An Unreliable Retrial Queue with Impatience and Preventive Maintenance

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Abstract. Retrial Queues are useful in the stochastic modeling of computer and telecommunication systems amongst others. In this paper, we study some problems connected with retrial phenomena involving by the unreliability of the server line which can be subject to physical breakdowns or computer attacks. The model considered here takes into account the corrective and preventive maintenance. Such policies are useful for example in many practical situations such as in production systems or for the maintenance of websites. We obtain the joint probability distribution of the server state and the number of orbiting customers in the system. This distribution is obtained in terms of Laplace and \( z \)-transforms.

Keywords: Retrial queues, Unreliable Server, Piece-Wise Markov Process, Laplace and \( z \) transforms.

1 Introduction

Queueing Systems are interesting stochastic modeling tools, particularly in computer systems. The server represents access of customers (or clients) to the available resources and queue represents the capacity of the system (available memory and other capacity storage) [5].

The classical Queueing Theory distinguishes two scenarios in the framework "client-server" to solve the conflict which occurs when an arrival finds the server blocked (busy or out of order): (i) In the first scenario, the arrival joins a queue with some service discipline (FIFO, LIFO or RANDOM); (ii) In the second one (Erlang model), the arrival is refused or denied (from the point of view of the client) or lost (from the point of view of the server).

In the Retrial Queueing Theory, the blocked customer or client is allowed to repeat successively his attempt until the server is able to provide service. Otherwise, if the server is available, the arriving customer begins service immediately. These retrial queueing models have been used in modeling Switching Networks, Wireless Sensor Networks, Call centers and so on [4], [3], [7].

The interesting reader can find an extensive bibliography covering the 1990 – 1999 and 2000 – 2009 periods [4], although the study of such problems begun with the Queueing Theory itself. The blocking of a customer is not due only to the conflict which occurs when the server is busy, but also when if it is out of order. This "breakdown" can be due to a "physical" incapacity of the material server to provide the required service or to the arrival of a priority...
client. The technology has now evolved and there is some other applications such as computer attacks as related in [2]. The stochastic model presented in this paper takes into account all of this aspects and also gives a new regard on the preventive aspect. Indeed, we can found in the literature some models trying to take into account the preventive maintenance aspect by introducing vacations after each (server or system) busy period (see for example [1]). In this paper, we present a more simple stochastic modeling approach to take into account such preventive actions in the case of linear retrial policy. In the following section we describe the mathematical model and we show that the evolution of the system can be described by a linear Markovian stochastic process in the sense of Gnedenko & Kovalenko [5]. In section 3 we derive the ergodicity condition and in section 4 we obtain the stationary distribution of the joint distribution of the server state and the number of orbiting customers.

2 Mathematical formulation

We consider an $M/G=1$ retrial queue with unreliable server and two types of primary customers, persistent and impatient. The flows generated by these calls form ordinary and independent Poisson processes with rate $\lambda > 0$ and $\gamma > 0$ respectively. There is no queue in the classical sense. If an arriving primary call (persistent or impatient) finds the server available and free of service, it immediately occupies the server and leaves the system after completion of service. If an arriving persistent call finds the server blocked (occupied by a service or out of order), it becomes a source of secondary call and return later to try again until it finds the server free and available; the collection of all secondary calls is called “orbit”. If an arriving impatient call finds the service blocked, it leaves the system forever. Any customer accepted for service upon arrival or on retrial leaves the system forever after service completion. We assume that each customer in orbit reapplies for service according to an exponential law with rate $\nu > 0$. The service times of the persistent customers are independent with common probability distribution function $H(x), H(0^+) = 0$, Laplace-Stieltjes transform $h(s), \Re(s) \geq 0$ and first order moments are denoted by $h_1$ and $h_2$.

The server is subject to two types of breakdowns. These breakdowns can be of physical nature (mechanical or electronical) or of software nature (bug or computer attack) and arrive according to Poisson process. We denote by $\theta_1$ (resp. $\theta_0$) the rate of breakdown given that the server is busy (resp. idle). We distinguish two types of maintenance (renewals): preventive and corrective.

- preventive maintenances, which occur randomly, but with a constant rate $\delta > 0$. Indeed, in practice it is difficult to implement a strictly constant periodic maintenance policy. If a preventive action occurs when a service is in course, then it is reported at a later date, and its duration is a random
variable with probability distribution function \( G(x), G(0^+) = 0 \), Laplace-Stieltjes transform \( g(s) \) and first order moments are denoted by \( g_1 \) and \( g_2 \).

- corrective maintenance, which is a random variable with probability distribution function \( R_1(x), R_1(0^+) = 0 \) (resp. \( R_0(x), R_0(0^+) = 0 \)) given that the breakdown occurs in busy state (resp. in free state), Laplace-Stieltjes transform \( r_1(s) \) (resp. \( r_0(s) \)) and first order moment are denoted by \( r_{11} \), \( r_{12} \) (resp. \( r_{01} \), \( r_{02} \)). If a breakdown occurs when a service is in course, the interrupted customer joins the orbit and retry his call according to the retrial linear policy.

Consider the following random process \( \zeta(t) = \{\alpha(t), \beta(t), R(t); \xi(t), t \geq 0\} \), where \( \{R(t), t \geq 0\} \) is the number of customers in orbit at time \( t \); \( \alpha(t) = 0 \), if the server is on at time \( t \); \( \alpha(t) = 1 \) (resp. \( \alpha(t) = 2 \)) if it is out of order at time \( t \) due to a preventive maintenance (resp. corrective maintenance); \( \beta(t) = 0 \), if the server is free at time \( t \), \( \beta(t) = 1 \) (resp. \( \beta(t) = 2 \)) if the server is busy by the service of persistent (resp. impatient customer). The last component \( \xi(t) \) is a positive real random variable, \( \xi(t) = 0 \), if \( \alpha(t) = 0 \) and \( \beta(t) = 0 \); \( \xi(t) \) is the residual service time if \( \beta(t) \neq 0 \) and \( \alpha(t) = 0 \); \( \xi(t) \) is the residual maintenance time if \( \alpha(t) \neq 0 \).

It is not difficult to show that the stochastic process \( \{\zeta(t), t \geq 0\} \) is a Markovian process with piecewise linear paths which describes the evolution of the server state and the number of orbiting customers. We establish the ergodicity condition for such a process and we obtain its stationary probability distribution.

### 3 Ergodicity condition

Let

\[
\rho = \frac{\lambda}{\theta_1} \left( 1 - h(\theta_1) \right) \left( 1 + \theta_1 (h_1 + r_{11}) \right).
\]

(1)

The following theorem gives a condition for the existence of a stationary regime.

**Theorem 1.** Assume that the following conditions

\[
\max\{h_1, f_1, r_{01}, r_{11}\} < \infty,
\]

(2)

\[
\rho < 1,
\]

(3)

are fulfilled, then the stochastic process \( \{\zeta(t), t \geq 0\} \) is ergodic.

**Proof.** We use the Smith’s theorem for regenerative processes with regeneration points \( T_i \) such that \( \zeta(T_{i-0}) > 0, \zeta(T_{i+0}) = 0, i=1,2,... \). An alternative proof is to use the Foster-Moustafa-Tweedie criterion. This condition appears also in the following section from the expression of the stationary probability distribution.
4 Joint distribution of the server state and the number of customers in orbit

In this section we derive the joint distribution of the server state and the number of customers in orbit in steady-state by its transform.

Under the assumption \( \rho < 1 \), the stochastic process \( \{ \xi(t), t \geq 0 \} \) is ergodic. As a consequence, the ergodic stationary probabilities

\[
P_{00}(m) = \lim_{t \to \infty} P\{ \alpha(t) = 0, \beta(t) = 0, R(t) = m \}, m \geq 0,
\]

\[
P_{ij}(m, x) = \lim_{t \to \infty} P\{ \alpha(t) = i, \beta(t) = j, R(t) = m; \xi(t) < x \},
\]

\( i, j = 0, 1, 2, (i, j) \neq (0, 0), m \geq 0, x \geq 0, \)

are solutions of the following system of differential equations

\[
(\lambda + \gamma + \theta_0 + \delta + \nu m)P_{00}(m) = \sum_{i=1}^{2} \left( \frac{dP_{i0}(m, 0)}{dx} + \frac{dP_{0i}(m, 0)}{dx} \right), m \geq 0,
\]

\[
\lambda P_{10}(m, x) = \frac{dP_{10}(m, x)}{dx} - \frac{dP_{00}(m, 0)}{dx} + \lambda(1 - \delta_{00})P_{10}(m - 1, x) + \\
+ \delta P_{00}(m)G(x), m \geq 0, x \geq 0,
\]

\[
\lambda P_{20}(m, x) = \frac{dP_{20}(m, x)}{dx} - \frac{dP_{00}(m, 0)}{dx} + \lambda(1 - \delta_{00})P_{20}(m - 1, x) + \\
+ \theta_0 P_{00}(m)R_0(x) + \theta_1[(1 - \delta_{00})P_{01}(m - 1, \infty) + P_{02}(m, \infty)]R_1(x),
\]

\( m \geq 0, x \geq 0, \)

\[
(\lambda + \theta_1)P_{01}(m, x) = \frac{dP_{01}(m, x)}{dx} - \frac{dP_{00}(m, 0)}{dx} + \lambda(1 - \delta_{00})P_{01}(m - 1, x) + \\
+ \lambda P_{00}(m)H(x) + \nu(m + 1)P_{00}(m + 1)H(x), m \geq 0, x \geq 0,
\]

\[
(\lambda + \theta_1)P_{02}(m, x) = \frac{dP_{02}(m, x)}{dx} - \frac{dP_{00}(m, 0)}{dx} + \lambda(1 - \delta_{00})P_{10}(m - 1, x) + \\
+ \gamma P_{00}(m)F(x), m \geq 0, x \geq 0,
\]

where \( \delta \) is the Kronecker function. We introduce the partial generating functions in \( z \),

\[
F_{00}(z) = \sum_{m=0}^{\infty} z^m P_{00}(m),
\]

\[
F_{ij}(z) = \sum_{m=0}^{\infty} z^m P_{ij}(m), i = 0, 1, 2; j = 0, 1, 2; (i, j) \neq (0, 0).
\]

Applying these transforms to the previous system, we obtain

\[
(\lambda + \gamma + \theta_0 + \delta)F_{00}(z) + \nu z \frac{dF_{00}(z)}{dz} = \sum_{i=1}^{2} \left( \frac{\partial F_{i0}(z, 0)}{\partial x} + \frac{\partial F_{0i}(z, 0)}{\partial x} \right), \quad (4)
\]
\[ (\lambda - \lambda z)F_{10}(z, x) = \frac{\partial F_{10}(z, x)}{\partial x} - \frac{\partial F_{10}(z, 0)}{\partial x} + \delta F_{00}(z)G(x), \quad (5) \]

\[ (\lambda - \lambda z)F_{20}(z, x) = \frac{\partial F_{20}(z, x)}{\partial x} - \frac{\partial F_{20}(z, 0)}{\partial x} + \theta_0 F_{00}(z)R_0(x) + \theta_1 [F_{01}(z, \infty) + F_{02}(z, \infty)]R_1(x), \quad (6) \]

\[ (\lambda - \lambda z + \theta_1)F_{01}(z, x) = \frac{\partial F_{01}(z, x)}{\partial x} - \frac{\partial F_{01}(z, 0)}{\partial x} + \left( \lambda F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right)H(x), \quad (7) \]

\[ (\lambda - \lambda z + \theta_1)F_{02}(z, x) = \frac{\partial F_{02}(z, x)}{\partial x} - \frac{\partial F_{02}(z, 0)}{\partial x} + \gamma F_{00}(z)F(x). \quad (8) \]

We apply now the Laplace transform to the second argument of the obtained partial generating functions (5)-(8)

\[ s(s - \lambda + \lambda z)f_{10}(z, s) = \frac{\partial F_{10}(z, 0)}{\partial x} - \delta F_{00}(z)g(s), \quad (9) \]

\[ s(s - \lambda + \lambda z)f_{20}(z, s) = \frac{\partial F_{20}(z, 0)}{\partial x} - \theta_0 F_{00}(z)r_0(s) - \theta_1 [F_{01}(z, \infty) + F_{02}(z, \infty)]r_1(s), \quad (10) \]

\[ s(s - \lambda + \lambda z - \theta_1)f_{01}(z, s) = \frac{\partial F_{01}(z, 0)}{\partial x} - \lambda \left( F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right)h(s), \quad (11) \]

\[ s(s - \lambda + \lambda z - \theta_1)f_{02}(z, s) = \frac{\partial F_{02}(z, 0)}{\partial x} - \gamma F_{00}(z)f(s). \quad (12) \]

The unknown functions \( \frac{\partial F_{ij}(z, 0)}{\partial x} \) can be determined as usual by using the fact that the functions \( F_{ij}(z, 0) \) are analytical functions in the domain \( ||z|| \leq 1 \). Consider for example the first equation of the previous system. Since \( F_{10}(z, 0) \) is analytic in the domain \( ||z|| \leq 1 \), and since the left right hand is equal to zero for \( s = \lambda - \lambda z \), then the right hand side must also be zero at this point, so we have the first condition

\[ \frac{\partial F_{10}(z, 0)}{\partial x} = \delta F_{00}(z)g(\lambda - \lambda z). \quad (13) \]

By repeating this procedure, we obtain all the functions \( \frac{\partial F_{ij}(z, 0)}{\partial x}, 0 \leq i, j \leq 2, \)

\[ \frac{\partial F_{20}(z, 0)}{\partial x} = \theta_0 F_{00}(z)r_0(\lambda - \lambda z) - \theta_1 [F_{01}(z, \infty) + F_{02}(z, \infty)]r_1(\lambda - \lambda z), \quad (14) \]

\[ \frac{\partial F_{01}(z, 0)}{\partial x} = \left( \lambda F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right)h(\lambda - \lambda z + \theta_1), \quad (15) \]

\[ \frac{\partial F_{02}(z, 0)}{\partial x} = \gamma F_{00}(z)f(\lambda - \lambda z + \theta_1). \quad (16) \]

Substituting now (13)-(16) in (9)-(12), we obtain the functions \( f_{ij}(z, s) \) in the following form

\[ f_{10}(z, s) = \delta \frac{g(\lambda - \lambda z) - g(s)}{s(s - \lambda + \lambda z)} F_{00}(z), \quad (17) \]
Similarly, we can rewrite the equation (14) under the form

\[ f_{20}(z, s) = \theta_0 \frac{r_0(\lambda - \lambda z) - r_0(s)}{s(s - \lambda + \lambda z)} F_{00}(z) + \]

\[ + \theta_1 [z F_{01}(z, \infty) + F_{02}(z, \infty)] \times \frac{r_1(\lambda - \lambda z) - r_1(s)}{s(s - \lambda + \lambda z)}, \]

(18)

Taking into account (23) and (24), the equation (22) become

\[ f_{01}(z, s) = \left( \lambda F_0(z) + \frac{dF_{00}(z)}{dz} \right) \frac{h(\lambda - \lambda z + \theta_1) - h(s)}{s(s - \lambda + \lambda z + \theta_1)} F_{00}(z), \]

(19)

\[ f_{02}(z, s) = \gamma \frac{f(\lambda - \lambda z + \theta_1) - f(s)}{s(s - \lambda + \lambda z - \theta_1)} F_{00}(z). \]

(20)

Using Tauberian theorem in formula (17), we get

\[ F_{10}(z, \infty) = \lim_{x \to \infty} F_{10}(z, \infty) = \lim_{s \to 0^+} s f_{10}(z, s) = \delta \frac{1 - g(\lambda - \lambda z)}{\lambda - \lambda z} F_{00}(z). \]

(21)

Similarly, we obtain from (18)-(20)

\[ F_{20}(z, \infty) = \theta_0 \frac{1 - r_0(\lambda - \lambda z)}{\lambda - \lambda z} F_{00}(z) + \theta_1 [z F_{01}(z, \infty) + F_{02}(z, \infty)] \frac{1 - r_1(\lambda - \lambda z)}{\lambda - \lambda z}, \]

(22)

\[ F_{01}(z, \infty) = \left( \lambda F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right) \frac{1 - h(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1}, \]

(23)

\[ F_{02}(z, \infty) = \gamma \frac{1 - f(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} F_{00}(z). \]

(24)

Taking into account (23) and (24), the equation (22) become

\[ F_{20}(z, \infty) = \theta_0 \frac{1 - r_0(\lambda - \lambda z)}{\lambda - \lambda z} F_{00}(z) + \]

\[ + \theta_1 \left( \lambda F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right) \frac{1 - h(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} \times \frac{1 - r_1(\lambda - \lambda z)}{\lambda + \lambda z} \]

\[ + \gamma \theta_1 \frac{1 - f(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} \times \frac{1 - r_1(\lambda - \lambda z)}{\lambda - \lambda z} F_{00}(z). \]

(25)

Similarly, we can rewrite the equation (14) under the form

\[ \frac{\partial F_{20}(z, 0)}{\partial x} = \theta_0 F_{00}(z) r_0(\lambda - \lambda z) + \]

\[ + \theta_1 \left( \lambda F_{00}(z) + \nu \frac{dF_{00}(z)}{dz} \right) \frac{1 - h(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} r_1(\lambda - \lambda z) \]

\[ + \theta_1 \gamma \frac{1 - f(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} r_1(\lambda - \lambda z) F_{00}(z). \]

(26)
Now, substitution of (13)-(16) in equation (4) and taking into account (26) gives

\[
\{ \lambda - \lambda v(\lambda - \lambda z) + \gamma - \gamma w(\lambda - \lambda z) + \theta_0 - \theta_0 r_0(\lambda - \lambda z) + \delta - \delta g(\lambda - \lambda z) \} F_{00}(z) = \\
= \nu \{ v(\lambda - \lambda z) - z \} \frac{dF_{00}(z)}{dz},
\]

where

\[
v(\lambda - \lambda z) = h(\lambda - \lambda z + \theta_1) + \theta_1 z \frac{1 - h(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} r_1(\lambda - \lambda z)
\]

and

\[
w(\lambda - \lambda z) = f(\lambda - \lambda z + \theta_1) + \theta_1 \frac{1 - f(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} r_1(\lambda - \lambda z).
\]

The solution of this homogeneous ordinary differential equation is of the form

\[
F_{00}(z) = k_0 \exp \left( \frac{\lambda}{\nu} \int_0^z 1 - \frac{v(\lambda - \lambda y)}{v(\lambda - \lambda y) - y} dy \right) \times \exp \left( \frac{\gamma}{\nu} \int_0^z 1 - \frac{w(\lambda - \lambda y)}{v(\lambda - \lambda y) - y} dy \right) \times \\
\times \exp \left( \frac{\theta_0}{\nu} \int_0^z 1 - \frac{r_0(\lambda - \lambda y)}{v(\lambda - \lambda y) - y} dy \right) \times \exp \left( \frac{\delta}{\nu} \int_0^z 1 - \frac{g(\lambda - \lambda y)}{v(\lambda - \lambda y) - y} dy \right).
\]

The constant $k_0$ can be determined by using the normalization condition.

So, we have proved the following result.

**Theorem 2.** If the condition $\rho < 1$ is fulfilled, then the joint distribution of the server state and orbit size is given by its transform

\[
f_{10}(z, s) = \delta \frac{g(\lambda - \lambda z) - g(s)}{s(\lambda - \lambda z)} F_{00}(z),
\]

\[
f_{20}(z, s) = \theta_0 \frac{r_0(\lambda - \lambda z) - r_0(s)}{s(\lambda - \lambda z)} F_{00}(z) + \\
+ \theta_1 \left\{ \frac{z g(\lambda - \lambda z)}{v(\lambda - \lambda z) - z} \frac{1 - h(\lambda - \lambda z)}{\lambda - \lambda z + \theta_1} + \\
+ \frac{1 - f(\lambda - \lambda z + \theta_1)}{\lambda - \lambda z + \theta_1} \right\} r_1(\lambda - \lambda z) - r_1(s) F_{00}(z),
\]

\[
f_{01}(z, s) = \frac{q(\lambda - \lambda z)}{v(\lambda - \lambda z) - z} \frac{h(\lambda - \lambda z + \theta_1) - h(s)}{s(\lambda - \lambda z + \theta_1)} F_{00}(z),
\]

\[
f_{02}(z, s) = \frac{q(\lambda - \lambda z)}{v(\lambda - \lambda z) - z} \frac{f(\lambda - \lambda z + \theta_1) - f(s)}{s(\lambda - \lambda z + \theta_1)} F_{00}(z),
\]

where

\[
q(\lambda - \lambda z) = \gamma - \gamma w(\lambda - \lambda z) + \theta_0 - \theta_0 r_0(\lambda - \lambda z) + \delta - \delta g(\lambda - \lambda z).
\]
The function $F_{00}(z)$ is given by formula (30) and the constant

$$k_0 = \frac{1}{F_{00}(1) \times \chi(1)}$$

$$\chi(1) = \frac{(1 - \rho)(\delta g_1 + \theta_0 r_{01}) + (1 - f(\theta_1)\Psi}{(1 - \rho)},$$

where

$$\Psi = \frac{\gamma}{\theta_1} + r_{11} + \frac{1}{2}(\lambda \gamma w_1 + \theta_0 r_{01} + \lambda \delta g_1)(\lambda r_{12} + r_{11} \chi^2).$$

**Remark.** We note that the ergodicity condition $\rho < 1$ appears here since the constant $k_0 > 0$.

5 Some performance measures

The obtained results allow us to obtain some performance measures of interest. We give only some of them for illustration.

- The probability that the server is available and idle
  $$p_{00} = F_{00}(1).$$

- The probability that the server is on and busy by the service of a persistent customer
  $$p_{02} = \frac{\gamma - \gamma f(\theta_1)}{\theta_1} p_{00}.$$

- The probability that the server is out of order and no customer in service
  $$p_{20} = \delta g_1 p_{00}.$$

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**References**


Limitations and assumptions of experience curves used as an instrument to evaluate the competitiveness of photovoltaic technologies in the energy market.

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Abstract. Experience curves describe the reduction in unit production cost with an increase in cumulative production. This concept is used to examine past price decreases in photovoltaic [PV] and to assess the potential economic impact of different PV growth scenarios. This article makes research in the literature on PV experience curves and their application to energy technology.

Before 2000, there have been published a few studies on PV experience curves. But in recent years an increase of literature on experience curve theory for energy technology can be noted. In both, scientific literature and policy documents of experience curves are partially mixed with the learning curves. But there is an important distinction, as a rule, the learning curves analyze only one factor, while experience curves include factors such as the costs of research, management, marketing or capital; they consider the total costs and cumulative production analysis of the entire market. This paper considers that care must be taken in the application of experience curves to evaluate the competitiveness and to forecast cost reductions in PV. In addition, we explain that special attention should be paid to the reference that are being used, because a lot of research was done on the development of the module prices, but only a little in the field of the experience curves of PV kWh [Kilowatt-hour] prices.

Keywords: Experience curves, energy technology, photovoltaic.

1 Introduction

In 1936 learning curves were first quantified and reported in the airplane industry (Wright [1]). Later, in 1962, Arrow [2] drew the economic implications from “learning-by-doing”. However, the experience effect was firmly established within the management sciences through the work of the Boston Consulting Group [3]. Working with a leading manufacturer of semiconductors, the consultants noticed that the company's unit cost of manufacturing fell by about 25% for each doubling of the volume that it produced. This relationship they called the experience curve: the more experience a firm has in producing a particular product, the lower is its costs.

Experience curves are classical econometric models in which the key explanatory variable is experience, as measured by cumulative production or, in this case, cumulative installed capacity. Therefore the experience formula in their basic form can be described as:
Cost(x) = a \cdot x^m \\
\log(Cost(x)) = \log(a) + m \cdot \log(x)

where:

- Cost(x) is the total cost of unit x.
- x is the cumulative (unit) production.
- a is the cost of the first unit produced.
- m is the experience (or learning) parameter, which is constant.

The Parameter ‘m’ is usually negative and is used to calculate the progress ratio (PR) and the learning rate (LR):

\[ PR = 2^m \]
\[ LR = 1 - 2^m \]

A learning rate of 0.1 means, for instance, that unit cost decreases by 10% for each doubling of experience. The progress ratio also measures the relationship between the increase in cumulative production and the decrease of unit costs. A progress ratio of 80%, which is equal to a learning rate of 20%, means that each doubling of cumulative production costs decreases by 20%.

![Experience Curve](image)

**Figure 1.1:** Example of an experience curve

In the following only the most relevant publications on PV experience curves are summarized. This summary does not intend to give a complete resume of the studies.

2 **International Energy Agency, IEA [4]**

This study is a very broad paper about experience curves and their relevance for energy technology policy. In the first part the author describes how the
cumulative break-even capacity and the corresponding learning investments are calculated. Assuming a break-even price of 0.5 USD/Wp (Watt peak) and a progress ratio of 80% for PV modules a cumulative production of 200 GW (Gigawatt) is required. This corresponds to 60 billion USD worth of learning investments.

In addition, this paper considers the development of the PV kWh price as an alternative measure of PV cost: a progress ratio of 65% was found in the literature. However, as this construction is only based on 3 data points at 5 year intervals, it is only a “very rough estimate”.

In the second part possible changes are described that can happen when constructing experience curves. For instance a “technology structural change” takes place, if a major technical shift in the production process lets the experience curve drop from the existing technology (variant A, e.g. crystalline PV) to a new technology (variant B, e.g. thin film PV). The progress ratio of the variants may be the same, but during the transition period there is a significant higher progress ratio.
Figure 2.2: Technology structural change.

The author gives a progress ratio of 84% for the PV module market in Europe in the years from 1976 to 1996. At 100 MW [Megawatt] cumulative capacity he finds a structural break with a progress ratio of 53% and afterwards the progress ratio levels back at 79%. The conclusion is that cost and price experience curves can differ, but in the long run they always come close to each other, mainly driven by competition among the market player.

A “market structural change” can happen as well. In this case a market player decreases his price below the cost. He protects his business and in the “Price Umbrella” period he profits from decreasing costs until the “Shakeout” period. There new entrants or competitors put pressure on the market. Prices decrease faster than costs and finally at the same progress ratio as the costs.
In the third part a seminal paper from Tsuchiya [6] is quoted, where the prospects for Japanese niche markets are analyzed. Without niche markets the Break-even Price (BEP) of ca. 10 Yen/kWh would be reached at a cumulative installed capacity of more than 100 GW for a progress ratio of 76%. However, in niche markets customers are willing to pay more for PV energy than for mature energy technologies as PV is somehow more competitive. And BEPs are accordingly different. A decreasing BEP line is constructed which reduces the cumulative capacity to 6 GW at similar progress ratio level. Once reached this level, a self-sustaining PV market is reached and the learning investments will be made by this market, without public support.

In the fourth section main results of a BEP study are presented. However, the assumption that different renewable technologies compete for the same learning investments is mentioned as questionable in other papers (Staffhorst [7]). Furthermore the data provided in this work appears difficult to verify as most of it is from workshops and seminal papers.

3 Wene [5]

The author is discussing the shift in the learning environment for energy technologies through three case studies, based on and described in a detail in IEA [4] and Wene et al. [8]: solar heated swimming pools, wind energy and residential photovoltaic systems. The author is pointing out, that learning investments and public RD&D (research, development & demonstration) measure different parts of the resources needed for technology learning and not surprisingly the RD&D spending on PV by the 28 IEA countries is twice as
large as the learning investments. Hence the conclusion is that energy technology policies should consider two distinct phases to bring energy technology to commercial maturity: in the first one direct R&D support is required, whereas in the second phase the focus should be on providing learning opportunities on the market. However, this paper does not offer consolidated findings of PV experience curves but emphasizes the relevance of government deployment programs.

4 Harmon [9]

Harmon is presenting “the longest experience curve for PV systems assembled to date”. Based on data from Maycock and Wakefield [10]; Thomas et al. [11] and Watanabe [12] an experience curve of module prices from 1968 to 1998 is constructed. The author is ending up with more than 13 cumulative doublings. The reliability of a progress ratio of 78.8% appears questionable. The Balance of System (BOS) is used in this paper as alternative measure of PV cost. However, there are no numbers given for the BOS experience curves, but only a few examples of price reductions. Break-even prices and learning investments are not further assessed. Although this paper is quite often quoted in literature the focus is more on combining research that was done before to one long experience curve. As there was very limited industrialized production of PV before 1976, the sense of this long experience curve is questionable.

5 Parente et al. [13]

This publication updates the experience curve for PV modules based on price data from Maycock and Wakefield [10] until the year 2000. A progress ratio of 77.2% was found for the years 1981 to 2000. After splitting this curve into two separate ones from 1981 to 1990 and 1991 to 2000, the authors explain and prove that these two new curves represent a better adjustment. They conclude, that the decrease of the progress ratio from 79.8% in the eighties to 77.4% in the nineties leads to lower future learning investments than expected. The paper is just a short update of PV experience curves. Only module price data and module progress ratios are presented. A more detailed scenario for the future learning investments is not presented.

6 Zwaan and Rabl [14]

This paper addresses the potential for PV cost reductions. At first the authors give an overview of current PV production costs which range for example from 2 to 8 USD/Wp for grid connected systems based on data from Turkenburg [15] and Oliver and Jackson [16]. Detailed assumptions for PV systems are done and end up with PV electricity costs from 0.091 to 0.182 USD/kWh (grid connected). Further on an overview of progress ratios is given based on studies from Williams and Terzian [17], Watanabe [11] and IEA [4]. Taking the
average price for grid connected systems of 5 USD/Wp the necessary cumulative production to reach a BEP of 1 USD/Wp is shown for progress ratios between 0.7 to 0.9 (see Figure 6.1). The authors emphasize that a progress ratio above 0.8 means that the BEP will become likely unrealistic. Even with a progress ratio of 0.8 the cumulative production needs to be 148 GW. The learning investments are calculated at about 211 billion USD for the 0.8 progress ratio, which means a learning investment of 64 billion USD. The authors do not provide an estimation of growth rates or time frames to happen as the progress ratio is the key element to determine at what cumulative capacities the BEP will be reached. However, in 2011 the world-wide power plant capacity was about 22.891 GW [Source: http://www.worldnuclearreport.org]. In 2012 the world’s solar PV electricity capacity surpassed 100 GW [Source: http://cleantechnica.com]. Hence cumulative production of 148 GW appears realistic as it covers less than 1% of the world-wide power plant capacity.

Table 7

<table>
<thead>
<tr>
<th>Progress ratio, pr</th>
<th>0.7</th>
<th>0.75</th>
<th>0.8</th>
<th>0.85</th>
<th>0.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>Break-even PV annual production, $P_{BEP}$ (GW)</td>
<td>23</td>
<td>48</td>
<td>144</td>
<td>957</td>
<td>39,700</td>
</tr>
<tr>
<td>Break-even annual production (% of 1300 GW, the present world capacity)</td>
<td>3.7%</td>
<td>1.5%</td>
<td>4.5%</td>
<td>29.0%</td>
<td>1200%</td>
</tr>
<tr>
<td>Cost of reaching break-even, $C_{BE}$ ($ billion)</td>
<td>37</td>
<td>74</td>
<td>211</td>
<td>1240</td>
<td>46,000</td>
</tr>
<tr>
<td>Cost of reaching break-even if cost were 10% of break-even, $(15/3.7)(C_{BE})$ ($ billion)</td>
<td>22</td>
<td>47</td>
<td>144</td>
<td>957</td>
<td>39,700</td>
</tr>
<tr>
<td>Cost gap, $C_{BE} - (15/3.7)(C_{BE})$ ($ billion)</td>
<td>15</td>
<td>27</td>
<td>64</td>
<td>219</td>
<td>710</td>
</tr>
<tr>
<td>Cost gap (% of cost of reaching break-even)</td>
<td>41%</td>
<td>36%</td>
<td>10%</td>
<td>25%</td>
<td>15%</td>
</tr>
<tr>
<td>Avoided damage of $P_{BEP} - P_{BE}$ in 25 years ($ billion)</td>
<td>4</td>
<td>12</td>
<td>37</td>
<td>239</td>
<td>99,600</td>
</tr>
<tr>
<td>Avoided damage (% of cost gap)</td>
<td>37%</td>
<td>44%</td>
<td>58%</td>
<td>23%</td>
<td>14%</td>
</tr>
</tbody>
</table>

7 Poponi [18]

The author analyses price development for PV modules between 1976 and 2002 based on price data from Maycock and Wakefield [10]. The performance ratio of his experience curve (75%) is significant lower than in other studies. This is caused by the big influence of the early years. Starting with the year 1989 the author gets a progress ration of 80.5% and confirms that this structural break is statistically significant.

In the next part of the paper, the author calculates the module-BEPs for two different electricity prices. Assumptions a 25 years system lifetime a generating cost of electricity of 0.05 USD/kWh (0.15 USD/kWh) the BEP for modules is 0.5 USD/Wp (1.9 USD/Wp) and for PV systems 0.9 USD/Wp (3.2 USD/Wp). However, no information is provided about the necessary learning investments to reach these BEPs.

Finally the author explains what cumulative shipments are necessary to ride down the experience curve to the BEP. In an optimistic scenario of a growth rate of 30% and a progress ratio of 80% a world’s solar PV electricity capacity of
1.440 GW (27 GW) could be reached in 2026 (2011) and could bring down the PV generating costs to 0,05 USD/kWh (0,15 USD/kWh).

8 Schaeffler et al. [19]

The key objective of this comprehensive and detailed work was to contribute on what energy policy can learn from the experience curve theory by researching the PV case. This final Photex-project report was published by an international research team, supported by the EU. Different to other publications this report is based on an own project database with more than 3,600 records, representing 26 MW of primary data from different countries. However, more than 80% of the installed capacity came from Germany, Italy and the Netherlands. The authors constructed not only typical experience curves for module prices, but for BOS and inverters as well.

Results of their own database were compared with PV module prices from Strategies Unlimited (SU) for the years 1976 to 2001. In this period the progress ratio of the SU data is 80±0,4% while 77±1,5% were obtained in the years 1987 to 2001 based on the Photex data base. Besides of results for BOS the authors provide progress ratios for an inverter experience curve for the years 1995 to 2002 which is 91% (Germany) and 93% (Netherlands).

In Chapter 4 the question is discussed whether policy programs in different countries can be related to the historical experience curve analyzed before. However, policies and programs are highly contextual and thereof difficult to copy. Different geographical backgrounds avoid that programs even within the Europe are exchanged and cannot be pasted.

Based on the target costs of 3,4 EUR/Wp for total systems in 2010 set by the European Photovoltaic Industry Association EPIA, some scenarios are provided to demonstrate that a growth rate of at least 20% and a progress ratio of 80% are necessary to obtain low PV prices (see Figure 8.1). Further sources of cost reductions before 2010 are examined.
In Chapter 6 the authors discuss about break-even analysis and future learning investments. However, this section is influenced by Zwaan and Rabl [14]. Based on a spreadsheet model a scenario for a solar-rich region is given and a BEP of 0.7 EUR/Wp is assumed. In this model a progress ratio of 80% and a growth rate of 20% will reduce PV costs down to 0.7 EUR/Wp in 2039 and the global cumulative learning investment will be 634 billion EUR. Assuming a progress ratio of 70% will result in learning investments of only 89 billion EUR reaching the same BEP in 2013. Hence the impact of the progress ratio is very high.

The authors assume that most likely PV will not initially compete in the bulk electricity market. The learning investment needed can be reduced by first targeting at competitive niche-markets. The idea of Poponi [18] is used to calculate the learning investments in higher-value markets.

Figure 8.1: Typical price and growth scenarios for PV systems, Schaeffler et al. [19]

Considering the characteristics for a residential electricity market in the Palermo region (Italy) and assuming a BEP of 4 EUR/Wp is resulting in a cumulative installed capacity of 8 GW in 2009 and learning investments of only 5 billion EUR.

9 Tour et al. [20]

This working paper is targeting to predict the cost of PV modules out to 2020 using experience curve models and its implications on the cost of PV electricity. As most of the experience curve models use the cumulative production (as a proxy for experience) as single explanatory variable, the author is adding other variables and creates a multifactor experience curve. It is outlined, that in the literature additional explanatory variables have been included in the experience curves (Isoard and Soria [21], Kobos et al. [22], Yu et al. [23]) but only little
attention on the influence of adding these variables (e.g. price, scale, R&D) on the predictive power of the experience model.

The author is exploring a set of 16 different variables and combinations of R&D, scale, silicon price and silver price using annual world average values and raw material prices (Yu [24], Nemet [25], Dechezleprêtre [26], Silver Institute website, Photon International magazines) from 1990 to 2011.

Contrary to what is suggested in mentioned literature, the addition of explanatory variables does not improve the accuracy of predictions as a matter of principle. However, the author recommends utilizing two models: the first one considers module cost by cumulative production only to be used for estimations before 2005 to avoid the influence of silicon shortage from 2005 to 2009. The second model includes silicon price as additional explanatory variable for estimations after 1989 to avoid the correlation of silicon price and cumulative production in old data.

Finally average world module prices are predicted: in a pessimistic outlook the price could move at 0,8 USD/Wp in 2020 and in the most optimistic it could end up at 0,63 USD/Wp (in the best case concerning silicon price development). The author is aware that his model can be improved as several aspects can impact the future development like market power, overproduction, incentive policies or module quality.

10 Conclusions

In the following table the results of the former publications are summarized and the key values are shown. They differ in terms of time frame used for the estimation, region, data source and reference capacity (if available). Studies before the year 2000 are not included.

<table>
<thead>
<tr>
<th>Author, Study (Data source)</th>
<th>PR [%]</th>
<th>Time Period</th>
<th>Region</th>
<th>Type of EC</th>
<th>cum. reference [MW]</th>
</tr>
</thead>
<tbody>
<tr>
<td>IEA (2000), (EU-Atlas and Nitsch)</td>
<td>84%</td>
<td>1976-1984</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 0,8-800</td>
</tr>
<tr>
<td></td>
<td>79%</td>
<td>1987-1996</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 0,8-800</td>
</tr>
<tr>
<td>Harmon (2000) (Maycock)</td>
<td>79,8%</td>
<td>1968-1998</td>
<td>Global</td>
<td>Modules</td>
<td>0,095-950</td>
</tr>
<tr>
<td></td>
<td>79,8%</td>
<td>1981-1990</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 10,5-250</td>
</tr>
<tr>
<td></td>
<td>77,4%</td>
<td>1991-2000</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 300-1500</td>
</tr>
<tr>
<td></td>
<td>80,5%</td>
<td>1989-2002</td>
<td>Global</td>
<td>Modules</td>
<td>238-2380</td>
</tr>
<tr>
<td>Photex (2004) (SU)</td>
<td>80±0,4%</td>
<td>1976-2001</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 0,3-1800</td>
</tr>
<tr>
<td></td>
<td>77±1,5%</td>
<td>1987-2001</td>
<td>Global</td>
<td>Modules</td>
<td>Ca. 100-1800</td>
</tr>
</tbody>
</table>
Table 10.1: Overview of published PV experience curves, refer to Staffhorst [7] and Tour [20]

While surveying the literature on experience curves, nearly all papers consider modules as a measure of PV cost. Price information is globally available (in USD/Wp) and it appears most suitable. Other alternative measures are dependent either on local conditions (e.g. installation cost, sunlight availability) or are not specific to the PV industry (e.g. inverter, batteries or wires) and therefore deemed unsuitable for the evaluation on global experience curves. Due to this only very few papers consider the development of the PV kWh price or inverter price as an alternative measure of PV cost.

Another finding is that in most of the papers the BEP is considered as constant over time. Several author mentions that the BEPs are highly sensitive to the assumptions made like system lifetime, interest, O&M cost, energy yield, etc. and presumably little attention is paid in this matter. However, changing energy prices could lead to recalculate the investment cost resulting in different BEP references.

Finally a technology policy geared only on market development which is based on the experience curve considering cumulative production as single explanatory variable may not be successful. Important drivers like R&D, scale effects or most relevant raw material price developments are not taken into...
account. This topic is even more important when scenarios are drawn for future price evolution and necessary learning investments.

References


Approximations for two-dimensional discrete scan statistics in some dependent models

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Abstract. We consider the two-dimensional discrete scan statistic generated by block factors from i.i.d. sequences. We present the approximation for the distribution of the scan statistics and error bounds. A simulation study illustrates our methodology.

Keywords: Scan statistics, m-dependent sequences, block-factor.

1 Introduction

Let $N_1$, $N_2$ be positive integers and \{\(X_{i,j} \mid 1 \leq i \leq N_1, 1 \leq j \leq N_2\)\} be a family of nonnegative integer random variables from a specified distribution. For $1 \leq i \leq N_1$ and $1 \leq j \leq N_2$, $X_{ij}$ represents the number of some events observed in the elementary square sub-region \([i, i + 1] \times [j, j + 1]\). Let $m_1$, $m_2$ be positive integers, $1 \leq m_1 \leq N_1$, $1 \leq m_2 \leq N_2$. For $1 \leq t \leq N_1 - m_1 + 1$, $1 \leq s \leq N_2 - m_2 + 1$ let

\[
\nu_{ts} = \nu_{t,s}(m_1, m_2) = \sum_{i=t}^{t+m_1-1} \sum_{j=s}^{s+m_2-1} X_{ij}.
\]  

(1)

The \textit{two-dimensional discrete scan statistic} is defined as the largest number of events in any $m_1 \times m_2$ rectangular scanning window within the rectangular region \([1, N_1] \times [1, N_2]\), i.e.

\[
S = S(m_1, m_2, N_1, N_2) = \max_{1 \leq t \leq N_1 - m_1 + 1} \nu_{ts}.
\]  

(2)

Most of research devoted to two-dimensional discrete scan statistics considers the i.i.d. model for $X_{i,j}$’s. Then, the statistic $S$ is used for testing the null hypothesis that the $X_{i,j}$’s are independent and identically distributed according to some specified probability law, in general Bernoulli, binomial or Poisson (see Glaz et al.[4]). Since there are no exact formulas for $P(S \leq n)$, various methods of approximation and bounds for $P(S \leq n)$ have been proposed by several authors. An overview of these methods as well as a complete bibliography on the subject are given in Chen and Glaz [3], Glaz et al. [4], Boutsikas and Koutras [2], Haiman and Preda [7] and references therein. In this paper...
we consider the two-dimensional discrete scan statistics generated by some particular dependent sequences \( \{X_{i,j} \mid 1 \leq i \leq N_1, 1 \leq j \leq N_2\} \). More precisely, we are interested in the case where the \( X_{i,j} \)’s are obtained as block-factors from an independent and identically distributed sequence of random variables \( \{Y_{i,j} \mid 0 \leq i \leq N_1 + 1, 0 \leq j \leq N_2 + 1\} \), in the following way:

\[
X_{i,j} = f(Y_{i,j}, Y_{i,j-1}, Y_{i,j+1}, Y_{i-1,j}, Y_{i-1,j-1}, Y_{i-1,j+1}, Y_{i+1,j}, Y_{i+1,j+1}),
\]

(3)

where \( f \) is a non-negative measurable function \( f : \mathbb{R}^9 \rightarrow \mathbb{R}_+ \) (see Figure 1).

\[
\begin{array}{cccccc}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{N_1+1,j-1} & Y_{N_1+1,j} & Y_{N_1+1,j+1} & \vdots & \vdots & \vdots \\
\end{array}
\]

\[
\begin{array}{cccccc}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{N_1+1,j-1} & Y_{N_1+1,j} & Y_{N_1+1,j+1} & \vdots & \vdots & \vdots \\
\end{array}
\]

\[
\begin{array}{cccccc}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{N_1+1,j-1} & Y_{N_1+1,j} & Y_{N_1+1,j+1} & \vdots & \vdots & \vdots \\
\end{array}
\]

\[
\begin{array}{cccccc}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i-1,j-1} & Y_{i-1,j} & Y_{i-1,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{i,j-1} & Y_{i,j} & Y_{i,j+1} & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
Y_{N_1+1,j-1} & Y_{N_1+1,j} & Y_{N_1+1,j+1} & \vdots & \vdots & \vdots \\
\end{array}
\]

Fig. 1. Two-dimensional block-factor model

The paper is organized as follows. In Section 2, we present the methodology for approximating the distribution of the scan statistics generated by the model (3) providing approximations and error bounds. Numerical results based on simulations are presented in Section 3 for particular block-factor functions, \( f \).

2 The scan statistics as an extremum of a 1-dependent stationary sequence of random variables

The methodology we use to approximate the distribution of scan statistics generated by the dependent model (3) follows closely to that presented in Haiman and Preda [7] for the i.i.d. model. Let us suppose that \( N_1 = (L_1 + 1)(m_1 + 1) - 2 \), \( N_2 = (L_2 + 1)(m_2 + 1) - 2 \) where \( L_1 \) and \( L_2 \) are positive integers and define

\[
Z_k = \max_{1 \leq t \leq L_1(m_1 + 1) \atop (k-1)(m_2+1)+1 \leq s \leq k(m_2+1)} \nu_{t,s}, \quad k \in \{1, 2, \ldots, L_2\}. \tag{4}
\]

The random variables \( Z_k \) represent the scan statistics on the overlapping \( N_1 \times 2m_2 \) rectangular regions

\[
\mathcal{R}_k = [1, N_1] \times [(k-1)(m_2 + 1) + 1, (k + 1)(m_2 + 1) - 2].
\]
From the independence of $Y_{ij}$ and

$$Z_{k-1} \in \sigma \left( X_{ij} \mid 1 \leq i \leq N_1, (k-2)(m_2+1) + 1 \leq j \leq k(m_2+1) - 2 \right)$$
$$\in \sigma \left( Y_{ij} \mid 0 \leq i \leq N_1 + 1, (k-2)(m_2+1) \leq j \leq k(m_2+1) - 1 \right),$$  \hspace{1cm} (5)

$$Z_k \in \sigma \left( X_{ij} \mid 1 \leq i \leq N_1, (k-1)(m_2+1) + 1 \leq j \leq (k+1)(m_2+1) - 2 \right)$$
$$\in \sigma \left( Y_{ij} \mid 0 \leq i \leq N_1 + 1, (k-1)(m_2+1) \leq j \leq (k+1)(m_2+1) - 1 \right),$$  \hspace{1cm} (6)

$$Z_{k+1} \in \sigma \left( X_{ij} \mid 1 \leq i \leq N_1, k(m_2+1) + 1 \leq j \leq (k+2)(m_2+1) - 2 \right)$$
$$\in \sigma \left( Y_{ij} \mid 0 \leq i \leq N_1 + 1, k(m_2+1) \leq j \leq (k+2)(m_2+1) - 1 \right),$$  \hspace{1cm} (7)

we can verify that the sequence $(Z_k)_{1 \leq k \leq L_2}$ is 1-dependent (see Figure 2 for the case $k = 2$). Since $Y_{ij}$ are also identically distributed we conclude that the sequence $Z_k$ is stationary.

![Fig. 2. Illustration of $Z_k$ emphasizing the 1-dependence](image)

Notice that from (2), (4) and the measurability of $f$, the following relation holds

$$S = \max_{1 \leq k \leq L_2} Z_k.$$

The relation described in (8) is the key idea behind our approximation. The methodology is based on the following result developed in Haiman [5, Theorem 4] and improved in Amarioarei [1, Theorem 2.6]:

Let $(T_k)_{k \geq 1}$ be a strictly stationary 1-dependent sequence of random variables and for $x < \sup \{ u \mid P(T_1 \leq u) < 1 \}$, consider

$$q_m = q_m(x) = P(\max(T_1, \ldots, T_m) \leq x).$$  \hspace{1cm} (9)
**Theorem 1.** Assume that \( x \) is such that \( q_1(x) \geq 1 - \alpha \geq 0.9 \) and define \( \eta = 1 + l\alpha \) with \( l = l(\alpha) > t_2^2(\alpha) \) and \( t_2(\alpha) \) the second root in magnitude of the equation \( \alpha t^3 - t + 1 = 0 \). Then the following relation holds

\[
q_m - \frac{2q_1 - q_2}{[1 + q_1 - q_2 + 2(q_1 - q_2)^2]^m} \leq mF(\alpha,m)(1-q_1)^2, \tag{10}
\]

with

\[
F(\alpha,m) = 1 + \frac{3}{m} + \left[ \frac{\Gamma(\alpha)}{m} + K(\alpha) \right](1-q_1), \tag{11}
\]

and where \( \Gamma(\alpha) = L(\alpha) + E(\alpha) \) and

\[
K(\alpha) = \frac{n! - 3\alpha}{(1-\alpha)^2} + 2l(1+3\alpha)^2 \frac{3\alpha(2-l\alpha)(1+l\alpha)}{1-(1-\alpha(1+l\alpha))^2}, \tag{12}
\]

\[
\begin{align*}
L(\alpha) & = 3K(\alpha) \left[1 + (1 + 3\alpha^2)[1 + (1 + 3\alpha^2)K(\alpha)\alpha^3] + \alpha^6 K^3(\alpha)\right] + 9\alpha(4 + 3\alpha + 3\alpha^2) + 55.1 \\
E(\alpha) & = \frac{\eta^5}{2(1 - \alpha\eta^2)^4} \frac{1 + (1 - 2\alpha)\eta^4}{(1 - \alpha\eta^2)^2 - \alpha\eta^2(1 - 2\alpha\eta^2)}. \tag{13}
\end{align*}
\]

Let define \( r \in \{2,3\}, \)

\[
Q_r = Q_r(n) = P \left( \bigcap_{k=1}^{r-1} \{ Z_k \leq n \} \right) = P \left( \max_{1 \leq s \leq (r-1)(m_2+1)} \nu_{ts} \leq n \right). \tag{15}
\]

For \( n \) such that \( Q_2(n) \geq 1 - \alpha_1 \geq 0.9 \), we can apply the result in Theorem 1 to obtain the first step approximation

\[
\left| P(S \leq n) - \frac{2Q_2 - Q_3}{[1 + Q_2 - Q_3 + 2(Q_2 - Q_3)^2]^{r_2}} \right| \leq L_2 F(\alpha_1, L_2)(1 - Q_2)^2. \tag{16}
\]

In order to evaluate the approximation in (16) one has to find approximations for the quantities \( Q_2 \) and \( Q_3 \). To achieve this, we will apply for the second time the result in Theorem 1. We define, as in (4), for each \( r \in \{2,3\} \) and \( l \in \{1,2,\ldots,L_1\} \) the sequences

\[
Z^{(r)}_l = \max_{1 \leq s \leq (r-1)(m_2+1)} \nu_{ts}, \tag{17}
\]

As for the sequence \( Z_k \), we deduce that the sequences \( Z^{(r)}_l \) in (17) are stationary, 1-dependent and the following relation holds:

\[
Q_r = P \left( \max_{1 \leq s \leq L_1} Z^{(r)}_l \leq n \right), \quad r \in \{2,3\}. \tag{18}
\]
Denoting, for \( u, r \in \{2, 3\} \)
\[
Q_{ur} = Q_{ur}(n) = \mathbb{P} \left( \bigcap_{l=1}^{u-1} \{ Z_l^{(r)} \leq n \} \right) = \mathbb{P} \left( \max_{1 \leq t \leq (u-1)(m_1+1)} \max_{1 \leq s \leq (r-1)(m_2+1)} u_{ts} \leq n \right) \quad (19)
\]
then, under the supplementary condition that \( Q_{23}(n) \geq 1 - \alpha_2 \geq 0.9 \), we apply Theorem 1 to obtain
\[
\left| Q_r - \frac{2Q_{2r} - Q_{3r}}{1 + Q_{2r} - Q_{3r} + 2(Q_{2r} - Q_{3r})^2} \right| \leq L_1 F(\alpha_2, L_1)(1 - Q_{2r})^2 \quad (20)
\]
Combining (16) and (20) we find an approximation formula for the distribution of the scan statistic depending on the values of \( \{Q_{22}, Q_{23}, Q_{32}, Q_{33}\} \). There are no exact formulas for \( Q_{ur}, \ u, r \in \{2, 3\} \), thus they will be evaluated by Monte Carlo simulation.

For the error computation we have to notice that there are three expressions involved: the first one is the theoretical error \( E_{app} \) obtained from the substitution of (20) in (16) and the other two are simulations errors, one corresponding to the approximation formula \( E_{af} \) and the other to the error formula \( E_{app} \). In what follows we will deal with each of them separately. To simplify the presentation it will be convenient to introduce the following notations;
\[
A(x, y, m) = \frac{2x - y}{[1 + x - y + 2(x - y)^2]^m}, \ \alpha_1 = 1 - Q_3, \ \alpha_2 = 1 - Q_{23},
\]
\[
F_1 = F(\alpha_2, L_1), \ F_2 = F(\alpha_1, L_2), \ R_s = A(Q_{2s}, Q_{3s}, L_1), \ s \in \{2, 3\}.
\]
It is not hard to see (based on mean value theorem in two dimensions) that if \( y_i \leq x_i, \ i \in \{1, 2\} \), then we have the inequality:
\[
|A(x_1, y_1, m) - A(x_2, y_2, m)| \leq m \left[ |x_1 - x_2| + |y_1 - y_2| \right]. \quad (21)
\]
From (16) and (21) we get
\[
|\mathbb{P}(S \leq n) - A(R_2, R_3, L_2)| \leq |\mathbb{P}(S \leq n) - A(Q_2, Q_3, L_2)| + |A(Q_2, Q_3, L_2) - A(R_2, R_3, L_2)| \leq L_2 F_2 (1 - Q_2)^2 + L_2 [|Q_2 - R_2| + |Q_3 - R_3|] \quad (22)
\]
If we substitute (20) in (22) and we take \( B_2 = 1 - R_2 + L_1 F_1 (1 - Q_{22})^2 \), then the theoretical approximation error is given by
\[
E_{app} = L_2 F_2 B_2^2 + L_1 L_2 F_1 \left[ (1 - Q_{22})^2 + (1 - Q_{23})^2 \right] \ . \quad (23)
\]
To compute the simulation error corresponding to the approximation formula let’s denote by \( \hat{Q}_{ur} \) the simulated values of \( Q_{ur} \) for each \( u, r \in \{2, 3\} \). Usually between the true and estimated values we have
\[
\left| Q_{ur} - \hat{Q}_{ur} \right| \leq \beta_{ur}, \quad (24)
\]
Indeed, if $\text{ITER}$ is the number of iterations used in the Monte Carlo simulation algorithm for estimation of $Q_{ur}$ then, one can consider, for example, the bound $\beta_{ur} = 1.96 \sqrt{\frac{Q_{ur}(1-Q_{ur})}{\text{ITER}}}$ with a 95% confidence level. Taking for $r \in \{2, 3\}$, $\hat{Q}_r = A \left( \hat{Q}_{2r}, \hat{Q}_{3r}, L_1 \right)$ to be the simulated values that corresponds to $Q_r$ and applying (19) whenever $\hat{Q}_3 \leq \hat{Q}_2$ we have

$$
\left| A \left( R_2, R_3, L_2 \right) - A \left( \hat{Q}_2, \hat{Q}_3, L_2 \right) \right| \leq L_2 \left[ \left| R_2 - \hat{Q}_2 \right| + \left| R_3 - \hat{Q}_3 \right| \right]
$$

$$
\leq L_1 L_2 \left[ \left| Q_{22} - \hat{Q}_{22} \right| + \left| Q_{23} - \hat{Q}_{23} \right| + \left| Q_{32} - \hat{Q}_{32} \right| + \left| Q_{33} - \hat{Q}_{33} \right| \right].
$$

(25)

From (25) and (24) we obtain the first simulation error

$$
E_{sf} = L_1 L_2(\beta_{22} + \beta_{23} + \beta_{32} + \beta_{33}).
$$

(26)

Finally, introducing

$$
C_{2r} = 1 - \hat{Q}_{2r} + \beta_{2r}, \quad r \in \{2, 3\},
$$

$$
C_2 = 1 - \hat{Q}_2 + L_1(\beta_{22} + \beta_{32}) + L_1 F_1 C_{22}^2,
$$

and substituting them in (23), we get the simulation error associated with the approximation error formula

$$
E_{sapp} = L_2 F_2 C_2^2 + L_1 L_2 F_1 \left[ C_{22}^2 + C_{23}^2 \right].
$$

(27)

Adding the expressions from (23), (26) and (27) we obtain the total error,

$$
E_{total} = E_{sapp} + E_{sf} + E_{sapp}.
$$

(28)

3 Simulation study

In order to illustrate the results presented in Section 2, we consider the following block-factor dependence model. Let $\{Y_{ij} \mid i = 0, \ldots, N_1 + 1, \ j = 0, \ldots, N_2 + 1\}$ be an i.i.d. sequence of Bernoulli r.v.’s with parameter $p$. For each $1 \leq i \leq N_1$ and $1 \leq j \leq N_2$, define the r.v.’s $X_{ij}$ by

$$
X_{ij} = \begin{cases} 
1, & \text{if } Y_{ij} = 1 \text{ and } \sum_{k \in \{-1,0,1\}} Y_{i+k,j+k} \geq 2, \\
0, & \text{otherwise.}
\end{cases}
$$

(29)

The model in (29) is a particular case of (3). Obviously $X_{ij}$’s are dependent Bernoulli r.v.’s with parameter $p' = p \left[ 1 - (1-p)^8 \right]$. A success of $X_{ij}$ occurs each time when $Y_{ij} = 1$ and there is at least one success in its neighborhood (horizon one).

In our setting we consider the scanning window of size $m_1 \times m_2 = 4 \times 6$ and the region to be scanned of size $53 \times 75$ ($L_1 = L_2 = 10$). The numerical results
presented in Table 1 corresponds to \( p \in \{0.01, 0.1\} \). The second column in Table 1 (\( \text{Sim Dep} \)) corresponds to the estimate of \( P(S \leq n) \) with \( 10^5 \) trials. The column Approx Dep presents the approximations obtained by our methodology. Columns 4 – 6 are the associated errors computed in Section 2 with \( ITER = 10^9 \). We compare the dependent model in (29) with the Bernoulli independent model with parameter \( p' \) using the results in Haiman and Preda [7]. The results are presented in the last two columns of Table 1. Figure 3 presents the ecdf of the scan statistic computed by simulation (\( \text{Sim Dep} \) and \( \text{Sim Indep} \)).

<table>
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<th>( n )</th>
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<th>( \text{Approx Dep} )</th>
<th>( E_{\text{app}} )</th>
<th>( E_{\text{sim}} )</th>
<th>( E_{\text{total}} )</th>
<th>( \text{Sim Indep} )</th>
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Table 1. Values for \( P(S \leq n) \) when \( m1 = 4, m2 = 6, L1 = 10, L2 = 10, ITER = 10^9 \)

![ECDF for dependent and independent scan statistics](image)

**Fig. 3.** Empirical cumulative distribution functions for \( p = 0.1 \).
References

Conditional density estimation based on a clustering procedure

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Abstract. This paper deals with nonparametric estimation of conditional densities in mixture models. The proposed approach consists to perform a preliminary clustering algorithm to guess the mixture component of each observation. Conditional densities of the mixture model are then estimated using kernel density estimates applied separately to each cluster. We investigate the expected $L_1$-error of the resulting estimates with regards to the performance of the clustering algorithm. In particular, we prove that these estimates achieve optimal rates over classical nonparametric density classes under mild assumptions on the clustering method used. Finally, we offer examples of clustering algorithms verifying the required assumptions.

Keywords: Nonparametric estimation, mixture models, clustering.

1 Introduction

Finite mixture models are widely used to account for population heterogeneities. In many fields such as biology, econometrics as well as social sciences, experiments are based on the analysis of a variable characterized by a different behavior depending on the group of individuals. A natural way to modeling heterogeneity for a real random variable $Y$ is to use a mixture model to characterize its density as

$$f(y) = \sum_{i=1}^{M} \alpha_i f_i(y), \quad y \in \mathbb{R}. \quad (1)$$

Here $M$ is the number of subpopulations, $\alpha_i$ and $f_i$ are respectively the mixture proportion and the probability density function of the $i^{th}$ subpopulation. We refer the reader to \cite{7,12,13} for a broader picture of mixture density models as well as for practical applications.

When the model (1) is identifiable, the statistical problem consists to find efficient estimates of the mixture proportions $\alpha_i$ and the density functions $f_i$. In the parametric case, some algorithms have been proposed such as maximum likelihood techniques (see \cite{15}) as well as Bayesian approaches (\cite{2,6}). When
the \( f_i \)'s belong to some nonparametric families, it is often assumed that training data are observed, \textit{i.e.}, the component of the mixture from which \( Y \) is distributed is available. In that case, the model is identifiable and some algorithms allow to estimate both the \( \alpha_i \)'s and the \( f_i \)'s (see \cite{3,8,9}). However, as pointed out by \cite{10}, inference in mixture nonparametric density models becomes more difficult without training data. These authors introduce consistent nonparametric estimators of the marginal distribution in a multivariate setting.

The framework we consider lies between the two above situations. More precisely, training data are not observed but we assume to have at hand some covariates that may provide information on the components of the mixture from which \( Y \) is distributed. Our approach consists to perform a preliminary clustering algorithm on these covariates to guess the mixture component of each observation. Density functions \( f_i \) are then estimated using a nonparametric density estimate based on the prediction of the clustering method.

Many authors have already proposed to perform a preliminary clustering step to improve density estimates. \cite{17} conduct a comprehensive simulation study to conclude that a preliminary clustering using the EM algorithm allows to some extent to improve performances of some density estimates (see also \cite{11}). However, to our knowledge, no work has been devoted so far to measure the effects of the clustering algorithm on the resulting estimates of the distribution functions \( f_i \). This work proposes to fill this gap, studying the \( L_1 \)-error of these estimates in terms of the performances of the clustering method used. In particular, we prove that these estimates achieve optimal rates over classical nonparametric density classes under mild assumptions on the clustering method used.

The paper is organized as follows. In Section 2, we present the statistical problem. In Section 3, we present the two-step estimator and give the main results. We finally provide an example of clustering algorithm and study its performances for disjoint connected compact supports in Section 4.

\section{The statistical problem}

Our focus is on the estimation of conditional densities in a univariate mixture density model. Formally we let \((Y, I)\) be a random vector taking values in \( \mathbb{R} \times [1, M] \) where \( M \geq 2 \) is a known integer. We assume that the distribution of \( Y \) is characterized by a density \( f \) defined, for all \( t \in \mathbb{R} \), by

\[
  f(t) = \sum_{i=1}^{M} \alpha_i f_i(t),
\]

where, for all \( i \in [1, M] \), \( \alpha_i = \mathbb{P}(I = i) \) are the prior probabilities (or the weights of the mixture) and \( f_i \) are the densities of the conditional distributions \( \mathcal{L}(Y | I = i) \) (or the components of the mixture).

If we have at hand \( n \) observations \((Y_1, I_1), \ldots, (Y_n, I_n)\) drawn from the distribution of \((Y, I)\) one can easily find efficient estimates for both the \( \alpha_i \)'s and the
$f_i$'s. For example, if we denote $N_i = \# \{ k \in [1,n] : I_k = i \}$, we can estimate $\alpha_i$ using the empirical proportion $\hat{\alpha}_i = N_i/n$ and $f_i$ using the kernel density estimate $\hat{f}_i$ defined for all $t \in \mathbb{R}$ by

$$f_i(t) = \frac{1}{N_i} \sum_{k=1}^{n} K_h(t,y_k)\mathbb{I}(I_k)$$

if $N_i > 0$ and $\hat{f}_i(t) = 0$ otherwise. Here $K : \mathbb{R} \to \mathbb{R}$ is a kernel such that $\int K = 1$, $h > 0$ is a bandwidth and

$$K_h(t,y) = \frac{1}{h} K \left( \frac{t-y}{h} \right),$$

is the classical convolution kernel located at point $t$ (see [14] and [16] for instance). Observe that $\hat{f}_i$ is just the classical kernel density estimate defined from observations in the $i$th subpopulation. It follows that, under classical assumptions regarding the smoothing parameter $h$ and the kernel $K$, $\hat{f}_i$ has similar properties as those of the well-known kernel density estimate. In particular, its expected $L_1$-error

$$\mathbb{E}\|f_i - \hat{f}_i\|_1 = \mathbb{E} \int_{\mathbb{R}} |f_i(t) - \hat{f}_i(t)|dt$$

achieves optimal rates when $f_i$ belongs to regular classes of densities such as Hölder or Lipschitz classes (see [4]).

Things turn out to be more complicated when the random variable $I$ is not observed. This is typically the case in mixture density model estimation. In this situation, $\hat{\alpha}_i$ and $\hat{f}_i$ are not computable and one has to find another way to define efficient estimates for both $\alpha_i$ and $f_i$. In this work, we assume that one can obtain information on $I$ through an other covariate $X$ which takes values in $\mathbb{R}^d$ where $d \geq 1$. This random variable is observed and its conditional distribution $\mathcal{L}(X | I = i)$ is characterized by a density $g_i = g_{i,n} : \mathbb{R}^d \to \mathbb{R}$ which could depend on $n$. The statistical problem with which we are faced is now to estimate both the components and the weights of the mixture based on the observations $(Y_1,X_1), \ldots, (Y_n,X_n)$ extracted from a $n$-sample $(Y_1,X_1,I_1), \ldots, (Y_n,X_n,I_n)$ randomly drawn from the distribution of $(Y,X,I)$.

3 Performances of a two-step estimator

To summarize the model so far, we observe a sample $(Y_1,X_1), \ldots, (Y_n,X_n)$ of random pairs extracted from $(Y_1,X_1,I_1), \ldots, (Y_n,X_n,I_n)$ and our goal is to estimate densities $f_i$ of the conditional distribution $\mathcal{L}(Y | I = i)$ for all $i \in [1,M]$. We propose the following two-step algorithm.

- First, we split the sample $X_1, \ldots, X_n$ into $M$ clusters to estimate the label $I_k$ of each observation $X_k$;
- Last, the conditional densities $f_i$'s are estimated using kernel density estimates in each cluster.
Formally, we first split the sample \( X_1, \ldots, X_n \) into \( M+1 \) clusters \( X_0, X_1, \ldots, X_M \) such that \( X_i \neq \emptyset \) for all \( i \in \{1, M\} \) according to a given clustering method. The clusters \( X_0, X_1, \ldots, X_M \) satisfy

\[
\bigcup_{i=0}^{M} X_i = \{X_1, \ldots, X_n\} \quad \text{and} \quad \forall i \neq j, \ X_i \cap X_j = \emptyset.
\]

We do not specify the clustering method here but provide an example in section 4. Observe that we define \( M+1 \) clusters instead of \( M \). The cluster \( X_0 \) (which could be empty) contains the observations for which the clustering procedure is not able to predict the label. For example, if the clustering procedure reveals some outliers, they are collected in \( X_0 \) and we do not use these outliers to estimate the \( f_i \)'s.

Once the clustering step is performed, we define the predicted labels \( \hat{I}_k, k \in [1, n] \) as

\[
\hat{I}_k = \hat{I}(X_k) = \begin{cases} i & \text{if } X_k \in X_i \\ 0 & \text{otherwise.} \end{cases}
\]

Remark that if \( I_k = i \) then \( X_k \) is not correctly affected to its group with probability

\[
P(X_k \notin X_i|I_k = i) = \mathbb{P}(\hat{I}_k \neq i|I_k = i).
\]

So the maximal misclassification error

\[
\phi_n = \max_{1 \leq k \leq n} \max_{1 \leq i \leq M} \mathbb{P}(\hat{I}_k \neq i|I_k = i).
\]  (4)

measures the performance of the clustering procedure. This misclassification error \( \phi_n \) will be evaluated in the example discussed in section 4.

We are now in position to define the estimates of both the \( \alpha_i \)'s and the \( f_i \)'s. The prior probabilities \( \alpha_i \) are estimated by

\[
\hat{\alpha}_i = \frac{\hat{N}_i}{n} \quad \text{where} \quad \hat{N}_i = \#\{k \in [1, n] : \hat{I}_k = i\}.
\]

For the conditional densities \( f_i \), we consider the kernel density estimator with kernel \( K : \mathbb{R} \to \mathbb{R} \) and bandwidth \( h > 0 \) defined by

\[
\hat{f}_i(t) = \frac{1}{\hat{N}_i} \sum_{k, Y_k \in X_i} K_h(t, Y_k) = \frac{1}{\hat{N}_i} \sum_{k=1}^{n} K_h(t, Y_k) \mathbb{1}_{(i)}(\hat{I}_k),
\]

where \( K_h \) is defined in (3). Observe that since for all \( i \in [1, M] \) the clusters \( X_i \) are nonempty, the estimates \( \hat{f}_i \) are well defined.

The kernel estimates \( \hat{f}_i \) are defined from observations in cluster \( X_i \). The underlying assumption is that, for all \( i \in [1, M] \), each cluster \( X_i \) collects almost all of the observations \( X_k \) such that \( Y_k \) is drawn from \( f_i \). Under this assumption, \( \phi_n \) is expected to be small and \( \hat{f}_i \) to be closed to the “ideal” estimates \( \hat{f}_i \) defined by equation (2). The following Theorem compares the expected \( L_1 \)-error of \( \hat{f}_i \) and \( \hat{f}_i \). In other words, it allows to measure the effects of the clustering method with regards to the performances of \( 
\hat{f}_i \).
Theorem 1 There exist positive constants $A_1 - A_4$ such that, for all $n \geq 1$ and $i \in [1, M]$

$$\mathbb{E}\|\hat{f}_i - f_i\|_1 \leq \mathbb{E}\|\bar{f}_i - f_i\|_1 + A_1 \varphi_n + A_2 \exp(-n)$$

and

$$\mathbb{E}|\hat{\alpha}_i - \alpha_i| \leq A_3 \varphi_n + A_4 \sqrt{n}.$$

We emphasize that inequality (5) is non-asymptotic, that is, the bound is valid for all $n$. We can first remark that if we intend to prove any consistency results regarding $\hat{f}_i$ and $\hat{\alpha}_i$, the misclassification error $\varphi_n$ should tend to zero. Moreover, inequality (5) says that if the misclassification error $\varphi_n$ tends to zero much faster than the $L_1$-error of $\bar{f}_i$, then we have asymptotically a performance that is guaranteed to be equivalent to the performance of the “ideal” estimate $\bar{f}_i$. The $L_1$-error of $f_i$, with properly chosen bandwidth $h$, is known to go to zero, under standard smoothness assumptions, at the rate $n^{-s/2s+1}$ where $s > 0$ is typically an index which represents the regularity of $f_i$. For example, when we consider Lipschitz or Hölder classes of functions, $s$ corresponds to the number of absolutely continuous derivatives of the functions $f_i$. In this context, when $\varphi_n = o(n^{-s/2s+1})$, the estimates $\hat{f}_i$ achieve the rate

$$\mathbb{E}\|\hat{f}_i - f_i\|_1 = O(n^{-s/2s+1}).$$

4 A clustering procedure for support disjoint densities

In this section, we propose an automatic clustering procedure and we study its performances for support disjoint densities. More precisely, we assume that supports $S_{i,n} \subset \mathbb{R}^d$ of $g_{i,n}$ are disjoint connected compact sets and we denote by

$$\delta_n = \min_{1 \leq i \neq j \leq M} d(S_{i,n}, S_{j,n})$$

the minimum Euclidean distance between these supports. Given $n$ i.i.d. observations $X_1, \ldots, X_n$ drawn from $g_n(x) = \sum_{i=1}^M \alpha_i g_{i,n}(x)$, the goal is to split $\{X_1, \ldots, X_n\}$ into $M$ clusters $X_1, \ldots, X_M$ such that the probability of the events $\{X_i \subset S_{i,n}\}$ is close to one as $\delta_n$ decreases to zero. In such a situation, one can expect the misclassification error associated with this clustering algorithm to be close to zero.

4.1 The clustering procedure

The method we propose is based on density support estimation tools developed by [5] and [1]. The main idea is to find a data-driven procedure to choose a radius $\hat{r}_n > 0$ such that the set

$$\bigcup_{k=1}^n B(X_k, \hat{r}_n)$$

is...
has exactly \( M \) connected components. Here \( B(x, r) \) stands for the closed Euclidean ball with center \( x \in \mathbb{R}^d \) and radius \( r > 0 \). Cluster \( X_i \) will then be naturally composed by observations \( X_k \) which belongs to the \( i \)th connected components of the set (7). We need to find on optimal way to select \( \hat{r}_n \) from the observations \( X_1, \ldots, X_n \).

To this aim, we define for each positive real number \( r \) the \( n \times n \) matrix \( A_r = (A_{k,\ell})_{1 \leq k,\ell \leq n} \) by

\[
A_{k,\ell} = \begin{cases} 
1 & \text{if } \|X_k - X_\ell\|_2 \leq 2r \iff B(X_k, r) \cap B(X_\ell, r) \neq \emptyset \\
0 & \text{otherwise.} 
\end{cases}
\]  

(8)

This matrix induces a non-orientated graph on the set \([1, n] \) and we say that two different observations \( X_k \) and \( X_\ell \) belong to the same cluster if \( k \) and \( \ell \) belong to the same connected component of the graph. We let \( \hat{M}_r \) be the number of connected components of the graph and we denote by \( X_1(\hat{r}_n), \ldots, X_{\hat{M}_r}(\hat{r}_n) \) the associated clusters. We select the radius as follows

\[
\hat{r}_n = \inf \{ r > 0 : \hat{M}_r \leq M \}.
\]

Note that \( \hat{r}_n \) is well defined since the random set \( \mathcal{R}_M = \inf \{ r > 0 : \hat{M}_r \leq M \} \) is lower bounded (by 0) and non-empty since \( r^* = \max_{k,\ell} \|X_k - X_\ell\|_2 \) always belongs to this set (\( \hat{M}_r \cdot r = 1 \)). Moreover, one can easily prove that \( M_{\hat{r}_n} = M \) almost surely when \( n \geq M \). We denote by \( X_1(\hat{r}_n), \ldots, X_M(\hat{r}_n) \) the \( M \) clusters induced by \( A_{\hat{r}_n} \) and the goal is now to study the misclassification error (4) of this clustering algorithm.

### 4.2 Basic assumptions

To study the misclassification error of the proposed clustering algorithm, we need the following assumptions.

#### Assumption 1

The density \( g_n(x) = \sum_{i=1}^{n} \alpha_i g_{i,n}(x) \) is bounded away from zero on its support. We define the sequence \( (t_n)_n \) by

\[
t_n = \inf_{x \in S_n} g_n(x) > 0 \quad \text{where} \quad S_n = \bigcup_{i=1}^{M} S_{i,n}.
\]

#### Assumption 2

Let

\[
r_n^d = \frac{(\log n)^2}{nM}.
\]

There exists a family of \( N \in \mathbb{N}^* \) Euclidean balls \( \{B_\ell\}_{\ell=1, \ldots, N} \) with radius \( r_n/2 \) and two positive constants \( c_1 \) and \( c_2 \) such that

\[
\begin{align*}
S_n &\subset \bigcup_{\ell=1}^{N} B_\ell \\
\text{Leb}(S_n) &\geq c_1 \sum_{\ell=1}^{N} \text{Leb}(S_n \cap B_\ell) \\
\forall \ell = 1, \ldots, N, \quad \text{Leb}(S_n \cap B_\ell) &\geq c_2 r_n^d.
\end{align*}
\]
where Leb denotes the Lebesgue measure on $\mathbb{R}^d$.

Assumption 1 implies that densities $g_{i,n}$ do not vanish on the interior of the supports $S_{i,n}$. This assumption ensures that, for $n$ large enough and a safe choice of radius $r$, all points $X_k \in S_{i,n}$ belong to the same connected component of the graph induced by the $n \times n$ matrix $A'$ defined in (8). Assumption 2 is more technical and is concerned with the diameter and the regularity of supports $S_{i,n}$. Roughly speaking, recall that our approach identify the supports $S_{i,n}$ by the connected components of $\bigcup_{k=1}^{n} B(X_k, r)$. It means that when the diameter of $S_{i,n}$ increases, large values or radius $r$ are necessary to connect observations in $S_{i,n}$. However for too large values of $r$, the number of connected components of $\bigcup_{k=1}^{n} B(X_k, r)$ becomes smaller than $M$ and the method fails. Consequently, we need to constraint the diameter of $S_{i,n}$. This is ensured by assumption 2 since it implies that $S_n$ can be covered by $N \leq n c_1 c_2 (\log n)^{2/d}$.

Finally, inequality $\text{Leb}(S_n \cap B_r) \geq c_2 r^d n$ in assumption 2 can be seen as a regularity constraint on $S_n$. In particular, it allows to avoid too sharp boundaries for the support $S_n$.

### 4.3 The misclassification error

The algorithm described in section 4.1 gives a partition of $\{X_1, \ldots, X_n\}$ into $M$ clusters $X_1(\hat{r}_n), \ldots, X_M(\hat{r}_n)$. The following theorem provides an upper bound for the misclassification error $\varphi_n$ of this clustering procedure.

**Theorem 2** Assume that Assumption 1 and Assumption 2 hold. Moreover, if

$$\delta_n > 2r_n = 2 \left( \frac{(\log n)^2}{nt_n} \right)^{1/d}$$

then, after a possible rearrangement of the indices, we can define $\hat{I}_k = i \iff X_k \in X_i(\hat{r}_n)$ such that for all $a > 0$ with $\log n \geq (1 + a)/c_2$, we have

$$\varphi_n = \max_{i=1, \ldots, M} \max_{k=1, \ldots, n} P(\hat{I}_k \neq i | I_k = i) \leq A_6 n^{-a}$$

where $A_6$ is positive constant.

This theorem establishes that the misclassification error of the proposed clustering procedure tends to zero at a polynomial rate. In particular, using Borel-Cantelli lemma, it implies that $\hat{I}_k = I_k$ almost surely for $n$ large enough, i.e., all the predictions are correct for $n$ large enough. Inequality (10) gives the minimum distance between the supports $S_{i,n}$ to make the clustering method efficient. Observe that this minimum distance could tend to zero as the sample size increases. For example, when $d = 1$ and $g_n(x) \geq c/n^\gamma$ with $\gamma \in [0, 1]$, inequality (11) holds provided $\delta_n$ tends to zero much slower than $(\log n)^2/n^{1-\gamma}$.
Remark 1 Even if the rate of convergence (11) does not depend on the dimension $d$, the curse of dimensionality appears in Theorem 2. Indeed, the minimum distance $\delta_n$ clearly increases with the dimension $d$. Consequently, even if we can obtain fast rates in large dimension, the assumption (10) becomes stronger as the dimension $d$ increases.

References

Cluster Model Selection using Minimum Cost Spanning Trees

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Abstract. Cluster model selection, often manifested as determination of the suitable number of clusters, is a crucial and ill-posed challenge in cluster analysis. Although many approaches have been proposed for solving this problem, none stands out as being the most effective for a general-purpose model selection problem. Our approach presented here is based on the perception that samples drawn from the source population have to be well mixed in the clusters if the model is correctly chosen. Consequently, their clustered occurrences can be interpreted as independent realizations of the same random variable. A natural tool to measure the realizations’ closeness is provided by simple probability metrics or two sample test multivariate statistics. In this paper we propose a method for cluster model selection, which is based on the minimum cost spanning tree approach. Our method is founded on a modified version of the Friedman and Rafsky two sample test which takes into account the edges’ lengths. This Minimal Spanning Tree based test is intended to determining whether two sets of data originate from the same source. In our modified version of Friedman-Rafsky’s algorithm, the statistic $J(x)$ uses not only the number of edges that connect points from different samples in a Minimal Spanning Tree that is constructed for each of the clusters, but also edge lengths in determining the suitability of a subset. Our approach for determining the number of clusters is summarized in a short Meta-algorithm. We then show how we adopted that meta-algorithm in the clustering process, in order to formulate our proposed approach to the cluster model selection. Finally, we present results of several numerical experiments which imply the ability of the suggested model to detect the true number of clusters.

Keywords: Clustering, Cluster Stability, Two sample test.

1 Introduction

The goal of clustering is to divide a given data set into distinct groups of objects, where similarity between objects belonging to the same group is much higher of than between objects that belong to other groups. Two types of methods are identified in the clustering process. First, the clustering method (or algorithm
type, e.g.: K-means), deals with finding of partition in the data elements into a certain number of clusters. No additional external information is available for such clustering procedure. The second type includes validation methods, aimed at determining the optimal (or "correct") number of clusters in the dataset. The general problem called cluster model selection involves evaluating the possible clustering solutions according to predefined rules and determining the optimal number of clusters as the one which yields the optimal result. This model selection problem is a crucial and ill-posed challenge in cluster analysis. Many approaches have been proposed for solving this problem. They are not reviewed here for space limitation reasons. However, we note that it has been proved difficult to assess the compatibility of any specific approach and none stands out as being the most effective for general-purpose model selection problem.

Attempting to breakthrough in a particular direction, we base our approach presented here on the perception that samples drawn from the source population have to be well mixed in the clusters if the model is correctly chosen. Consequently, their clustered occurrences can be interpreted in this case as independent realizations of the same random variable. A natural tool to measure the realizations’ closeness provides by simple probability metrics or two sample test multivariate statistics. This general point of view has been proposed in previous authors’ papers. We refer to Volkovich et al. [14] paper where a general cluster stability methodology was introduced in order to reformulate many existing approaches from a new generic point of view and to offer a new cluster stability criteria. Clustered samples elements are considered in the framework of this methodology as realizations of random variables such that the partition quality is measured by probability metrics between these instances. The perception suggests a statistical homogeneity, of the clustered samples, in the case of the "correct" number of clusters. I.e., it is presumed that sample occurrences in a cluster appear to be, in this situation, independent realizations of the same random variable. This point of view conceptually generalizes several methods, introduced in [9], [6], [7] and [10]. This general cluster stability methodology has been implemented in several ways by [13], [1], [11], [15] and [12], applications of variants of the goodness of fit tests based on the "well mingled samples" concept in the case of the "correct" number of clusters were implemented.

A geometrical stability of a partition was considered in [15] and [1] with respect to inner stability model based on the Friedman and Rafsky two sample test statistic [4]. This statistic is expressed by the number of edges that connect points from different samples in the Minimal Spanning Tree (MST) that is constructed for each of the clusters. This number is sufficiently large if the samples, within each cluster, are well mingled. Under this null hypothesis on the homogeneity of the source data, this statistic is approximately normally distributed. So, the case of well mingled samples within the clusters leads to a normal distribution of the considered statistic. It means that, a provided stability model assumes a normal distribution of the mentioned amount and a similarity of the actual distribution to a normal one exhibits cluster goodness.
However, the edges' lengths are totally ignored that can lead to inaccurate conclusions in cases of partitions with overlapping clusters.

In this paper we propose a method for cluster model selection, which is based on the minimum cost spanning tree approach. Our method is founded on a modified version of the Friedman and Rafsky two sample test which takes into account the edges' lengths. This Minimal Spanning Tree based test is intended to determining whether two sets of data originate from the same source. A tree is constructed across the data from two sources such that edges which join samples of different data sets are removed. So, if many edges are detached, then the two samples are expected to originate from the same source. However, the edges' lengths are ignored. This modified version additionally suggests in the case of well mingled a large number of short edges connecting samples of the same class and a small number of long edges connecting samples of different sets. This measure is expected to perform better; on the other hand it can be more sensitive to the data outliers. Thus we initially smooth the data in order to reduce the outliers' impact.

The rest of the paper is organized in the following way: section 2 is devoted to establishing the initial modification to the Friedman and Rafsky statistic. In section 3 we present the application of the proposed new method to the modified algorithm. Section 4 includes a description of the numerical experiments conducted in order to test the ability of our methodology to find the "correct" number of clusters. We conclude with a general discussion and outlook in section 5.

2 The Enhanced Friedman-Rafsky MST two-sample test

As mentioned earlier, a cluster stability model is based here on the Friedman-Rafsky MST two-sample test within the general methodology stated in [14]. Recall that a spanning tree is a graph which reaches out to all \( n \) vertices of the graph and has no loops. Among all the spanning trees of a weighted and connected graph, the one (or possibly more) with the least total weight is called a Minimal Spanning Tree (MST). A MST can be built in \( O(n^2) \) time (including distance calculations) using the Prim’s, Kruskal’s, Borůvka’s or Dijkstra’s algorithms (e.g., [8]). MSTs are widespread for several reasons: they can be quickly and easily computed, and they are capable to create sparse sub-graphs which reflect some essence of the given set.

To apply The Friedman-Rafsky’s test we consider \( S = S_1 \cup S_2 \) the disjoint union of the samples \( S_1 := \{z(1), z(2), ..., z(n)\} \) and \( S_2 := \{z(n+1), z(n+2), ..., z(n+m)\} \). Let \( D := \{d_{ij} = d(z^{(i)}, z^{(j)}) \mid i, j = 1, 2, ..., n + m\} \) be the Euclidean distances between all points of \( S \). If all values of \( d_{ij} \) are distinct, then the set is called nice. For the nice set a unique MST exists. On this MST, we define a test statistic \( R_{mn} \) which equals to the number of the MST elements connecting points belonging to different samples. Friedman and Rafsky actually offered the statistic \( 1 + R_{mn} \), which counts the number of disjoint sub-trees resulting from removing all edges that unite vertices of different samples. Henze and Penrose [5] analyzed the asymptotic behavior of \( R_{mn} \).
Our approach suggests to use the modified Friedman-Rafsky statistic offered in [3] and defined by

\[ J(x) = 0.5 \cdot \left( 1 - \frac{NEB}{NEB + NEW} + \frac{Avg(LEB)}{Avg(LEB) + Avg(LEW)} \right), \quad (1) \]

where

- \( NEB \) denotes the cardinality of the set of edges which connect elements of different samples;
- \( NEW \) denotes the cardinality of the set of edges which connect elements of the same sample;
- \( LEB \) denotes the total lengths of edges connecting points from different samples;
- \( LEW \) denotes the total lengths of edges connecting points from the same sample;
- \( Avg(e) \) denotes the function on the set of edges \( e \) which returns the average of the lengths of the edges in the set \( x \).

The statistic \( J(x) \) uses not only the number of edges connecting points from different samples in a Minimal Spanning Tree (MST) constructed for each of the clusters but also edge lengths in determining the suitability of a subset. A good subset will have a large number of short edges connecting samples of the same class and a small number of long edges connecting samples of different classes.

Meta-algorithm for determining the number of clusters can be described as follows.

- Pairs of samples are drawn from the data source and the clusters obtained from each one of the samples are assessed;
- A Minimal Spanning Tree is constructed in each cluster in order to obtain edges that connect points originating from both samples;
- The modified Friedman-Rafsky statistics is calculated, aiming to construct its empirical distribution for any number of clusters in the considered range;
- The true number of clusters is obtained according to the calculated distribution which is mostly concentrated at the origin.

### 3 The Model Selection Procedure

In this section we describe how we adopted the meta-algorithm presented above in the clustering process, in order to formulate our proposed approach to the cluster model selection.

**Input parameters:**

- \( X \) – the dataset;
- \( c \) – the tested number of clusters;
- \( C^* \) – the maximal number of clusters to be tested;
• $T$— number of the drawn samples;
• $m$— the samples size;
• $K$— the number of the neighbors in KNN method.

Output:

• $\tilde{c}$— an estimated number of clusters in the dataset.

1. In order to overcome the noise sensitivity of the MST method and minimize the impact of outliers by improving the geometric structure of the data collection we construct a smoothen version $\tilde{X}$ of the original dataset $X \subseteq R^d$. This is achieved by using the $K$–NearestNeighbors approach (KNN) and replacing each point $x$ by the average of its $K$ Nearest Neighbors $\bar{x}$.

2. We draw samples $S_1$ and $S_2$ from the smoothened version data source $\tilde{X}$ and assess the clusters with reference to each of the drawn samples.

3. The samples which are used in the Friedman-Rafsky MST test have to be independent. To provide it we model the samples occurrences in the clusters with the help of clustering algorithm rerunning, as was offered by the second simulation method described in [14].

4. We apply $k$-means algorithm clustering algorithm to obtain a partition $\Pi_k(S)$ of the simulated union $S = S_1 \cup S_2$ into $c$ clusters and construct a minimal spanning tree (MST) within each cluster. Note that drawbacks of the $k$-means algorithm together with the complexity of the dataset structure add to the uncertainty of the process outcome. To overcome this ambiguity, a sufficient quantity of data has to be used. This is achieved by drawing many pairs of samples (denoted here by $T$).

5. We quantify the goodness of the partition by calculating for each cluster $i = 1, 2, ..., c$ the modified Friedman-Rafsky’s index score $J_i(x)$ according to equation (1).

6. The partitions quality is represented by its worst cluster corresponding to the maximal score value obtained $J^{(c)}(x) = \max_{1 \leq i \leq c} J_i(x)$.

7. We study the series of values $J^{(c)}(x)$; $1 \leq t \leq T$ (Recall that $T$ denotes the number of drawn pairs of samples for a given number of clusters $c$).

8. It is natural to expect that the correct number of clusters is delivered by the distribution of $J^{(c)}(x)$; $2 \leq c \leq C^*$ ($C^*$ denote the maximal number of possible clusters to be examined) that is most concentrated at the origin because well mixed samples in the clusters produce small values of the employed statistics $J$. 
4 Numerical Experiments

In order to evaluate the ability of our proposed methodology, we have carried out several numerical experiments on synthetic and real datasets. Due to space limitations we demonstrate the performance of our methodology by comparing our experiments results to the known structure, of three datasets. We have set $C^*$, in all the tests, and ran 10 trials for each experiment. The results are presented by the error-bar plots of the sample percentiles mean within the trials. The sizes of the error bars are equal to two standard deviations, found inside the trials of the results. For clustering, the standard version of the k-means algorithm has been used.

4.1 Synthetic Data

The synthesized dataset is a mixture of five two dimensional Gaussian distributions with independent coordinates owning the standard deviation $\sigma = 0.2$. Mean values of the components are placed on the unit circle on the angular neighboring distance $2\pi/5$. The dataset contains 1000 items. Using our method with the parameters: $T = 200$, $m = 300$ and $K = 10$, we succeeded to find the true number of clusters, as shown in figure 1.

![Fig. 1. Error-bar plot of the percentiles for the synthetic dataset.](image)

4.2 Three text collection dataset

This dataset has been obtained from the text collection $http://ftp.cs.cornell.edu/pub/smart/$. It includes the following three text collections:

- DC0–Medlars Collection (1033 medical abstracts);
- DC1–CISI Collection (1460 information science abstracts);
- DC2–Cranfield Collection (1400 aerodynamics abstracts).

Following the well-known ”Bag of Words” method, 600 best terms were selected (see, [2] for term selection details). So, the dataset was mapped into Euclidean spaces with dimensions 600. A dimension reduction is provided by
the Principal Component Analysis (PCA). The considered dataset is recognized to be well-separated by means of the two leading principal components. We use this data representation in our experiments. Here we choose $T = 200$, $m = 400$ and $K = 10$. Figure 2 depicts the results and exhibits that a three cluster configuration is properly determined.

![Fig. 2. Error-bar plot of the percentiles for the Three text collection dataset.](image)

### 4.3 The Iris Flower Dataset

Another considered real dataset is the well-known Iris flower dataset or Fisher’s Iris dataset available, for example, at [http://archive.ics.uci.edu/ml/datasets/Iris](http://archive.ics.uci.edu/ml/datasets/Iris). The collection includes 50 items presented by four features originated from each of three species of Iris flowers:

- 0 - Iris Setosa;
- 1 - Iris Versicolour;
- 2 - Iris Virginica.

These species compose three clusters situated in a manner that one cluster is linearly separable from the others, but the other two are not. This dataset was analyzed in many papers. A two cluster structure was detected in [9]. As can be seen in figure 3, the true cluster structure has been detected with the parameters $T = 100$, $m = 50$ and $K = 5$.

### 5 Summery and Conclusions

In this paper we propose a new method for cluster model selection, which is based on the minimum cost spanning tree analysis. Our method is founded on a modified version of the Friedman and Rafsky two sample test [4]. We modified the Friedman-Rafsky statistic (which originally expresses the number of edges that connect points from different samples in the Minimal Spanning Tree ($MST$) that is constructed for each of the clusters) to takes into account the edges’ lengths, as we believe it would perform better. According to our proposed method, pairs of samples are drawn from the smoothened version of the data.
source and for each cluster in the partition of the simulated union of those samples we construct a MST. The value of the modified Friedman and Rafsky statistics are calculated in each clusters aiming to construct its empirical for each considered number of clusters. We have conducted several experiments in order to validate our proposed clustering methodology. The results show that it performs well on several known datasets. As continued research we intend to perform additional numerical experiments to examine the stability of the suggested method for additional simulated and real databases and compare the results obtained with those obtained for other known methods, in particular those based on the use of the standard Friedman-Rafsky MST two-sample test described in section 2.

References


Survey of the Euro Currency Fluctuation by Using Data Mining

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Abstract. Data mining or Knowledge Discovery in Databases (KDD) is a new field in information technology that emerged because of progress in creation and maintenance of large databases by combining statistical and artificial intelligence methods with database management. Data mining is used to recognize hidden patterns and provide relevant information for decision making on complex problems where conventional methods are inefficient or too slow. Data mining can be used as a powerful tool to predict future trends and behaviors, and this prediction allows making proactive, knowledge-driven decisions in businesses. Since the automated prospective analyses offered by data mining move beyond the analyses of past events provided by retrospective tools, it can answer the business questions which are traditionally time consuming to resolve. Based on this great advantage, it provides more interest for the government, industry and commerce. In this paper we have used this tool to investigate the Euro currency fluctuation. For this investigation, we have three different algorithms: K*, IBK and MLP and we have extracted Euro currency volatility by using the same criteria for all used algorithms. The used dataset has 21,084 records and is collected from daily price fluctuations in the Euro currency in the period of 10/2006 to 04/2010.

Keywords: Euro Currency Fluctuation, Data Mining, Stock Market, Knowledge Discovery in Databases.

1 Data Mining

The act of data mining is divided into several marked stages database. in this paper we confine to introduce and a brief description of each of these steps:

1. Define the problem.
2. Data recognition:
   • Data warehouse formation: This stage is where performed for the formation of continuous and integrated environments are performed in order to perform the next steps and data mining on it. In general, the data warehousing is continuous; collection and classified constantly changing and a new is dynamic that ready to explore.
   • Data Selection at this stage, in order to reduce costs of data mining operations, data that have been studied are selected from the database. Data mining aims to give results about them. Data conversion: is determined for data mining operations and should be performed on
necessary transformations for certain data. These transformations may be very convenient and concise as byte to integer conversion or very complex and time consuming with high costs, such as defining new attributes and extracting or converting data from string values.

3. Pre-processing.
4. Explore in data: at this stage the data mining is done. At this stage data is being explored by using data mining techniques. What is extracted is hidden knowledge of them and modeling is done.
5. Results Interpretation: At this stage, results and patterns offered by data mining tools investigated and useful results is determined. Also used in data mining, are genetic algorithms and neural networks. Neural networks are used due to their efficiency are useful in solving large complex problems. The application of genetic algorithms in data mining for search and build an optimal model among the models is achieved. Such that the initial models are placed on some chromosomes and competition over the transfer of traits to the next generation. The best and most worthy models are and most worthy to be presented to the user [1] [2].

2 Data collection

Our data set includes 21,084 records from 10/2006 to 4/2010 [3]; and have been gathered based on daily price fluctuations in the euro exchange forex Sponsored Europe. This includes the following classifications:

- Time, date: day, month, year: Each 24 record is a day.
- New Price in specific hours- Open: Euros Price at Arrival time in hours. For example, at 12:01 How much is the euro price.
- Out Price in an hour- Close: EUR Price per hour at the time of departure. For example, at 12:59 How much is the euro price.
- Lowest price per hour- Low: It is the Lowest Euros price in that time.
- The highest price at the time- High.
- Average price: Average price in that hour.

3 Data Pre-processing

In order to obtain better results when sorting through data, we applied the following changes:

- Add weekdays category to evaluate excitement of the first days of the week after weekend and holidays in the market. - Rounding the total data to get a better result.
- Add seasons Category to evaluate the market fluctuations in different seasons. Separated the day, month and year to better access to data.
- Open and Close is possible nearly equal and difference of them is in the decimal range. So to simplify the data we have decided to remove the exit price.
- Methods used in modeling.
4 Neural Network

Neural network have three concepts: 1 - Data Analysis System 2 - neurons or nerve cells 3 - neurons Labor Law Group, or Network. In a classical definition, neural networks, are a set of simple processing elements that are connected. Processing elements in neural networks are much easier than conventional processors with numerous differences. [4] Each neuron with a number of other neurons to connect directly and is independent and weight of the connections will determine their relationship, the data are placed in weights. Neural network has the following features:

1. Do Processing units.
2. No virtual memory Part And information are saved in a set of weights.
3. Loss of parts of networks and failure are not causes of the networks failure to resist the noise ratio and hardware failures.

Compared with artificial neural networks, the Vector Machine method is to support relatively new Methods, that have shown good performance than the perceptron neural networks in recent years. To find the solution equation Optimum Line for data by quadratic programming methods the known methods in solving problems are significant limitations is done. Support Vector Machine is basically a linear machine. From human neurons to artificial neurons: Setting aside some of the critical properties of neurons, and internal communications can be simulated a primary model of neurons by computer.

5 Neural Networks Structure

A neural network consists of components and weights of layers. Behavior of the network is dependent on the relationship between members. In general neural networks have three neuronal layers: 1. Input layer: the raw information is fed to the network. 2. Hidden layer: These layer performances are determined by relationship between input and weights and hidden layers. Weights between input and hidden units sets when a hidden unit that must be activated. 3. Output layer: Outputs Unit performances are depending on the hidden unit activity and weight between the hidden and output units. [5] There are also Single-layer and multi-layer networks that single-layer organization where all units have a connectivity layer, the most used has Greater computational potential than the multiple layers organization. Units in multi-layer networks are numbered by the layers (Instead of pursuing overall numbering). [4] Both layers of a network communicate with each other by weights, In fact connections. In neural networks are some types of connection or link weight: Pioneer: More links of this type in which signals are only in one direction. Does not exist any feedback from output to input (loop). The output of each layer has no effect on the layer. Backward: [4] Peripherals: Output nodes of each layer are used as input nodes.
6 K* algorithm

An Instance-based Learner Using an Entropic Distance Measure selecting values for the parameters x and s, and a way of using the values returned by the distance measure to give a prediction. Choosing values for the arbitrary parameters for each dimension we have to choose values for the parameters x (for real attributes) and s (for symbolic attributes). The behavior of the distance measure as these parameters change is interesting. Consider the probability function for symbolic attributes as s changes.

7 IBK algorithm

IBK is an implementation of the k-nearest-neighbors classifier that employs the distance metric discussed. If more than one neighbor is selected, the predictions of the neighbors can be weighted according to their distance to the test instance.[6]

8 Decision Tree; Association Rules

Two different formulas have been implemented for conversion between weight and distance. Number of training samples that are kept by the classifier may be limited to window size by setting options. When new samples are added and old samples deleted the old samples remain as the total number of samples in training set size [7] [8].

9 Results and Discussion

In this paper we used three classification algorithms to forecast the euro currency fluctuation. Multi-layer Perceptron procedure neural network, K* and IBK were the models which used to forecast the euro currency fluctuation. Five layers show input that has duty to get raw information which feed the networks. Table 1 compares same criteria of each algorithm: This index is the root mean square approximation. Root Mean Square Error index for good models is 0.05 or less. The models which there RMSEA is 0.1 have a week processes. This index is a relative absolute error. Relative absolute error index is better to have a higher value. This index is expressed as a percentage.

<table>
<thead>
<tr>
<th></th>
<th>IBK</th>
<th>K*</th>
<th>MLP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Root Squared Error</td>
<td>0.051</td>
<td>0.42</td>
<td>0.52</td>
</tr>
<tr>
<td>Relative Absolute Error</td>
<td>1.078</td>
<td>82.75</td>
<td>100.1189</td>
</tr>
</tbody>
</table>

Table 1. Compares criteria of RSE and RAE

Also association rules and classification rules which induction of decision trees used for conclusion. Some simple of association rules and classification
rule are shown below follows C5 algorithm in Clementine software. For example, analyses of the 5 roll are discussed below:

First roll:

If first month
And first day, then price decreases.

If second day and the average price is less than 1.745 and
on Monday and Thursday, the price decreases.

if Tuesday and
the average price is smaller than 432 or less then price decreases.
The average price is greater than 432, the price increases.
on Wednesday, the price increases.
on Friday, the price decreases.

the average price is greater than 1.745, the price increases.
on day nine, on Monday, Tuesday, Wednesday, Thursday and Friday, the prices decrease

Second roll:
on days 10, 15, 17, 20, 21, 22, 29, the price increases.

If on first month, 9.48 percent done shopping that 18.01 percent are on Monday. Trading volume in January was higher. It seems after the holidays ensure the relative movement at the end of the year causes the market itself shows good mobility. 9.48 percent for trades made in January, confirmed it. Statistics show that on Mondays in January, more trading takes place during the week than the rest of. On Fridays we also have a relative increase in trading volume and price fluctuation. It is well because it could be time to declare the U.S. unemployment statistics attributed. The listed statistics affected more on the trend of equality exchange between dollars to euro rate. Since it shows the strength of the U.S. economy and future prospects in the short term. Successful transaction is not so simple and easy and needs several components such as extensive knowledge, understanding market conditions and confidence and composure. In currency markets, the timing and on time entering into the trade are the most important factor in successful deal but sometimes determine the right time to deal is unknown. Never expect that every transaction could earn profits. Trading in foreign exchange markets based on conjecture and estimates and can be caused losses. However, these transactions can be exciting, teaser and even addictive. Whatever you have more dependence on your money and investment, making decisions with a comfortable mind about it would be more difficult. Your money is worth so with the money that you need to live, you should never be traded. Before the transaction you should know what the market situation. Whether the process has upside, downside, or is neutral. Whether this trend is strong or weak? And did so before the start of the process or process is new? Obtain the clear and accurate picture of market position, cause to the successful transaction. Many traders attempted to transaction without specifying the time out of the transaction. Of course not doubt that the first goal is profit; however the trader should be focused his mind on exactly what to predict the market movements. For the transac-
tion, carefully considered and determined on the anticipated market moves in a certain period of time is essential. One of the cases in this area should be considered is the deal time. Importance of this issue is that your mind would be ready to make it. Although specifying the exact time of departure of the transaction is not possible, but to specify the time before entering the trade is very important. If your number of transactions is high during the day, technical analysis on the daily charts is less important and is better to use 30-minute charts or an hour ones. Moreover, you should know start and end of working hours of financial and economic centers of the world. You should keep in mind these times when doing the trading. Since hours, volatility, liquidity and market movements are noticeably changed. Can be speculated synchronize on with the potential of market. But it may be too early or too late to do. Attention to the time of transaction can be effective in the result. The news will be announced in the market, such as CPI (Consumer Price Index), announced retail sales or the central banks decide to increase interest rates, can stabilize the previous market movement. Due to the timing transaction means that know what to expect before the transaction and you can specify them in advance. Technical analysis can help you to detect when and how the prices will be changed. If you have doubt about doing a deal correctly and you are not sure, do not enter the market. Generally, adjusting and measuring transactions in the way to re-enter the market and trading with other currencies are more rational. In short, with large quantities that may destroy your account do not deal. And with a slang words; do not put all your eggs in one basket. What the majority of market plan for situation and movement or would do in future are called market trends. Which means you will successful if you go to the right direction for trading market. It should be mansion that this removal is a very simple and basic image as a process may take in any time and move in the opposite direction. Technical and fundamental analysis can determine when to start the process and whether this trend is strong or weak. Market expectations are indicating tendencies that most traders and analysts of the market and the news will be announced in the near future. If they expect that interest rates rise then it will. A lot of changes in market movements will not be seen because the market already announced this change to react and prepare for it but if the news is announced unlike forecasts, market will inevitably react strongly to it. Attractive Association Rules Extracted:

- If it is 13th day and 3.15 percent of the purchase is done then 28.87 percent is on Tuesday.
- If it is 4th month and 7.57 percent of the purchase is done then 22.63 percent is on Wednesday.
- If it is 5th month and 3.75 percent of the purchase is done then 22.88 percent is on Friday.
- If it is 12th day and 3.38 percent of the purchase is done then 22.88 percent is on Friday.
- If it is first month and 9.48 percent of the purchase is done then 18.01 percent is on Monday.
- If it is 3th day and 3.28 percent of the purchase is done then 16.64 percent is on Friday.
• If it is 12th day and 3.38 percent of the purchase is done then 16.69 percent is on Wednesday.
• If it is 4th day and 3.39 percent of the purchase is done then 16.81 percent is on Tuesday.
• If it is 11th day and 3.39 percent of the purchase is done then 16.81 percent is on Tuesday.
• If it is 3th month and 5.01 percent of the purchase is done then 17.98 percent is on Thursday.
• If it is second month and 4.57 percent of the purchase is done then 17.96 percent is on Wednesday.
• If it is first month and 4.46 percent of the purchase is done then 17.75 percent is on Friday.
• If it is second month and 9.14 percent of the purchase is done then 20.29 percent is on Friday.

10 Conclusion

K* algorithm has a less Root Squared error. MLP algorithm has e more Relative absolute error than the rest. In order to make a better understanding in the classification, classification techniques based on the Association Rules, i.e. the association classification. The main purpose of classification is a prediction in terms of class. While the discovery of association rules describe relationships between items in transaction database. In association classification, classifier made section on a subset of association rules called association rules classification. In association rules classification, after every law is a class attributes. Classifier studies a rule or set of compatible laws with the object to predict an object tag. The results of work performed in this field show that association classification act better than Machine learning Classification algorithms [9] However, association rules algorithms has challenges such as determine the minimum values, For extracted association rules because first, the algorithm produces a large number of laws and storage, retrieval, pruning and sorting of these laws is difficult. Also, to find the best subset of rules for building strong and accurate classification is challengeable. [9] However, association rules algorithms has challenges such as determine the minimum values for extracted association rules because first, the algorithm produces a large number of laws and storage, retrieval, pruning and sorting of these laws is difficult. Also, to find the best subset of rules for building strong and accurate classification is challengeable. [9] In recent years a number of association classification such as CPAR (Han J.; Pei J. Yin Y.; 2000), CMAR (Li W.; Han J.; Pei J.; 2001), MCAR (Thabtah, F.; Cowling P.; 2005), MMAC (Thabtah F.; Cowling P.; 2004) is presented. These algorithms are used various ways in the discovery, ranking, pruning, prediction and evaluation of interest. To construct classifier with association rules algorithms, first found complete set of association rules from training data set and select a subset to make a classifier. Selecting such a subset has different methods. For example CBA (Liu B.; Hsu W.; Ma Y.; 1998) [10] and CMAR algorithms, this method occurs of selection based on coverage
heuristic method. In this method we evaluate complete set of CARs on educational data sets and considered laws that cover certain number of educational data. When the classifier made, it evaluate the power of predictive the test data for predicting class labels. Several AC techniques are presented in recent years. [9] These methods make different approaches in discover frequent item collection, extraction rules, classification rules, sorting rules; pruning waste and harmful laws - that leads to the wrong classification -and classification of new educational samples. The first finding from this study is to understand the complexity of mechanisms in stock price changes. Neural networks models in recent research got success to predict the indicators. Neural network designed to predict the index of input data interrupt such interruption of economic factors, along with some of their interrupt has a better performance than neural networks that have only input index. But this situation not found when the interrupt input was removed from the index. This shows that macroeconomic variables associated with stock market indices in this study does not determine a relationship and indicators applied the most effective from their historical values. Partially adding macroeconomic variables to the model increases power of provider distribution models, and no decisive role. Contents stated above indicate that psychological climate prevailing stock market price changes. Stock market is not yet prices to determine principally but Chartyst theory is based on yesterday price changes to determine today price changes.

References

3. Used Data from: http://ch.saxobank.com
6. M. Nasiri, B. Minaei, A. Hadian, 2007, Comparison-Find Closest distance, SV-M and C.5, Third Conference on Data Mining, Iran University of Science and Technology
A nonlinear mixed effects model to explain inter-individual variability in plant populations

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Abstract. It is common knowledge that the genetic variability of plants, even of the same variety, can be very important and, if we add locally varying climatic effects, the development of two neighboring similar plants could be highly different. This is one of the reasons why population-based methods for modeling plant growth are of great interest. A highly promising individual-based plant growth model is the GreenLab model [4] which was recently shown to have a good predictive capacity among competing models [1]. In this study, we extend the GreenLab formulation to the population level. In order to model the deviations from some fixed but unknown important biophysical and genetic parameters we introduce into the GreenLab model appropriate random effects. Under some assumptions, the resulting model can be cast into the framework of nonlinear mixed effects models. A stochastic variant of an EM-type algorithm (Expectation-Maximization) is generally needed to perform MLE for this type of incomplete data models and the interest is focused on the design of an efficient algorithm. In this direction, we propose a suitable Monte-Carlo EM (MCEM) algorithm for our model, where at each EM-iteration, MCMC is used to draw from the hidden states given the observed data. Data consist in organ mass measurements and are treated sequentially as first proposed in [11]. The performance of the algorithm is illustrated on simulated data from the sugar beet plant. Some possible extensions and improvements are also discussed.

Keywords: plant growth model, nonlinear mixed effects model, stochastic EM algorithm, MCMC methods, sugar-beet plant.

1 Introduction

Plants, as any other living organisms, are in constant interaction with each other. Genetic variability, even for plants of the same variety, as well as locally varying environmental conditions in a given field, can lead to the development of two different neighboring plants. This inter-individual variability can have a major impact at the agrosystem level, as shown for example by [3], who demonstrated that soil and crop micro-variability can have an impact on final yield, as some parts of the field can be more adapted to dryness, and can thus compensate less good performances of other parts of the field.

Individual-based plant growth models such as functional-structural plant models (FSPM) have gained a lot of success over the past years. These models describe the evolution of the 3D architecture of the plant over time, driven by the underlying ecophysiological processes (e.g., [13]), at the organ level. However, extrapolation to the field scale is still at its early stages. It mostly
concerns competition for light (e.g., [5]), and the calibration process is made from an average individual plant. If the level of description available in FSPMs made these approaches very appealing, their calibration on averaged individuals is not fully satisfactory as it only gives a partial representation of the field production.

In this study, we propose an extension of the individual-based Greenlab model, based on a bottom-up approach: the growth of each individual plant in a given field can be characterized by the same set of equations from the Greenlab model, but some of the model parameters are specific to this individual, and can therefore be considered as random effects. The resulting model can thus be cast into the framework of nonlinear mixed-effects models [7]. In this context, maximum likelihood estimators of the parameters can be obtained using an appropriate stochastic variant of an EM-algorithm (Expectation-Maximization) [10]. Due to the nonlinearity of the model, the E-step is in general analytically intractable, and an approximation of the Q-function should be done, but on the other hand, under suitable assumptions, the M-step can be resolved explicitly.

The methodology was developed here in the specific case of sugar beet crops, which have a very simple structure, as only three types of organs need to be considered (blades, petioles and root), but it can of course be applied to more complex plant structures, like maize or oilseed rape. The Greenlab model is introduced in Section 2.1, while the methodology is described in Section 2.3. Results from simulated data are presented in Section 3.

2 Material and Methods

2.1 The Greenlab model

The Greenlab model is a functional-structural model, combining rules for (i) biomass (mass for living organisms) production and allocation (functional part), and (ii) architectural development at the organ level (structural part). It was introduced by [8], and represented as a discrete dynamic system in [4]. Parameter estimation methods for this model are reviewed in [6]. Some recent advances for parameter estimation in the presence of modeling errors can be found in [11] and [12].

The first description of the Greenlab model as a discrete dynamic system was possible by taking advantage of the modular architectural development of plants. Indeed, the plant structure can be considered as the result of the accumulation of elementary botanical entities, called metamers, which usually correspond to some specific combinations of organs, characteristic for each plant species. The discretization of time is therefore possible by taking into account the time instants where metamers appear. The time interval between the appearance of two successive metamers is known as a growth cycle.

Despite the relative benefits of this inherent discretization, the choice of the growth cycle as a time step bears some limitations, especially for the functional part of the model and the handling of environmental data, since the latter are usually collected on a daily basis, while the growth cycle can vary from several days to one year in trees. To overcome these difficulties, a daily time step was
chosen to compute biomass production and allocation, but we still rely on the growth cycle for the creation of new organs.

In this paper we present in some detail the case of sugar beet which consists of three type of organs, that we denote by \( \mathcal{O} = \{ b, p, r \} \), where \( b \) stands for blade, \( p \) for petiole and \( r \) for root. Each blade and each petiole is defined by its rank, corresponding to the growth cycle at which it was preformed. The interest is focused on the functional part since the structural development is known and corresponds to the creation of one blade and one petiole at each growth cycle. The inter-individual variability of organogenesis has been studied by [2], who showed that it can be important in sugar beet populations.

**Biomass production.** The seed mass corresponds to the first biomass. After the appearance of the first leaf, biomass production is assumed to be given by:

\[
F(t; p^*) = u_t \mu s^{pr} \left( 1 - \exp \left( -k_b s^{act}(t; p_{al}) \right) \right),
\]

where \( u_t \) stands for an environmental condition on day \( t \) (usually, the photosynthetically active radiation), \( s^{pr} \) an empirical coefficient related to the space occupied by the plant on the ground, \( \mu \) an efficiency coefficient, \( s^{act}(t; p_{al}) \) the photosynthetically active foliar surface at the beginning of day \( t \) (see [11] for further details) depending on the allocation parameters \( p_{al} \) described in the next paragraph, and \( p^* = (\mu, s^{pr}, k_b, p_{al}) \).

**Biomass allocation.** A basic assumption of the Greenlab model is that biomass allocation to all expanding organs is proportional to organ specific functions, called sink functions and denoted by \( s_{o,k}(u; p_{al}) \). At a given time \( u \), these functions depend on the type of the organ, and its expansion stage, i.e., the number of growth cycles that have elapsed since its creation. The basic factor determining the duration of a growth cycle, and consequently, organs demand for growth, is the temperature. For this reason it is very convenient to introduce the notion of thermal time, which is defined as follows:

\[
\tau(u) = \int_0^u \max(0, T(s) - T_b) \, ds, \quad u \geq 0,
\]

and represents at calendar time \( u \), the accumulated sum of temperatures above a base temperature \( T_b \) until time \( u \). In the sequel, for a leaf of rank \( k \), we denote by \( \tau_k \) its thermal time of initiation, \( \tau^e_k \) its expansion period, and \( \tau^s_k \) its lifetime. The thermal time of initiation of root is thus equal to \( \tau_1 \), and we denote by \( \tau^e_k \) its corresponding expansion period. We assume that root do not get senescent, and that initiation, expansion and lifetime of blades and petioles from the same leaf are identical.

After a first phase of initiation where the seed biomass is distributed uniformly in time, the produced biomass (due to photosynthesis) given by (1) is distributed to all expanding organs proportionally to

\[
s_{o,k}(u; p_{al}) = c_{p_0} \left( \frac{\tau(u) - \tau_k}{\tau^e_k} \right)^{a_0-1} \left( 1 - \frac{\tau(u) - \tau_k}{\tau^e_k} \right)^{b_0-1} 1_{\tau_k \leq \tau(u) \leq \tau_k + \tau^e_k},
\]
where $p_{al} = (p_o, a_o, b_o)$ for $o \in \mathcal{O}$ and $c$ is the normalizing constant of a discrete beta law $B(a_o, b_o)$.

The sum of all sink functions on day $u$ defines the total biomass demand $d(u; p_{al})$ on day $u$, and the ratio $s_{o,k}(u; p_{al})/d(u; p_{al})$ determines the percentage of the produced biomass $F(t; p^*)$ which is allocated to the organ of type $o$ and rank $k$ at the end of day $u$.

### 2.2 A two-stage formulation of the model

To account for inter-individual variability, random effects are introduced in the Greenlab model, which can then be seen as a two-stage hierarchical one.

**First-stage: intra-individual variation.** We denote by $\bar{z}_{i,n} = (\bar{z}_{i,n})_{1 \leq i \leq s, 0 \leq n \leq n_i}$ the theoretical biomasses of organs of rank $n + 1$ for plant $i$. The theoretical biomasses $\bar{z}_{i,n}$ can be obtained as a function of the sequence of produced biomasses:

$$\bar{z}_{i,n} = G_n(\phi_i) = \left(\frac{\sum_{\tau(t) = \tau(n+1)} s_{o,n}(t; p_{al})}{d(t; p_{al})} F(t; \phi_i)\right)_{o \in \mathcal{O}}, \quad (2)$$

where $\phi_i$ is the vector of parameters specific to plant $i$, $G_n$ is the vector-valued function of the theoretical biomasses of organs of rank $n + 1$, and $\tau_{\text{max}}$ is the thermal time at which observations are made.

To account for positivity in mass measurements we define $\bar{y}_{i,n} = \log(\bar{z}_{i,n})$.

If we denote by $y_{i,n} = (y_{i,n})_{1 \leq i \leq s, 0 \leq n \leq n_i}$ the vector of mass measurements in the log-scale and by $\Sigma_{b,p}$ and $\sigma_r^2$ a two-dimensional covariance matrix and variance parameter respectively, then we assume that:

$$y_{i,n} = \bar{y}_{i,n} + \epsilon_{i,n}, \quad \epsilon_{i,n} \sim \mathcal{N}_{d_n}(0, \Sigma_n), \quad 1 \leq i \leq s, \quad 0 \leq n \leq n_i, \quad (3)$$

where $(\epsilon_{i,n})_{1 \leq i \leq s, 0 \leq n \leq n_i}$ are mutually independent random variables and

$$\Sigma_n = \begin{cases} \text{diag}(\Sigma_{b,p}, \sigma_r^2) & \text{if } n = 0, \\ \Sigma_{b,p} & \text{if } n \geq 1. \end{cases} \quad (4)$$

In this way, the measurement errors from organs of two different plants or of the same plant but with different ranks are assumed to be independent.

**Second-stage: inter-individual variation.** In this second stage, the variability of the subject-specific parameters defined in the previous stage, $\phi_i$, is assessed.

We assume the following model for the vector $\phi_i = (\phi_{i,1}, \ldots, \phi_{i,P})^t$, with $P$ the number of random parameters:

$$\phi_i = \beta + \xi_i, \quad \xi_i \sim \mathcal{N}_P(0, \Gamma),$$

where $\beta$ is the vector of fixed effects and $\Gamma$ a diagonal covariance matrix.
2.3 Parameter estimation

We denote by $\theta = (\theta_1, \theta_2)$, where $\theta_1 = (\beta, \sigma_1^2, \ldots, \sigma_P^2)$ and $\theta_2 = \Sigma_{b,p}$, the vector of unknown parameters. To compute the maximum likelihood estimator of $\theta$, we need to compute the likelihood of the model, which will be in general analytically intractable due to the nonlinearity of $G_n$ given by (2). However, our model can be seen as an incomplete data model, with $y = (y_{i,n}, 1 \leq i \leq s, 0 \leq n \leq n_i)$ the observed data, the random effects $\phi = (\phi_i, 1 \leq i \leq s)$ being the unobserved data. The complete data of the model is $(y, \phi)$, and in such cases, an appropriate variant of an EM-algorithm [9] (Expectation-Maximization) can be implemented to approximate the maximum likelihood estimator of $\theta$.

Each iteration of this algorithm consists in two steps: the expectation step (E-step) in which the conditional expectation of the complete data log-likelihood given the observed data is computed under the current parameter value, and the maximization step (M-step) in which the parameters are updated by maximizing the $Q$-function obtained in the E-step. The two steps of the EM-algorithm are described below:

**E-step.** At iteration $k$, the E-step of the algorithm consists in the computation of the $Q$-function given the current value of the parameter $\theta^k$. Due to the independence between plants and between organs of different ranks within the same plant, the $Q$-function can be decomposed as follows:

$$Q(\theta; \theta^k) = \sum_{i=1}^{s} E_{\theta^k}(\log f(\phi_i; \theta_1) \mid y) + \sum_{i=1}^{s} \sum_{n=0}^{n_i} E_{\theta^k}(\log f(y_{i,n} \mid \phi_i; \theta_2) \mid y)$$

$$= Q_1(\theta_1; \theta^k) + Q_2(\theta_2; \theta^k). \quad (6)$$

**M-step.** In the M-step of the algorithm, we maximize the $Q$-function with respect to $\theta$. Thanks to the decomposition of the $Q$-function given by (6), maximizing $Q(\theta; \theta^k)$ with respect to $\theta$ is equivalent to maximizing $Q_1(\theta_1; \theta^k)$ with respect to $\theta_1$ and $Q_2(\theta_2; \theta^k)$ with respect to $\theta_2$. The update equations can be obtained easily and are given by:

$$\hat{\beta}_j = \frac{1}{s} \sum_{i=1}^{s} E_{\theta^k}(\phi_{i,j} \mid y_i), \quad (7)$$

$$\hat{\sigma}_j^2 = \frac{1}{s} \sum_{i=1}^{s} E_{\theta^k}(\phi_{i,j}^2 \mid y_i) - \hat{\beta}_j^2, \quad (8)$$

$$\hat{\Sigma}_{b,p} = \frac{1}{s + \sum_{i=1}^{s} n_i} \sum_{i=1}^{s} \sum_{n=0}^{n_i} E_{\theta^k} \left[ (y_{i,n} - \log G_n(\phi_i)) (y_{i,n} - \log G_n(\phi_i))^t \mid y_i \right], \quad (9)$$

where $y_{i,0}$ is restricted to blade and petiole only.

From these equations, we can see that at each iteration of the EM-algorithm, the problem of maximization is reduced to the problem of computing conditional expectations given $y_i$, under the current parameter value $\theta^k$. 

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Approximation of the E-step  
Due to the nonlinearity of the model the E-step given by (6) cannot be performed explicitly. However, many stochastic variants of the EM algorithm are available to approximate a non-explicit E-step. In this paper, as a first implementation we tried a Monte Carlo EM (MCEM, [14]) algorithm, where the Q-function is approximated via Monte Carlo simulations. In particular, hidden data are drawn via an MCMC (Markov Chain Monte Carlo) algorithm like Metropolis-Hastings or Gibbs Sampling. At iteration $k$ of the algorithm, we simulated for each individual plant a Markov Chain of size $M$, with stationary distribution our target distribution $f(\phi_i | y_i; \theta^k)$.

3 Results

The methodology was first applied to a set of 50 simulated plants. Thanks to a preliminary sensitivity analysis, the two most influential parameters were shown to be $\mu$ and $s^{pr}$. Consequently, as a first approach, random effects were only used for these parameters. The other parameters were assumed to be known. Concerning $s^{pr}$, we assumed that $\log s^{pr} \sim N(\beta_2, \sigma^2_2)$. Finally, $\theta_1 = (\beta_1, \beta_2, \sigma_1, \sigma_2)$ and $\theta_2 = (\sigma^2_b, \sigma^2_p, \rho)$, where the latter vector corresponds to the variance parameters and the correlation coefficient of the covariance matrix $\Sigma_{b,p}$ (see, (4)). In the tests that we present, the parameter $\sigma^2_2$ was fixed.

In Table 1 we present the parameter estimation results that we obtained. We used two different initializations and three independent runs for each one of them. At each iteration, a Markov chain of size 1000 was generated for each plant. The proposal distribution was set equal to the prior distribution of the hidden data under the current parameter value. For these tests, the algorithm stopped manually after 60 iterations. Table 1 gives as well the values that we used to generate the data, and the MLE if the data were fully observed. Two different sets of initial values were tested: for the first three runs (columns 4 to 6), the initial values were 4.5 for $\mu$ and -4 for $s^{pr}$, and for the last three runs (columns 7 to 9) the initial values were 5.5 for $\mu$ and -2 for $s^{pr}$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>True value</th>
<th>Fully-observed</th>
<th>Run 1</th>
<th>Run 2</th>
<th>Run 3</th>
<th>Run 4</th>
<th>Run 5</th>
<th>Run 6</th>
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<td>5.512</td>
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<tr>
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<tr>
<td>$\sigma_1$</td>
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<td>0.074</td>
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<tr>
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<td>0.010</td>
<td>0.010</td>
<td>0.009</td>
<td>0.009</td>
</tr>
</tbody>
</table>

Table 1. Parameter estimation results.

Figure 1 shows that the convergence was reached quickly for $\beta_1$ and $\beta_2$, but more iterations are needed for the variance of the random effects, especially for $\sigma_1$. The results from different initializations and independent runs were also very encouraging (Table 1), even for the estimations of observation noises.
Fig. 1. Parameter estimation for 60 iterations of the Metropolis-Hastings algorithm: (top) estimation of $\beta_1$ and $\beta_2$, (bottom) estimation of $\sigma_1$ and $\sigma_2$. The solid lines represent the values used to generate the data and the dotted line correspond to the maximum likelihood estimators if the data were fully observed.

4 Discussion

The methodology that we presented in this paper to account for inter-individual variability in plant populations is suitable for a large number of crop plants. Results from simulated data were encouraging, and we are currently working with real data and with more random parameters. Different MCMC versions of the current MCEM algorithm will be compared in the sequel and the latter will be compared with a Stochastic Approximation EM (SAEM, see [10]) algorithm. An automated MCEM algorithm can easily be implemented (see, [12]). The latter paper presents a parameter estimation method by including modeling errors in biomass production for a single plant. As a future step, we will extend our population based approach to account for modeling errors as well.
Finally, it is noteworthy that with the proposed methodology, approximated confidence intervals can be easily obtained as a by-product of the algorithm.

References


Determination of the optimal strategy of a quarry in Algeria using the Three Phase Discrete-Event Simulation: A case study

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Abstract This work investigates how Turbo Pascal Three Phase Discrete-Event Simulation Routines and its libraries can be used in optimizing the number of loaders and trucks in the aggregate production, at a minimum cost. A model is developed using the activity cycle diagram and the performance measures of the system are evaluated. Inefficiencies of the studied problem are identified and improvement is proposed for the quarry managers by determining the optimal strategy.

Keywords Modeling , Activity Cycle Diagram ,Discrete-Event Simulation , Monte Carlo

1 Introduction

Civil Engineering is a branch of engineering dealing with the optimization of complex processes or systems which can be modelled and simulated using computers. Then, Civil engineers use simulation software to make simulation an easy to use, especially, A REsource based Simulation system for construction process planning (Resque) [1], STate and ResOurce Based Simulation of COnstruction ProcEsses (STROBOSCOPE) [2], Resource-Interacted Simulation Modelling in Construction (RISim) [3], along with extensive mathematical tools, modelling, evaluation, and optimization.

Simulation involves the development of an imitation on a computer of the system under study, followed by experimentation to understand and investigate improvements to the system. Discrete-event simulation can help to identify inefficiencies and examine how these may be addressed.

This paper examines Civil Engineering problem throughout a three phase discrete-event simulation systems and focuses on a case study of Bejaia quarry in Algeria at the operational level, considering the random behaviour, the resource characteristics and dynamic interactions during operations. The behaviour of this case-study depends on input random variables with known probability density functions. A logical model for the quarry aggregates using an expanded Activity Cycle Diagram (ACD) is built from which we have simulated the behaviour of the quarry on a computer. The ACD expresses the logic of complex simulation models effectively and is used as a vehicle for experimentation. So, experiments are carried out on the model built and unknown parameters of the output random variables of interest are estimated. Hence, Monte Carlo methods [4,5] are usually used for such problems. That is, in a simulation experiment, defined by $M$ replicated runs, input random variables are replaced by random samples such that the unknown parameters can be estimated by the sample mean of the samples results obtained by the $M$ runs. Then, our system is simulated and the purpose of the simulation is to improve the system being studied by determining the optimal strategy. The three phase simulation system is based on specific libraries of the three phase approach; these libraries are available
in different programming languages, Turbo Pascal, C, C++ and Visual Basic v3. The Turbo Pascal Three Phase Simulation Routines and its libraries (PSim) [6] has been selected for a better simulation programming of the aggregates quarry problem. The selected three phase approach in discrete-event simulation fits well our requirements; nevertheless we can find other methods like the Activity based approach, the Event based approach and the Process interaction approach.

Section 2 is devoted to the description of the studied problem. By then, a discrete-event simulation model is given in section 3. The performance measures of the aggregates quarry system are established by developing a simulator using PSim language. In the design of the simulator, we used the modified built in random number generator "Rnd". Indeed, given the problem of the integrated "Rnd" function in TURBO Pascal, this function was improved to support the different replications.

Finally, experiments and software interface are described in section 5 followed by a conclusion section.

2 Description of the problem

The manufacture of a certain volume of aggregates at Bejaia quarry must go through a sequence of operations that are:

- Drilling of boreholes: A round is defined by 60 boreholes and its drilling is performed by a driller and a drilling team. The time for making a hole is estimated at 30 minutes (mn), so, for a round, we need 1800 mn.
- Mining: Introduction of primers in boreholes and connecting all the mines of the round shooting. The holes are about to be fired and for safety reasons, there will be the setting away of the drilling team, the driller and the loader.
- Firing: The successive explosions of drilled holes roughly break the rock and bring it down.
- Inspection: The blaster performs the recognition site for a possible presence of a fire incident and gives the signal of the guard lifting; there will be then the return on site of the drilling team, the driller and the loader.
- Loading the rock into the truck, this activity is done by the loader.
- Transporting the rock by the truck. It is a process of paramount importance in the mining process because it provides the link between the place of extraction of raw materials and the place of transformation where the distance between them is 03 kilometres.
- Unloading the truck at the site of crushing.
- The Return of the truck to the quarry site for possible reloading.
- The Crushing of the rock which is made by the crusher reduces to small parts (up to a few millimeters) the obtained rock, hence, the production of aggregates.

3 Modelling the quarry in discrete-event simulation

Modelling is representing the important interactions in a model which has a form useful for simulation. To express the main concepts of our system, we built a model of the studied problem described in section 2 by drawing the Activity Cycle Diagram (ACD). To do so, we need to identify the classes of entities, the activities, the conditions under which these activities can occur and their results once these activities are executed. For this quarry aggregates, we have identified:

- Five (5) classes of entities that are, Driller, Crusher, Drilling Team, Truck and Loader identified respectively by two characters Dr, Cr, DT, Tr and Lo.
- Fifteen (15) activities that are, drilling, mining, drilling team shelter, loader shelter, driller shelter, firing, inspection, drilling team return, loader return, driller return, loading, transport, unloading, truck return and crushing.
- Conditions to start the different activities and their results. They are
numerous and to not mention them all, we will give just those related to the truck entity which are represented in a tabular form given in table 2 and the corresponding ACD is represented in figure 1.

- The quarry aggregates defined in section 2 is then, represented by its ACD in figure 2.

### 3.1 The assumptions of the quarry

Once the quarry system has been modeled, we need to make certain assumptions for its simulation. The quarry operates in two shifts of five hours each, one morning and one afternoon daily with a lunch break of one hour making the working day to 10 hours and the day to 11 hours. In this case, drilling a round is done in approximately 3 days which is the longest time of all activities.

As long as the system performance is the aggregates production, the operations of loading and transporting that provide the rock to the crusher never stop during working hours except in the case of force majeure. Thus, the optimal strategy for the quarry’s operation is to carry out firing only during the lunch break when the operations of loading and transportation stop anyway. The various activities that begin to approach the break are not allowed unless it remains at least 20 mn for the end of a shift, this offset adjusts operations in the breaks.

For that firing can take place during the break, all conditions must be met 20 mn before the break. The decision and the announcement of the firing cannot take place if there is not at least 30 mn before the break. Firing during working hours can only occur when there is not enough rock to be loaded and transported, and there are 60 holes already loaded with explosives. In this case, it is unnecessary to await the next break to fire, because all operations are already stopped (with the exception of drilling extra holes).

### 4 The three phase program structure

In this section, we present the software "Quarry Simulator" developed for the simulation of Bejaja quarry problem that evaluates the performance measures of the system in the three phase discrete event simulation. The "quarry Simulator" software is realized under Turbo Pascal 7 (TP7) and implemented under the Windows environment using the source code of the program Turbo Pascal PSim Three Phase Simulation Routines and its libraries. After building the ACD, this information, together with activity durations, attributes, branching conditions and any other additional data that might be necessary is fed into the PSim environment. Its implementation requires the generation of artificial samples of known distribution variables.

#### 4.1 B and C activities

Two types of activity are identified, B and C activities. B for Bound activities are executed whenever the time at which they are scheduled is reached. C for Conditional activities whose initiation depends on either the co-operation of different entities, or the satisfaction of certain specified conditions, or both.

One or several activities of either type will be initiated whenever the system changes state, i.e. whenever an event occurs. The system of the quarry may change state at any of the following points: Beginning and end of drilling, mining, drilling team shelter, driller shelter, loader shelter, firing, inspection, drilling team return, driller return, loader return, loading, transport, unloading, truck return and crushing.

#### 4.2 Variables and estimates
To simulate the quarry problem, we consider fifteen (15) input random variables which are, the different service times of loading, transport, unloading, crushing, truck return, drilling, mining, drilling team shelter, drilling team return, loader shelter, loader return, driller shelter, driller return, firing and inspection. We observe seven (7) output variables through simulation which are, the occupancy rates of different entities having all one parameter, the mean to be respectively estimated by DrRate, CrRate, DTRate, TrRat, LoRate. The cost and the required time to produce a scheduled aggregates volume are both computed for choosing the best strategy. We suppose that the different input processes follow all Poisson distributions with different rates $\lambda_i, i = 1, ..., 15$.

4.3 The three phase activity approach

We first present the three phase approach which is the basic principle of this particular implementation. This is due to Tocher [7] and is as follows:

Repeat

A phase: Determine when the next event occurs and move simulated time to that point.

B phase: Execute any B activities due to occur at this time.

C phase: Execute any C activities whose conditions are now satisfied

4.4 Simulation executive

In a three phase simulation, we have an executive or control program to ensure that the entities are properly scheduled for future activities (known as Bs) and also to ensure that current activity (often known as Cs) are properly sequenced. In the actual case, this is managed by representing the entities in the following simple form like in PSim.

Each entity forms a single row of a Control Array, known as Details. As provided in the libraries, the Details array contains the five information needed to run a sensible three phases simulation. An extra field named Lo used only for trucks is added to the Details array to make the system well simulated. Thus, the design of details is available in Table 1.

The Details array is examined during the A Phase, so as to find the time of the next event. This involves a simple search for the minimum TimeCell, disregarding any rows in which Avail is True. The row numbers, referred to as the entity ID, of entities with minimum Time Cells are placed in the CurrEntArray.

During the B Phase, the focus is on the CurrEntArray. This is worked through, one element at a time and the B Phase procedure takes the entity ID and then executes the B indicated by the entity’s NextAct field in the Details array.

<table>
<thead>
<tr>
<th></th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Name</td>
<td>A String ID that may be useful to identify an entity in a report of some kind.</td>
</tr>
<tr>
<td>2</td>
<td>Avail</td>
<td>A Boolean type that indicates whether the entity is available for committal to a B. True means the entity is available, False means it is not.</td>
</tr>
<tr>
<td>3</td>
<td>TimeCell</td>
<td>The time at which the entity is next due to change state. This is only meaningful if Avail = False for this entity</td>
</tr>
<tr>
<td>4</td>
<td>NextAct</td>
<td>The next activity in which the entity is due to engage at the time indicated by TimeCell. This activity must be a B. This field is only meaningful if Avail= False for this entity</td>
</tr>
<tr>
<td>5</td>
<td>Util</td>
<td>The total time that this entity has been active since the start of the simulation</td>
</tr>
<tr>
<td>6</td>
<td>Lo</td>
<td>It indicates the loader that deals with the loading of this truck.</td>
</tr>
</tbody>
</table>

Table 1: Representation of an entity in the Details array
4.5 The main units of the software

4.5.1 The routines provided

PSim or the main program "PasExec" contains the 3 phase executive and other procedures needed for the processing and is based around the following, each of which represents a Turbo Pascal unit. "GenLib" contains useful functions for frequently needed tasks such as input/output. "ExecVars" contains global variables needed by "PasExec", "ExecUtils" and "model". "ExecUtils" contains functions that are used mainly by the simulation executive and the "model". Finally, the "model" contains the simulation model. The run-time program is produced by compiling and linking these files within the Turbo Pascal Interactive Development Environment.

4.5.2 The routines proposed

For better programming, some changes were made to "PasExec" unit. Stopping the simulation is not supported by the duration of simulation but by the produced volume of aggregates, this parameter is fixed by the user. Execution of "PasExec" was extended to N scenarios and M replicated simulation runs for each scenario. The number N and M are also fixed by the user. After the run-time of all scenarios, a call to a new procedure entitled "Finalisation2" is executed.

The latter procedure defined in "Model" unit allows the computation of mean, variances and finding the best scenario according to averages of the production cost. To do this, two two-dimensional ResArray and A arrays and two one-dimensional V and Vmin arrays were used and then added to the area of global variables of "model". The first two are arrays of real contain 9 rows and M columns. In the first five lines are stored the different occupancy of the five entities and in the last four, the time taken to produce the scheduled volume of aggregates, the total cost, the number of trucks and loaders. The A array contains the temporary results, while ResArray contains the results for the best scenario. The last two V and Vmin arrays contain respectively the jth scenario averages and averages for the best scenario. Another "Entity" array has been added to the area of global variables "model" which is used for printing the results.

The unit "Model" contains the constants, types and variables necessary for processing the program, as well as procedures such as, all B and C activities procedures, initialization, finalization and finalisation2.

On the other hand, some changes to the unit "ExecVars" were also made. As already mentioned in 4.4 we added a field to the registration of array "Details". Another array called "Etat" is added to handle the truck’s entity. This array has two fields "Ind" and "Tonn". The field "Ind" is a character that will inform us if the truck can be loaded, transported, unloaded or returned. The "Tonn" field of real type will include the volume of the truck.

5 Experiments and software interface

We carried out N = 6 different scenarios of different number of trucks and loaders, for the production of 31520 m³ volume of aggregates, each scenario with M = 30 replicated simulation runs, using the same following simulation input parameters.

- The cost of mining a round is assumed to 7372 DA. A round provides an average volume of rock, after firing, equal to 7920 m³.
- The cost of the drilling team in activity is assumed to 400 DA/h. Indeed, we assumed a team of 4 people where each person is paid 1100 DA/ working
day. Therefore, the awaiting cost of the team is estimated to 400 DA/working day i.e. 36.36 DA/h.

- The cost of the driller in activity and awaiting is respectively assumed to 9171 DA/h and 7492 DA/h.
- The cost of the crusher in activity and awaiting is respectively assumed to 4087 DA/h and 1000 DA/h.
- The cost of the truck in activity and awaiting is respectively assumed to 1328 DA/h and 548 DA/h. We assumed that all trucks have the same volume.
- The cost of the loader in activity and awaiting is respectively assumed to 4734 DA/h and 1000 DA/h.

All these parameters are given by the quarry of ALGRAN-Bejaia and any others could be used to predict the future behaviour of the system or to simulate another optimization quarry problem.

For each simulation experiment defined by a scenario, the variables representing the return of Dr and DT entities are initialized to one (1) i.e both entities are ready for drilling.

5.1 Data inputs

For the first window, we kept the external appearance of the program Psim. So, when running the program PasExec, a first window appears prompting the user to enter system data, in the following order: The number of scenarios, replicated simulation runs, loaders and trucks, the smallest capacity of trucks, the capacity of the crusher, the average amount of rock spilled after firing, the volume of aggregates to produce, the mean time of the different input variables. See figure 3. After that, a second window appears and invites the user to enter the costs per hour of activity and awaiting of different entities, the cost of mining, the delay for a possible stop of the simulation duration and an invitation to keep or not the trace of the execution. If yes, please give a name to the file. From the second scenario, the program will require just the number of loaders, trucks and display delay since the rest is unchanged. See figure 4.

5.2 Results output

For each scenario, the following results will be displayed. The number of loaders and trucks of the current scenario which does not change throughout the execution of the $M$ replicated simulation runs. The volume (in cubic meter) of available rock. The simulation duration (in minutes). The number of the current simulation run. The use, the shelter and the return number of the driller. The mining, the shelter, the firing, the inspection and the return number made by the drilling team. The use, the shelter and the return number of loaders. The use number of the crusher. The transport, the unloading and the return number of the trucks. The volume (in m$^3$) of the achieved aggregates. All these results change throughout the simulation experiments. Once, all $M$ simulation runs are carried out, the cost of the current scenario is compared to the previous scenario’s cost and the one with a minimum cost is kept, after that, another scenario will start. Once all simulation runs and all scenarios are carried out, the best strategy to produce the scheduled volume of aggregates is displayed indicating the mean cost, the mean time, the number of trucks and the number of loaders, and the mean and variance of the occupancy rates averages of different entities for the best strategy. According to the best scenario given in figure 5, the production of 31520 m$^3$ volume of aggregates is obtained at minimum cost of 4,390,268.51 monetary unit and a minimum time of 19613.58 mn.
<table>
<thead>
<tr>
<th>Activities</th>
<th>Conditions</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Loading</td>
<td>- Lo free</td>
<td>- Lo free</td>
</tr>
<tr>
<td></td>
<td>- Tr free (empty ready to be loaded)</td>
<td>- Tr loaded (ready for transportation)</td>
</tr>
<tr>
<td></td>
<td>- RC receipt (Rock available)</td>
<td></td>
</tr>
<tr>
<td>Transport</td>
<td>- Tr loaded (ready for transportation)</td>
<td>- Tr arrived (ready for unloading)</td>
</tr>
<tr>
<td>Unloading</td>
<td>- Tr arrived (ready for unloading)</td>
<td>- RC unloaded (ready for crushing)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Tr unloaded (empty ready for the return)</td>
</tr>
<tr>
<td>Tr Return</td>
<td>- Tr unloaded (empty ready for the return)</td>
<td>- Tr free (empty ready to be loaded)</td>
</tr>
</tbody>
</table>

Table 2: Activities, conditions and results related to the truck entity Tr in a quarry aggregates.

6 Conclusion

According to the different scenarios carried out, inefficiencies of the studied problem were identified and it has been shown through the three-phase discrete-event simulation that the quarry system can be improved to 2 loaders and 6 trucks for the production of 31,520 m³ of aggregates at a minimum cost. Finally, the best performance of the quarry is demonstrated using MC method through the mean occupancy rates of different entities and their variance values strongly support the efficiency of MC method on a civil engineering problem.

References

7 Annexes

![Diagram of the ACD representing the loop truck (Tr).](image)

**Fig. 1** The ACD representing the loop truck (Tr).

![Diagram of the ACD representing the ALGRAN Quarry of Bejaia](image)

**Fig. 2** The ACD representing the ALGRAN Quarry of Bejaia
Quarry Simulation

Input Parameters of Simulation

- How many Loader(s)? 1
- How many Truck(s)? 5
- Smallest Truck Capacity? 1.50: 14
- Crusher capacity? 1.50: 40
- Amount of Rock spilled after fire/m³? 1.50: 7920
- Volume of aggregates to Produce/m³? 1.50: 31580

Input mean Service times / min

- Truck Loading (1.50): 3
- Truck Transport (1.50): 4
- Truck unloading (1.50): 1
- Rock Cruching (1.50): 1
- Truck Return (1.50): 7
- Holes Drilling (1.50): 1800
- Holes Mining (1.50): 19
- Drilling Team Shelter (1.50): 1
- Drilling Team Return (1.50): 1
- Loader Shelter (1.50): 3
- Loader Return (1.50): 3
- Driller Shelter (1.50): 6
- Driller Return (1.50): 15
- Holes Fire (1.50): 15
- Site Inspection (1.50): 10

Fig. 3 The 1st window summarizing the input data of the quarry simulation

different Input Costs

- Truck in activity (1.3275): 1328
- Truck awaiting (1.3275): 548
- Crusher in activity (1.3275): 4000
- Crusher awaiting (1.3275): 1000
- Drilling Team in activity (1.3275): 480
- Drilling Team awaiting (1.3275): 37
- Loader in activity (1.3275): 4734
- Loader awaiting (1.3275): 1000
- Driller in activity (1.3275): 9171
- Driller awaiting (1.3275): 7422
- Mining Cost (1.3275): 7322

Set up event trace file? (Y/N)

Fig. 4 The 2nd window summarizing the input data of the quarry simulation

Number of Loader: 2
Number of Truck: 6
rock available: 124
Simul. clock: 17525

Driller: 4
Shelter: 4
Use: 4
Mining: 4
Use: 2254
Transport: 2252

Loader: 4
Sewer: 8
Use: 788
Unload: 2252
Return: 2256
Return: 8
Simul. number: 60

Inspection: 4

Return: 5

the best strategy to produce 31580.00 m³ of aggregates is achieved with

- Mean Cost = 4390265.51
- Mean Time = 19613.50
- Trucks number = 6
- Loaders number = 2

Mean Variance
- DrRate 89.88 3.77
- DRate 11.25 0.35
- DTRate 0.91 0.01
- IrRate 22.24 1.13
- LoRate 16.30 0.72

Press any key to continue

Fig. 5 Simulation results related to the quarry problem using MC
Extreme value copulas and marginal effects

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Abstract. In this paper we estimate the risk in an auto insurance company by the theory of copulas. This leads us to consider two fundamental issues. First we propose a goodness-of-fit test for extreme value copulas to selecting which the best copula reveals the dependence structure. The empirical results show that copula belongs to the family of extreme values. Second, we adjusted marginals based on the graphic evidence and we incorporate the Champernowne distribution function modified, with gave a high capital requirement using the level required by Solvency II. Finally we treat to bounding the measure value at risk VaR for the aggregate loss by several methods in order to control the risk.

Keywords: Copula, VaR, Extreme Value.

1 Introducción

The use of copulas have been in recent years an essential tool considered by analysts to measure risk in financial and actuarial field. By revealing the dependence structure, is revealed the relationship between the joint distribution and the marginals. Therein lies its importance for adjustment.

In other words they are intimately related to the study of marginals distributions with "fixed" or "given", Nelson [11]. This relationship is decrypted by the fundamental theorem proposed by Sklar [2]. Specifically it is shown that each bivariate function $H$ of a vector of variables $(X, Y)$ with marginal $F$ and $G$ contains within a copula $C$, that isolate the dependence with the representation:

$$H(x, y) = C(F(x), G(y)) \forall x, y \in \mathbb{R}. \quad (1)$$

The unknown of the joint distribution of the variables involved the unknown of the dependence structure between them, and the problem of the most time lies in choosing the class of copulas that best reflects its structure.

Tests of adequacy of copula are today an effective tool for building the goodness-of-fit, and lately the lines research is increasingly focusing its development. It is worth mentioning the works of Fern\'an\'an [8] finding the weak convergence of the empirical copula and then the contrast of Scalliet [9] for the positive quadrant dependence hypothesis, and ultimately the test of symmetry in bivariate copulas introduced by Genest\ et al. [10]. For the contrast to the extreme value copulas we can mention the test introduced by Goudi \textit{et al.} [12] derived from the transformation of the bivariate distribution of extreme values, and the proposed by Kojadinovic \textit{et al.} [7], using the definition of max-stable as null hypothesis. In our study we found a similar result in the bivariate case and we got the weak convergence of the statistic proposed in the general case.

1.1 Test for Extreme Value Copulas

One way to know if our data have an extreme copula behavior or not, is contrast the property of the $\text{max} = \text{stable}$. The copula is said max-stable if for every positive real number $r$ and all $u, v$ in $[0, 1]$, $C(u, v) = C^r(u^{1/r}, v^{1/r})$, then we formulate the null hypothesis and its alternative like:

\[\begin{align*}
H_0^\prime : \quad & C(u, v) = C^r(u^{1/r}, v^{1/r}), \quad \forall u, v \in [0, 1], \forall r > 0 \\
H_1^\prime : \quad & C(u, v) \neq C^r(u^{1/r}, v^{1/r}), \quad \exists u, v \in [0, 1], \exists r > 0.
\end{align*}\]
We consider the functions:
\[
\mathbb{D}_n^r(u, v) = \sqrt{n} \left( C_n(u, v) - C^r_n(u^{1/r}, v^{1/r}) \right)
\]
\[
\mathbb{D}(u, v) = \sqrt{n} \left( C(u, v) - C^r(u^{1/r}, v^{1/r}) \right),
\]
where \( C_n(u, v) \) is the empirical copula defined as:
\[
C_n(u, v) = \frac{1}{n} \sum_{i=1}^{n} I(F_n(X_i) \leq u, G_n(Y_i) \leq v), \quad u, v \in [0, 1]^2. \tag{2}
\]
To find the convergence of the difference \( \mathbb{D}_n^r(u, v) - \mathbb{D}(u, v) \), we rely on the result of Fernanian [8] for the weak convergence of the empirical copula \( C_n \) towards the Gaussian process \( \mathbb{G} \) in \( L^\infty([0, 1]^2) \), which is expressed as follows:
\[
\mathbb{G}(u, v) = \mathbb{B}(u, v) - \partial_1 C(u, v) \mathbb{B}(u, 1) - \partial_2 C(u, v) \mathbb{B}(1, v), \tag{3}
\]
such that \( \mathbb{B} \) is a Brownian bridge on \([0, 1]^2\) with the covariance functions:
\[
E[\mathbb{B}(u, v) \mathbb{B}(u', v')] = C(u \wedge u', v \wedge v') - C(u, v)C(u', v').
\]

**Proposition 1.** If the partial derivatives of a copula \( C(u, v) \) are continuous then for any \( r > 0 \) we have:
\[
\mathbb{D}_n^r(u, v) - \mathbb{D}(u, v) \Rightarrow C^r(u, v) = \mathbb{G}(u, v) - r C^{-1}(u^{1/r}, v^{1/r}) \mathbb{G}(u^{1/r}, v^{1/r}), \tag{4}
\]
in \( L^\infty([0, 1]^2) \).

Under the hypothesis \( H_0 \) we have \( \mathbb{D}(u, v) = 0 \) and in this case \( \mathbb{D}_n^r(u, v) \) converges weakly towards the process (4). I should mention that the same convergence get it the authors Kojadinovic et al. [7] in the multivariate case but is the inverse of our (negative sign). To calculate de critical values we refer to the results obtained in their article based on the method **Multiplier**. Van der Vaart [4], and that consists in generating independent copies of a distribution with the same behavior. In particular the statistic used is Cramer-von Mises and can not affect the significance of the test by its quadratic expression:
\[
S_n^r = \int_0^1 \int_0^1 (\mathbb{D}_n^r(u, v))^2 \, du \, dv, \tag{5}
\]

## 2 Marginals

The first two marginal are the Gumbel and Weibull distribution resulting from the generalized theory of extreme values **GEV**. We include the log-normal distribution that has interesting theoretical properties, and finally, we analyze the modified Champernowne distribution who has been studied by Budi-Larsen et al. [3] in the context to estimate the density with the kernel function for the extremes variables.

**Definition 1.** The modified Champernowne distribution is defined for \( x \geq 0 \) and its density function:
\[
f_{\alpha, M, c}(x) = \frac{\alpha (x + c)^{\alpha-1} ((M + c)^\alpha - c^\alpha)}{(x + c)^\alpha + (M + c)^\alpha - 2c^\alpha},
\]
with parameters \( \alpha > 0, \ M > 0, \ y \ C \geq 0 \) and distribution function:
\[
F_{\alpha, M, c}(x) = \frac{(x + c)^\alpha - c^\alpha}{(x + c)^\alpha + (M + c)^\alpha - 2c^\alpha},
\]
The asymptotic behavior of the distribution Champernowne modified is the same as the original and also converges towards a Pareto distribution.
3 Bounds of the VaR

One of the most commonly used risk measures in the field of finance and actuarial is the VaR (Value-at-Risk). Statistically the VaR represents the quantile of a distribution to a level fixed previously.

**Definition 2.**

$$\text{VaR}_\alpha(X) = \inf\{x \in \mathbb{R} | F_X(x) \geq \alpha \}.$$  

Next we find the bounds of the VaR for two reasons, first because this risk measure violates the subadditivity condition, and in the general we do not know the joint distribution function. We use two methods to solve these problems. The Bootstrap method wish gives us confidence intervals and the technique proposed by Mesfanni y Quessay [6] in the case that the marginal are unknown.

Finally, when the dependence structure is unknown and the marginals are known we can use the resulting limits of Fréchet bounds.

$$W = \max(u + v - 1, 0) \leq C(u, v) \leq M = \min(u, v) \quad \forall u, v \in [0, 1].$$

The upper bound M is always a copula in any dimension, however, lower bound fails as the distribution in the multivariate case. Overall in the bivariate case, for $F_1$ y $F_2$ two marginal of $X$ and $Y$ is met, see Embrechts et al. [1]:

$$\underline{\text{VaR}}(\alpha) \leq \text{VaR}_\alpha(S) \leq \overline{\text{VaR}}(\alpha),$$

where

$$\underline{\text{VaR}}(\alpha) = \sup_{u+v=\alpha} (F_1^{-1}(u) + F_2^{-1}(v))$$

$$\overline{\text{VaR}}(\alpha) = \inf_{u+v=\alpha+1} (F_1^{-1}(u) + F_2^{-1}(v)).$$

In the case that we have Champernowne distribution function as marginal with parameters $\alpha_i > 0, M_i > 0$ y $c_i \geq 0$ for i=1,2:

$$F_i^{-1}(u) = \left( \frac{u[M_i + c_i \alpha_i - 2c_i \alpha_i]}{1 - u} \right)^{-1} - c_i \quad \forall u \in [0, 1].$$

Using the fact that the density of Champernowne is nonincreasing after a certain point (have the same behavior in a Pareto tail) we can deduce using the convexity of $F_i^{-1}$ that:

$$\underline{\text{VaR}}(\alpha) = \max(F_1^{-1}(\alpha) + F_2^{-1}(0), F_2^{-1}(\alpha) + F_1^{-1}(0))$$

$$= \max(F_1^{-1}(\alpha), F_2^{-1}(\alpha)), \quad (6)$$

and the upper bound is equal:

$$\overline{\text{VaR}}(\alpha) = \inf_{\alpha \leq u \leq 1} h(u), \quad (7)$$

such that $h(u) = F_1^{-1}(u) + F_2^{-1}(\alpha + 1 - u).$

4 Results

This section put on approval the theoretical concepts that we have seen and our goal is to decipher the structure of dependency between the data corresponding to a sample of claims relating to insurance a major car company that operates in Spain. The sample is random and contains two costs: Cost1, presenting own damages and compensation of the loss, and Cost2, which corresponds to the expenses related to medicine and hospitalization. In general, the injuries are covered by the National Institute of Health, however, some medical expenses and rehabilitation, technical assistance, drugs, etc... are going to account of the insured, including compensation for pain, suffering and loss of income. Although bodily injury claims typically take years, all related cases
Proceedings, 15th Applied Stochastic Models and Data Analysis (ASMDA2013)
International Conference, Mataró (Barcelona), Spain 25 - 28 June 2013

<table>
<thead>
<tr>
<th>Cost</th>
<th>Media</th>
<th>Dev.std</th>
<th>Kurtosis</th>
<th>Asimetría</th>
<th>Min</th>
<th>Max</th>
<th>Mediana</th>
<th>J-B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost 1</td>
<td>182.8</td>
<td>686.8</td>
<td>297.1</td>
<td>15.65</td>
<td>13</td>
<td>137900</td>
<td>677</td>
<td>1941868.27</td>
</tr>
<tr>
<td>Cost 2</td>
<td>293.92</td>
<td>863.17</td>
<td>82.02</td>
<td>8.04</td>
<td>1</td>
<td>11853</td>
<td>88</td>
<td>1549697.73</td>
</tr>
<tr>
<td>Cost Total</td>
<td>211.2</td>
<td>752</td>
<td>286.4</td>
<td>15.27</td>
<td>32</td>
<td>149800</td>
<td>789</td>
<td>1804742.8</td>
</tr>
</tbody>
</table>

Table 1. Descriptive statistics and normality test.

![Q-Q Plot for "log-normal" distribution](image1)

**Fig. 1. Log-Normal QQ-Plot.**

![Champernowne QQ-Plot](image2)

**Fig. 2. Champernowne QQ-Plot.**

were liquidated in 2002, according to the company, Bolancé et al. [13]. Lastly, the compensation may include payments to third parties that have been damaged in one way or another.

In the Table 1 we summarize the descriptive statistics of the sample, which has a size n=518. The data are all positive with one big difference between Min and Max. The kurtosis and skewness are very high if we compare them with a normal distribution. The hypothesis of non-normality of the data is rejected by the Jarque-Bera test which gives a p-value < $2.10^{-16}$ too small for the three costs. The QQ-plot graphs help us to look the behavior of the empirical distribution in the tails of distributions. Specifically theoretical quantiles of a supposed distribution are compared with the empirical quantiles. When there is a good fit the empirical quantiles coincide with the theoretical. Using a log-normal distribution (Figure 1), we note that the values set on the left side and then deviate upwards indicating the existence of extreme values and therefore heavy tailed distribution may be a good fit for data as shows the adjustment of QQ-Plot respect to the quantile of a Champernowne distribution in the Figure 2.

4.1 K-Plot and Test of extreme value copula

In Figure 3 of K-Plot we note that costs have a positive association (which mark values of K-plot are above the diagonal that indicates independence). The points are almost all between the straight line and curve boundary that marks perfect positive dependence. It seems that according the $W_k$ (Pseudo-observationes modified) growing, data approach a perfect positive dependence. This means that the amounts in medical costs and compensation are more correlated, as the incident is more severe.

The statistic of Cramer-Von Mises (5) gives us a value 0.26795 and a p-value equal to 0.1773227. We do not reject the null hypothesis that the copula associated with this type of data is the extreme values at level 10%.

If in addition we use the information criteria for selecting the copula in this classe, we have the Akaike information criterion:

$$AIC = -2 \log L(\theta, u, v) + 2k,$$
and Bayesian information criterion,

\[ BIC = -2 \log L(\theta, u, v) + \log(n)k \]

(where \( k \) is the number of parameters to be estimated and \( L \) the maximum likelihood function). Therefore, from the Table 2 we deduce that the Gumbel copula reflect the best structure of dependence for our data.

<table>
<thead>
<tr>
<th>Copula</th>
<th>AIC</th>
<th>BIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gumbel</td>
<td>-246.8053</td>
<td>-241.8621</td>
</tr>
<tr>
<td>Galambos</td>
<td>-243.9354</td>
<td>-238.9922</td>
</tr>
<tr>
<td>Husler-Reiss</td>
<td>-239.6841</td>
<td>-234.741</td>
</tr>
</tbody>
</table>

Table 2. Information Criteria.

4.2 Bounding the empirical VaR

In the following Table 3 we present first the empirical values with different VaR confidence levels \( \alpha \) to the aggregate loss \( S = X_{Cost1} + Y_{Cost2} \). In the second and third rows are located the confidence intervals at level of 95\% of the VaR \( S(\alpha) \) using a Bootstrap. In the last rows we bounds the measure of the risk using the upper and lower limits from the Mesfioui method and Quesay [6].

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>0.90</th>
<th>0.91</th>
<th>0.92</th>
<th>0.93</th>
<th>0.94</th>
<th>0.95</th>
<th>0.96</th>
<th>0.97</th>
<th>0.98</th>
<th>0.99</th>
<th>0.95</th>
</tr>
</thead>
<tbody>
<tr>
<td>VaR(( \alpha ))</td>
<td>0.959</td>
<td>0.964</td>
<td>0.969</td>
<td>0.974</td>
<td>0.979</td>
<td>0.984</td>
<td>0.989</td>
<td>0.994</td>
<td>0.999</td>
<td>1.000</td>
<td>0.959</td>
</tr>
<tr>
<td>bootstrap.IC.Inf(95%)</td>
<td>0.956</td>
<td>0.961</td>
<td>0.966</td>
<td>0.971</td>
<td>0.976</td>
<td>0.981</td>
<td>0.986</td>
<td>0.991</td>
<td>0.996</td>
<td>1.001</td>
<td>0.956</td>
</tr>
<tr>
<td>bootstrap.IC.Sup(95%)</td>
<td>0.953</td>
<td>0.958</td>
<td>0.963</td>
<td>0.968</td>
<td>0.973</td>
<td>0.978</td>
<td>0.983</td>
<td>0.988</td>
<td>0.993</td>
<td>1.000</td>
<td>0.953</td>
</tr>
<tr>
<td>VaR.Inf(( \alpha ))</td>
<td>0.954</td>
<td>0.959</td>
<td>0.964</td>
<td>0.969</td>
<td>0.974</td>
<td>0.979</td>
<td>0.984</td>
<td>0.989</td>
<td>0.994</td>
<td>1.000</td>
<td>0.954</td>
</tr>
<tr>
<td>VaR.Sup(( \alpha ))</td>
<td>0.951</td>
<td>0.956</td>
<td>0.961</td>
<td>0.966</td>
<td>0.971</td>
<td>0.976</td>
<td>0.981</td>
<td>0.986</td>
<td>0.991</td>
<td>1.000</td>
<td>0.951</td>
</tr>
</tbody>
</table>

Table 3. Bounding the empirical VaR.

Figure 4 displays the confidence bands for the empirical VaR. We note that the method and Quesay Mesfioui provides a large bounds, especially in the upper bound, while the Bootstrap technique provides narrower intervals accompanying empirical VaR. If we plot the VaR of Cost 1 plus the VaR of Cost2 [cut red lines] we first note that their numbers are within the confidence interval level 95\% of the aggregate loss, and secondly we clearly see that the condition of Sub-additivity is violated.
4.3 Simulation of the VaR

In Table 4 we calculate the VaR of the total Costs by simulation and with 10,000 repetitions. The simulation was performed with Itau approximation for parameters of various copula and using the maximum likelihood estimation for marginal parameters. We note that only using the Normal copula with Champenowne marginal we obtain a higher value of the VaR at the level 95%, however we note that the highest VaR comes from Gumbel copula with marginal Champenowne if we increase the level at 99.5% as required Solvency II. Precisely the only copula used in the table and it extreme values is Gumbel copula, and this result coincides with the selection tests done before for the structure dependence of the data.

Given the VaR as a risk measure for the solvency of the insurance cover, we can say that the Champenowne distribution ensures greater capital requirement at level required by Solvency II.

<table>
<thead>
<tr>
<th>Copula</th>
<th>Marginals</th>
<th>Normal</th>
<th>Gumbel</th>
<th>Champenowne</th>
</tr>
</thead>
<tbody>
<tr>
<td>VaR (95)</td>
<td>6477.471</td>
<td>11751.43</td>
<td>5189.154</td>
<td>7769.814</td>
</tr>
<tr>
<td>VaR (99.5)</td>
<td>22718.02</td>
<td>26762.99</td>
<td>8377.31</td>
<td>44748.02</td>
</tr>
<tr>
<td>Copula t-Student</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VaR (95)</td>
<td>6600.84</td>
<td>11889.94</td>
<td>5167.743</td>
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</tr>
<tr>
<td>VaR (99.5)</td>
<td>21361.53</td>
<td>29476.47</td>
<td>8007.314</td>
<td>39424.63</td>
</tr>
<tr>
<td>Copula Gumbel</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VaR (95)</td>
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<td>5301.551</td>
<td>7462.712</td>
</tr>
<tr>
<td>VaR (99.5)</td>
<td>21433.02</td>
<td>32434.25</td>
<td>7397.997</td>
<td>45381.0</td>
</tr>
<tr>
<td>Copula Clayton</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>VaR (95)</td>
<td>6484.238</td>
<td>12332.19</td>
<td>5109.727</td>
<td>7331.435</td>
</tr>
<tr>
<td>VaR (99.5)</td>
<td>19674.56</td>
<td>23716.97</td>
<td>8064.769</td>
<td>39971.79</td>
</tr>
<tr>
<td>Copula Frank</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>VaR (95)</td>
<td>6818.795</td>
<td>12879.43</td>
<td>5043.886</td>
<td>7501.679</td>
</tr>
<tr>
<td>VaR (99.5)</td>
<td>22912.35</td>
<td>26298.98</td>
<td>8074.56</td>
<td>35644.29</td>
</tr>
</tbody>
</table>

Table 4. VaR with the estimate marginals.

In Figure 5 (part left) we note that the VaR of aggregate loss with marginal Champenowne (red line) can violate confidence intervals empirical VaR (black lines) but in this case does not reach the limits calculated from the method of Mestafion and Quessy [6]. Finally in the right figure we plot the lower and upper bounds when the copula associated is unknown by solving numerically the limits (7) and (8). We add in the same graph the VaR resulting of simulation with a Gumbel copula and marginal Champenowne (green lines). We observe that the simulated VaR is identical to the lower bound to some degree, and when we increase the confidence levels its is located within the limits established by a unknown copula.
5 Conclusions

In the present work we have attempted to solve the unknown adjustment of the two components that form part of a bivariate distribution that are the associated copula and marginals. The adequacy test on extreme value copula introduced assures us the possible class copula, and especially when the data have extreme values.

Graphs as K-Plot and QQ-Plot are also good tools to help us explore the structure of dependence between variables. In our case the K-Plot revealed a positive and growing dependence between variables Auto Insurance and the incorporation of the new test of extreme value copulas that we have constructed confirms that our copula associated is the extreme values as Gumbel copula.

In the selection of marginal distribution we have incorporated modified Champernowne, who gave an interesting result in the simulation of copulas, due, firstly, to its similarity to the Log-Normal at low values of the variable and, secondly, by their convergence toward Pareto in the right tail. Indeed, in order to ensure the required capital requirement and solvency II we find that using Gumbel copula and marginal Champernowne yields a high value of the VaR at level 99.5% followed by the value of VaR with marginals Weibull.

Non-coherence of some measures of risk led some statisticians to try to bounding the aggregate VaR loss. Noteworthy are the results of Embrechts and Puccetti [5] using the Fréchet bounds when the marginal distributions are known and the copula is unknown.

We have used some of these results and we have compared them with the confidence intervals provided by Bootstrap method. In our study we found that the empirical VaR violates at some points the subadditivity condition, but is always inside the confidence interval (using Bootstrap) at the level 95% of the VaR for the aggregate losses. Moreover, by means of simulation and using the Gumbel copula with marginal Champernowne, we have found that can be given the case that the VaR goes out of the at the top of confidence interval, but would always be within the lower and upper bounds used when the marginal are unknown. Finally, we contrast in the case unknown associated copula and using the Champernowne marginal, the VaR simulated is within the limits resulting from the bounds developed by Embrechts et al. [5].

References

The Risk of Poverty Model in EU Population

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Abstract. In the time of economic crisis the questions of poverty become of the great importance. In order to discover groups affected strongly by this problem it appears to be important to analyze factors influencing the situation at-risk-of-poverty. The contribution presents a generalized linear model (namely the multifactor logistic ANOVA model with mixed effects) of risk-of-poverty in EU countries in years 2004 to 2008. The analysis is based on EU SILC survey data and focuses on the study of the impact of age group, sex, EU country and the year of survey on the risk-of-poverty.

Keywords: Multifactor Logistic ANOVA, Mixed Effects, Risk-of-poverty, EU SILC.

1 Introduction

The problems of poverty in EU appear to be of the great interest particularly in the contemporary situation of Global economic crisis which is characterized by a high unemployment rate and significant uncertainty of business together with the increasing public and private indebtedness. Such climate appears to be very demanding for the management and cooperation of EU states. In this difficult situation the governments constantly operating in the regime of the budget deficit are forced to introduce the austerity measures in order to stop or decelerate the increase of the debt. Moreover, these problems are accompanied by an adverse demographic development, namely the threat of growing average age demanding the continuing growth of mandatory expenses as well as high proportion of unemployed youth appearing in several countries and ranking to the so called Ninja generation. Such factors even increase the load of mandatory expenses and thus deepen the adverse social and political climate in Europe. This development necessitates not only the economical changes but also the transformation of social, social cohesion and unemployment policies.

The European Union and its particular bodies, primarily European Commission, provide certain programs and recommendations for individual EU members. Among the primary program documents ranks the EU’s strategy for current decade Europe 2020, the smart, sustainable and highly inclusive strategy for the increasing of employment, productivity, innovation and social cohesion. Contemporarily, two important initiatives are devoted to the situation of youth
and seniors. Namely, the project of *European Year for Active Ageing and Solidarity between Generations 2012*\(^1\) and current EU *Strategy for Youth (2010 – 2018)*\(^2\).

The contribution thus stems from the defined partial aims of EU and focuses on the modeling of the influence of sex, age category and region where the individual lives on his or her economic situation according to the possible threat of the monetary poverty. Yet another effect taken into the account in the modeling of risk-of-poverty is the year of survey. In our analysis the five year period 2005 – 2009 of EU SILC surveys is used.

## 2 Surveys of incomes, living conditions and poverty in EU

Information on incomes and household sizes originate from the data files of EU SILC survey (*European Union – Statistics on Income and Living Conditions*). The objective of this survey is to acquire representative data concerning the income distribution of particular household types about the style, quality and financial demands on housing, long-term household equipment and material and health conditions of adults living in the household. The EU SILC survey is performed once a year from February to May and has a form of so called rotational panel survey, where the same households are surveyed repeatedly in an annual interval for four consecutive years. In the Czech Republic and in Slovakia the first EU SILC survey was organized in 2005 and therefore the data files from 2005 to 2009 were used.

For the sake of comparison of incomes in case of different types of households, usually the average incomes per individual (resp. per household) were used. Presently, the conversion of incomes on the equalized scale using a so called consuming unit is employed. This process reflects the size of household and the type of its members. The enumeration of consuming unit itself takes into the consideration the economies of scale in multi-member households\(^3\). In EU the modified OECD scale is used which assigns the weight to of 1.0 to the (adult) head of household, other members aged over 13 obtain the weight of 0.5 and children under 13 years get the weight 0.3.

The calculation of a measure called *at-risk-of-poverty rate* is according to the EU methodology based on an equalized income, i.e., the ratio of a disposable income of a household and number of its consuming units. Such equalized income is assigned to all household members\(^4\). The set of all individuals ranked

---


\(^3\) These economies of scale concerns the savings on objects and services used by several household members (household equipment, energies, etc.).

\(^4\) The value is assigned uniformly to all household members.
increasingly according to their disposable income is used as a basis for the computation of a poverty threshold (Ravallion [13]). As a poverty threshold most frequently serves the limit 60% of median of the equalized income. Other possible definitions can be based on thresholds given by 40%, 50% or 70% of median. The measure of monetary poverty is given by a proportion of individuals with equalized incomes lower the chosen poverty threshold among all members of considered group of individuals5. Such measure is relative and belongs among the additive Foster-Greer-Thorbecke poverty measures (Foster et al. [6]). The common methodology comprises a prerequisite for the necessary international comparisons among EU countries.

To the analyses of the monetary poverty and material deprivation as well as to the modeling of income distribution and prediction of the age structure of chosen population an immense amount of articles is devoted. As an illustration we can mention a few chosen sources concerning particularly the situation in the Czech Republic and Slovakia. See, e.g., works of Bartosova and Bina [1], Bartosova and Forbeska [2], Bartosova and Zelinsky [3], Bilkova [4], Fiala and Langhamrova [5], Labudova et al. [8], Longford and Pittau [9], Mala [10], Marek [11], Rezankova and Loster [14], Smrcka and Arltova [15], Stankovicova and Bartosova [16], Vecernik [17], Vecernik [18], Zelinsky [19] and others.

3 Mathematical model

The analyzed data sets concern the inhabitants of EU member states in years 2004 – 2008. The data are thus dependent in different groups and, moreover, observed in several years. Therefore the classical linear models with fixed effects cannot be used, because they require independence of particular observations. The modeling itself is performed using the linear models with mixed effects enabling to take into account the influence of particular experimental units (groups, subjects) on the repeated measurements (Hosmed and Lemeshow [7]). The insertion of individual effects allows the estimation not only of the total common influence but also the particular changes of each group (each subject). The model utilizes the following notation: index \( i \); \( i = 1, \ldots, N \), denotes independent experimental units (groups), pair of indices \( ij \); \( j = 1, \ldots, n_j \), stands for the correlated observation on the \( i \)-th experimental unit.

The modeled variable, the risk of monetary poverty, is of a dichotomic type (it takes the values of \{0;1\}). Therefore, we will apply the model from a broad class of Generalized Linear Mixed Models (GLMMs) enabling to handle the response with exponential type of distribution6 (McCulloch and Searle [12]).

5 As a group the incomes of individuals are compared with, the inhabitants of particular state are concerned.

6 The class of exponential distributions comprises large scale of discrete and continuous distributions including also, e.g., the alternative, binomial, Poisson, negative binomial, normal, exponential, gamma, etc.
For such purposes we employ the multifactor logistic ANOVA model with mixed effects. In the logistic model with the random effects the conditioned mean response \( \mu_{ij,k} \) is tied together with the linear predictor \( \eta_{ij,k} \) via the logit link function \( g(\mu_{ij,k}) = \logit = \ln[\mu_{ij,k} / (1 - \mu_{ij,k})] \), thus

\[
\eta_{ij,k} = \ln \frac{\mu_{ij,k}}{1 - \mu_{ij,k}}.
\]

The conditioned mean value \( \mu_{ij,k} = E(\mu_{ij,k} | \nu_i, x_{ij,k}) \) of an alternative distribution of response is equal to the conditional probability \( P(Y_{ij,k} = 1 | \nu_i, x_{ij,k}) \), and therefore

\[
\mu_{ij,k} = g^{-1}(\eta_{ij,k}) = F_{\text{logist}}(\eta_{ij,k}),
\]

where \( F_{\text{logist}}(\eta_{ij,k}) \) is a CDF of a logistic distribution with the shape given by

\[
F_{\text{logist}}(\eta_{ij,k}) = \frac{1}{1 + \exp(-\eta_{ij,k})}.
\]

Nice property of the logistic distribution stems from the fact that its density can be simply calculated using the distribution function

\[
f_{\text{logist}}(\eta_{ij,k}) = \frac{F_{\text{logist}}(\eta_{ij,k})}{1 - F_{\text{logist}}(\eta_{ij,k})}.
\]

4 Logistic ANOVA model of risk of monetary poverty in EU

The considered paper presents a construction of model with two variables comprising the group effect – country and AgeGroup, this provides a possibility to consider the influence of both types of groups simultaneously. According to the fact that both variables are correlated with the year of EU SILC survey (variable year), the model will contain also interaction factors combining pairs year, country and year, AgeGroup. Only variable sex will be considered as a fixed effect. Thus, all explanatory variables are categorical and the presented model can be described by following formula

\[
\eta_{ij,k} = \beta_{sex} \cdot sex_{ij,k} + (\beta_{year} + v_{year,AgeGroup} + v_{year,country}) \cdot year_{ij,k},
\]

where \( i = 1, \ldots, 27 \) denotes the EU member state, \( j = 1, \ldots, 4 \) age category and \( k \) means the \( k \)-th observation (individual) within the \( ij \)-th subgroup. Parameters

\( \beta_{sex} \), where \( sex \in \{ \text{male; female} \} \), and \( \beta_{year} \), where \( year \in \{ 2005; \ldots; 2009 \} \).
express the fixed effects of sex and year of EU SILC survey. Parameters \( \nu_{\text{year}, \text{AgeGroup}} \) and \( \nu_{\text{year}, \text{country}} \) represent a combination of the year of survey and age group of a person, resp. the combination of the year and country where the person lives.

Table 1. Estimates of the fixed effects in the logistic model of risk of monetary poverty for individuals. (Own computation according to EU-SILC 2005 – 2009)

Table 2 contains particular variance components of the estimated logistic model, namely standard deviations of random effects for both group variables \( \text{country} \) and \( \text{AgeGroup} \). The description of estimate variability for \( \text{AgeGroup} \) is augmented by a matrix of year-on-year correlations. The following Table 3 presents maximum likelihood estimates of random effects of the group variable \( \text{AgeGroup} \) indicating the increase (+), respectively the decrease (–) of the individual chance on the slide under the poverty threshold.

<table>
<thead>
<tr>
<th>Fixed effects</th>
<th>point estim.</th>
<th>std. deviation</th>
<th>z-statistics</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Intercept)</td>
<td>-1.866300</td>
<td>0.105672</td>
<td>-17.661300</td>
<td>8.3 \cdot 10^{-70}</td>
</tr>
<tr>
<td>2006</td>
<td>0.021417</td>
<td>0.020804</td>
<td>1.029437</td>
<td>0.303275</td>
</tr>
<tr>
<td>2007</td>
<td>-0.000850</td>
<td>0.025171</td>
<td>-0.033670</td>
<td>0.973137</td>
</tr>
<tr>
<td>2008</td>
<td>0.005567</td>
<td>0.030181</td>
<td>0.184438</td>
<td>0.853670</td>
</tr>
<tr>
<td>2009</td>
<td>0.012454</td>
<td>0.041332</td>
<td>0.301329</td>
<td>0.763164</td>
</tr>
<tr>
<td>female</td>
<td>0.153820</td>
<td>0.000126</td>
<td>1225.332</td>
<td>0.000000</td>
</tr>
</tbody>
</table>

Table 1. Estimates of the fixed effects in the logistic model of risk of monetary poverty for individuals. (Own computation according to EU-SILC 2005 – 2009)

<table>
<thead>
<tr>
<th>Standard deviations of random effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>group variable – ( \text{AgeGroup} )</td>
</tr>
<tr>
<td>EU-SILC 2005</td>
</tr>
<tr>
<td>AgeGroup 2006</td>
</tr>
<tr>
<td>2007</td>
</tr>
<tr>
<td>2008</td>
</tr>
<tr>
<td>2009</td>
</tr>
</tbody>
</table>

| group variable – \( \text{country} \) |
|EU-SILC 2005 | 0.322875 | 0.093479 | 0.125959 | 0.152537 | 0.175405 |
| Country 2006 | 0.093479 | 0.322875 | 0.125959 | 0.152537 | 0.175405 |
| 2007 | 0.125959 | 0.322875 | 0.152537 | 0.175405 |
| 2008 | 0.152537 | 0.322875 | 0.175405 |
| 2009 | 0.175405 |

<table>
<thead>
<tr>
<th>Correlation components of random effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>group variable – ( \text{AgeGroup} )</td>
</tr>
<tr>
<td>EU-SILC 2006</td>
</tr>
<tr>
<td>Intercept 2007</td>
</tr>
<tr>
<td>Intercept 2008</td>
</tr>
<tr>
<td>Intercept 2009</td>
</tr>
</tbody>
</table>

\(^7\) Reference group consist of the variant \( \text{year} = 2005, \text{sex} = \text{male} \).
For the categorization of individuals into age groups the half-closed intervals (15,30], (30,50], (50,60], (60,100] were used.
The Predicted random effects for considered age groups and studied years are depicted on the Fig. 1.

**Fig. 1.** Random effects of the model for particular age groups and years in EU countries. (Own computation according to EU-SILC 2005 – 2009)
Conclusions

The estimates of fixed effects in the model showed that the risk of poverty among women is significantly higher than among men. In contrary, the year of EU SILC survey is not statistically significant. Thus, their influence can be neglected and probability of slide below the poverty threshold can be considered as constant in the whole five year period.

The values of correlation coefficients in case of group variable $AgeGroup$ shows in the most cases small or medium correlation (from 0.1469 to 0.5765). An exception can be observed in case of pair EU SILC 2006 and 2007 and EU SILC 2008 and 2009, where the strength of correlation exceeded values of 0.79156 and 0.96621.

The constructed model showed significant influence of particular age categories on the chance of slide below the poverty threshold. It is apparent, that the growth of risk appear in the groups of youngest and oldest individuals, (15;30] and (60;100], where the estimates of constant components of the random effects (related to the survey of 2005) are positive and indicate the growth of chance on the slide under poverty threshold in comparison with an average. In general, during the years the changes were insignificant, but the course shows an obvious worsening of situation in the group of “juniors”. In the “oldest” group (with the majority of retired people) the trend was opposite – the situation appears to get slightly better. Therefore, the chance of slide below the poverty threshold in 2009 was lower than in 2005. Yet another, much more positive, situation appears in this period in the group of “older” individuals (usually economically active) between 50 and 60 years. This can be inferred from the negative value of an intercept of the random effect, which indicate the decrease of risk-of-poverty in 2004 (EU SILC 2005) in comparison to the European average. Also the situation of “middle aged” individuals (from 30 to 50 years) appears to be satisfying.

According to the results of generalized linear model with mixed effects it is apparent that the Czech Republic in 2004 – 2008 ranks among the countries with the lowest risk of monetary poverty. The situation remains unchanged even in more detailed perspective of different age groups and years of EU SILC survey.

References

A generalization of some quantile-based measures commonly used in financial and insurance applications

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Abstract We propose a new family of risk measures -GlueVaR- which belongs to the class of distortion risk measures. This family is devised to reach a risk assessment lying between that provided by common quantile-based risk measures, namely value at risk and tail value at risk. A straightforward relationship between GlueVaR and these standard quantile-based risk measures is shown. It provides an easy procedure to obtain analytical closed-form expressions of GlueVaR for several distribution functions. Additionally, the concept of tail-subadditivity for distortion risk measures is introduced and investigated. A proof that a subfamily of GlueVaR risk measures satisfies tail-subadditivity is provided. An application to insurance claim data is presented.

Keywords: quantiles, subadditivity, tails, risk management.

1 Introduction

Value at risk (VaR) has been adopted as a standard tool to assess the risk and to calculate capital requirements in the financial industry. Value at risk at level $\alpha$ is the $\alpha$-quantile of a random variable $X$, i.e. $\text{VaR}_\alpha (X) = \inf \{ x \mid F_X (x) \geq \alpha \} = F_X^{-1} (\alpha)$, where $F_X$ is the cumulative distribution function (cdf) of $X$ and $\alpha$ is the confidence level $0 \leq \alpha \leq 1$. However, VaR is known to present a number of pitfalls when applied in practice.

Tail value at risk (TVaR) may be interpreted as the mathematical expectation beyond VaR, and is defined as $\text{TVaR}_\alpha (X) = \frac{1}{1 - \alpha} \int_{\alpha}^{1} \text{VaR}_\lambda (X) d\lambda$.

The TVaR risk measure does not suffer the two drawbacks mentioned for VaR and, as such, would appear to be a more powerful measure for assessing the actual risks faced by companies and financial institutions. However, TVaR has not been widely accepted by practitioners in the financial and insurance industries.

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1 Often called tolerance level.
2 A risk measure is subadditive when the aggregated risk is less than or equal to the sum of individual risks. Subadditivity is an appealing property when aggregating risks in order to preserve the benefits of diversification. The subadditivity of VaR cannot be generalized as it has been shown, for instance, in Artzner et al. [2] and Acerbi and Tasche [1]. In addition, capital requirements based on VaR can be underestimated for catastrophic losses.
We propose a new family of risk measures (GlueVaR) which forms part of a wider class referred to as distortion risk measures. We analyze the subadditivity properties of these GlueVaR risk measures and show that a subfamily of GlueVaR risk measures satisfies tail-subadditivity.

2 Distortion risk measures

Consider a probability space and the set of all random variables defined on this space. Any risk measure $\rho$ is a mapping from the set of random variables to the real line $\mathbb{R}$, $X \mapsto \rho(X) \in \mathbb{R}$. Distortion risk measures were introduced by Wang [16, 17] and are closely related to the distortion expectation theory (see Yaari [20]). There are two key elements to define a distortion risk measure: first, the associated distortion function; and, second, the concept of the Choquet Integral. A detailed literature review of distortion risk measures is available in Denuit et al. [9] and Balbás et al. [3]. The distortion function, Choquet Integral and the distortion risk measure can be defined as follows:

- **Distortion function.** Let $g : [0, 1] \rightarrow [0, 1]$ be a function such that $g(0) = 0$, $g(1) = 1$ and $g$ is non-decreasing. Then $g$ is called a distortion function.

- **Choquet Integral.** The (asymmetric) Choquet Integral with respect to a set function $\mu$ of a $\mu$-measurable function $X : \Omega \rightarrow \mathbb{R}$ is denoted as $\int X d\mu$ and is equal to $\int X d\mu = \int_{-\infty}^{0} [S_{\mu,X}(x) - \mu(\Omega)] dx + \int_{0}^{+\infty} S_{\mu,X}(x) dx$ if $\mu(\Omega) < \infty$, where $S_{\mu,X}(x) = \mu(\{X > x\})$ denotes the survival function of $X$ with respect to $\mu$.

- **Distortion risk measure.** Let $g$ be a distortion function. Consider a random variable $X$ and its survival function $S_X(x) = P(X > x)$. Function $\rho_g$ defined by $\rho_g(X) = \int_{-\infty}^{0} [g(S_X(x)) - 1] dx + \int_{0}^{+\infty} g(S_X(x)) dx$ is called a distortion risk measure.

From the previous definitions, it is straightforward to see that for any random variable $X$, $\rho_g(X)$ is the Choquet Integral of $X$ with respect to the set function $\mu = g \circ P$, where $P$ is the probability function associated with the probability space in which $X$ is defined.

$^3$ VaR is currently the risk measure contemplated in the European solvency regulation for the insurance sector (Solvency II). This is also the case of solvency regulation for the banking sector (Basel accords).

$^4$ See Szégo [13], for instance, for an extensive introduction to risk measures.

$^5$ In honour of Gustave Choquet who introduced the concept of the integral for non-additive measures [6].

$^6$ $\Omega$ denotes a set, which in financial and insurance applications is the sample space of a probability space. A set function $\mu$ in this context is a function defined from $2^\Omega$ (the set of all subsets of $\Omega$) to $\mathbb{R}$. A $\mu$-measurable function $X$ is, widely speaking, a function defined on $\Omega$ so that expressions like $\mu(\{X > x\})$ or $\mu(\{X \leq x\})$ make sense. See Denneberg [8] for more details.
The mathematical expectation is a distortion risk measure whose distortion function is the identity function, \( \rho_{id}(X) = \mathbb{E}(X) \) (see, for instance, Denuit et al. [9]). Therefore, a straightforward way to interpret a distortion risk measure is as follows: first, the survival function of the random variable is distorted \((g \circ S_X)\); second, the mathematical expectation of the distorted random variable is computed.

Based on their distortion functions, once \( \alpha \) is fixed it can be proved that \( \text{VaR}_\alpha(X) \leq \text{TVaR}_\alpha(X) \) for any random variable \( X \).

3 A new family of risk measures: GlueVaR

We define a new family of risk measures, named GlueVaR. Any GlueVaR risk measure can be described by means of its distortion function. Given a confidence level \( \alpha \), the distortion function for GlueVaR is:

\[
\kappa_{\beta,\alpha}^{h_1,h_2}(u) = \begin{cases} 
\frac{h_1}{1-\beta} \cdot u & \text{if } 0 \leq u < 1-\beta \\
\frac{h_2-h_1}{\beta-\alpha} \cdot [u-(1-\beta)] & \text{if } 1-\beta \leq u < 1-\alpha \\
1 & \text{if } 1-\alpha \leq u \leq 1
\end{cases}
\]

where \( \alpha, \beta \in [0,1] \) so that \( \alpha \leq \beta \), \( h_1 \in [0,1] \) and \( h_2 \in [h_1,1] \). Parameter \( \beta \) is the additional confidence level besides \( \alpha \). The shape of the GlueVaR distortion function is determined by the distorted survival probabilities \( h_1 \) and \( h_2 \) at levels \( 1-\beta \) and \( 1-\alpha \), respectively. We call parameters \( h_1 \) and \( h_2 \) the heights of the distortion function.

If the following notation is used, \( \omega_1 = h_1 - \frac{(h_2-h_1)(1-\beta)}{\beta-\alpha} \), \( \omega_2 = \frac{h_2-h_1}{\beta-\alpha}(1-\alpha) \) and \( \omega_3 = 1-\omega_1-\omega_2 = 1-h_2 \), then

\[
\text{GlueVaR}_{\beta,\alpha}^{h_1,h_2}(X) = \omega_1 \cdot \text{TVaR}_\beta(X) + \omega_2 \cdot \text{TVaR}_\alpha(X) + \omega_3 \cdot \text{VaR}_\alpha(X). 
\] (2)

Thus, an interesting interpretation in the context of decision making and risk management is that GlueVaR risk measures arise as a linear combination of three possible scenarios. So, two levels of severity can be fixed, namely \( \alpha \) and \( \beta \), with \( \alpha < \beta \). Then, the risk can be measured in the highly conservative scenario with TVaR at level \( \beta \); in the conservative scenario with TVaR at level \( \alpha \); and in the less conservative scenario with VaR at level \( \alpha \) (more details can be found in [4]).

Illustration: GlueVaR expression for Student \( t \) distribution. If \( X \) is a random variable such that \( \tilde{X} = \frac{X - \mu}{\sigma} \) is distributed as a Student \( t \) random variable with \( \nu \) degrees of freedom (df) \( \nu \) then \( \text{VaR}_\alpha(X) = \mu + \sigma \cdot t_\alpha \)

7 In a case such as this, \( X \) has \( \mu \) mean and a standard deviation equal to \( \sqrt{\frac{\nu \cdot \sigma^2}{\nu - 2}} \)
and \( \text{TVaR}_\alpha (X) = \mu + \sigma \cdot \frac{\tau (t_\alpha)}{1 - \alpha} \left( \frac{\nu + t_\alpha^2}{\nu - 1} \right) \), where \( t_\alpha \) is the \( \alpha \)-quantile of a Student \( t \) distribution with \( \nu \) df and \( \tau \) is its density function.

Using (2) the GlueVaR of \( X \) random variable is

\[
\text{GlueVaR}^{h_1, h_2}_{\beta, \alpha} (X) = \mu + \sigma \cdot \left[ \left( \frac{h_1}{1 - \beta} \cdot \frac{h_2 - h_1}{\beta - \alpha} \right) \cdot \tau \left( t_\beta \right) \cdot \left( \frac{\nu + t_\alpha^2}{\nu - 1} \right) + \frac{h_2 - h_1}{\beta - \alpha} \cdot \tau \left( t_\alpha \right) \cdot \left( \frac{\nu + t_\alpha^2}{\nu - 1} \right) + \left( 1 - h_2 \right) \cdot t_\alpha \right].
\]

Analytical expressions of GlueVaR for Normal (\( N \)), Log-normal (\( LN \)) and Generalized Pareto (\( GP \)) distributions have simple closed-form expressions of GlueVaR, as shown in Belles-Sampera et al. [4].

4 Subadditivity in the tail

This section is devoted to an analysis of the properties of the GlueVaR family of risk measures, with special attention to subadditivity. Artzner et al. [2] established the following set of axioms that a risk measure should satisfy: positive homogeneity, translation invariance, monotonicity and subadditivity. They referred to such risk measures as “coherent risk measures”. Distortion risk measures always satisfy the first three properties [8], but subadditivity is only guaranteed when the distortion function is concave [8, 18, 19]. Therefore, VaR, unlike TVaR, is not coherent [9].

GlueVaR risk measures may be interpreted as a linear combination of VaR and TVaR risk measures. Therefore, a GlueVaR risk measure is coherent when the weight assigned to VaR is zero and the weights of TVaR are non-negative. In terms of the parameters of the distortion function, GlueVaR is subadditive (and thus coherent) if \( h_2 = 1 \) and \( \frac{1 - \beta}{1 - \alpha} \leq h_1 \). More generally, any property satisfied by TVaR but not by VaR will be inherited by GlueVaR if \( \omega_1 \geq 0 \) and \( \omega_3 = 0 \).

Subadditivity in the whole domain is a strong condition. When dealing with fat tail risks (i.e. low-frequency and large-loss events), risk managers are especially interested in the tail region. We introduce the concept of subadditivity in the right tail for a pair of risks. This property is defined in this discussion for distortion risk measures. Consider a probability space with sample space \( \Omega \). Let \( s_\alpha (Z) \) the \( \alpha \)-quantile of random variable \( Z \), \( s_\alpha (Z) = \inf \{ z \ | \ S_Z (z) \leq 1 - \alpha \} \). Let \( Q_{\alpha, Z} \) be defined by \( Q_{\alpha, Z} := \{ \omega \ | \ Z (\omega) > s_\alpha (Z) \} \subseteq \Omega \), so \( Q_{\alpha, Z} \) means here the tail region of random variable \( Z \) given a confidence level \( \alpha \). Let \( X, Y \) be two risks defined on the same probability space. When aggregating two risks, the common tail for both risks

\[8\] Additional properties for distortion risk measures can be found in Jiang [13] and Balbás et al. [3].

\[9\] Criticisms regarding requirements for risk measures to be coherent can be found, for example, in Dhaene et al. [10].
must be taken into account. This common tail region is defined here as follows:

\[ Q_{\alpha,X,Y} := Q_{\alpha,X} \cap Q_{\alpha,Y} \cap Q_{\alpha,X+Y}. \]

**Definition 1** Given a confidence level \( \alpha \in [0,1] \), a distortion risk measure \( \rho_g \) is subadditive in the tail for the pair \( X,Y \) if \( Q_{\alpha,X,Y} \neq \emptyset \) and

\[
\int_{Q_{\alpha,X,Y}} (X + Y) d(g \circ P) \leq \int_{Q_{\alpha,X,Y}} X d(g \circ P) + \int_{Q_{\alpha,X,Y}} Y d(g \circ P),
\]

where the integral symbol stands for Choquet Integrals with respect to the set function \( g \circ P \).

**Theorem 1** Given a confidence level \( \alpha \) and a pair of risks \( X \) and \( Y \) so that \( Q_{\alpha,X,Y} \neq \emptyset \), a GlueVaR risk measure is tail-subadditive if its associated distortion function \( \kappa_{h_1,h_2}^{h_1,h_2} \) is concave in \([0,1-\alpha)\).

The proof is provided in Belles-Sampera et al. [4]. Tail-subadditivity is a desirable property, because it implies that the benefits of diversification may not be valid in every situation but, at least, they hold in extreme cases.

5 Geometrical discussion on risk attitudes

Given \( \alpha \) and \( \beta \), the shaded areas in Figure 1 delimit feasible weights \((\omega_1,\omega_2)\) for GlueVaR\(^{h_1,h_2}_{\beta,\alpha} \) and the corresponding risk manager’s attitude towards risk. For example, the point \((1/3,1/3)\) corresponds to a balanced risk attitude on the part of risk managers when faced by the three components shown in (2). If \( \omega_1 < 0 \), risk managers are optimistic regarding the impossibility of the occurrence of the worst case scenario, and so attach a negative weight to it. Note that any pair of weights \((\omega_1,\omega_2)\) on the boldest line in Figure 1 leads to \( \omega_3 = 0 \). This means that a zero weight is allocated to the less conservative scenario, i.e. the one associated with the VaR\(_{\alpha} (X) \). This is indicative of the decision makers’ conservative approach. Nonetheless, differences in just how restrictive this conservative attitude is can be found among the weights lying on this line: the nearer to \((\omega_1,\omega_2) = \left( \frac{\beta - 1}{\beta - \alpha}, \frac{1 - \alpha}{\beta - \alpha} \right)\), the less restrictive it is, while the nearer to \((\omega_1,\omega_2) = (1,0)\), the more conservative it is.

6 Illustration

Data for the cost of claims for medical expenses from a major Spanish motor insurer are used to illustrate the applicability of these results. These data contain \( n = 519 \) observations of the cost of individual claims in thousands of euros, and were analyzed in Bolancé et al. [5] and Guillén et al. [11]. The risk measures for these data are displayed in Table 1. In the first row, our results obtained using the empirical distribution are presented. In subsequent rows Normal, Log-normal, Student t with 4 df and Generalized Pareto distributions are fitted and their respective risk values are shown. Calculations have been made in R. R commands are available from the authors.
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Figure 1. Given $\alpha$ and $\beta$, the shaded areas delimits feasible weights $(\omega_1, \omega_2)$ for GlueVaR$_{h_1,h_2}^{\beta,\alpha}$. The corresponding distortion function $\kappa_{h_1,h_2}^{\beta,\alpha}$ is concave in $[0, 1 - \alpha)$ in the lightly shaded area and, thus, the associated GlueVaR risk measure can be tail-subadditive. Yet, the distortion function is not concave in $[0, 1 - \alpha)$ in the darkly shaded area and, thus, the associated GlueVaR risk measure cannot be tail-subadditive. The distortion function is concave in $[0, 1]$ in the boldest continuous segment and, thus, the associated GlueVaR risk measure is subadditive.

Table 1. Example of calculating GlueVaR as a linear combination

<table>
<thead>
<tr>
<th></th>
<th>VaR$_{95%}$ (X)</th>
<th>TVaR$_{95%}$ (X)</th>
<th>TVaR$_{99.5%}$ (X)</th>
<th>GlueVaR$_{1/3,3/3,3/3}^{1/3,3/3,3/3}$ (X)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical</td>
<td>6.4</td>
<td>18.4</td>
<td>54.3</td>
<td>26.3</td>
</tr>
<tr>
<td>Normal</td>
<td>10.2</td>
<td>12.4</td>
<td>16.7</td>
<td>13.1</td>
</tr>
<tr>
<td>Log-normal</td>
<td>6.5</td>
<td>14.5</td>
<td>44.6</td>
<td>21.8</td>
</tr>
<tr>
<td>Student $t$ (4 df)</td>
<td>12.8</td>
<td>18.3</td>
<td>34.5</td>
<td>21.9</td>
</tr>
<tr>
<td>Pareto</td>
<td>5.9</td>
<td>12.4</td>
<td>38.5</td>
<td>18.9</td>
</tr>
</tbody>
</table>

$X$ stands for “cost of individual claims in thousands of euros”. For $\alpha = 95\%$, $\beta = 99.5\%$, $\omega_1 = 1/3$, $\omega_2 = 1/3$ and $\omega_3 = 1/3$.

7 Conclusions

We have shown that GlueVaR measures can be expressed as linear combinations of standard risk measures and that, similarly, they can be defined based on a straightforward distortion function. Concavity of the distortion function on the subrange $[0, 1 - \alpha)$ assures tail-subadditivity for GlueVaR measures. This condition in the distortion function might be a sufficient requisite for risk measures when fat right-tail risks are assessed: the benefits of diversification are attained in adverse scenarios but capital requirements are not excessively high.

The ideas provided in this article are directly applicable in the industry. We encourage regulators and financial and insurance risk managers to seek an equilibrium between their different demands. The two levels of qualitative
information that GlueVaR risk measures incorporate (one related to the confidence levels of bad and worst-case scenarios; the other related to the plausibility of those scenarios) can help achieve this goal.

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Bibliography


On some interrelations of generalized $q$-entropies and a generalized Fisher information, including a Cramér-Rao inequality

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Abstract In this communication, we describe some interrelations between generalized $q$-entropies and a generalized version of Fisher information. In information theory, the de Bruijn identity links the Fisher information and the derivative of the entropy. We show that this identity can be extended to generalized versions of entropy and Fisher information. More precisely, a generalized Fisher information naturally pops up in the expression of the derivative of the Tsallis entropy. This generalized Fisher information also appears as a special case of a generalized Fisher information for estimation problems. Indeed, we derive here a new Cramér-Rao inequality for the estimation of a parameter, which involves a generalized form of Fisher information. This generalized Fisher information reduces to the standard Fisher information as a particular case. In the case of a translation parameter, the general Cramér-Rao inequality leads to an inequality for distributions which is saturated by generalized $q$-Gaussian distributions. These generalized $q$-Gaussians are important in several areas of physics and mathematics. They are known to maximize the $q$-entropies subject to a moment constraint. The Cramér-Rao inequality shows that the generalized $q$-Gaussians also minimize the generalized Fisher information among distributions with a fixed moment. Similarly, the generalized $q$-Gaussians also minimize the generalized Fisher information among distributions with a given $q$-entropy.

Keywords: Cramér-Rao inequality, generalized $q$-entropy, generalized Gaussians, de Bruijn identity.

Let $f(x)$ be a probability distribution defined on $X \subseteq \mathbb{R}^n$. If $M_q[f] = \int_X f(x)^q dx$, $q \geq 0$ is the information generating function, then $S_q[f] = \frac{1}{1-q} (M_q[f] - 1)$ is the so-called Tsallis entropy, or $q$-entropy (which can be easily related to the Rényi entropy). Both entropies reduce to the standard Shannon-Boltzmann entropy for $q = 1$. It is well-known that the maximum of the Rényi-Tsallis entropy, among all distributions with a fixed moment $m_\alpha = E_g[\|X\|^n]$, is obtained for a generalized $q$-Gaussian distribution

$$G_q(x) \propto (1 - (q - 1) \gamma \|x\|^n)^\frac{1}{q-1} \text{ for } q \neq 1$$

which reduces to a generalized Gaussian for $q = 1$. It is also well-known that the classical Fisher information, which is derived from considerations in estimation theory, is linked to the Shannon entropy via the de Bruijn identity, and that this Fisher information is minimized by a Gaussian distribution, among all distributions with a fixed moment or entropy. It is the main objective of this
paper to show that such results can be extended to the $q$-entropy and a suitable extension of Fisher information. Incidentally, we derive an interesting new generalized Cramér-Rao inequality in estimation theory, which might prove useful in its own right.

1 An extended de Bruijn identity

A fundamental connection between the Boltzmann-Shannon entropy, Fisher information, and the Gaussian distribution is given by the de Bruijn identity [8]. We show here that this important connection can be extended to the $q$-entropies, a suitable generalized Fisher information and the generalized $q$-Gaussian distributions.

The de Bruijn identity states that if $Y_t = X + \sqrt{2t}Z$ where $Z$ is a standard Gaussian vector and $X$ a random vector of $\mathbb{R}^n$, independent of $Z$, then

$$\frac{d}{dt} H[f_{Y_t}] = I_{2,1}[f_{Y_t}] = \phi_{2,1}[f_{Y_t}],$$

where $f_{Y_t}$ denotes the density of $Y_t = X + \sqrt{2t}Z$, and $I_{2,1}[f_{Y_t}]$, $\phi_{2,1}[f_{Y_t}]$ are two notations for the classical Fisher information (the meaning of which will be made clear in the following). Although the de Bruijn identity holds in a wider context, the classical proof of the de Bruijn identity uses the fact that if $Z$ is a standard Gaussian vector, then $Y_t$ satisfies the well-known heat equation \( \partial f / \partial t = \Delta f \), where $\Delta$ denotes the Laplace operator.

Nonlinear versions of the heat equation are of interest in a large number of physical situations, including fluid mechanics, nonlinear heat transfer or diffusion. Other applications have been reported in mathematical biology, lubrication, boundary layer theory, etc; see the series of applications presented in [9, chapters 2 and 21] and references therein. The porous medium equation and the fast diffusion equation correspond to the differential equation \( \partial f / \partial t = \Delta f^m \), with $m > 1$ for the porous medium equation and $< 1$ for the fast diffusion. These two equations have been exhaustively studied and characterized by J. L. Vazquez, e.g. in [9,10].

These equations are included as particular cases in the doubly nonlinear equation, which involves a $p$-Laplacian operator $\Delta_p f := \text{div} (|\nabla f|^{p-2} \nabla f)$, and the power $m$ of the porous medium or fast diffusion equation. This doubly nonlinear equation takes the form

$$\frac{\partial}{\partial t} f = \Delta_{\beta} f^m = \text{div} (|\nabla f|^\beta - 2 \nabla f^m),$$

where we use $p = \beta$ for convenience and coherence with notation in the paper. The $\beta$-Laplacian typically appears in the minimization of a Dirichlet energy like $\int |\nabla f|^\beta dx$ which leads to the Euler-Lagrange equation. It can be shown, see [10, page 192], that for $m(\beta-1) + (\beta/n) - 1 > 0$, (3) has a unique self-similar solution, called a Barenblatt profile, whose initial value is the Dirac mass at the origin. This fundamental solution is usually given as a function of $m$. Here, if
we put $q = m + 1 - \frac{\alpha}{\beta}$, the solution can be written as a $q$-Gaussian distribution:

$$f(x,t) = \frac{1}{t^\frac{\alpha}{2}} B\left(\frac{x}{t^\frac{\beta}{2}}\right), \quad \text{with } B(x) = \begin{cases} (C - k|x|^{\alpha})^\frac{1}{\alpha} & \text{for } q \neq 1 \\ \frac{1}{\beta} \exp\left(-\frac{1}{\beta} \frac{|x|^\alpha}{m}\right) & \text{for } q = 1 \end{cases}$$

with $\delta = n(\beta - 1)m + \beta - n > 0$, $k = \frac{m(\beta - 1)}{\beta - 1} (\frac{1}{2})^{\frac{1}{\beta - 1}}$ and $\alpha = \frac{\beta}{\beta - 1}$.

As mentioned above, the doubly nonlinear diffusion equation allows to derive a nice extension of the de Bruijn identity (2), and leads to a possible definition of a generalized Fisher information. This is stated in the next Proposition. The case $\beta = 2$ of this result has been given in a paper by Johnson and Vignat [6].

**Proposition 1.** [Extended de Bruijn identity [2]] Let $f(x,t)$ a probability distributions defined on a subset $X$ of $\mathbb{R}^n$ and satisfying the doubly nonlinear equation (3). Assume that the domain $X$ is independent of $t$, that $f(x,t)$ is differentiable with respect to $t$, is continuously differentiable over $X$, and that $\frac{\partial}{\partial t} f(x,t)^q$ is absolutely integrable and locally integrable with respect to $t$. Then, for $\beta > 1$, $\alpha$ and $\beta$ Hölder conjugate of each other, for $q = m + 1 - \frac{\alpha}{\beta}$, $M_q[f] = \int f^q$ and $S_q[f] = \frac{1}{\beta} (M_q[f] - 1)$ the Tsallis entropy, we have

$$\frac{d}{dt} S_q[f] = q m^{\beta - 1} \phi_{\beta,q}[f] = \left(\frac{m}{q}\right)^{\beta - 1} \frac{\beta}{M_q[f]^{\beta}} I_{\beta,q}[f]$$

(5)

with $\phi_{\beta,q}[f] = \int_X f(x)^{\beta(q - 1) + 1} \left(\frac{\nabla f(x)}{f(x)}\right)^\beta \text{dx}$ and $I_{\beta,q}[f] = \frac{\phi_{\beta,q}[f]}{M_q[f]^{\beta}}$.

(6)

In (6), $\phi_{\beta,q}[f]$ and $I_{\beta,q}[f]$ are two possible generalization of Fisher information. Of course, the standard Fisher information is recovered in the particular case $\alpha = \beta = 2$, and $q = m = 1$, and so is the de Bruijn identity (2). The proof of this result relies on integration by part (actually using the Green identity) along the solutions of the nonlinear heat equation (3). This proof can be found in [2] and is not repeated here. A variant of the result for $\beta = 2$, which considers a free-energy instead of the entropy above, is well-known in certain circles, see e.g. [5,4]. More than that, by using carefully the calculations in [5], it is possible to check that $\frac{d}{dt} \phi_{\beta,q}[f] \leq 0$ for $q > 1 - \frac{\alpha}{m}$, which means the Tsallis entropy is a monotone increasing concave function along the solutions of (3). In their recent work [7], Savaré and Toscani have shown that in the case $\beta = 2$, $m = q$, the entropy power, up to a certain exponent, is a concave function of $t$, thus generalizing the well-known concavity of the (Shannon) entropy power to the case of $q$-entropies. This allows to obtain as a by-product a generalized version of the Stam inequality, valid for the solutions of (3). We will come back to this generalized Stam inequality in Proposition 6.

2 Extended Cramér-Rao inequalities

Let $f(x; \theta)$ be a probability distribution, with $x \in X \subseteq \mathbb{R}^n$ and $\theta \in \mathbb{R}^k$. We will deal here with the estimation of a scalar function $h(\theta)$ of $\theta$, with $T(x)$ the
corresponding estimator (the more general case where \( h(\theta) \) and \( T(x) \) are vector valued is a bit more involved; some results are given in [3] with general norms). We extend here the classical Cramer-Rao inequality in two directions. Firstly, we give results for a general moment of the estimation error instead of the second order moment, and secondly we introduce the possibility of computing the moment of this error with respect to a distribution \( g(x; \theta) \) instead of \( f(x; \theta) \): in estimation, the error is \( T(X) - h(\theta) \), and the bias can be evaluated as \( \int_X (T(x) - h(\theta)) f(x; \theta) \, dx = E_f [T(X) - h(\theta)] = \eta(\theta) - h(\theta) \), while a general moment of the error can be computed with respect to another probability distribution \( g(x; \theta) \), as in \( E_g \left[ (T(x) - h(\theta))^r \right] = \int_X |T(x) - h(\theta)|^r \, g(x; \theta) \, dx \).

The two distributions \( f(x; \theta) \) and \( g(x; \theta) \) can be chosen very arbitrary. However, one can also build \( g(x; \theta) \) as a transformation of \( f(x; \theta) \) such as to highlight, or on the contrary scores out, some characteristics of \( f(x; \theta) \). An important case is when \( g(x; \theta) \) is defined as the escort distribution of order \( q \) of \( f(x; \theta) \):

\[
f(x; \theta) = \frac{g(x; \theta)^q}{\int g(x; \theta)^q \, dx} \quad \text{and} \quad g(x; \theta) = \frac{f(x; \theta)^q}{\int f(x; \theta)^q \, dx},
\]

where \( q \) is a positive parameter, \( q = 1/q \), and provided of course that involved integrals are finite. These escort distributions are an essential ingredient in the nonextensive thermostatistics context. It is in the special case where \( f(x; \theta) \) and \( g(x; \theta) \) are a pair of escort distributions that we will find again the generalized Fisher information (6) obtained in the extended de Bruin identity.

Our previous results on generalized Fisher information can be found in [3,1] in the case of the direct estimation of the parameter \( \theta \). We propose here a novel derivation, introducing in particular a notion of generalized Fisher information matrix, in the case of the estimation of a function of the parameters. Let us first state the result.

**Proposition 2.** Let \( f(x; \theta) \) be a multivariate probability density function defined for \( x \in X \subseteq \mathbb{R}^n \), and with \( \theta \in \Theta \subseteq \mathbb{R}^k \) is a parameter of the density. Let \( g(x; \theta) \) denote another probability density function also defined on \( (X; \Theta) \). Assume that \( f(x; \theta) \) is a jointly measurable function of \( x \) and \( \theta \), is integrable with respect to \( x \), is absolutely continuous with respect to \( \theta \), and that the derivatives with respect to each component of \( \theta \) are locally integrable. Let \( T(x) \) be an estimator of a function \( h(\theta) \) and set \( \eta(\theta) = E_f[T(X)] \). Then, for any estimator \( T(x) \) of \( h(\theta) \), we have

\[
E_g \left[ (T(X) - h(\theta))^\alpha \right] \geq \sup_{A > 0} \frac{\bar{\eta}(\theta)^T A \bar{\eta}(\theta)}{E_g \left[ |\bar{\eta}(\theta)^T A \psi_g(X; \theta)|^2 \right]^{\frac{\alpha}{2}}}. \tag{8}
\]

with equality if and only if \( \eta(\theta)^T A \psi_g(X; \theta) = c(\theta) \mathrm{sign} (T(x) - h(\theta)) \left| T(x) - h(\theta) \right|^{\alpha - 1} \), \( c(\theta) > 0 \) and where \( \alpha^{-1} + \beta^{-1} = 1, \alpha > 1, A \) is a positive definite matrix and \( \psi_g(x; \theta) \) a score function given with respect to \( g(x; \theta) \):

\[
\psi_g(x; \theta) := \frac{\nabla \theta f(x; \theta)}{g(x; \theta)}. \tag{9}
\]
Proof. Let $\eta(\theta) = E_f[T(X)]$. Let us first observe that $E_g[\psi_g(x; \theta)] = \frac{\partial}{\partial \theta} \int_X f(x; \theta) dx = 0$. Differentiating $\eta(\theta) = E_f[T(X)]$ with respect to each $\theta_i$ we get
\[
\dot{\eta}(\theta) = \nabla_\theta \eta(\theta) = \nabla_\theta \int_X T(x) f(x; \theta) dx = \int_X T(x) \frac{\nabla_\theta f(x; \theta)}{g(x; \theta)} g(x; \theta) dx = \int_X (T(x) - h(\theta)) \psi_g(x; \theta) g(x; \theta) dx.
\]
For any positive definite matrix $A$, multiplying on the left by $\dot{\eta}(\theta)^T A$ gives
\[
\dot{\eta}(\theta)^T A \dot{\eta}(\theta) = \int_X (T(x) - h(\theta)) \dot{\eta}(\theta)^T A \psi_g(x; \theta) g(x; \theta) dx,
\]
and by the Hölder inequality, we obtain
\[
E_g ||T(x) - h(\theta)||^\alpha \leq E_g \left[ ||\dot{\eta}(\theta)^T A \psi_g(x; \theta)||^\beta \right]^{\frac{\alpha}{\beta}} \geq \dot{\eta}(\theta)^T A \dot{\eta}(\theta),
\]
with equality if and only if $T(x) - h(\theta) = \dot{\eta}(\theta)^T A \psi_g(x; \theta) > 0$ and $T(x) - h(\theta) = k(\theta) ||\dot{\eta}(\theta)^T A \psi_g(x; \theta)||^\beta$, $k(\theta) > 0$. This inequality, in turn, provides us with the lower bound (8) for the moment of order $\alpha$ and computed wrt to $g$ of the estimation error. \hfill \Box

The inverse of the matrix $A$ which maximizes the right hand side is the Fisher information matrix of order $\beta$. Unfortunately, we do not have a closed-form expression for this matrix in the general case. Two particular cases are of interest.

Corollary 3. [Scalar extended Cramér-Rao inequality] In the scalar case (or the case of a single component of $\theta$), the following inequality holds
\[
E_g [||T(X) - h(\theta)||^\alpha]^{\frac{1}{\alpha}} \geq \frac{||\dot{\eta}(\theta)||}{E_g [||\psi_g(X; \theta)||^\beta]^{\frac{1}{\beta}}}, \tag{10}
\]
with equality if and only if $\psi_g(x; \theta) = c(\theta) \text{sign}(T(x) - h(\theta)) |T(x) - h(\theta)|^{\alpha - 1}$.

In the simple scalar case, we see that $A > 0$ can be simplified in (8) and thus that (10) follows. Note that for $\alpha = 2$, the equality case implies that $E_g[\psi_g] = 0 = E_g[T(X) - h(\theta)]$, which means that $E_g[T(X)] = \eta(\theta) = h(\theta)$, i.e. the estimator is unbiased (with respect to both $f$ and $g$). Actually, this inequality recovers at once the generalized Cramér-Rao inequality we presented in the univariate case [1]. The denominator plays the role of the Fisher information in the classical case, which corresponds to the case $g(x; \theta) = f(x; \theta)$, $\beta = 2$. As mentioned above, an extension of this result to the multidimensional case and arbitrary norms has been presented in [3] but it does not seem possible to obtain it here as particular case of (8).

A second interesting case is the multivariate case $\alpha = \beta = 2$. Indeed, in that case, we get an explicit form for the generalized Fisher information matrix and an inequality which looks like the classical one.
Corollary 4. [Multivariate Cramér-Rao inequality with $\alpha = \beta = 2$] For $\alpha = \beta = 2$, we have

$$E_g \left[ |T(X) - h(\theta)|^2 \right] \geq \eta(\theta)^T J_\beta(\theta)^{-1} \eta(\theta)$$

(11)

with $J_\beta(\theta) = E_g \left[ \psi_g(X;\theta) \psi_g(X;\theta)^T \right]$, and with equality if and only if $|T(X) - h(\theta)| = k(\theta) |\eta(\theta)^T J_\beta(\theta)^{-1} \psi_g(X;\theta)|$.

Proof. The denominator of (8) is a quadratic form and we have

$$E_g \left[ |T(X) - h(\theta)|^2 \right] \geq \sup_{A > 0} \frac{(\eta(\theta)^T A \eta(\theta))^2}{E_g \left[ \left| \eta(\theta)^T A \psi_g(X;\theta) \right|^2 \right]}$$

$$\geq \sup_{A > 0} \frac{(\eta(\theta)^T A \eta(\theta))^2}{\eta(\theta)^T A E_g \left[ \psi_g(X;\theta) \psi_g(X;\theta)^T \right] A^T \eta(\theta)}.$$  (12)

Let $J_\beta(\theta) = E_g \left[ \psi_g(X;\theta) \psi_g(X;\theta)^T \right]$ and set $z(\theta) = A^{1/2} \eta(\theta)$. With these notations, and using the inequality $(z^T z)^2 \leq (z^T B z) (z^T B^{-1} z)$ valid for any $B > 0$, we obtain that

$$\eta(\theta)^T J_\beta^{-1} \eta(\theta) \geq \sup_{A > 0} \frac{(z(\theta)^T z(\theta))^2}{z(\theta)^T A z(\theta)}.$$  \hspace{1cm} \text{(13)}$$

Since it can be readily checked that the upper bound is attained with $A = J_\beta(\theta)^{-1}$, we finally end with (11). Of course, for $g = f$, the inequality (11) reduces to the classical multivariate Cramér-Rao inequality.$\square$

An important consequence of these results is obtained in the case of a translation parameter, where the generalized Cramér-Rao inequality induces a new class of inequalities. Let $\theta \in \mathbb{R}$ be a scalar location parameter, $x \in X \subseteq \mathbb{R}^n$, and define by $f(x; \theta)$ the family of density $f(x; \theta) = f(x - \theta)$, where $1$ is a a vector of ones. In this case, we have $\nabla_x f(x; \theta) = -1^T \nabla_x f(x - \theta)$, provided that $f$ is differentiable at $x - \theta$, and the Fisher information becomes a characteristic of the information in the distribution. If $X$ is a bounded subset, we will assume that $f(x)$ vanishes and is differentiable on the boundary $\partial X$. Without loss of generality, we will assume that the mean of $f(x)$ is zero. Set $h(\theta) = \theta$ and take $T(X) = 1^T X/n$, with of course $\eta(\theta) = E[T(X)] = \theta$ and $\dot{\eta}(\theta) = 1$. Finally, let us choose the particular value $\theta = 0$. In these conditions, the generalized Cramér-Rao inequality (10) becomes

$$E_g \left[ |T(X)|^\alpha \right] ^{\frac{1}{\alpha}} \leq E_g \left[ \left| \frac{\nabla_x f(X)}{g(X)} \right| ^\beta \right] ^{\frac{1}{\beta}} \geq n,$$

(13)

with equality if and only if $1^T \frac{\nabla_x f(x)}{g(x)} = c(\theta) \text{sign}(1^T X) \left| 1^T X \right|^{\alpha - 1}$. In[3], we have a slightly more general result in the multivariate case:

$$E_g \left[ \left| X \right|^{\alpha} \right] ^{\frac{1}{\alpha}} \leq E_g \left[ \left\| \frac{\nabla_x f(X)}{g(X)} \right\| _\alpha ^\beta \right] ^{\frac{1}{\beta}} \geq n,$$

(14)
where $||.||$ is a norm, and the corresponding dual norm is denoted by $||.||_*$. Finally, let $f(x)$ and $g(x)$ be a pair of escort distributions as in (7). In such a case, the following recovers the generalized Fisher information (6) and yields a new characterization of $q$-Gaussian distributions.

**Corollary 5.** [q-Cramér-Rao inequality] Assume that $g(x)$ is a measurable differentiable function of $x$, which vanishes and is differentiable on the boundary $\partial X$, and finally that the involved integrals exist and are finite. Then, for the pair of escort distributions (7), the following q-Cramér-Rao inequality holds

$$q^2 E_q[||X||^\alpha]^\frac{1}{\beta} I_{\beta,q}[g]^\frac{1}{\beta} \geq n,$$

with $I_{\beta,q}[g] = \left(1/M_q[g]\right) E \left[\left(g(x)^{\beta(q-1)} \left|\nabla_x g(x)\right|_{{\parallel.\parallel}_*}\right)^{\beta}\right]$, and with equality if and only if $g(x)$ is a generalized $q$-Gaussian, i.e. $g(x) \propto (1 - \gamma ||x||^\alpha)^{\frac{1}{\gamma q}}$, with $\gamma > 0$.

**Proof.** The result follows from (14), or (13) with $n = 1$, and the fact that

$$\frac{\nabla_x f(X)}{g(X)} = \frac{q}{M_q[g]} g(X)^{q-1} \frac{n \nabla_x g(X)}{g(X)}.$$

The case of equality is obtained by solving the general equality conditions in the special case where $f(x)$ and $g(x)$ form a pair of escort distributions. \qed

As a direct consequence of the $q$-Cramér-Rao inequality (15), we obtain that the minimum of the generalized Fisher information among all distributions with a given moment of order $\alpha$, say $m_\alpha = E_q[||X||^\alpha]$, is obtained when $g$ is a generalized $q$-Gaussian distribution, with a parameter $\gamma$ such that the distribution has the prescribed moment. This parallels, and complements the well known fact that the $q$-Gaussians maximize the $q$-entropies subject to a moment constraint, and yields new variational characterizations of the generalized $q$-Gaussians. As mentioned earlier, the generalized Fisher information also satisfies an extension of Stam’s inequality, which links the generalized Fisher information and the $q$-entropy power, defined as an exponential of the Rényi entropy $H_q[f]$ as

$$N_q[f] = M_q[f]^\frac{2}{n} = \exp\left(\frac{2}{n} H_q[f]\right) = \left(\int \! f(x)^q \, dx\right)^\frac{2}{n - \alpha},$$

for $q \neq 1$. For $q = 1$, we set $N_q[f] = \exp\left(\frac{2}{n} H_1[f]\right)$, where $H_1[f]$ is the Boltzmann-Shannon entropy. The generalized Stam inequality is given here without proof (see [2]).

**Proposition 6.** [Generalized Stam inequality] Let $n \geq 1$, $\beta$ and $\alpha$ be Hölder conjugates of each other, $\alpha > 1$, and $q > \max\{(n-1)/n, n/(n+\alpha)\}$. Then for
any probability density on $\mathbb{R}^n$, that is continuously differentiable, the following generalized Stam inequality holds

$$I_{\beta,q}[f]^{\frac{1}{2}} N_q[f]^{\frac{1}{2}} \geq I_{\beta,q}[G]^{\frac{1}{2}} N_q[G]^{\frac{1}{2}},$$

(17)

with $\lambda = n(q-1) + 1 > 0$ and with equality if and only if $f$ is any generalized $q$-Gaussian \((1)\).

The generalized Stam inequality implies that the generalized $q$-Gaussian minimize the generalized Fisher information within the set of probability distributions with a fixed $q$-entropy power.

To sum up and emphasize the main results, let us point out that we have exhibited a generalized Fisher information, both as a by-product of a generalization of de Bruijn identity and as a fundamental measure of information in estimation theory. We have shown that this allows to draw a nice interplay between $q$-entropies, generalized $q$-Gaussians and the generalized Fisher information. These interrelations yield the generalized $q$-Gaussians as minimizers of the $(\beta,q)$-Fisher's information under adequate constraints, or as minimizers of functionals involving $q$-entropies, $(\beta,q)$-Fisher's information and/or moments. This is shown through inequalities and identities involving these quantities and generalizing classical information relations (Cramér-Rao’s inequality, Stam’s inequality, De Bruijn’s identity).

References


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Abstract. This paper sketches a novel meta-heuristic evolutionary approach for the optimal deployment of aerial firefighting aircrafts based on predictive fire risk estimations over a certain geographical areas. In particular, the problem can be formulated as how to properly allocate firefighting resources to capacity-constrained aerodromes in such a way that the utility of the deployed resources with respect to fire forest risk predictions is maximized. On the purpose of efficiently tackling this optimization problem, the proposed meta-heuristic solver inspires from the well-known Harmony Search algorithm, whose operators mimic the way musicians improvise new melodies in an aesthetically optimum fashion. Preliminary simulation results are presented and discussed, showing the effectiveness of the designed algorithm when handling problems of increasing dimensionality. This noted promising performance calls for new research lines towards considering further constraints and including new aspects for a more realistic problem formulation.

Keywords: Firefighting aircrafts, FWI, optimal deployment, Harmony Search.

1 Introduction

During the last years many regions around the world have undergone intensive and seasonally severe forest fire periods. Wildfires may occur on every continent (except Antarctica), but they have been notably frequent in the southern part of Europe where, unfortunately, the intensity and spread of such wildfires has occasionally lead to casualties and extensive damages to civil infrastructures. In this context, intensive efforts are being taken in the research community on novel advances that enhance the speed and effectiveness of prevention, detection and suppression techniques, in a technological attempt at minimizing the severity and frequency of wildfires.

One of the most widely adopted fire combating strategies relies on the direct human intervention in the form of firefighting brigades, which have traditionally shown to be effective in small-to-moderate wildfires over areas with scarce
vegetation density. However, fighting wildfires may become deadly dangerous due to life-threatening hazards including disorientation, heat stress, fatigue, smoke and dust, as well as the risk of other injuries such as burns, cuts and scrapes. Other side dangers in human intervened fire suppressing campaigns include faults in communication facilities and issues in the logistics and operational procedures, as exemplified by the Australian Victorian bushfires in 2009 (where at least 173 people died and over 2000 homes and 3,500 structures were destroyed due to fire ambush). This motivates the use of fire retardants and water dropped onto wildfires by planes and helicopters, by virtue of which the risk for human casualties is dramatically decreased.

Of particular interest for the scope of this work is the natural wildfire happened in Guadalajara (Spain) in July 2005, where 11 fire fighters died due to a documented lack of effectiveness in the timing and deployment of the necessary aerial firefighting vehicles. From the operational perspective, the pre-emergency deployment of this fire combating fleets over aerodromes happens to be in general uncoordinated with respect to well-known and accurate predictive numerical methodologies such as the FWI (Fire forest Weather Index). The FWI quantifies, in a user-defined scale, the fire risk of a certain geographical coordinate based exclusively in weather-related parameters (see Figure 1). Following this rationale, a tool capable of dynamically matching the pre-emergency deployment of aerial firefighting fleets with the risk predictions offered by national weather services would eventually entail an improved speed and effectiveness when dealing with massive wildfires, as well as reduce the number of casualties due to the minimum human intervention necessitated in land.

Fig. 1. Predicted Fire forest Weather Index (FWI) for the Spanish mainland and Balearic Islands, corresponding to 26 July 2012.

This paper addresses this need by elaborating on the formulation of an optimization problem with cost constraints that blends together predictive fire weather risk quantification and operational fleet deployment over available
aerodromes. In its simplest form, the derived formulation takes into account the number of aerial vehicles, the number and position of existing aerodromes, available operational budget and the predicted fire weather risk metrics of the area under study, based on which a fitness function assessing the utility of a fleet deployment with respect to all the geographical coordinates with predicted risk is described and maximized. To the knowledge of the authors, this operational logistics field has not been so far tackled from an analytical, formal standpoint.

In order to lessen the computational complexity incurred when solving the aforementioned problem in a nation-wide scale, we propose the use of novel evolutionary meta-heuristics that allow trading optimality of the produced solutions for a lessened complexity required for their computation. Specifically, the designed evolutionary approaches incorporate a solution encoding strategy representing the airport to which each aerial firefighting vehicle is assigned, which is well suited for the problem at hand. Computer experiments are performed so as to shed light on the excellent results attained by the proposed heuristics, which pave the way to further research aimed at extending this problem with new factors such as e.g. the relative position of water resources with respect to any given wildfire.

2 System model

We assume that both the number $M$ and location $\{p_m\}_{m=1}^M$ of the available aerodromes are known a priori. The same assumption holds for the number $N$ of firefighting aircrafts. However, the location of the aircrafts is not fixed and can be selected according to different changing criteria. In this work we assume that this criterion hinges on the aforementioned FWI, which is usually computed over a number $Z$ of points arranged on a square lattice grid over the geographic area under consideration. The model and characteristics of each of such aircrafts must be also taken into account; note that such characteristics establish the coverage area of the aircraft at hand, a necessary parameter to determine its effect on the fire risk estimated for the $Z$ points. It is further assumed that:

- Water resources are unlimited in any location, i.e. the utility of each aircraft with respect to every single point of the risk grid depends exclusively on the distance from the assigned aerodrome to the point itself.
- Only one model of firefighting aircraft is considered.
- The aircraft capacity may vary between different aerodromes, but for any given aerodrome it falls within the range $[0, N]$.

This being said, the optimization problem can be summarized as to maximize the aggregate fire risk covered by the allocated aircrafts subject to resource and budget constraints. On the one hand, resource constraints are determined by the total number of available aircrafts, whereas budget constraints are set by a maximum operational budget assigned to each aerodrome to cover maintenance, fuel distribution and facilities for the pilots. Therefore, the budget $B_m$
for aerodrome $m$ also drives the maximum of aircrafts that could be located at a certain aerodrome.

Mathematically, the problem can be cast as follows:

Maximize $\sum_{z=1}^{Z} r_z \cdot \left( \sum_{m=1}^{M} n_m \cdot f(d_{m,z}) \right)$

subject to $\sum_{m=1}^{M} n_m = N$, $\sum_{n=1}^{N} C \cdot n_m \leq B_m \forall m = 1, \ldots, M$,

where $f(d_{m,z})$ stands for a strictly decreasing function accounting for the utility of an aircraft deployed on aerodrome $m$ on a given point $z$ at a distance $d_{m,z}$ ($f(d_{m,z}) = 0 \forall d_{m,z} > R$, where $R$ denotes the coverage radius); $r_z$ represents the FWI index value at point $z$; $C$ represents the operational cost of an aircraft, which is assumed to be constant for this work; and $n \rightarrow m$ denotes the assignment of aircraft $n$ to aerodrome $m$. In general, the optimization variable of this optimization problem is the assignment of aircrafts to aerodromes; however, in this initial research aircrafts are assumed to be equal to each other, thus such optimization variables collapse to the number of aircrafts assigned to each aerodrome.

3 Proposed Heuristic Procedure

The heuristic utilized for efficiently solving this optimization problem grounds on the Harmony Search (HS) algorithm [1], which is combined with a greedy algorithm. HS is a population-based evolutionary solver that has shown to provide an excellent performance in a number of combinatorial and continuous-variable optimization problems arising from diverse disciplines such as engineering [2–4], telecommunications [5–7], energy [8] and economics [9], among many others.

From a general perspective, the algorithm operates on a set of $K$ candidate vectors or harmonies representing candidate solutions or harmonies, which are iteratively refined by successive applications of HS and the aforementioned greedy procedure, and evaluated so as to select and filter the worst harmonies out from the $K$-sized population according to the metric in Expression (1). The solution encoding for the evolutionary process is set to be a vector of $N$ integer variables corresponding to each aircraft, whose value indicates the aerodrome to which the aircraft at hand is assigned. Note that the proposed encoding makes the iteratively produced solutions meet the resource constraint in Expression (2). Therefore, while the HS plays the role of a global search procedure driven by its constituent improvisation operators (HMCR and a subtly modified PAR based on distance vicinity criterion, see [1]), the greedy algorithm is used to repair the solutions that do not comply with the budget constraints.
During the evolutionary process, aircrafts are assigned to aerodromes in a directed yet random fashion, which may go against the imposed maximum budget constraints \( \{B_m\}_{m=1}^{M} \). Assuming that all aircraft models and their associated operational costs are equal, it does not matter which aircraft is assigned to which aerodrome, but it all depends on the amount of aircrafts assigned to each aerodrome. Based on this rationale, budget constraint \( B_m \) establishes how many aircrafts could eventually be assigned to aerodrome \( m \). If any aerodrome happens to be over its capacity, the first aircraft assigned to this aerodrome is swapped to the nearest aerodrome whose occupancy (i.e. number of assigned aircrafts) falls below its capacity.

4 Simulation Results

In order to assess the performance of the proposed heuristic solver, different synthetically-generated simulations scenarios have been arranged over a 500 \( \times \) 500 rectangular area, built on combinations of the number of aircrafts (\( N \)) and aerodromes (\( M \)) jointly with 5 different risk estimation maps composed by distinct values for \( \{r_z\}_{z=1}^{Z} \). The objective is to lay a sufficiently diverse simulation benchmark from where to extract well-reasoned generalized conclusions on the performance and scalability of the proposed algorithm. To this end, simulation scenarios will be denoted by \([N, M, S]\), where \( S \) indexes the risk estimation grid under consideration: namely, \( \{[4, 9, s]\}_{s=1}^{5} \), \( \{[7, 13, s]\}_{s=1}^{5} \), \( \{10, 25, s]\}_{s=1}^{5} \), \( \{13, 36, s]\}_{s=1}^{5} \) and \( \{16, 49, s]\}_{s=1}^{5} \). Statistics (minimum, maximum, standard deviation, mean) of the value of the best fitness after 150 iterations of the solver are computed over 20 independent runs over each of such scenarios. In particular, the value obtained for the fitness standard deviation will shed light on the stability of the algorithm as the scales of the underlying optimization problem increase. Regarding the budget constraint \( B_m \) per airdrome, all have been assigned the same budget without loss of generality. Considering that the cost per aircraft is also assumed to be constant, the maximum number of aircrafts per airport is \( B_m = 3 \) for all the scenarios. Based on a previous simulative optimization stage, the parameters controlling the HS solver are set to \( \text{HMCR} = 0.5, \text{PAR} = 0.05 \) and \( K = 25 \) for all the simulated scenarios. As for function \( f(d_{m,z}) \), it is assumed to decrease linearly from the center to the boundary of a circular coverage area with radius \( R = 100 \).

Having said this, the obtained statistics are summarized in Table 1. It can be observed that the proposed algorithm renders a very stable performance behaviour for the simulated scenarios of lowest dimensionality, showing a negligible (even null, in some instances) standard deviation of the fitness over the executed 20 runs of the algorithm. Noteworthy is to mention that for the scenarios with highest dimensionality, the scale order of the resulting standard deviation is well below that of the average metric value, which further buttresses the conclusion that the HS-based solver results to be quite stable. Not shown for the sake of space, it has been noted that in the easiest scenarios the results converge very quickly. The convergence speed slows down for the complex scenarios, but as mentioned before, the variance between the results in each run is negligible with respect to the obtained mean.
Table 1. Results’ statistics computed over 20 runs of the algorithm for each scenario.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Min</th>
<th>Max</th>
<th>Std. Deviation</th>
<th>Mean</th>
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<td>3.112,10</td>
<td>9.3312E-13</td>
<td>3.112,10</td>
</tr>
<tr>
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<td>3.928,40</td>
<td>1.8662E-12</td>
<td>3.928,40</td>
</tr>
<tr>
<td>[4, 9, 5]</td>
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<td>4.220,50</td>
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<td>4.220,50</td>
</tr>
<tr>
<td>[7, 16, 2]</td>
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<td>6.642,30</td>
<td>53.75</td>
<td>6.630,30</td>
</tr>
<tr>
<td>[7, 16, 4]</td>
<td>7.166,90</td>
<td>7.185,20</td>
<td>5.36</td>
<td>7.182,00</td>
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<tr>
<td>[10, 25, 1]</td>
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<td>7.042,50</td>
<td>22.41</td>
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</tr>
<tr>
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<td>8.059,70</td>
<td>23.18</td>
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</tr>
<tr>
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<td>11.447,00</td>
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</tr>
<tr>
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<tr>
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<td>16.022,00</td>
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<td>15.972,00</td>
</tr>
<tr>
<td>[16, 49, 5]</td>
<td>17.778,00</td>
<td>17.953,00</td>
<td>64.24</td>
<td>17.927,00</td>
</tr>
</tbody>
</table>

Figure 2 exemplifies one of the produced solutions for the [16, 49, 5] scenario, that is, the scenario consisting of \( N = 16 \) aircrafts and \( M = 49 \) aerodromes. The risk map is plotted as a two-dimensional contour map, where coloured lines indicate the boundaries between regions with different risk level, from red (boundary between \( r_z = 5 \) and \( r_z = 4 \)) to orange (\( r_z = 4 \) and \( r_z = 3 \)), green (\( r_z = 3 \) and \( r_z = 2 \)) and blue (\( r_z = 2 \) and \( r_z = 1 \)). Black crosses identify those points where aerodromes are located in the area, whereas airdromes with aircrafts assigned are surrounded with a circle along with a number denoting their number. As can be seen from the plot, the assignment is correctly realized: airdromes close to risk peaks are assigned more aircrafts, always respecting their budget-driven capacity constraints.

5 Conclusions and Future Research Lines

This paper has sketched the preliminary design of a meta-heuristic algorithm for the optimal deployment of firefighting aircrafts over airdromes based on weather-based predictive fire risk information. The paper has gone through the motivation of the research and the formal statement of the underlying optimization problem, to its solving via a combination of the HS algorithm and
Fig. 2. Assignment of aircrafts to aerodromes for a $[16, 49]$ risk estimation map.

A greedy repair procedure to account for budget-related capacity constraints. Results obtained in a set of synthetically-generated scenarios confirm that the performance of the meta-heuristic solver scales up nicely. This conclusion paves the way for further research aimed at validating this algorithm in realistic scenarios by incorporating further aspects such as different aircraft models.

References

Fractional Brownian Motion in SP500 and NASDAQ Market Indices

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Abstract. The potential presence of stochastic long memory process in economic and financial time series has been an important subject of both theoretical and empirical research. The long−memory or long time dependence property describes the high−order correlation structure of a series. The lack of memory is checked by using $R/S$ statistic and Lo’s modified $R/S$ statistic and adequate fractional Brownian motion (fBm) are simulated. The main contribution of this paper is fractal analysis of the selected financial time series.

Keywords: correlation, fractional Brownian motion, long memory process, simulation.

1 Introduction

In this paper we study a random process fractional Brownian motion that can be used to model the financial times series better than the classical models. The phenomenon of long−range dependence (or long memory or the Joseph effect first used by Mandelbrot and Wallis [14]) has a long history and has remained a topic of active research in the study of economic and financial time series (see e.g. [13], [11], [12], [20], [21], [22], [3]).

It is known that financial time series like real interest rates, real exchange rates are very persistent, it means that unexpected shock to the underlying variable has long lasting effects. Persistence can occur in the first or higher order moments of a time series. The persistence in the first moment of a time series can be confirmed by applying either unit root test or stationarity test. If we take into account the class of the stationary ARMA processes, these processes cannot capture the high degree of persistence in financial time series and if we consider the class of non−stationary unit root or $I(1)$ processes, thus $I(1)$ processes have some unattractive properties for financial economists.

In recent years, there have been preferred processes with long memory, which lie halfway between traditional stationary $I(0)$ processes and the non-stationary $I(1)$ processes. There is substantial evidence that long memory processes can provide a good description of many highly persistent financial time series. The long memory can be empirically observed, e.g. by a slowly decaying autocovariance function (ACF) (see [2], [18], [3]). The classic example of a long−range dependent process is the fractional autoregressive integrated
moving average (FARIMA) model with a power-law ACF. It appears that the values of FARIMA with Gaussian noise, for the memory parameter $d > 0$, have such a slowly decaying ACF that it is not absolutely summable. This behaviour serves as a classical definition of the long-range dependence (see [2]). When $d < 0$, the ACF still follows a power law, hence exhibiting more significant dependence than any other process with exponentially decaying ACF, such as, e.g. an autoregressive moving average (ARMA) time series, but the rate of decay is slower than for the $d$-positive case making the ACF absolutely summable. This negative memory phenomenon can be described as follows: increases in the values of the time series are likely to be followed by decreases and, conversely, decreases are more likely to be followed by increases (negative correlation). Such a time series is called short memory or antipersistent.

The study of non-Gaussian FARIMA processes was initiated more recently, see e.g. [2], [20], [21], [11]. Starting with the memorable work written by Mandelbrot [15], stable processes have enjoyed great popularity as flexible modeling tools in economics and natural sciences, see e.g. [19], [5], [22], [20], [21], [3]. In the infinite variance case there is no standard definition of short and long memory as the autocovariance function does not exist (is infinite). Therefore, definitions used in the literature incorporate other measures of dependence, e.g. codifference, or different functionals such as partial sums and maxima [11]. Analogously to the Gaussian case, we say that the FARIMA process with $\alpha$-stable noise has a long memory if $d > 0$ and short (negative) memory if $d < 0$. FARIMA with $\alpha$-stable noise is related via a limit theorem to a fractional stable motion (fSm) with self-similarity exponent $H = d + \frac{1}{\alpha}$, see [3], and it is a generalization of the fBm. The fractional stable motion has an infinite variance.

Since the short and long memory have been observed in many real world phenomena there have been developed many different methods for assessing type of dependence and estimating the memory parameter $d$, see e.g. [2], [11], [22]. It is important to know what are the assumptions and limitations of various tools and what is the exact result of different estimators, see [3]. For example, the classic rescaled range ($R/S$) method (see [20]), in the general $\alpha$-stable case, does not return the self-similarity parameter $H$, which is true only in the Gaussian case, but the value $d + \frac{1}{2}$, where $d = H - \frac{1}{\alpha}$ and $\alpha$ is the index of stability. Estimating the parameters of the FARIMA process seems a more complex task. Since the case $d > \frac{1}{2}$ can be reduced to the case $-\frac{1}{2} < d \leq \frac{1}{2}$ by taking appropriate differences, the latter case is particularly interesting. Long-range dependence occurs for $0 < d < \frac{1}{2}$, implying that the process is also asymptotically second order self-similar in this case. The corresponding Hurst parameter is $H = \frac{1}{2} + d$.

Fractional Brownian motion accepts global determinism and local randomness of the behaviour of the financial time series. In this paper we will analyse and simulate the selected financial time series as fractal processes. This paper is organized as follows: in section 2 we define fractional Brownian motion and we describe its basic properties, we recall basic facts about a classic example of long-range dependent processes. In section 3 we will describe empirical
analysis of the selected financial time series. The paper ends with a summary of our results.

2 Fractional Brownian motion and its basic properties.

2.1 Self–similarity and long–range dependence

Firstly we define self–similarity and long–range dependence in the framework of general stationary stochastic processes (see [10]). Let \( X = \{ X_k : k = 0, 1, 2, \ldots \} \) be a stationary discrete–time stochastic process, meaning that the vectors \( (X_{k_1}, \ldots, X_{k_d}) \) and \( (X_{k_1+n}, \ldots, X_{k_d+n}) \) have the same distribution for all integers \( d, n \geq 1 \) and \( k_1, \ldots, k_d \geq 0 \). For Gaussian processes, it is equivalent to require that \( \gamma(k) := \text{Cov}(X_n, X_{n+k}) \) does not depend on \( n \). These two notions are sometimes referred to as strict stationarity and second–order stationarity, respectively. The function \( \gamma(\cdot) \) is called the autocovariance function.

Let \( m \geq 1 \) be the general factor, not necessarily a power of 10. For every \( k \geq 0 \),

\[
X_{km} + \cdots + X_{(k+1)m-1} = a_mX_k, \tag{1}
\]

where the equality is in the sense of equality in distribution. Although the scaling factor \( a_m > 0 \) is still not defined by this intuitive reasoning, we first define a new process \( X^{(m)} = \{ X^{(m)}_k : k = 0, 1, 2 \ldots \} \) for every \( m \geq 1 \):

\[
X^{(m)}_k = \frac{1}{m} (X_{km} + \cdots + X_{(k+1)m-1}). \tag{2}
\]

Following Cox ([6], or [10]), we call a discrete–time stochastic process \( X \) self–similar with Hurst exponent \( 0 < H < 1 \) if \( X \) and \( m^{1-H}X^{(m)} \) have the same finite–dimensional distributions for all \( m \geq 1 \). This means that for every \( d \geq 1 \) and \( 0 \leq k_1 < \ldots < k_d \) the vector

\[
(X_{k_1}, \ldots, X_{k_d})
\]

has the same distribution as the vector

\[
(m^{1-H}X^{(m)}_{k_1}, \ldots, m^{1-H}X^{(m)}_{k_d})
\]

implying that the correlation function \( \rho(\cdot) = \frac{\gamma(\cdot)}{\text{Var}(X_1)} \) of \( X \) equals the correlation function \( \rho^{(m)}(\cdot) \) of \( X^{(m)} \) for all \( m \). Thus, (1) holds with \( a_m = m^H \) if \( X \) is self–similar with Hurst parameter \( H \).

The above definitions can easily be extended to continuous–time stochastic processes. A continuous time stochastic process \( Y = \{ Y(t) : 0 \leq t < \infty \} \) is called self–similar with Hurst parameter \( 0 < H < 1 \) if \( \{ a^HY(t) : 0 \leq t < \infty \} \) and \( \{ a^HY(t) : 0 \leq t < \infty \} \) have identical finite–dimensional distributions for all \( a > 0 \). Weaker notions than self–similarity also exist. A process is second–order self–similar if the finite dimensional distributions of \( X \) and \( m^{1-H}X^{(m)} \) have equal mean and covariance structure. If this is only true as \( m \to \infty \), the process is called asymptotically second–order self–similar, see [6], [10].
Presently we introduce the definition of long–range dependence. A stationary discrete–time processes \( X \) is said to be a process with long–range dependence, long memory, or strong dependence when its autocovariance function \( \gamma(\cdot) \) decays so slowly that \( \sum_{k=0}^{\infty} \gamma_k = \infty \) (in contrast to processes with summable covariances, which are called processes with short–range dependence, short memory, or weak dependence). Intuitively, when long–range dependence is present, high–lag correlations may be individually small, but their cumulative effect is significant.

As pointed out by Beran [1], [2], such a covariance structure has an important impact on usual statistical inference. As an example, assume that we have \( n \) observations of some random variable \( X \) with finite variance. The standard deviation of the mean is then proportional to \( \sqrt{n} \) if the observations are uncorrelated. If the covariances decay exponentially (as is the case with a so–called AR(1) process), the covariances are summable and similar behaviour is observed: the standard deviation of the mean is proportional to \( n^{\frac{1}{2}} \) for sufficiently large \( n \), although the proportionality constant is different. Under this long–range dependence, the standard deviation of the mean is proportional to \( n^{-\alpha} \). This affects the confidence intervals for the mean of \( X \) and all related test statistics. Moreover, the standard estimator for the variance of \( X \) becomes biased. This bias does not disappear when the sample size increases, as is the case for short–range dependent processes. It is very well possible that there are some specific lags for which \( (k) \) is particularly large, which makes the detecting of long–range dependence more difficult. In fact, it is theoretically impossible to conclude that long–range dependence is present in a finite sample.

In general, self–similarity and long–range dependence are not equivalent. As an example, the increments of a standard Brownian motion are self–similar with Hurst parameter \( H = \frac{1}{2} \), but clearly not long–range dependent (the increments are even independent). However, under the restriction \( \frac{1}{2} < H < 1 \), long–range dependence is equivalent to asymptotic second–order self–similarity for stationary processes.

If a system is independently distributed, then \( H = \frac{1}{2} \). When \( H \) differed from \( \frac{1}{2} \), the observations are not independent. Each observation carried a memory of all the events that preceded it. What happens today influences the future. Where we are now is a result of where we have been in the past. Time is important. The impact of the present on the future can be expressed as a correlation:

\[
C = 2^{(2H-1)} - 1,
\]

where \( C \) is correlation measure and \( H \) is Hurst exponent.

There are three distinct classifications for the Hurst exponent ([21], p.64):

1. \( H = 0.50 \): time series is random, events are random and uncorrelated. Equation (3) equals zero. The present does not influence the future. Its probability density function can be normal curve, but it does not have to be. \( R/S \) analysis can classify an independent series, no mater what the shape of the underlying distribution.

2. \( 0 \leq H < 0.50 \): time series is antipersistent, or ergodic. If the time series has been up in the previous period, it is more likely to be down in the
next period. Conversely, if it was down before, it is more likely to be up in the next period. The strength of this antipersistent behaviour depends on how close $H$ is to zero. The closer it is to zero, the closer $C$ in equation (3) moves toward 0.50, or negative correlation. This time series is more volatile than a random series.

3. $0.50 \leq H < 1.00$: time series have a persistent or trend-reinforcing character. If the series has been up (down) in the last period, then the chances are that it will continue to be positive (negative) in the next period. Trend is apparent. The strength of the trend-reinforcing behaviour, or persistence, increases as $H$ approaches 1.0. The closer $H$ is to 0.5, the noisier it will be, and the less defined its trends will be. Persistent series are fractional Brownian motion, or biased random walk. The strength of the bias depends on how far $H$ is above 0.50. A high $H$ value shows less noise, more persistence and clearer trends than does lower value. A high $H$ means less risk.

### 2.2 Fractional Brownian motion

Fractional Brownian motion is defined by its stochastic representation (see Mandelbrot and van Ness [15]):

$$B_H(t) = \frac{1}{\Gamma(H + \frac{1}{2})} \left( \int_{-\infty}^{0} \left[ (t-s)^{H-\frac{1}{2}} - (-s)^{H-\frac{1}{2}} \right] dB(s) + \int_{0}^{t} (t-s)^{H-\frac{1}{2}} dB(s) \right),$$

(4)

where $\Gamma$ represents the Gamma function $\Gamma(\alpha) := \int_{0}^{\infty} x^{\alpha-1} \exp(-x) dx$ and $0 < H < 1$ is called the Hurst parameter (we will soon see the connection with the Hurst parameter for self-similar processes). The integrator $B$ is a stochastic process, defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$, ordinary Brownian motion. Note that $B$ is recovered by taking $H = \frac{1}{2}$ in (4).

A normalized fractional Brownian motion $B_H = \{B_H(t) : 0 \leq t < \infty\}$ with $0 < H < 1$ is uniquely characterized by the following properties, (see [10]):

- $B_H(t)$ has stationary increments;
- $B_H(0) = 0$, and $\mathbb{E}(B_H(t)) = 0$ for $t \geq 0$;
- $\mathbb{E}(B_H^2(t)) = t^{2H}$ for $t \geq 0$;
- $B_H(t)$ has a Gaussian distribution for $t > 0$.

From the first three properties it follows that the covariance function is given by

$$\gamma(s, t) = \mathbb{E}(B_H(s)B_H(t)) = \frac{1}{2} \left\{ t^{2H} + s^{2H} - (t-s)^{2H} \right\}$$

(5)

for $0 < s \leq t$. For Gaussian processes, the mean and covariance structure determine the finite-dimensional distributions uniquely. Therefore, we conclude from (5) that $\{B_H(at) : 0 \leq t < \infty\}$ and $\{a^H B_H(t) : 0 \leq t < \infty\}$ have the same finite-dimensional distributions: fractional Brownian motion with Hurst exponent $H$ is self-similar process. In fact, fractional Brownian motion is the only Gaussian process with stationary increments that is self-similar ([6], [10]).
3 Empirical study

We analyse time series consisting of the daily close price data of the two American market indices: SP500 and NASDAQ since April 24, 1981 until March 27, 2013 presented in the Figure 1. The observations were obtained from Bloomberg. We denote the given 8053 observations by \( \{Y_n : n = 1, 2, \ldots, 8053\} \). Our computations were done using Wolfram Mathematica and SAS IML software.

Since the data have clearly nonstationary structure and fitting the distribution requires stationarity, we compute daily logaritmic returns for both price series denominated in USD, see Figure 2. A sample plot is enough to observe volatility clustering for all return series. Table 1 provides summary statistics as well as the Jarque–Bera value based on the daily return series. In all cases, the null hypothesis of normality is rejected at any level of significance, and there is evidence of significant excess kurtosis of the return series. This indicates that the distributions of these return series are nonGaussian. The stationarity of the returns was tested using Dickey–Fuller unit root test. Both return series are stationary (\( p \)-value of Unit Root test equals to 0.0).

For the logarithmic returns of the price data, we check the hypothesis of the lack of long memory in SP500 and NASDAQ time series. We estimate the self–similarity parameter \( H \) using the \( R/S \) statistic and Lo's modified \( R/S \) statistic (see Tables 3, 4 and Figures 3, 4). In the case of Gaussian (i.e., finite variance) time series the result of the method is indeed an estimate of \( H \). During period 04/24/1981–03/27/2013 the Hurst coefficient \( H \) for the daily SP500 index log return is equal to 0.53636 and for NASDAQ daily log return is equal to 0.58803. Expected Hurst exponent is equal to \( E(H) = 0.5407 \) (Table 2). The variance of \( E(H) \) is \( 1/n = 1/8050 = 0.000124 \), for Gaussian random variables. Standard deviation of \( E(H) \) is 0.0111. The Hurst exponent for SP500 daily log return time series is -0.3894 standard deviations away from its expected value and it is insignificant (see Figures 3, 4). This time series exhibits random behaviour. The Hurst exponent for daily NASDAQ log return time series is 4.2465 standard deviations away from its expected value. This is a highly significant result at the 95% level. The time series has persistent character. We also plotted \( E(R/S_n) \) (dashed line) as a comparison against the null hypothesis that the system is an independent process (Figures 3, 4). Figure 5 shows simulated (we used equation 4) future log returns for both time series and for estimated values of the Hurst coefficients (Table 2).

4 Conclusion

In this paper, we propose a fractal analysis of the selected financial time series. SP500 log return exhibits random behaviour and NASDAQ log return shows persistent character. SP500 market index is effective index, but the market index NASDAQ shows intervention character.

Information obtained by fractal analysis can be used as the basis of momentum analysis and other forms of technical analysis. The second use is in
choosing periods for model development, particularly for back testing. Fractal analysis offers an alternative to conventional risk measure.

References

Appendix

<table>
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<th>NASDAQ</th>
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<tr>
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<tr>
<td>Unit Root test</td>
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Table 1. Descriptive statistics based on the daily log return series, (April, 24 1981 – March, 27 2013)

Fig. 1. SP 500 and NASDAQ indices daily price series from 24. 4. 1981 to 27. 3. 2013

Fig. 2. SP 500 and NASDAQ indices daily log return series from 24. 4. 1981 to 27. 3. 2013
Fractal analysis | SP500 | NASDAQ
---|---|---
Hurst coefficient H | 0.53636 | 0.58803
R - Square | 0.99992 | 0.9987
Expected Hurst coefficient | 0.54070 | 0.54070
R - Square | 0.999198 | 0.999198

Table 2. Hurst exponent based on the daily log return series, (April, 24 1981 – March, 27 2013)

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<th>V stat</th>
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Table 3. R/S statistics and Modified R/S statistics for SP500 index daily log return series from 24. 4. 1981 to 27. 3. 2013

Fig. 3. R/S statistics and Modified R/S statistics for SP 500 index daily log return series from 24. 4. 1981 to 27. 3. 2013
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<th>V stat</th>
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Table 4. R/S statistics and Modified R/S statistics for NASDAQ index daily log return series from 24. 4. 1981 to 27. 3. 2013

**Fig. 4.** R/S statistics and Modified R/S statistics for NASDAQ index daily log return series from 24. 4. 1981 to 27. 3. 2013

**Fig. 5.** SP 500 and NASDAQ simulated log return series
Assessing the Importance of Risk Factors in Distance-Based Generalized Linear Models

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Abstract. Predictions with distance-based linear and generalized linear models rely upon latent variables derived from the distance function. This key feature has the drawback of adding a non-linearity layer between observed predictors and response which shields one from the other and, in particular, prevents us from interpreting linear predictor coefficients as influence measures. In actuarial applications such as credit scoring or a priori rate-making we cannot forgo this capability, crucial to assess the relative leverage of risk factors. Towards the goal of recovering this functionality we define and study influence coefficients, measuring the relative importance of observed predictors. Unavoidably, due to inherent model non-linearities, these quantities will be local -valid in a neighborhood of a given point in predictor space.

Keywords: Distance analyses, nonlinear regression, influence coefficients, risk factors, actuarial science.

1 Introduction

Assessing the relative importance of each predictor and calibrate its influence on the response, a straightforward operation in linear prediction, becomes a non trivial issue for non linear or non parametric methods.

In distance-based (DB) prediction this difficulty is compounded due to the indirect relationship between predictors and response through a metric. This indirect relationship prevents us from interpreting linear predictor coefficients as is done in ordinary linear models (LM) or generalized linear models (GLM).

A partial approach has been proposed to this problem for DB regression (DB linear model, DB-LM, with a continuous response). There is a version of the $F$-test statistic for selecting explanatory variables, with bootstrapped $p$-values (see Boj et al.[1]). In this article, we analyze a set of influence coefficients, that is, local -valid in a neighborhood of a given point in the predictor space- which measures the relative importance of each observed variable. This procedure is applied to DB generalized linear models, DB-GLM (Boj et al.[4]).
The reach and performance of these influence coefficients are demonstrated on case studies drawn from actuarial (insurance) problems, in which quantify the relative leverage of risk factors is of utmost importance. Computations are made using a newly developed R package (R Development Core Team[20]), called dbstats (Boj et al.[5]) which implements several distance-based procedures.

The paper is structured as follows. In Section 2 we define -local- influence coefficients for the DB-LM and DB-GLM models. In Section 3 we propose a bootstrap methodology for the calculation of confidence intervals. In Section 4 we provide an empirical example using R. Finally, in Section 5 we include a discussion with some further research.

2 Influence Coefficients: Definition

DB-LM was introduced by Cuadras[7] and has been developed in Cuadras and Arenas[6], Cuadras et al.[8] and in Boj et al.[1],[2],[3]. DB-GLM has been defined in Boj et al.[4] where we refer for a detailed description. In this article we define influence coefficients for the DB-GLM. These coefficients are also valid for the DB-LM because DB-LM is a particular case of DB-GLM when it is supposed Gaussian error distribution jointly with the Identity link.

In ordinary GLM (see McCullagh and Nelder[19]) we have the relation between response and linear predictor:

\[ \hat{y} = g^{-1}(\hat{\eta}) = g^{-1}(\hat{\beta}_0 + F_1 \cdot \hat{\beta}_1 + F_2 \cdot \hat{\beta}_2 + \cdots + F_p \cdot \hat{\beta}_p) \]

If we want to measure the influence of each \( F_j \) in GLM we can use the numerical estimated coefficients \( \hat{\beta}_j \) for \( j = 1, \ldots, p \) of the linear predictor. But in DBLM and DB-GLM the relation of each observable predictor \( F_j \) is not linear in predictions. The idea of our definition of influence will be comparable to the measured influence coefficients \( \hat{\beta}_j \) for \( j = 1, \ldots, p \) of LM or GLM.

Let \( f_0 \) be the \( p \) predictor values of a reference/virtual individual, being \( f_0 \) a new individual or one of the average population, \( f_0 = (f_0^1, f_0^2, \ldots, f_0^p) \). It is important to point out, that the influence of each \( F_j \) that we want to quantify will depend on the chosen reference individual which we will use as origin. We need to specify a representative \( f_0 \), for example the mean or the median in the numerical coordinates and the mode in the binary or qualitative coordinates.

2.1 Influence coefficients for categorical (or binary) predictors

Suppose that we have categorical (or binary) predictors, then we define the influence coefficients \( \hat{\beta}_j \) for \( j = 1, \ldots, p \) as the increment of the link prediction when the \( j \)-th predictor value of \( f_0 \) changes to another level:

\[ \beta_j = \nabla_j \hat{\eta}_{f_0} \quad j = 1, \ldots, p. \]
2.2 Influence coefficients for quantitative predictors

Suppose that we have quantitative predictors, then we define the influence coefficients \( \hat{\beta}_j \) for \( j = 1, \ldots, p \) as

\[
\beta_j = \left. \frac{\partial \hat{\eta}}{\partial F_j} \right|_{F_0} \quad j = 1, \ldots, p,
\]

the speed of the link prediction change when \( F_0 \) is modified with the values

\[
f_0 + t \times s_j \left( 0, \ldots, 0, 1_{j-th}, 0, \ldots, 0 \right), \quad t \in (-\varepsilon, +\varepsilon),
\]

where \( s_j \) is the standard deviation of the \( j \)-th quantitative predictor. This calculation is inspired in the nonlinear biplots of Gower and Harding[14].

In practice, to this end we use the smooth.spline function of the stats package for R to fit a cubic smoothing spline for some values of (3). E.g., in the application of Section 4 we use 201 values, by a sequence varying \( t \) from \(-1\) to \(1\) by \(0.01\). Then, to estimate the influence coefficient we use the command predict to fit the first derivative of the spline evaluated at the \( t \) zero point.

3 Bootstrapping pairs and Confidence Intervals

We propose to use the resampling technique bootstrapping pairs or resampling cases in which each bootstrap sample consists of \( n \) response-predictor pairs from the original data (see, e.g. Efron and Tibshirani[10], Davidson and Hinkley[9] or Boj et al.[1]). In this way we can generate \( B \) bootstrap samples from which we can estimate the matrix \( Beta \) of coefficients

\[
Beta = \begin{bmatrix} \hat{\beta}_1 & \hat{\beta}_1^1 & \cdots & \hat{\beta}_1^B \\ \vdots & \vdots & \ddots & \vdots \\ \hat{\beta}_p & \hat{\beta}_p^1 & \cdots & \hat{\beta}_p^B \end{bmatrix}_{p \times (B+1)},
\]

where in the first column we have the estimated coefficients of the original sample, \( \hat{\beta}_j \) for \( j = 1, \ldots, p \), and in the next \( B \) columns we have the estimated coefficients for the \( B \) bootstrapped samples, \( \hat{\beta}_j^b \) for \( j = 1, \ldots, p \) and for \( b = 1, \ldots, B \). To estimate the influence coefficients \( \text{standard errors} \) we can use the usual formula:

\[
\text{std}^* \left( \hat{\beta}_j \right) = \sqrt{\text{var}^* \left( \hat{\beta}_j \right)} = \sqrt{\frac{1}{B-1} \sum_{b=1}^{B} \left( \hat{\beta}_j^b - \bar{\hat{\beta}}_j \right)^2},
\]

where

\[
\bar{\hat{\beta}}_j = \frac{1}{B} \sum_{b=1}^{B} \hat{\beta}_j^b.
\]
To construct *simple bootstrap confidence intervals* related to the bootstrap hypothesis testing $H_0 : \beta_j = \beta_0$ with $\beta_0$ a fixed numerical value, we can apply the formula:

$$
\left[ \hat{\beta}_j - \text{std}^* \left( \hat{\beta}_j \right) \times z_{1 - \alpha/2}, \hat{\beta}_j + \text{std}^* \left( \hat{\beta}_j \right) \times z_{1 - \alpha/2} \right],
$$

(6)

where $z_{1 - \alpha/2}$ denotes the $1 - \alpha/2$ quantile of the standard normal distribution. If e.g. $\alpha = 0.05$ this is equal to 1.96.

The simple bootstrap interval (6) can be modified so that it will be centred on a bias-corrected estimate $\tilde{\beta}_j$. One can simply replace $\hat{\beta}_j$ in (6) by

$$
\tilde{\beta}_j = \hat{\beta}_j - \left( \bar{\hat{\beta}}^*_j - \hat{\beta}_j \right) = 2\hat{\beta}_j - \bar{\hat{\beta}}^*_j.
$$

(7)

There is no theoretical reason to believe that the simple interval (6) will work better, or any worse, than a similar interval based purely on asymptotic theory. However, it can be used when there is no way to calculate a standard error analytically or when asymptotic errors are unreliable. Another advantage of (6) is that the number of bootstrap samples, $B$, does not have to be very large, as we verify in the next Section. We refer to MacKinnon[16],[17],[18] for more details.

4 Application

In the computations of this Section we use the function `dbglm` of the `dbstats` package for R (Boj et al.[5]). This function fits DB-GLM.

We use a data set on Swedish third-party motor insurance in 1977 described in Hallin and Ingenbleek[15] and also used in Boj et al.[4]. Data are incorporated in the package `faraway` of R and named `motorins`. The total number of observations is $n = 295$ corresponding to different non-empty risk groups. We analyze claim frequency, defined by the number of claims and the exposure variable number of insured in policy-years. There are three risk factors: Distance (kilometers travelled per year), Bonus (level in the scale of Bonus, with numerical values from 1 to 7) and Make (with 9 nominal categorical classes). We treat Distance and Bonus as numerical variables and Make as categorical nominal. We code Distance as numerical using its class marks as in Boj et al.[4]. As distance function for the DB-GLM we use the Gower’s similarity index (Gower[13]), taking into account all the relative geometric variability, i.e., the model named `dbglm1` in the Appendix A of Boj et al.[4], with a residual deviance of 454.05 on 276 degrees of freedom.

We want to estimate eleven coefficients: nine for the classes of Mark applying the definition (1), and two for the numerical factors Distance and Bonus applying (2). In this way we could interpret the linear predictor:

$$
\eta = \beta_0 + F_1 \cdot \beta_1 + F_2 \cdot \beta_2 + \cdots + F_{10} \cdot \beta_{10} + \varepsilon = \\
\beta_{\text{Make1}} + F_{\text{Make2}} \cdot \beta_{\text{Make2}} + F_{\text{Make3}} \cdot \beta_{\text{Make3}} + F_{\text{Make4}} \cdot \beta_{\text{Make4}} \\
+ F_{\text{Make5}} \cdot \beta_{\text{Make5}} + F_{\text{Make6}} \cdot \beta_{\text{Make6}} + F_{\text{Make7}} \cdot \beta_{\text{Make7}} + F_{\text{Make8}} \cdot \beta_{\text{Make8}} \\
+ F_{\text{Make9}} \cdot \beta_{\text{Make9}} + F_{\text{Km}} \cdot \beta_{\text{Km}} + F_{\text{Bon}} \cdot \beta_{\text{Bon}} + \varepsilon.
$$
We define the reference individual $f_0 = (\text{Make} = 1, \bar{Km} = \bar{Bon} = (1.9683.82, 5.58)$ being the class $\text{Make} = 1$ the corresponding to the intercept term, $\hat{\beta}_0$.

The results of the estimated influence coefficients for this model, $dbglm1$, are in the first column of Table 1. In parenthesis, below of each value, there are the results of the estimation of influence coefficients of model $dbglm4$ of Appendix A of Boj et al.[4]. The $dbglm4$ is estimated using the Euclidean distance in the DB-GLM. We observe that the results of the estimated influence coefficients for $dbglm4$ coincide with those of glm1 of Appendix A of [4]. We refer to the `summary` command of glm1 (pp. 23-24 in [4]). For that classical model (glm1) one can compute the significance of each predictor in the regression with the glm function of the stats package for R. We observe that the less significant p-values are for $\hat{\beta}_{\text{Make}_7} \hat{\beta}_{\text{Make}_8}$ and $\hat{\beta}_{\text{Make}_9}$ with a values of 0.02508, 0.10762 and 0.17618 respectively. Then, one could conclude that for glm1 the three factors could be entered in the model.

We estimate standard errors with formula (4) using a size $B = 1000$ for the bootstrap, but we divide it into two subsets of sizes $B_1 = B_2 = 500$. In Table 1 we show the results. We observe that using a size of 500 will be enough for the bootstrap results. As an illustration of the bootstrapped distributions we show in Figure 1 the histograms of four betas.

Finally, we construct simple bootstrap confidence intervals using the standard error calculated with the total size $B$ and formulas (6) and (7). The results are shown in Table (2). If we use the confidence intervals to test that $H_0 : \beta_j = 0$, for $j = 0, \ldots, 10$, we can conclude that all coefficients are significant at the confidence level of the 95%.

<table>
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<td>$6.465381e-03$</td>
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<tr>
<td>$\hat{\beta}_{\text{Make}_4}$</td>
<td>$-4.976677e-01 (-5.162e-01)$</td>
<td>$2.668724e-03$</td>
<td>$2.672244e-03$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\text{Make}_5}$</td>
<td>$1.238671e-01 (1.270e-01)$</td>
<td>$3.360581e-03$</td>
<td>$3.347443e-03$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\text{Make}_6}$</td>
<td>$-3.880247e-01 (-3.976e-01)$</td>
<td>$2.383127e-03$</td>
<td>$2.377103e-03$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\text{Make}_7}$</td>
<td>$-1.303605e-01 (-1.320e-01)$</td>
<td>$5.395997e-03$</td>
<td>$5.412965e-03$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\text{Make}_8}$</td>
<td>$1.362958e-01 (1.396e-01)$</td>
<td>$1.504232e-02$</td>
<td>$1.508169e-02$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\text{Make}_9}$</td>
<td>$-2.360768e-02 (-3.079e-02)$</td>
<td>$1.317354e-03$</td>
<td>$1.311761e-03$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\bar{Km}}$</td>
<td>$1.068948e-05 (1.431e-05)$</td>
<td>$9.231468e-08$</td>
<td>$9.298712e-08$</td>
</tr>
<tr>
<td>$\hat{\beta}_{\bar{Bon}}$</td>
<td>$-3.732707e-02 (-2.165e-01)$</td>
<td>$1.791164e-03$</td>
<td>$1.792390e-03$</td>
</tr>
</tbody>
</table>

Table 1. Estimated coefficients and bootstrap standard errors for two resamples of sizes $B_1 = B_2 = 500$ and the total $B = 1000$ using Gower’s distances.
Fig. 1. Histograms of bootstrap distributions of influence coefficients for factors Make1, Make2, Kilometers and Bonus for the DB-GLM using Gower’s distances.

<table>
<thead>
<tr>
<th></th>
<th>Confidence interval with $\alpha = 0.05$ using (6)</th>
<th>Bootstrapped mean (5), $\hat{\beta}_i^*$</th>
<th>Confidence interval with $\alpha = 0.05$ using (7)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{\text{Make1}}$</td>
<td>$[-1.859852e+00, -1.853354e+00]$</td>
<td>$[-1.85662e+00, -1.853337e+00]$</td>
<td>$[-1.859835e+00, -1.853337e+00]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make2}}$</td>
<td>$[1.248679e-01, 1.374383e-01]$</td>
<td>$[1.311534e-01, 1.374380e-01]$</td>
<td>$[1.248676e-01, 1.374380e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make3}}$</td>
<td>$[-2.268812e-01, -2.015370e-01]$</td>
<td>$[-2.150491e-01, -2.006970e-01]$</td>
<td>$[-2.260412e-01, -2.006970e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make4}}$</td>
<td>$[-5.029018e-01, -4.924336e-01]$</td>
<td>$[-4.976958e-01, -4.928055e-01]$</td>
<td>$[-5.028737e-01, -4.928055e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make5}}$</td>
<td>$[1.172881e-01, 1.304461e-01]$</td>
<td>$[1.238302e-01, 1.304830e-01]$</td>
<td>$[1.173002e-01, 1.304830e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make6}}$</td>
<td>$[-3.928970e-01, -3.833597e-01]$</td>
<td>$[-3.881282e-01, -3.832562e-01]$</td>
<td>$[-3.925862e-01, -3.832562e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make7}}$</td>
<td>$[1.409533e-01, 1.197677e-01]$</td>
<td>$[1.306013e-01, 1.195269e-01]$</td>
<td>$[1.407125e-01, 1.195269e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make8}}$</td>
<td>$[-1.067743e-01, 1.658173e-01]$</td>
<td>$[1.35706e-01, 1.664071e-01]$</td>
<td>$[1.073641e-01, 1.664071e-01]$</td>
</tr>
<tr>
<td>$\beta_{\text{Make9}}$</td>
<td>$[-2.618421e-02, -2.103115e-02]$</td>
<td>$[-2.363303e-02, -2.100580e-02]$</td>
<td>$[-2.615866e-02, -2.100580e-02]$</td>
</tr>
<tr>
<td>$\beta_{\text{Km}}$</td>
<td>$[1.050788e-05, 1.087108e-05]$</td>
<td>$[1.068304e-05, 1.087752e-05]$</td>
<td>$[1.051432e-05, 1.087752e-05]$</td>
</tr>
</tbody>
</table>

Table 2. Confidence intervals with the standard error calculated using the total size $B = 1000$ and assuming $\alpha = 0.05$ using Gower’s distances.
5 Discussion

In this paper we propose a definition of -local valid- influence coefficients for the DB-GLM. Additionally, we use a bootstrap methodology to estimate standard errors and to calculate simple bootstrap confidence intervals. The proposed bootstrap methodology is bootstrapping pairs which could be adequate when we use DB regression models (see Boj et al.[1]).

The pairs bootstrap is very easy to implement and it can be applied to an enormous range of models. However it sufers from two major deficiencies (see MacKinnon[16],[17],[18]). The first is that the bootstrap data generation process (DGP) does not impose any restriction on $\beta_j$. Then, if we are testing restrictions on $\beta_j$, as opposed to estimating standard errors or forming confidence intervals, we need to modify the bootstrap test statistic so that it will test something that will be true in the bootstrap DGP. Or, alternatively, we can modify the resampling scheme so that the null hypothesis will be respected in the bootstrap DGP (see Boj et al.[1] and Flachaire[11],[12]). The other deficiency of the pairs bootstrap is that, compared with the residual bootstrap (when it is valid) and with the wild bootstrap, the pairs bootstrap generally does not yield very accurate results. But the pairs bootstrap is less sensible to the hypotheses of the model than the residual bootstrap. And the estimated standard error via the pairs bootstrap offers reasonable results when the hypotheses of the model are not satisfied.

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References


Breast Cancer Survival at Braga’s Hospital - Portugal

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³ Senology Unit of Braga’s Hospital, Portugal

Abstract. The present work intends to describe the survival rate of breast cancer patients of the Senology Unit of Braga’s Hospital, located in the north of Portugal. Data consists in 540 female patients, diagnosed with a malignant tumour in the corresponding period of 1998 up to 2012, whose age at the time of diagnosis varies between 20 to 89 years. We performed a survival analysis in order to describe the survival rate of these patients as a function of possible risk factors. Making use of Flexible Parametric Survival Models to estimate hazard ratios over time since diagnosis by a set of statistical significant covariates. Covariates triple negative (yes vs no), age at diagnosis, tumour stage and tumour grade have a significant statistical effect on the global survival rate of these patients. Results were also compared to those obtained when adjusting to the well known Cox proportional hazard model, and were quite similar for both models. There is an improvement of survival rate at 1, 3 and 5 years when compared to results from earlier studies.

Keywords: Breast Cancer, Survival, Flexible Parametric Survival model.

1 Introduction

Oncological diseases are the second highest cause of death in Portugal, and they have a big social impact in patients and their families [8]. In Europe breast cancer is the tumor with highest incidence in women [1]. In Portugal there are not many published studies on breast cancer over the years. However, the publication of 2003 by Pinheiro et al [8], refers that since 1995 mortality, due to breast cancer, has been decreasing in Portugal. They argue that this improvement, is a consequence of earlier diagnostic and better quality of treatment.

Accordingly to results presented by the European Cancer Observatory, the estimated incidence for Breast Cancer in Portuguese women in 2012 is 29.41% and the estimated mortality rate due to this type of cancer is 16.01%, both values lower than the European average (85.6% and 18.4% respectively).

At the moment, the existing recommendations and guidelines from the National Health Service are mainly based on European studies. However, it is not clear that the behaviour of the disease is similar among European countries. Therefore, it is of great importance the continuous investment on statistical and epidemiological studies in oncological diseases for understanding the progression of the disease in Portugal.
This study aims to answer at least some of the questions on the Portuguese population specificity, particularly the population of the Senology Unit of Braga Hospital, located in the north of Portugal, that have been diagnosed with malignant breast cancer.

Our main purpose is to describe the survival rate of the patients who were followed and treated in that hospital, as a function of possible risk factors. For that, we analysed how the overall and cause-specific risk of dying from breast cancer of these patients is related with possible risk factors by adjusting multivariate survival models.

In section 2 we will briefly describe the data source and study cohort as well the methods used in the statistical analysis. Section 3 intends to describe some of the important results. And the last section will present a discussion of the results and a comparison of these with results from earlier studies.

2 Methodology

Data were collected directly from the medical records of each patient, listed in the computer system of Braga’s Hospital - Glintt HS. We therefore have access to baseline and clinical history of each patient (a roll of information such as diagnosis; pre-surgery, post-surgery, group meetings; follow-up and medical exams). The authorization for collect and use of senology data was approved by the Ethical Committee of Hospital de Braga. From the information gathered in the medical reports we were able to collect 50 variables (Table 1) that can be grouped into two categories: (i) the explanatory variables at individual level, that are a group of demographic characteristics that include a set of prognostic factors reported by Rodrigues [10], such as, for example: age, menopause, age at first full term pregnancy; (ii) and a second group of variables, explanatory variables at tumour level, that include characteristics of the tumour, some of them important prognostic factors already reported in the literature and resumed by Fitzgibbons et al. [5] and Cianfrocca and Goldstein [2], such as TNM stage, histological type of tumour, hormonal receptors or vascular or lymphatic invasion, among others.

We analysed overall survival times for 540 female patients, diagnosed with a malignant tumour in the corresponding period of 1998 until 2012, whose age at the time of diagnosis varies between 20 and 89 years. Bilateral breast cancer cases, in this case 19 of them, were treated as independent cases. Therefore, a total number of 559 cases were analysed. The total number of deaths from breast cancer is 55.

The response variable is time from date of diagnosis to death from breast carcinoma (cause-specific), or right censored date if lost to follow-up, or last observed date of March 1, 2013. We handled all missing values as missing completely at random.

In order to estimate the relative risk of death from breast cancer we proceeded initially with the calculation of the Kaplan Meier estimates stratified by category, and compared these through their graphical representation and the logrank test to evaluate the statistical significance of differences among the survival
Using the statistically significant variables obtained in log rank tests we adjusted several multivariate models to estimate the joint effect of several independent variables on patients survival. We made use of Flexible Parametric Survival, in particular a flexible Royston-Parmar survival model (FRPM) [12], to estimate hazard ratios over time since diagnosis by a set of statistical significant covariates. Also the, well known, Cox Proportional Hazards Model [3] (CPHM), was fitted only for the purpose of comparing estimates. The CPHM defines the probability of survival, under the assumption of proportional hazards, as a function of time $t$, for a vector of covariates $x_i$, as it follows:

$$S(t|x_i) = [S_0(t)]^{\exp(x_i\beta)}$$
where $S_0(t)$ is the baseline survival function and $\beta$ the vector of coefficients estimated.

The corresponding hazard function can be written as:

$$h(t|x_i) = h_0(t) \exp(x_i \beta)$$

where $h_0(t)$ is the baseline hazard function. The particularity of this model, which can be viewed as one of its advantages, is that the estimation of the coefficients does not require the formulation of the baseline cumulative survival function as it gets absorbed when the coefficients are estimated by the method of partial log likelihood.

However, as Royston and Parmar [12] stress out it is often of interest, in medical studies, the smoothly estimation of the baseline hazard function as it is directly related to the time-course of an illness. Also the incorporation of time varying regression coefficients on the CPHM, when the assumption of proportional hazards is violated, results in a complex practical interpretation of the coefficients and in the robustness of the resulting model. So it’s of interest the use of a more flexible model where the visualization of the hazard function is much easier.

For that, we choose to work with the approach proposed by Royston and Parmar [12] where they model the logarithm of the baseline cumulative hazard function as a natural cubic spline function of log time.

The FRPM comes from the family of functions that are based on transformation of the survival function by a link function $g(.)$:

$$g[S(t|x_i)] = g[S_0(t)] + x_i \beta$$

Since we are interested in estimating hazard ratios, and as Royston and Parmar [3] suggest, we use natural cubic splines to model $g[S_0(t)]$ within the Aranda-Ordaz family of link functions: $g(x; \theta) = \log \left( \frac{x^\theta - 1}{\theta} \right)$. Choosing to work with hazards scaling by making $\theta \to 0$, rather than with more general values of $\theta$ as they refer that the interpretation of covariate effects would turn out obscure.

Thus, the model transformation may be written as it follows:

$$g[S(t|x_i)] = \ln[H(t|x_i)] = \eta_i = s(ln(t)|\gamma, k) + x_i \beta$$

where $H(t|x_i)$ is the cumulative hazard function and $s$ is a natural cubic spline acting on a log scale of time $t$, with adjustable parameter $\gamma$ vector and $k$ knots. The choice of number of knots can be made using the minimum combination of Akaike Information Criterion (AIC). The respective survival function can be formulated as: $S(t|x_i) = \exp(-\exp(\eta_i))$. And the hazard function as: $h(t|x_i) = \frac{ds[ln(t)|\gamma, k] \exp(\eta_i)}{dt}$. Since both CPHM and FRPM rely on the assumption of proportional hazards we preformed a statistical test proposed by Grambsch and Therneau [6] based on the Schoenfeld residual calculation.

The final model (adjusted) was estimated by "step-wise backwards", starting
with the saturated model with all the significant variables, and then eliminat-
ing one-by-one the variables with lower significance (p-value).
The entire analysis was preformed with open source statistical software R.

3 Results

As already referred we analysed 50 variables. Given the impracticality of sum-
marize and describe all variables in this study, we present in Table 2 the distri-
bution of explanatory variables which reflected significant effect on the survival
of patients, accordingly to the results obtained in the log rank test (Table 3),
by vital status and their respective percentage of missing values.

As we can tell from Table 2, the majority of cases present an early-stage
breast cancer, as the frequency distributions concentrate its values on the first
categories of tumour stage, size and grade. This can be related to an increased
screening leading to early detection of the tumour. It is an important result
as it may translate in a high probability of survival of these patients. In a
first exploratory analysis in terms of survival one can observe that the Kaplan
Meier estimate for 10-year survival of these patients (Figure 1), is quite near
of 80%. Also, it seems that for the entire observed follow up time the survival
probability is above the 50%.

![Kaplan-Meier estimate with 95% confidence bounds](image.png)

**Fig. 1.** Kaplan Meier curve estimates of Breast Cancer patients of Bragas Hospital.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Alive or death by other causes (%)</th>
<th>Dead from breast cancer (%)</th>
<th>(%) of NA’s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tumor Stage</td>
<td>0</td>
<td>26 (5.4)</td>
<td>1 (1.8)</td>
</tr>
<tr>
<td></td>
<td>I</td>
<td>182 (37.9)</td>
<td>11 (20.0)</td>
</tr>
<tr>
<td></td>
<td>II</td>
<td>195 (40.6)</td>
<td>18 (32.7)</td>
</tr>
<tr>
<td></td>
<td>III</td>
<td>74 (15.4)</td>
<td>24 (43.6)</td>
</tr>
<tr>
<td></td>
<td>IV</td>
<td>3 (0.6)</td>
<td>1 (1.8)</td>
</tr>
<tr>
<td>Neoadjuvant Treatment</td>
<td>Without</td>
<td>452 (90.6)</td>
<td>40 (66.7)</td>
</tr>
<tr>
<td></td>
<td>With</td>
<td>47 (9.4)</td>
<td>20 (33.3)</td>
</tr>
<tr>
<td>Type of surgery</td>
<td>No Surgery</td>
<td>9 (1.8)</td>
<td>5 (8.3)</td>
</tr>
<tr>
<td></td>
<td>Conservative</td>
<td>213 (42.7)</td>
<td>11 (18.3)</td>
</tr>
<tr>
<td></td>
<td>Mastectomy</td>
<td>277 (55.5)</td>
<td>44 (73.3)</td>
</tr>
<tr>
<td>Venous Vascular Invasion</td>
<td>No Images</td>
<td>479 (96)</td>
<td>54 (90)</td>
</tr>
<tr>
<td></td>
<td>Images</td>
<td>20 (4)</td>
<td>6 (10)</td>
</tr>
<tr>
<td>Sentinel Lymph Node Biopsy</td>
<td>Without</td>
<td>261 (52.3)</td>
<td>51 (85)</td>
</tr>
<tr>
<td></td>
<td>With</td>
<td>238 (47.7)</td>
<td>9 (15)</td>
</tr>
<tr>
<td>Estrogen Receptor</td>
<td>Negative</td>
<td>51 (11.8)</td>
<td>15 (29.4)</td>
</tr>
<tr>
<td>Expression</td>
<td>Positive</td>
<td>380 (88.2)</td>
<td>36 (70.6)</td>
</tr>
<tr>
<td>Progesteron Receptor</td>
<td>Negative</td>
<td>91 (22.3)</td>
<td>23 (45.1)</td>
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<tr>
<td>Expression</td>
<td>Positive</td>
<td>317 (77.7)</td>
<td>28 (54.9)</td>
</tr>
<tr>
<td>Triple</td>
<td>No</td>
<td>418 (97.4)</td>
<td>41 (80.4)</td>
</tr>
<tr>
<td></td>
<td>Yes</td>
<td>11 (2.6)</td>
<td>10 (19.6)</td>
</tr>
<tr>
<td>Tumor Grade</td>
<td>G1</td>
<td>162 (35.1)</td>
<td>6 (12)</td>
</tr>
<tr>
<td></td>
<td>G2</td>
<td>203 (43.9)</td>
<td>21 (42)</td>
</tr>
<tr>
<td></td>
<td>G3</td>
<td>95 (20.6)</td>
<td>23 (46)</td>
</tr>
<tr>
<td></td>
<td>Gx</td>
<td>2 (0.4)</td>
<td>0 (0)</td>
</tr>
<tr>
<td>Size of primary tumor</td>
<td>T1</td>
<td>248 (50.7)</td>
<td>16 (29.1)</td>
</tr>
<tr>
<td></td>
<td>T2</td>
<td>181 (37.0)</td>
<td>23 (41.8)</td>
</tr>
<tr>
<td></td>
<td>T3</td>
<td>17 (3.5)</td>
<td>6 (10.9)</td>
</tr>
<tr>
<td></td>
<td>T4</td>
<td>13 (2.7)</td>
<td>5 (9.1)</td>
</tr>
<tr>
<td></td>
<td>Tis</td>
<td>26 (5.3)</td>
<td>2 (3.6)</td>
</tr>
<tr>
<td></td>
<td>Tx</td>
<td>4 (0.8)</td>
<td>3 (5.5)</td>
</tr>
<tr>
<td>Spread</td>
<td>N0</td>
<td>252 (52.1)</td>
<td>17 (30.9)</td>
</tr>
<tr>
<td></td>
<td>N1</td>
<td>144 (29.8)</td>
<td>18 (32.7)</td>
</tr>
<tr>
<td></td>
<td>N2</td>
<td>37 (7.6)</td>
<td>8 (14.5)</td>
</tr>
<tr>
<td></td>
<td>N3</td>
<td>24 (5.0)</td>
<td>9 (16.4)</td>
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<td></td>
<td>Nx</td>
<td>27 (5.6)</td>
<td>3 (5.5)</td>
</tr>
<tr>
<td>Hormonotherapy</td>
<td>Without</td>
<td>48 (9.8)</td>
<td>15 (28.3)</td>
</tr>
<tr>
<td></td>
<td>With</td>
<td>440 (90.2)</td>
<td>38 (71.1)</td>
</tr>
<tr>
<td>Age at Diagnosis</td>
<td>[15-44]</td>
<td>65 (13.0)</td>
<td>18 (30.0)</td>
</tr>
<tr>
<td></td>
<td>[44-54]</td>
<td>132 (26.5)</td>
<td>13 (21.7)</td>
</tr>
<tr>
<td></td>
<td>[54-64]</td>
<td>120 (24.0)</td>
<td>12 (20.0)</td>
</tr>
<tr>
<td></td>
<td>[64-74]</td>
<td>84 (16.8)</td>
<td>6 (10.0)</td>
</tr>
<tr>
<td></td>
<td>&gt;74</td>
<td>98 (19.6)</td>
<td>11 (18.3)</td>
</tr>
<tr>
<td>Lymph Invasion</td>
<td>No Images</td>
<td>414 (83)</td>
<td>47 (78.3)</td>
</tr>
<tr>
<td></td>
<td>Images</td>
<td>85 (17)</td>
<td>13 (21.7)</td>
</tr>
</tbody>
</table>

Table 2. Distribution of explanatory variables with significant effect on the survival of patients by vital status and percentages of missing values
A total of 14 variables turned out to have significant differences in their categories survival curves (Table 3).

<table>
<thead>
<tr>
<th>Variable</th>
<th>p-value</th>
<th>Variable</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tumor Stage</td>
<td>&lt; 0.001</td>
<td>Triple Negative</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>Neoadjuvant treatment</td>
<td>&lt; 0.001</td>
<td>Tumor Grade</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>Venous vascular invasion</td>
<td>&lt; 0.001</td>
<td>Spread lymph nodes</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>Biopsy of sentinel lymph node</td>
<td>0.02</td>
<td>Hormonotherapy</td>
<td>&lt; 0.001</td>
</tr>
<tr>
<td>Type of surgery</td>
<td>&lt; 0.001</td>
<td>Age at diagnosis categorized</td>
<td>0.017</td>
</tr>
<tr>
<td>Estrogen receptor expression</td>
<td>&lt; 0.001</td>
<td>Images of lymph invasion</td>
<td>0.04</td>
</tr>
<tr>
<td>Progesterone receptor Expression</td>
<td>&lt; 0.001</td>
<td>Size of primary tumor</td>
<td>0.005</td>
</tr>
</tbody>
</table>

Table 3. P-values obtained from Log-rank test for variables with significant effect on the survival of patients

As Dawson et al [4] explain triple negative breast cancers (TNBC) are defined by the absence of estrogen, progesterone and HER2 expression. Although the prognostic significance of triple negative tumours remains unclear we decided to create a binary variable to indicate the cases with TNBC and the ones with non TNBC. It turns out, that there’s a significant difference on the survival rates as shown in Figure 3 and confirmed in the log rank test results (Table 3), being, as expected the TNBC the ones with lower survival rate. Although age at diagnose treated as a continuous variable it was not statistically significant in terms of survival, the result was not the same when categorized into two categories: patients younger than 44 years and patients older than 44. As we verified that the lower category (younger women) has a lower survival probably than the other category, and this difference is statistically significant (Table 3). Cianfrocca and Goldstein [2] point out, many studies evaluating the influence of age on outcome in breast cancer had conflicting results but two relatively large trials have, also, demonstrated a worse prognosis for patients younger than 35 years of age, even after adjustment for other prognostic factors. It is important to clarify that we categorized age at diagnosis as it is done in studies reported by North Region Cancer Registry of Portugal (RORENO) [11], as shown in Figure 3. We then were able to group categories that were not statistically different in terms of survival.

Cianfrocca and Goldstein [2] explain that tumour grade, specifically the grading system adopted by Braga’s Hospital - the Bloom-Richardson classifica-
tion -, does have prognostic significance and is primarily used to make decisions for lymph node-negative patients with borderline tumour sizes. And, also, a higher grade is related to a higher risk of recurrence. Our results, as shown in Figure 3, confirms that there is significant difference between the survival rate of the three grade categories (G1, G2 and G3). The survival rate of patients with tumour grade G3 is lower comparing to the other two categories, and the cases with tumour diagnosed in grade G1 have a higher survival rate.

The staging system adopted is the one proposed by the America Joint Committee on Cancer (AJCC), and stage categories are in a scale of 0 to IV. Actually, it groups into categories several tumour characteristics such as tumour size, ganglion situation and metastasis situation. All three pointed out by several authors [5][7][10], as important prognostic factors.

Our results, as shown in Figure 3, confirms that there’s no significant difference between the survival rate between the first three categories (0, I and II), and also between the last two categories (III and IV). Hence we were able to group the first three categories into only one category (0/I/II) and to group the two last categories into one (III/IV). The results suggest that the cases diagnosed in stage III or IV have lower probability of survival compared to tumours in stage 0, I or II, for these patients.

After the multivariate analysis, as already mentioned, with the saturate model, we ended up with a zero knots FRPM with the four, described covariates, with highly significant effect on the survival of these patients. Table 4 compares the estimates obtained (and respective 95% confident intervals) when adjusting to the FRPM with the ones obtained when adjusting to the CPHM. As we can see, the estimates values are identical for both models, and confirms the results pointed out above.

Fig. 2. Kaplan Meier curves for variables Triple Negative and Age at Diagnosis.
Note that, we did not considered the variables related to any kind of treatment, as treatment decisions by the medical team are made upon tumour characteristics (such as, for example, size, staging, grade). This would result into a strong correlation between treatment type of variables and variables related to tumour characteristics.

As expected, the hazard of dying from breast cancer is significantly higher in women with triple negative breast cancer (HR = 7.10). Also it seems that the hazard ratio for the ones younger than 44 years at the time of diagnose is higher (HR = 0.41). The risk of dying from breast cancer is 3.94 times higher for the cases with tumour stage III or IV compared to cases with tumour on stage 0, I or II. Also, the risk of dying from a tumour with G2 type of grade is 3.86 times higher than G1 type grade of tumour, and the risk increases for the ones with G3 type of grade (HR = 5.75).

![Kaplan Meier estimates by Tumour Grade](image1)

![Kaplan Meier Estimates by Stage categories](image2)

**Fig. 3.** Kaplan Meier curves for variables *Tumour Grade* and *Tumour Stage*.

<table>
<thead>
<tr>
<th>Covariates</th>
<th>Parmar-Royston Model</th>
<th>Cox Model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HR 95% CI</td>
<td>HR 95% CI</td>
</tr>
<tr>
<td>Triple Negative</td>
<td>7.10 [2.80; 17.99]</td>
<td>8.07 [3.27; 19.96]</td>
</tr>
<tr>
<td>Age at diagnosis (≤ 44)</td>
<td>0.41 [0.22; 0.78]</td>
<td>0.39 [0.20; 0.73]</td>
</tr>
<tr>
<td>Tumour Stage (III/IV)</td>
<td>3.94 [2.13; 7.24]</td>
<td>3.89 [2.09; 7.25]</td>
</tr>
<tr>
<td>Tumor Grade (G2)</td>
<td>3.86 [0.96; 15.33]</td>
<td>4.51 [1.04; 19.47]</td>
</tr>
<tr>
<td>Tumor Grade (G3)</td>
<td>5.75 [1.38; 24.05]</td>
<td>6.14 [1.37; 27.65]</td>
</tr>
</tbody>
</table>

**Table 4.** Hazard Ratios for each significant effect covariates for baseline combination: Without Recurrence; Without Neoadjuvant Treatment; No surgery; Non Triple Negative.
In order to graphically assess how well FRPM fits the data, and its estimates are identical to those obtained in the CPHM, Figure 4 presents the plot of the Kaplan Meier estimates, the FRPM and the CPHM for a subject with following characteristics: non triple negative; age at diagnosis < 44, tumor stage III/IV and tumor grade G2.

Note that, as Royston and Parmar [12] explain, by convention the zero knot model means that no internal and no boundary knots are specified and so, the baseline distribution is no other but the Weibull.

![Kaplan-Meier vs Cox Model vs Flexible Parametric Model](image)

**Fig. 4.** Cox Proportional Hazards Curve versus Kaplan Meier curve versus Flexible Royston-Parmar Survival Curve for Combination of covariates: Non Triple Negative; Age at diagnosis < 44, Tumor Stage III/IV and Tumor Grade G2.

As shown in Table 5, the proportional hazards assumption for these variables was not violated.

<table>
<thead>
<tr>
<th>Variables</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Triple Negative</td>
<td>0.38851</td>
</tr>
<tr>
<td>Age at diagnosis (≤ 44)</td>
<td>0.06215</td>
</tr>
<tr>
<td>Tumour Stage (III/IV)</td>
<td>0.57214</td>
</tr>
<tr>
<td>Tumour Grade (G2)</td>
<td>0.17272</td>
</tr>
<tr>
<td>Tumor Grade (G3)</td>
<td>0.42385</td>
</tr>
</tbody>
</table>

**Table 5.** P-values obtained from testing the proportional hazards assumption.
4 Discussion

Although many of 50 variables obtained are recognized as potential prognostic factors only four are shown to have a statistically significant effect on survival of the 540 patients of the Unity of Senology of Braga Hospital when adjusted to other prognostic factors, namely: triple negative (yes vs no); age at diagnosis (>44 vs ≤44); tumor stage (0/I/II vs III/IV) and tumor grade (G1 vs G2 vs G3). The resulting adjusted FRPM, with 0 knots, reveals that the patients with triple negative type of tumor, younger than 44 years at diagnose, with tumor in stage III or IV and grade G3, are the ones with higher risk of dying from breast cancer.

To compare the results obtained with previous studies we calculated the survival rate at 1, 3 and 5 years for the adjusted FRPM for the combination of variable values: Non Triple Negative; Age at diagnosis ≤44, Tumor Stage III or IV and Tumor Grade G2. Table 6 presents these results and the last results reported by the North Region Cancer Registry of Portugal (RORENO) [11] for the districts of North of Portugal and also for Bragas district itself, which points out to an improvement of the survival rate for the Unity of Senology of Bragas Hospital.

Further work includes an analysis of risk factors for recurrence for these patients and also longitudinal analysis of tumor markers such as Carcinoma Antigen 15-3 (CA 15.3) and the Carcinoembryonic antigen (CEA).

<table>
<thead>
<tr>
<th>Years after diagnosis</th>
<th>Braga’s Hospital FPM</th>
<th>Braga’s Hospital Cox PH</th>
<th>RORENO North of Portugal 2000/2001</th>
<th>RORENO Braga 2000/2001</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 year</td>
<td>99.2%</td>
<td>98.3%</td>
<td>97%</td>
<td>97%</td>
</tr>
<tr>
<td>3 years</td>
<td>94.2%</td>
<td>93.4%</td>
<td>89%</td>
<td>90%</td>
</tr>
<tr>
<td>5 years</td>
<td>84.9%</td>
<td>87.6%</td>
<td>83%</td>
<td>84%</td>
</tr>
<tr>
<td>Number of cases</td>
<td>540</td>
<td>2320</td>
<td>470</td>
<td></td>
</tr>
</tbody>
</table>

Table 6. Relative Survival (%) for breast tumors for the North Districts of Portugal and for Braga’s district of residence.

References


Demography: only quantity or quality as well?

Grigori Brekhman, Rivka Yahav, Yuli Volchkov

Interdisciplinary Clinical Center, Faculty of Social Welfare and Health Studies, University of Haifa, Israel. Mazra Mental Health Medical Center, Acre, Israel

The analysts of the International Monetary Fund in their presentation to the UN reported with concern: in the last 60 years the population of Earth is increased not only due to the birth rate, but also due to the increase in life expectancy. They predict the collapse of the financial system, because of increased spending on pensions, treatment and care for the elderly, if this trend will continue to 2050\(^1\). The analysts, focusing their attention on the costs for retirees, did not discuss the huge costs for the people born now and those who will be born in future. However not the number of born children is a problem, but their quality - physical and mental because the new posterity already from the moment of birth requires significant resources of a society on them care, raising, and then - constant health and/or psychological service, and also costs of police, penitentiary systems, armies etc.

The purpose of presentation: to involve attention both the scientists and public to mental and physical health of the generation of people, which be born now in order to find ways to improvement of its quality from a position of modern knowledge.

1. The extragenital diseases of the pregnant women and health of born posterity. The statistical analysis of morbidity in the different countries shows, that a condition of health of the pregnant women, as a rule, bad. The diseases of circulatory, endocrine, urinary, immune and other systems in many women are finding. This means that children are born with a predisposition to diseases

of like systems and organs. These diseases are found out in childhood, they have propensity to chronic current and accompany the individual in his lifetime, periodically aggravated. They require constant treatment, they reduce both mood and work capacity of the man.

As an example we shall consider a problem of diabetes. It is known, that the children who born at parents with diabetes have a genetic predisposition to it, and/or to the disorders of carbohydrate metabolism. In subsequent the damages of various organs at them are formed that requires the help of the various specialists (ophthalmologist, nephrologist, hepatologist, and neurologist). How many children are born with such pathology? Let's address to statistics.

As of 2002 in the World about 120 millions man had the diabetes. On the data the WHO by 2012 in the world the diabetes type-1 was sick already about 366 millions the man. Annually the diabetes at 78 000 children are diagnosed. The disorders of carbohydrate metabolism at 2-3 of 100 pregnant women are found. On the data of United Nations Population Fund (UNFPA) each year in the world occurs approximately of 130 millions labor, that is the opportunity of birth annually 2 millions 600 thousand babies with obvious or latent diabetes. Approximately half of them are girls, future pregnant women - mothers with this pathology.

Another problem binding to above: Research showed the chronic kidney diseases (CKD) risk was 69% higher for children whose mothers had diabetes before pregnancy. The CKD risk was 28 percent higher for children whose mothers developed gestational diabetes, and children whose mothers were obese had only a 22 percent higher risk of CKD. It is known, that the disease the urinary system occupies one of conducting places in structure of an extragenital pathology of pregnant women: their frequency reaches 10-12%. On the most rough calculations from 130 million of laboring women approximately 13 million of them suffer by a

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2 http://www.idf.org/diabetesatlas/5e/the-global-burden
3 http://www.funtrivia.com/askft/Question75884.html
5 http://urotoday.ru/issue/4-2012/article/beremennost-i-imvp-taktika-urologa
pathology of kidneys and they can give birth per one year 11 million 700 thousand children with predisposition to diseases of urinary system. The researches carried out in Russia have shown that the frequency of diseases of urinary system changes depending on ecological conditions from 66 up to 187 on 1000 children\textsuperscript{6}. It is possible to assume, that the ecological situation promotes display of genetic predisposition at growing up generation to diseases of urinary system, which in subsequent render at them negative influence on their health, pregnancy and labor, and also can form predisposition to these diseases at the following generation.

We have mentioned only one pathology but it is known the women and men, including those who giving life to the following generation, have also other diseases.

2. Prematurity of pregnancy and immature children. Infants born with low weight face a number of serious health risks. The children born with low weight of a body have a high risk of a psychomotor and social retardation (Hediger et al 2002, Reichman 2005), and in case of mental and physical infantilism the imperfection of functioning of organs and systems is observed. It is considered as chronic diseases. Immature children have a high probability of inability to training at usual school, to have low IQ, and inability to study in high school (Reichman 2005. Jackson 2006). The risk of all this is increased with reduction of weight of a body and sizes of a skull (at microcephaly) (Stoler-Porias et al 2010). It is necessary also to mean, that children with low and extremely low weight of a body require long reanimation measures without reliance, that good mental and physical health of the born child will be saved. The survived children are injured by surrounding circumstances during reanimation and care. And it is saved in their unconscious, defining their thinking and behaviour in the future life.

How many children are born before term and with low weight? The birth of children with low weight (less than 2 kg) with 2006 on 2011 гг in the world is at a level 8.1 - 8.3% of all births\textsuperscript{7}.

\textsuperscript{6}http://nature.web.ru/db/msg.html?mid=1171062&uri=index.html
\textsuperscript{7}http://www.childtrendsdatabank.org/?q=node/67
It is approximately 10 million 906 thousand babies annually, and approximately half of immature children are girls. The researches which have been carried out in Canada (Boivin et al. 2012), have shown: in case of birth of the girls before or about 32 weeks of pregnancy at approach at them of pregnancy more often such complications appear: gestation diabetes (in 2.34 times), pregnancy hypertension (in 1.56 times), preeclampsia or eclampsia (in 1.79 times). By other words, prematurity is a risk of pathology of pregnancy and damage of the following generation. The children born with low weight bring the huge economic costs: on medical needs, on special education and social charges on service, and also they have the reduced efficiency in mature age.

3. The socio-economic conditions of life (famine, poverty), in which the pregnancy is passed promotes "the birth of children biologically distinct from those who was born under favorable circumstances" (Barker et al. 2001) even in case of birth of children in time. The heavy conditions of development after conception can create predisposition to diseases cardiovascular system (coronary heart disease, hypertension), which are shown in younger age, and people which have experienced the famine together with the mothers up to birth are more sensitive at occurrence of similar stressful situations (Barker 1995; Painter et al. 2006). It relates not only to the women from the poorly advanced countries, but also to the women of western countries, and in an equal measure having superfluous weight or low weight, as according to a modern style many women have a unbalanced diet and continue it to do after conception. And thus women involuntarily bring in this world of children with illnesses or with predisposition to various diseases inclined to chronic current.

4. Prenatal mental trauma and its consequences. From a beginning of XX century the prenatal and perinatal psychology began are developed. It scientific direction connected to study of mental life of the unborn child and influence of impressions perceived up to birth on his thinking and behavior in subsequent after birth of life. The researches have shown, that:
   • The unborn child (prenate) has emotional perception,
   • The unborn child has actively functioning memory,
• The memory of prenate includes events, most emotionally experienced together with the mother,
• At the child and adult the prebirth impressions of the man make their unconscious,
• These unconscious feelings can operate thinking, emotions and behaviour of the man after birth,
• The quiet condition of the mother during pregnancy promotes display of the depositions and talents received by a child with genes from the mother and the father.
• Distress of the pregnant mother can put irreparable damage to a unborn child, his health and development after birth, his destiny in future.

As the researches have shown prenatal mental trauma received by child through his mother becomes a source of various mental condition and disorders: fears, phobias, persuasive conditions, anxiety, panic, neurosis, sexual problems, and also psychosomatic disorders: asthma, megrim, neurodermitis, disorders of speech, stammering, pyloristenosis, enuresis, and such mental disorders as autism, syndrome ADHD, unipolar and bipolar disorder, psychomotor retardation, oth. They show themselves with various intensity in different terms of life after birth.

**Autism** is one of displays of a prenatal trauma. He is characterized by deviations in social interaction and dialogue, and also limited, repeating behaviour. All specified attributes occur in the age of till three years. The related conditions, at which softer attributes and symptoms are marked, carry to disorders of the autistic spectrum. The reasons of autism in many respects connect with genetic aberrations, which result to the prebirth infringement of development both cerebellum and brain as a whole. Last years the significance of emotional distress of a prenate experienced together with his mother has found. It is high meaningful stressors (death of the husband, loss of job, moving, other), which rendered their action in the period 21-32 weeks of pregnancy with peak at 25-28 of weeks (Beversdorf et al 2001).

The majority of the recent reviews converge that the level of autism prevalence makes 1-2 on 1000 man in a population and about 6 man on 1000 for disorders of the autistic spectrum, though
admits, that the real quantity can be even more. Unfortunately, a little of autists can live by high-grade life in a community (Howlin et al 2004, Tidmarsh et al 2003, Billstedt et al 2005). The majority of children with autism need the social support, steady relations with other people, prospects of career, feeling of self-determination (Burgess et al 2007). Some symptoms smooth out with age, the moderate improvements in communicative sphere are observed, but the basic problems remain, and at many number of mature autists the line of skills, unfortunately, even are worsened (Helt et al 2008).

**ADHD Syndrome** (Attention deficit hyperactivity disorder) also connect with prenatal stress (Van den Bergh a. Marcoen 2004). ADHD's global prevalence is estimated at 3-5% in people under the age of 19. Rates of ADHD diagnosis and treatment have increased in both the UK and the USA since the 1970s. In the UK an estimated 0.5 per 1,000 children had ADHD in the 1970s, while 3/1,000 in the late 1990s. In the USA in the 1970s 12 per 1,000 children had the diagnosis, while in the late 1990s 34/1,000 had the diagnosis and the numbers continue to increase\(^8\): in 1997 only in USA the syndrome ADHD had 3.3 million children (Polanczyk et al 2007). About half of children with ADHD becoming the adults still will have concentration problems and impulsivity, though the adults are more capable to supervise their behaviour and to mask difficulties.

**Depression** approximately twice more often is found out in the women, than at the men [Kuehner 2003 249]. Depression (major and minor) in the various periods of pregnancy and in the postnatal period comes to light with high frequency - from 6.5% up to 12.9% (Gavin et al., 2005, Le Strat 2011). It often promotes interruption of pregnancy: the frequency of premature labor exceeds 20% at the pregnant women with depression (Wisner et al 2009). The depressive condition of the pregnant woman renders influence even on still unborn child that can be found out already after his birth. Newborn children, born from the mothers with depression, had a low estimation on an Apgar scale and more often have required reanimation for their revival. They more often cried, [\(\text{http://www.nice.org.uk/nicemedia/pdf/CG72FullGuideline.pdf}\)](http://www.nice.org.uk/nicemedia/pdf/CG72FullGuideline.pdf)
and it was more difficult to console them. Than more expressed there was a depression at the mother then angrier were children. These children in subsequent were more inclined to smoking, use of alcohol and drugs. The scientists of the different countries support the idea about pathogenic role of maternal depression concerning occurrence of depression at born posterity (Bettes 1988; Zuckerman et al 1990, Ponirakis et al 1998; Hernandez-Reif et al., 2002, Verny 2002).

The relative increase of frequency of depression begins from pubertal period of development, and by 15-18 of years reaches the frequency, which is present at the adults. Prevalence of depression changes over a wide range, from 3% in Japan up to 17% in USA (Andrade et al 2003). As of 2010 depression suffered approximately 298 million the man (4,3 % from an aggregate number of the population of the Earth) (Vos, 2012). The depression (major and minor) is one of the basic reasons morbidity all over the world. (WHO 2001). It is important also that the depression during pregnancy and after labor often is not the isolated condition, and it is connected to a wide spectrum of accompanying mental disorders. On the data of researches in Germany 2000 - 2004 гг., in 53-61% of the persons suffering by depression, other psychiatric disorders also were observed: generalized anxiety disorder, panic attacks, agoraphobia and posttraumatic stressful disorders. They had in 11 times more days of invalidity, than non depressed patients. The total cost of expenses has increased by the patients with this pathology on the data of the American researchers from 16 billions dollars per 1986 up to 44 billions dollars in 1993.

The monoamine theory of development of depression was dominant until recently and according with it the disease is connected to deficiency in a brain the biogenic amines: serotonin, noradrenalin, and dopamine and the serotonin transporter (5-HTTLPR) polymorphism (Surtees et al. 2006), which ensure the communications between nervous cells. The newest researches have shown, that the deficiency can be caused by feature of a gene (5-HTT), carrier serotonin, and it reveal oneself in case of very stressful vital events for the person (Kuehner 2003). The researches carried out in Sweden have confirmed hereditability of
depression (Kendler et al 2006). The genetic roots of depression explain, why the depression is run in family and why the child gets propensity to depression from the conception, and suffer from it during lifetime, even after it would seem of insignificant stressful events, sometimes so insignificant, that occurrence of depression consider as a "spontaneous". Frequency of such depression, which consider as endogenic, i.e. without any external influences, is rather high (about 35 % of all cases) (Tiganov et al 1999).

The similar mechanisms of pathogenesis are found out not only at unipolar disorders, but also at bipolar affective disorders and even schizophrenia (Lake 1979; Benedetti 1983; Janus 2001; Brekhman et al, 2010).

Psychomotor retardation involves a slowing-down of thought and a reduction of physical movements in an individual, including speech and affect (Tryon 1991). Psychomotor impairment can accompany children with mental disorders mentioned above (major depression, bipolar disorder), and as the clinical researches have shown the prenatal stress itself can cause the motormental retardation of children (Maldonado-Duran et al 2000; O'Connor et al 2002; Huizink et al 2003). These researches were confirmed experimentally by scientists of Wisconsin - Madison University (USA), who have found that the disorders of psychomotor development were more expressed, if the influence of stressor occurred in early terms of pregnancy (Schneider et al 2005, 2008). Moreover, the scientists from Haifa University (Israel) in their experiments have shown that the stress exposure before conception results in to pathological social behaviour at born offspring (Shachar-Dadon et al 2009).

5. The unwanted pregnancy is the important factor of breaking quality of the born people. The prenatal psychologists have opened, that children, who born from unwanted pregnancies, have a line of psychological peculiarities that bring sufferings both to them and surrounding people. They experience the psychological discomfort, complex of inferiority which induces them to special, sociopathic, and sometimes even psychopathic behaviour. Specialists also have found in them different psychosomatic diseases or syndromes. More over, they have found a high frequency of aggression, violent behaviour and auto-
aggression among the people which have experienced the attempt of an abortion, and in subsequent, after birth, the rejection of them as a confirmation of their undesirability (David et al. 1988; Matejchek et al. 1994; Sonne 2005). These children require often the medical aid and psychological support, and their destructive behaviour can put serious damage to a society depending on the position in a society. Last example - the massacre in December 2012 at school of State Connecticut (USA), where psychopath has killed 26 men.

Whether it is a lot of undesirable pregnancy in the world? The data on quantity of abortions could give some representation about it. On the data of the experts the WHO in 2003 in the world more than 42 million of abortions have made. Frequency of abortions on the average on the world 31 abortions on 100 live births, highest frequency in East Europe - 105 abortions on 100 live births. On the data National Center for Health Statistics (USA) follows, that for 15 years (1973-1988) from all fixed labor 35% (5,8 million) were undesirable. Among these 30% of born children - were definitely unwanted, and 70% - were not planned, i.e. they have come to this world at the improper moment of time.

6. Birth and everything, that surrounds it, also can leave at unborn children injuring impressions. These impressions are result of a complex of influencing factors such as: increasing fears of the mothers in connection with approximation and beginning of labor, disorders of labor activity because of stress or other reasons, medical measures directed on regulation of pains, etc. The recent research in the USA showed the electronic fetal monitoring used at 93% of mothers; epidurals – at 63%; membranes ruptured - 55%; oxytocin to stimulate labor progress received 53%; episiotomies received 52% of mothers. The cesarean section often is a speedy way (at the woman's request or at the obstetrician's suggestion), its
frequency in different countries varies from 25 to 70%. The researches have shown, children, born by such way, in subsequent have various psychological and psychosomatic problem (Odent 2004). According to the statistical data in Russia in 2001 the number of natural labor (labor without any intervention) was on the average at 31,2% of the women, with limits of fluctuations in various regions from 10,8% up to 54,8%\(^\text{12}\). All these factors cause trauma both the mothers and the children that are transformed at them as the psychological and psychosomatic problems, which often requiring the psychiatric and psychotherapeutical help (Grof 1975, 1985; oth.).

**Discussion.** We showed the incomplete list of the factors influencing the unborn child during his intrauterine period of development when genetic program is realized. These occur not always correct because it includes some mutations that parents accumulated before the conception. The mutations continue pile up also during nine month of prenatal life together with mother. Adding to it prenate has opportunity to receive new information from outside, from social and ecological environment. This information can be constructive and destructive unfortunately. The constructive information promotes the positive development of prenate, which after birth manifests as talents of individual. The destructive information can partially to break the genetic program.

The researches in the field of prenatal and perinatal psychology have shown, that the mental trauma received before birth becomes a source various mental and psychosomatic disorders of the child after birth. The reason of his prenatal trauma is the emotional stress of prenate experienced together with the mother. She is stressed because her way of responding on psycho-traumatic situation connected with her psychological features, by her attitude to pregnancy and to the unborn child, by her attitude to environmental circumstances and people. The disputed situations arise at participation nearest (nuclear family, extended family) and of remote (school, job, religion, state) social surrounding. One of the most often influence is violence (mental and/or physical) – domestic, street, terror, war. The war causing stress in the mother

can put a serious mental trauma in the unborn child (DeMause 1996; Janus 2001, oth.).

Modern philosophy and technology of delivery, in fact, reflect the status of society with its accelerated rhythm of life, a pragmatic approach, psychological illiteracy and "emotional deafness." Today everything that surrounds the birth, even obstetricians called as "an obstetrical aggression" (Radzinsky 2011). The events during birth can also saved in prenate’s memory, and, as researches showed - in genetic memory. But even described here consequences of prenatal trauma are enough for the asserting that quality of the new generation is bad: it is burdened with illnesses and mental traumas, which prevent them normally to develop and function. The part from the saved experience is passed to the following generation, forming "vicious circle". How to stop process of traumatizing of the following generation of people?

What possible ways non-admission, elimination or even if easing of the influencing factors breaking health of born generation? We do not assume to give the final recommendations. We bring in our offers, meaning, that the subsequent discussion will allow finding optimum ways and mechanisms to make healthier the future generation of the people.

At the first stage it would be necessary: а) wide informing of the population on mental life of the child before his birth, about his emotional perception, and actively functioning memory, б) about influence of the information received up to birth on thinking and style of behaviour of the individual in the subsequent life, в) about prenatal and perinatal roots of mental and psychosomatic disorders of individuals, and at last г) about opportunities of preventive maintenance of prenatal and perinatal traumas.

**Conclusion.** The demography studies the quantitative characteristic of a given population\(^\text{13}\). However it is necessary to develop other party of this science - qualitative characteristic of a population in order to receive more volumetric picture of the social world. Now there is an expansion of people quota with the genetic caused diseases at the expense of birth of generation, which

\(^{13}\) http://en.wikipedia.org/wiki/Demographics
received the gene mutations from parents. Besides it, social and ecological environments create a high risk of reception of a mental trauma of the child even before his birth. In subsequent, in process of maturing, this is transformed and is manifested as mental and psychosomatic disorders, from which suffer both they and society. Many from them from the moment of birth require the constant medical and social help that demands significant expenses from public fund.

References


45. Sonne J. Abortion Survivors. In: Phenomenon of Violence (From domestic to global). View from the position of prenatal and perinatal psychology and medicine. Eds. Prof. G.

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A fuzzy regression model for non-convex fuzzy numbers: the \textit{crisp input - fuzzy output} case

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Abstract. In this contribution we propose a least square approach to fuzzy linear regression analysis for non-convex data which generalizes a previous proposal for convex data (see: D'Urso and Gastaldi[1], Coppi et al.[4]). A formal definition of non-convex fuzzy number is provided and a fuzzy linear regression model for this type of fuzzy data is introduced. We also applied our fuzzy regression model to a simulated dataset. Finally, some relevant comments about limitations, potential new applications, and extensions of this approach are presented.

Keywords: Fuzzy data analysis, fuzzy regression model, non-convex fuzzy data.

1 Introduction

There is now a vast literature about the conceptualization of fuzzy data and their data analysis modeling (such as regression analysis, cluster analysis, principal component analysis, etc). We can recognize two main approaches in the fuzzy data analysis literature. The first is based on a standard statistical framework (fuzzy information as crisp-data) with standard estimation methods (such as least squares, variance decomposition, etc. See: D’Urso and Gastaldi[1], Coppi et al.[4]). The second approach is more related to a non-standard data analysis framework which is directly based on Fuzzy Set Theory (FST) principles (for example: Tanaka et al.[6]). In general both approaches have placed more attention on a specific type of fuzzy data, namely \textit{convex fuzzy data} which are traditionally related to the definition of \textit{LR-convex fuzzy number} (Dubois and Prade[3]). Convex fuzzy data may be considered as the simplest representation for a fuzzy set as it can be easily described by using only a triplet of real numbers. However, in real empirical contexts observed data can easily show some degree of non-convexity (e.g., in cognitive ratings, object evaluations, fuzzy control systems, etc.) and, therefore, \textit{non-convex fuzzy data} are needed (Garibaldi and John[5]). In this paper we describe a method to perform analysis with this more complex type of fuzzy data.

2 Non-convex fuzzy number: a first proposal

To provide a self-contained exposition, the first part of the paper briefly recapitulates the main properties of a LR fuzzy-number together with some key concepts of fuzzy set theory.
2.1 Preliminary definitions

Let $U \subset \mathbb{R}$ and $\mu$ be a universal set and a function $\mu : U \to [0,1]$, respectively. A fuzzy set $\tilde{A}$ is a subset of $U$ having $\mu$ as its characteristic function. More precisely, $\tilde{A} = \{x, \mu_{\tilde{A}}(x)\}$, where $\mu_{\tilde{A}}$ informs us about the membership-degree of $x_i$ in $U$. Under the possibility theory framework $\mu_{\tilde{A}}$ can be understood as the degree of possibility that $x$ belongs to $\tilde{A}$. A fuzzy set can be described as a family of nested crisp subsets, called $\alpha$-sets, where a generic set is written as $\tilde{A}_\alpha = \{x \in U | \mu_{\tilde{A}}(x) \geq \alpha\}$. By using this definition, it is easy to describe some relevant features of a fuzzy set. In particular, the core of $\tilde{A}$ is defined as $\tilde{A}_\alpha = \{x \in U | \mu_{\tilde{A}}(x) = 1\}$, whereas its support is $\tilde{A}_\alpha = \{x \in U | \mu_{\tilde{A}}(x) \geq 0\}$. Another important feature is called the high of $\tilde{A}$: $\text{hgt}(\tilde{A}) = \max[\mu_{\tilde{A}}(x)]$ which informs us about the normality condition of the fuzzy set (if $\text{hgt}(\tilde{A}) = 1$, $\tilde{A}$ is considered 'normal' otherwise $\tilde{A}$ is called 'subnormal'). $\tilde{A}$ is a convex fuzzy set if the following property holds:

$$\forall a, b, c \in \tilde{A}_\alpha \geq 0 \quad | a \leq b \leq c : \quad \mu_{\tilde{A}}(b) \geq \min[\mu_{\tilde{A}}(a), \mu_{\tilde{A}}(c)]$$

or alternatively if its $\alpha$-cut is a compact and convex interval. Now, following Dubois and Prade [3] we can define several types of fuzzy numbers (e.g., triangular, trapezoidal, etc.). In particular, for the case of a triangular fuzzy set, if $\tilde{A}$ is (i) normal, (ii) convex, and (iii) $\tilde{A}$ has a unique core, then it is also a fuzzy number, say $\tilde{a}$, which can be described by two smooth functions:

$$L : \mathbb{R}^+ \to [0,1] \quad \text{and} \quad R : \mathbb{R}^+ \to [0,1]$$

called the shape functions of $\tilde{A}$:

$$L(v) \begin{cases} 
= 0 & \text{if } v = 1 \\
= 1 & \text{if } v = 0 \\
> 0 & \text{if } v < 1 \\
< 1 & \text{if } v > 0 
\end{cases} \quad R(v) \begin{cases} 
= 0 & \text{if } v = 1 \\
= 1 & \text{if } v = 0 \\
> 0 & \text{if } v < 1 \\
< 1 & \text{if } v > 0 
\end{cases} \quad \forall v \in \mathbb{R}^+$$

The membership function of $\tilde{a}$ is defined as follows:

$$\mu_{\tilde{a}}(x) = \begin{cases} 
L \left( \frac{m-x}{l} \right) & \text{if } x \leq m \\
R \left( \frac{x-m}{r} \right) & \text{if } x \geq m 
\end{cases}$$

where $m$ is the modal value (or the core), whereas $l$ and $r$ are the left and the right spread, respectively.1 The fuzzy number $\tilde{a}$ can be represented by a triple:

$$\tilde{a} = (m, l, r)_{LR}$$

defining the main information about a fuzzy data, namely, its precision (through the core or modal value $m$) and fuzziness (by means of $l$ and $r$). If we are able to represent the analytic expressions of $L$ and $R$ together with $m$, $l$ and $r$ we can exactly reconstruct the fuzzy number $\tilde{a}$. For a graphical representation of a convex fuzzy number see figure 1-a.

1 Note that: $l = (m - lb)$ and $r = (m + ub)$ where $ub$ is the upper-bound of the set $\tilde{A}$ and $lb$ is the lower-bound of the set $\tilde{A}$. 
2.2 Non-convex fuzzy numbers

Let $\tilde{B} = \{x, \mu_{\tilde{B}}(x)\}$ be a fuzzy set. We recall that $\tilde{B}$ can always be represented faithfully by its family of nested $\alpha$-sets as well as its core (or eventually several cores). If $\tilde{B}$ is a non-convex fuzzy set, Property 1 does not necessarily hold and must be replaced by a more general property satisfying the non-convexity condition as follows:

$$\forall a', b', c' \in \tilde{A}_{\alpha \geq 0} \mid a' \leq b' \leq c' : \mu_{\tilde{A}}(b') \leq \min \{\mu_{\tilde{A}}(a'), \mu_{\tilde{A}}(c')\}$$ (2)

We can define different types of non-convex fuzzy numbers, however, for the sake of simplicity in this first proposal, we decided to consider only a simple instance of non-convex fuzzy number. In particular, if $\tilde{B}$ is (i) normal, (ii) non-convex and (iii) $\tilde{B}$ has at least a core with membership function equal to one, then it can be called a type-2 non-convex fuzzy number, say $\tilde{b}$. By extending the previous definition of LR-fuzzy numbers, we can now define this new type of fuzzy number by using the following shape functions:

$$L : \mathbb{R}^+ \rightarrow [0, 1] \quad H : \mathbb{R}^+ \rightarrow [0, 1] \quad I : \mathbb{R}^+ \rightarrow [0, 1] \quad \text{and} \quad R : \mathbb{R}^+ \rightarrow [0, 1]$$

with properties

$$L(v) = \begin{cases} = 0 & \text{if } v = 1 \\ = t & \text{if } v = 0 \\ > 0 & \text{if } v < 1 \\ < t & \text{if } v > 0 \end{cases}$$

$$H(v) = \begin{cases} = t & \text{if } v = 1 \\ = k & \text{if } v = 0 \\ > k & \text{if } v < 1 \\ < t & \text{if } v > 0 \end{cases}$$

$$I(v) = \begin{cases} = k & \text{if } v = 1 \\ = t & \text{if } v = 0 \\ > k & \text{if } v < 1 \\ < t & \text{if } v > 0 \end{cases}$$

$$R(v) = \begin{cases} = 0 & \text{if } v = 1 \\ = t & \text{if } v = 0 \\ > 0 & \text{if } v < 1 \\ < t & \text{if } v > 0 \end{cases}$$

Like for the convex fuzzy numbers, also the membership function of $\tilde{b}$ can be derived by the shape functions as follows:

$$\mu_{\tilde{b}}(x) = \begin{cases} L \left( \frac{x - m_1}{l} \right) & \text{if } x \leq m_1 \\ H \left( \frac{x - m_0}{h} \right) & \text{if } m_1 \leq x \leq m_0 \\ I \left( \frac{x - m_2}{i} \right) & \text{if } m_0 \leq x \leq m_2 \\ R \left( \frac{x - m_2}{r} \right) & \text{if } x \geq m_2 \end{cases}$$

where $m_1$ and $m_2$ are the cores; $m_0$ is the median value carrying information about the non-convexity condition of $\tilde{B}$; $l$ and $r$ (resp. $h$ and $i$) are the external (resp. internal) left and right spreads. A type-2 non-convex fuzzy number can be represented as follows:

$$\tilde{b} = \{ (m_0, m_1, m_2, l, r, h, i); (\mu_{m_1}, \mu_{m_0}, \mu_{m_2}) \}_{LHIR}$$

---

\(^{2}\) Where $h = (m_0 - m_1)$ and $i = (m_0 + m_2)$. 
where $\mu_{m1}$, $\mu_{m0}$, $\mu_{m2}$ are the membership functions of the cores and the median point, respectively. When $L$, $H$, $I$ and $R$ as well as $m1$, $m0$, $m2$, $l$, $h$, $i$, $r$ and $\mu_{m1}$, $\mu_{m0}$, $\mu_{m2}$ are known we can reconstruct the exact non-convex fuzzy set on the basis of this set of information. Figure 1-b shows an example of type-2 non-convex fuzzy number.

![Type-2 Fuzzy Number](image)

**Fig. 1.** (a) Convex fuzzy number (triangular type) and (b) non-convex fuzzy number (type-2)

## 3 A fuzzy regression model for non-convex fuzzy numbers

Following the rationale adopted by [1] and [2] we can define a novel fuzzy regression model for non-convex fuzzy data.

### 3.1 Fuzzy Data

Let $X_{n \times k}$ and $\tilde{Y} = \{m_1, m_0, m_2, l, h, i, r\}$ be a matrix with $n$ cases and $k$ predictor variables (the crisp input matrix) and a fuzzy dependent variable, respectively. The components of $\tilde{Y}$ are $n \times 1$ vectors.

### 3.2 Model definition

In order to manage information related to non-convex fuzzy numbers we need to define a hierarchical model based on two independent components (sub-models). The first sub-model represents the support of the fuzzy dependent variable. The second sub-model characterizes the membership function values of the cores of the fuzzy dependent variable. Notice, however, that this rationale is absent in the case of regression with convex fuzzy data. In particular, in this

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3 We can adopt a similar rationale for the definition of a convex fuzzy number as follows: $\tilde{a} = \{(m, l, r); (\mu_m)\}_{LR}$. Because the core membership function of a convex fuzzy number is always equal to 1, we can omit the second part of the formula thus obtaining the standard notation $\tilde{a} = \{m, l, r\}$ for convex fuzzy numbers.
latter (and more simplified) context we can reconstruct the fuzzy representation by using the first sub-model only. The two sub-models can be defined as follows:

\[
\begin{align*}
    m_0^* &= Xa \\
    m_1^* &= m_0^*b + 1r_1 \\
    l^* &= m_1^*c + 1r_2 \\
    m_2^* &= m_0^*d + 1r_3 \\
    r^* &= m_2^*e + 1r_4
\end{align*}
\]

where \( X \) is a \((n \times k + 1)\) matrix (with a column of ones for the intercept), \( a \) and \( \alpha \) are \((k + 1 \times 1)\) vectors of regression coefficients, \( b, c, d, r_1, r_2, r_3, \beta, \gamma, \xi_1 \) and \( \xi_2 \) are scalars, \( 1 \) is a vector of all ones. The left-side of Equation (3) describes the model for the support whereas the right-side represents the model for the membership function. Notice that the first sub-model represents a hierarchical structure where the median point \( m_0^* \) generates the centers \( m_1^* \) and \( m_2^* \) and, subsequently, \( m_1^* \) and \( m_2^* \) generate their external spreads \( l^* \) and \( r^* \). In a similar way, in the second sub-model the membership value for the median point \( \mu_{m_0}^* \) generates the other two points \( \mu_{m_1}^* \) and \( \mu_{m_2}^* \). In this way our model is able to take into account possible relations between the median point and the centers as well as the relationships between the centers and the spreads. By contrast, the components \( h^* \) and \( i^* \) can be indirectly derived by the other estimated components (see note 2). It is worthwhile noticing that both models work in parallel and in an independent fashion. However, if one has not got information about eventual relationships between the cores and the support of the fuzzy set, then it is always possible to modify the model in order to take into account this additional prior details in the estimation process. Because our proposal is mainly exploratory, in this paper we will limit our attention to the independent case only.

### 3.3 Parameters estimation: unconstrained version

The goal of the estimation procedure is to look for the best parameter estimates for \( a, b, c, d, r_1, r_2, r_3, \alpha, \beta, \gamma, \xi_1, \xi_2 \). The first sub-model estimation procedure is based on the minimization of the following weighted dissimilarity measure:

\[
\| m_0 - m_0^* \|^2 \omega_1 + \| m_1 - m_1^* \|^2 \omega_2 + \| m_2 - m_2^* \|^2 \omega_3 + \| l - l^* \|^2 \omega_4 + \| r - r^* \|^2 \omega_5 
\]

where \( \omega_1, \ldots, \omega_5 \) are positive weights for the external spreads, the median point and the centers. Next, by computing its partial derivatives and setting up them to zero, we obtain the following analytic solutions:

\[
\hat{a} = \frac{1}{k} (X^TX)^{-1} X^T [m_0\omega_1 + (m_1 - 1r_1)bw_2 + (m_2 - 1r_3)e\omega_3 + (l - 1r_2)cb\omega_4 + (r - 1r_4)cd\omega_5] 
\]

\[
\mu_{m_0}^* = X\alpha \\
\mu_{m_1}^* = \mu_{m_0}^*\beta + 1\xi_1 \\
\mu_{m_2}^* = \mu_{m_0}^*\gamma + 1\xi_2 
\]

If we are not interested in investigating these relationships we can still set up a model with estimated components which are only related with the crisp input matrix.
\[
\hat{b} = \frac{1}{(\omega_2 + c^2\omega_4)} (a^T X^T X a)^{-1} a^T X^T [(m_1 - 1r_1)\omega_2 + (l - 1r_2)c\omega_4]
\] (6)

\[
\hat{c} = \frac{1}{b^2} (a^T X^T X a)^{-1} a^T X^T (l - 1r_2)b
\] (7)

\[
\hat{r}_1 = \frac{1}{n} (1^T m_1 - a^T X^T 1b) \quad \hat{r}_2 = \frac{1}{n} (1^T l - a^T X^T 1bc)
\] (8)

\[
\hat{e} = \frac{1}{(\omega_3 + d^2\omega_5)} (a^T X^T X a)^{-1} a^T X^T [(m_2 - 1r_3)\omega_3 + (r - 1r_4)d\omega_5]
\] (9)

\[
\hat{d} = \frac{1}{c^2} (a^T X^T X a)^{-1} a^T X^T (r - 1r_4)e
\] (10)

\[
\hat{r}_3 = \frac{1}{n} (1^T m_2 - a^T X^T 1c) \quad \hat{r}_4 = \frac{1}{n} (1^T r - a^T X^T 1de)
\] (11)

Note that \(k = \frac{1}{(\omega_1 + b^2\omega_2 + c^2\omega_4 + d^2\omega_5)} \). The above solutions can be used to provide the best estimates for the model parameters via an iterative algorithm. Similarly, for the second submodel we look for the best parameters’ values to minimize the following dissimilarity measure:

\[
\|\vec{\mu}_m - \vec{\mu}_m^*\|^2\omega_1 + \|\vec{\mu}_m - \vec{\mu}_m^*\|^2\omega_2 + \|\vec{\mu}_m - \vec{\mu}_m^*\|^2\omega_3
\] (12)

with solutions:

\[
\hat{\alpha} = \frac{1}{(\omega_1 + \beta^2\omega_2 + \gamma^2\omega_3)} (X^T X)^{-1} X^T [\mu_m + (\mu_m - 1\xi_1)\beta\omega_2 + (\mu_m - 1\xi_2)\gamma\omega_3]
\] (13)

\[
\hat{\beta} = (\alpha^T X^T X \alpha)^{-1} \alpha^T X^T (\mu_m - 1\xi_1)
\] (14)

\[
\hat{\gamma} = (\alpha^T X^T X \alpha)^{-1} \alpha^T X^T (\mu_m - 1\xi_2)
\] (15)

\[
\hat{\xi}_1 = \frac{1}{n} (\alpha^T X^T 1\beta - 1^T \mu_m) \quad \hat{\xi}_2 = \frac{1}{n} (\alpha^T X^T 1\gamma - 1^T \mu_m)
\] (16)

and finally we apply an iterative algorithm to obtain the best parameter estimates for our data.

### 3.4 Properties of the model

The model satisfies some useful properties: i) the sums of residuals for the components are zero, ii) the estimation components and the proper residuals are uncorrelated and iii) the residuals among the components are uncorrelated. These properties allow us to place our method within the general family of least squares method of estimation. In particular, because the variance decomposition lemma holds for our model, the standard \(R^2\) goodness of fit index can be nicely used. However, due to space limitation we preferred to omit the analytic evidences from this short contribution.
4 Application

Suppose we are interested in studying the relation between economic resources (in million) and perceived life satisfaction (rating scale). Table 1 and Table 2 report the data set together with the best parameters’ estimates and the reconstructed data, respectively. We can provide a substantive interpretation for the results reported in the two tables. In particular, perceived life satisfaction increased by increasing levels of economic resources ($\hat{a} = 1.76$). Similarly for the fuzziness measure, the external spreads moderately increased their values by increasing levels of economic resources ($\hat{d} = 0.26$ and $\hat{c} = 0.38$).

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Table 1. Illustrative example: original dataset and parameters estimation for the model

The goodness-of-fit was excellent for the first submodel ($R^2 = 0.97$) and fairly good for the second submodel ($R^2 = 0.60$). In sum, economic resources seem to increase perceived life satisfaction although this evidence is related to an increase of uncertainty.

5 Conclusion

In this paper we have presented a novel fuzzy linear regression model for non-convex fuzzy numbers. To keep the dimension of the parameter space to a reasonable size we set up a regression model based on a generative hypothesis for the model parameters. The algorithm developed for the unconstrained model adopted an iterative procedure with a stopping criteria based on the minimum changes property whereas the starting criteria were based on a random initialization procedure. In order to evaluate the convergence stability of the algorithm, is a good rule to try several starting points. However, it is important to note that our model could not be able to fit highly perturbed data. To
this end it would be better to adopt a modified regression model with a more sophisticated optimization procedure (e.g., non-linear programming) capable to consider also the natural constraints of the model (namely \( m_1^* \leq m_0^* \leq m_2^* \) and \( l^* \geq 0_n \), \( r^* \geq 0_n \) for the first model while \( \mu_{m_1}^* \leq \mu_{m_0}^* \leq \mu_{m_2}^* \) for the second model). We are currently working on this line and future results will be presented in a forthcoming publication.

References

Stochastic models for the chemostat

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Abstract. The evolution of the state of a single species/single substrate chemostat is usually described by a set of ordinary differential equations (ODE) derived from a mass balance principle. In this case, the modeling process relies on the fact that the stochastic effects can be neglected thanks to the law of large numbers. This is possible only at macroscopic scale, for high population sizes, and under homogeneity conditions. At all other scales or when the homogeneity conditions are not met, random effects cannot be neglected. Our goal is to establish a set of stochastic models that are valid at different scales: from the small population scale to the scale immediately preceding the one corresponding to the deterministic model. At a microscopic scale we present a pure jump stochastic model that gives rise, at the macroscopic scale, to the ordinary differential equation model. At an intermediate scale, an approximation diffusion allows us to propose a model in the form of a system of stochastic differential equations. The convergence of the pure jump model or of the diffusion approximation to the deterministic model can be rigorously established. We expound the mechanism to switch from one model to another, together with the associated simulation procedures. Three associated simulation algorithms that will be valid at different scales are presented. We also describe the domain of validity of the different models. The pure jump model can be exactly simulated thanks to the Gillespie algorithm, also called stochastic simulation algorithm. In standard cases, that is for high population levels, this procedure is not feasible as it requires us to simulate too many events. In this case, we present the Poisson approximation and the normal approximation, both in discrete-time.
A comparison of artificial neural networks to forecast nitrogen dioxide concentrations

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Abstract. A comparison of artificial neural network models is presented to forecast hourly nitrogen dioxide concentrations 24 hours in advance, from local pollutant concentrations, traffic, meteorological data, and periodic components (sine and cosine terms for the daily and weekly cycles). The methods applied are: feed-forward multilayer perceptron networks, radial basis function networks and generalized regression networks. Bootstrap estimates of standard errors of model evaluation criteria are calculated. The radial basis approach provides the most accurate forecasts.

Keywords: Neural networks, Bootstrap, Air quality prediction.

1 Introduction

Air pollution may cause pernicious effects on human health, and is a widespread problem in the world. There are many air pollution indicators affecting human health. One of the important indicators is nitrogen dioxide (NO₂). How to monitor and predict the air quality indicators has become a problem in the environmental management (WHO [12]). Modelling variations in pollutants concentrations is useful when evaluating the effectiveness of plans and regulations to reduce pollutant emissions.

There is nowadays a considerable challenge to air quality forecasting. Tools to forecast pollution levels can be used in two different ways. 3-dimensional air quality models can be applied to integrate chemistry, transport and dispersion. This approach is time-consuming and requires very large databases to initialize and run the model. As the complexity of a problem increases, the theoretical understanding decreases (due to ill-defined interactions between systems) and statistical approaches are required. Statistical models generally directly connect meteorological conditions to level of pollutants. The autoregressive models are often used to analyze the seasonality, trend and autocorrelation of the pollutant variability (Box et al. [1], Prada-Sanchez et al. [8]), but they are limited by the weakness of the modeling of non-linear temporal variations. Regression models and automatic classification with the classification and regression tree (CART) have also been applied to model pollutant variability (Ryan [9], Gardner and Dorling [3]). The possible presence of chaotic dynamics in pollutant concentrations allows the performing of non-linear time series modeling (Kocak et al.[7]).
Neural networks have been shown to be effective alternatives to more traditional statistical techniques (Shalkoff [10]). The neural network models can be trained to approximate virtually any smooth, measurable function (Hornik et al. [5]). Unlike other statistical techniques the neural network models make no prior assumptions concerning the data distribution. They can model highly non-linear functions and can be trained to accurately generalize when presented with new, unseen data (Bishop [2]). These features of neural networks make them an attractive alternative to developing numerical models, and also when choosing between statistical approaches.

During the last decade the use of neural networks, and in particular the multilayer perceptron, has been developed to forecast pollutant concentrations. Ibarra-Berastegi et al. [6] focused on the prediction of hourly levels up to 8 h ahead for five pollutants using the multilayer perceptron. Caselli et al. [4] compared feedforward neural networks and multivariate regression models to predict critical pollution events. The objective of this work is to investigate the forecasting capability of the following methods: feed-forward multilayer perceptron networks, radial basis function networks and generalized regression networks. A time series of nitrogen dioxide (NO$_2$) concentrations is used as an example.

2 Data set and method

The study area is in Valencia (Spain), which has around 1 million inhabitants. It is a typical Mediterranean city in terms of its urban structure and climatology. Air pollution in Valencia mainly derives from motor vehicle emissions. In this work we consider the prediction of hourly NO$_2$ concentrations (expressed in µg/m$^3$). Previous studies in this city have shown a significant connection between a 10 µg/m$^3$ increase in NO$_2$ level and asthma, measured as a relative risk of emergency visits (Tenias et al. [11]). Other works have reported that daily levels of NO$_2$ in Valencia are associated with cardiovascular admissions. For monitoring and control purposes an automatic air pollution network is operated in the whole urban area by the local government. The network design and monitoring criteria follow the Air Quality Framework Directive and subsequent Daughter Directives (1996/62/EC, 1999/30/EC and 2000/60/EC). The network is subject to quality assurance and quality control procedures, which ensure the reliability of data.

Hourly pollutant and meteorological observations are available in one background monitoring station: P.Silla. The P.Silla station site is a roadside site located a few meters from a motorway. The meteorological variables are: wind direction (degrees), wind speed (m/s), temperature (°C), relative humidity (%), pressure (mbar) and solar radiation (W/m$^2$). In this site there are traffic data available (hourly number of vehicles).

The period analyzed is 1st January 2003-31st December 2005. The hourly means of NO$_2$ have not exceeded at P.Silla during the study period, neither the limit value nor the alert threshold set by the European Council Directive 1999/30/EC.
However the limit value of this pollutant for the protection of human health in a calendar year has been exceeded in 2003, 2004 and 2005. The highest annual NO$_2$ mean was observed in 2003.

In this work, an application of artificial neural network models is presented to predict hourly NO$_2$ concentrations 24 hours in advance, from local pollutants concentrations, traffic, meteorological data, and periodic components (sine and cosine terms for the daily and weekly cycles). The predictions produced by three different methods are compared: feed-forward multilayer perceptron networks (MLP), radial basis function (RBF) networks and generalized regression (GR) networks. The number of neurons in the hidden layer for the MLP networks is the optimum found by experimentation, and the transfer functions selected are the sigmoid and the hyperbolic tangent for the hidden layer, and linear for the output layer. The MLP model is applied using the Levenberg-Marquard (LM) and the scaled conjugate gradient learning (SCGL) algorithms. The spread parameter for RBF and GR networks are also found by experimentation.

The output of the models is NO$_2$ prediction 24 hours in advance. The inputs are nitrogen monoxide (NO) concentrations, traffic and meteorological data, and periodic components (sine and cosine terms for the daily and weekly cycles). The models are trained on data from 2003. Data from 2004 are used as the validation set and observations from 2005 are the test data set. The model evaluation criteria are the mean absolute error (MAE), the root mean square error (RMSE), the mean absolute percentage error (MAPE) and the correlation coefficient ($r$) between the pollutant observations and the predictions. Bootstrap estimates of standard errors of these criteria are calculated. These estimates were obtained by randomly resampling the test data 1000 times, with replacement.

### 3 Results

As an example of the distribution of the performance criteria observed by bootstrapping the test data set, Figure 1 shows the histogram of the RMSE values of the predictions obtained with the MLP network. The MLP network was applied with the sigmoid transfer function for the hidden layer and the scaled conjugate gradient algorithm. The shape of the RMSE histogram is asymmetric and therefore, the median of the 1000 bootstrap resamples will also be used to characterize the performance of the model. A similar result is obtained with the other performance criteria and methods (asymmetric distributions).

Figure 2 represents the RMSE observed for the RBF and GR networks as a function of the spread. Experimentation was used to select the value of the parameter for the neural network models. Table 1 shows the medians and means of the performance statistics of the trained networks when used to predict pollutant concentrations for 2005. The standard deviations of the means are given in brackets.
**Fig. 1.** Histogram of RMSE values obtained by bootstrapping with the MLP (sigmoid transfer function and SCGL algorithm)

**Fig. 2.** RMSE as a function of spread using a) RBF networks b) GR networks
The application of a RBF network to the test data gave the best results according to all the indicators. Table 1 also contains the 2.5% and 95.5% percentiles of the performance criteria obtained by bootstrapping. This method gives the smallest values of mean absolute error, root mean square error and mean absolute percentage error, and the highest value of the correlation coefficient.

The MLP network with the sigmoid transfer function for the hidden layer and the scale conjugate gradient learning algorithm, performed slightly better than the other MLP network models.

Table 1. Medians and means of the criteria results. Standard error of the mean in brackets.

<table>
<thead>
<tr>
<th>Model</th>
<th>MAE</th>
<th>RMSE</th>
<th>MAPE</th>
<th>r</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLP Logsig</td>
<td>Median=18,53, Mean=18,72</td>
<td>Median=22,70, Mean=22,94</td>
<td>Median=0,48, Mean=0,49</td>
<td>Median=0,57, Mean=0,55</td>
</tr>
<tr>
<td>SCGL</td>
<td>(0,04)</td>
<td>(0,04)</td>
<td>(0,001)</td>
<td>(0,002)</td>
</tr>
<tr>
<td>P2.5% = 16,83</td>
<td>P2.5% = 20,83</td>
<td>P2.5% = 0,44</td>
<td>P2.5% = 0,56</td>
<td></td>
</tr>
<tr>
<td>P97.5% = 21,61</td>
<td>P97.5% = 26,24</td>
<td>P97.5% = 0,56</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MLP Tansig</td>
<td>Median=17,69, Mean=17,81</td>
<td>Median=21,81, Mean=21,93</td>
<td>Median=0,46, Mean=0,46</td>
<td>Median=0,61, Mean=0,59</td>
</tr>
<tr>
<td>SCGL</td>
<td>(0,02)</td>
<td>(0,03)</td>
<td>(6,5 10^-5)</td>
<td>(0,001)</td>
</tr>
<tr>
<td>P2.5% = 16,59</td>
<td>P2.5% = 20,57</td>
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</tr>
<tr>
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<td>P97.5% = 24,24</td>
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</tr>
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<td>MLP Logsig</td>
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<td>Median=21,45, Mean=21,65</td>
<td>Median=0,45, Mean=0,45</td>
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<tr>
<td>LM</td>
<td>(0,16)</td>
<td>(0,17)</td>
<td>(6,5 10^-4)</td>
<td>(9,5 10^-7)</td>
</tr>
<tr>
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<td>P2.5% = 0,57</td>
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</tr>
<tr>
<td>P97.5% = 18,56</td>
<td>P97.5% = 22,84</td>
<td>P97.5% = 0,57</td>
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<td></td>
</tr>
<tr>
<td>MLP Tansig</td>
<td>Median=17,35, Mean=17,38</td>
<td>Median=21,50, Mean=21,54</td>
<td>Median=0,45, Mean=0,45</td>
<td>Median=0,63, Mean=0,62</td>
</tr>
<tr>
<td>LM</td>
<td>(0,05)</td>
<td>(0,06)</td>
<td>(0,001)</td>
<td>(0,001)</td>
</tr>
<tr>
<td>P2.5% = 15,99</td>
<td>P2.5% = 19,93</td>
<td>P2.5% = 0,42</td>
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<td>P97.5% = 18,66</td>
<td>P97.5% = 22,93</td>
<td>P97.5% = 0,58</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RBF</td>
<td>Median=15,50, Mean=15,65</td>
<td>Median=19,92, Mean=20,09</td>
<td>Median=0,36, Mean=0,36</td>
<td>Median=0,64, Mean=0,64</td>
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<tr>
<td>(0,03)</td>
<td>(0,04)</td>
<td>(8,7 10^-3)</td>
<td>(3,7 10^-3)</td>
<td></td>
</tr>
<tr>
<td>P2.5% = 14,25</td>
<td>P2.5% = 18,16</td>
<td>P2.5% = 0,34</td>
<td>P2.5% = 0,62</td>
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</tr>
<tr>
<td>P97.5% = 17,86</td>
<td>P97.5% = 23,04</td>
<td>P97.5% = 0,62</td>
<td></td>
<td></td>
</tr>
<tr>
<td>GG</td>
<td>Median=16,07, Mean=16,07</td>
<td>Median=20,83, Mean=20,73</td>
<td>Median=0,37, Mean=0,37</td>
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</tr>
<tr>
<td>(0,03)</td>
<td>(0,05)</td>
<td>(7 10^-4)</td>
<td>(2,8 10^-4)</td>
<td></td>
</tr>
<tr>
<td>P2.5% = 14,56</td>
<td>P2.5% = 18,46</td>
<td>P2.5% = 0,35</td>
<td>P2.5% = 0,62</td>
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<tr>
<td>P97.5% = 17,96</td>
<td>P97.5% = 23,17</td>
<td>P97.5% = 0,62</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 3 shows the time series plot of the first NO₂ observations of the test data set (1st January- 10th April year 2005) and the predictions obtained with the RBF network.

![Figure 3. NO₂ predictions using the radial basis function network.](image)

**Conclusions**

The aim of this research is to develop a predictive model to forecast hourly pollutant values 24 hours in advance in the urban area of Valencia (Spain). Air quality forecasting is an adequate method to plan a health warning system. The neural network models have become an alternative to conventional methods, because the relationship between air pollutants and meteorology is complex and extremely non-linear. They are an important instrument to model air pollution distribution. In the last decade the feedforward multilayer perceptron networks have been applied to analyze different pollutant levels. In this work a comparison of this method with other neural network models is developed. The study is based on data obtained at an official monitoring station in the city of Valencia, in an area with high traffic density.
The results showed that good forecast estimates of air quality can be achieved by applying neural networks methods to the prediction of time series of NO$_2$ concentrations. As the signal studied shows periodicity, a reasonable estimate can be recovered by using periodic components as estimators. Meteorological, traffic and nitrogen monoxide observations are also used as input variables to the models. The relative importance of meteorological and vehicle emission variable son the surface pollutant prediction is of great interest to establish the legislative measures that permit to reduce the pollutant levels.

The parameters of the models were chosen by experimentation, to optimize the values of several criteria. The forecasting capability of the models was evaluated using the mean absolute error, the root mean square error, the mean absolute percentage error and the correlation coefficient between the pollutant observations and the predictions. Bootstrap was applied to analyze the distribution of these criteria, by randomly resampling the test data 1000 times with replacement. The radial basis function networks performed better than the other models, giving satisfactory result for the prediction of pollutant 24 h in advance. The developed model is a potential tool for predicting air quality parameters inside the city, making the proposed forecaster a powerful tool for pollution management systems. The study involves the following inherent limitations. We model pollutant concentrations at one specific spatial location in Valencia. The city is situated in a fairly flat terrain. The input variables and the architecture of the neural network models may be different in other geographic regions.

References


A Novel Pointer-Encoding Genetic Programming Algorithm for Classification Problems

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Abstract. This paper presents a novel Genetic Programming (GP) algorithm to solve classification problems. The proposed GP includes a novel encoding of trees in the form of pointers, defined over a matrix structure, with several levels (rows). The advantages of this novel encoding is that it allows defining trees of any deep, in a simple way, and it is robust and compact, perfect to apply crossover operators in a straightforward manner. The proposed encoding also allows a very fast evaluation of subtrees, which is of interests in different applications. We have tested this novel GP in several classification problems, obtaining important advantages versus the classical GP and different classes of neural networks.

Keywords: Genetic Programming, Encoding, Classification problems.

1 Introduction

Genetic programming (GP) is one of the methods in the broad field of Genetic and Evolutionary Computation. GP is able to automatically create a computer program which solves a complex problem by using the evolution paradigm and the survival of the fittest concept. The research in the area of Genetic Programming (GP) took off in the early 1990’s, mainly driven by the key publication of J.R. Koza [1]. Today, there are dozens of excellent books on GP and its numerous and varied applications [2]-[7].

The basic steps that define the way GP works are:

1. Randomly create an initial population of programs from the available primitives—the set of allowed functions, variables and constants.
2. Repeat
3. Run each program and compute its fitness (a numerical measure of how well it solves the problem).
4. Select, with a probability based on such fitness, one or two program(s) from the population to participate in genetic operations.
5. Create new candidate program(s) by applying genetic operators with specified probabilities.
6. until an suitable solution is found or some other stopping condition is achieved.
7. Return the best-so-far program for solving the considered problem.
Among others, a key distinguishing feature of GP is that programs are usually represented by using syntax trees rather than as lines of code. The direct-tree encoding of individuals in GP has different disadvantages, such as complicated initializing procedures and operators or the necessity to establish a maximum depth in trees in order to avoid overtraining. Thus, in the last few years, different GP encodings have been investigated, some of them producing good and robust GP approaches. Some examples are the Binary Genetic Programming [8], the British Telecom Genetic Programming [9] or the Cartesian Genetic Programming [10]. All these alternative GP methods exploit a genotype-phenotype mapping, and particularly the effect of this mapping in evolutionary dynamics. A genotype-phenotype mapping is a non-linear function between the encoding of a solution in the algorithm (chromosome), and the solution upon which a fitness value is calculated (a final syntax tree in this case).

In this paper we propose a novel Genetic Programming algorithm, that also exploits a genotype-phenotype mapping. We have called Pointer Genetic Programming (PGP), and it is based on a compact encoding using a matrix, and on an easy decoding algorithm. In the paper, we detail the encoding and decoding procedures, and some characteristics of the algorithm. We test its performance in several regression and classification problems.

The remainder of the work has been structured as follows: next Section details the PGP algorithm proposed, its characteristics and peculiarities. Section 3 shows the performance of the proposed PGP in different regression and classification problems. Section 4 closes the paper by giving some final remarks.

2 Pointer-based Genetic Programming

The proposed PGP algorithm is based on a completely new encoding, shown in Figure 1. A four-levels (rows) matrix is used, in such a way that the first level (row), includes inputs (may not include all the available inputs, and can be repeated, as in the figure). The second level includes weights that will be used to modify the inputs in the first level. The third level is reserved for functions and the last level (fourth row in this case), is the pointers level. Figure 1 also shows the final tree graph obtained, after the decoding of the matrix.

The decoding algorithm is robust and easy, and it is mainly based on the pointers in the last level of the matrix. In a first step, the weights of the second level are multiplied by the inputs in the first level, and included in a memory, as shown in the initialization step of Figure 2. Then, the first decoding step is taken: starting from the leftmost column of the encoding matrix, the corresponding element in the memory is related to another one given by the pointer in level 4, using the function given by level 3. As an example, in this case, the function given by level 3 is a +, and the pointer in level 4 is the number 2, this means that the leftmost element in the memory is related to the element 2 positions to the right, by means of the function +, as can be seen in the figure, producing \( S_1 \) element of the tree. The decoding procedure continuous by the next element, in this case the function is a \( \times \), and the pointer is also the number 2. The result is shown in the step 2 of Figure 2, and produces the element \( S_2 \).
Fig. 1. Example of PGP encoding (genotype and phenotype (tree) are shown).

of the tree. Finally, the step 3 in this example produces \( S_3 \) element of the tree graph, by means of relating \( S_1 \) and \( S_2 \).

Several points have to be taken into account:

- In the last column of the matrix, levels 3 and 4 are always void (no pointer is allowed there, since it is the final element of the matrix).
- A maximum offset \( \phi \) is defined in the algorithm, so elements in the pointers levels cannot be larger than \( \phi \). In the example of Figure 2, \( \phi = 2 \).
- No pointer can aim at positions larger than the maximum number of columns in the matrix. A correction mechanism must be included to ensure this point.

In the PGP, the final result given by the tree is stored in the memory after the decoding process. Note, however, that other subtrees also keep stored in the memory after the decoding. We therefore can evaluate the remaining subtrees in the decoding memory in such a way that, if any of these subtrees obtains a better result than the complete tree, the subtree is used instead of the complete tree. Note that not all subtrees can be evaluated at the end of the decoding process, but only the ones remaining in the decoding memory after the last pointer operation.

2.1 Evolutionary operators

One of the main advantages of using a compact genotype for GP instead of the classical syntax tree encoding, is that the evolutionary operators of the algorithm can be simplified, and in many cases, standard operators can be used. In this case, we apply a selection mechanism based on the well-known tournament procedure, as is described in [11]. The crossover operator used is as follows: first, two individuals (matrices) are paired at random. A binary template, of the same length than the encoding matrix, is randomly generated. Then, the columns of both individuals are interchanged if there is a 1 in the corresponding position of the binary template (columns coinciding with a 0 in the template are not modified). The mutation operator is applied to each level independently. In this operator, we mutate one element of each level, randomly chosen. This process consists of substituting it by an alternative element for the
Decoding algorithm

<table>
<thead>
<tr>
<th>Initialization</th>
<th>Memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.2</td>
</tr>
<tr>
<td>+</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Step 1

<table>
<thead>
<tr>
<th>Initialization</th>
<th>Memory</th>
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</thead>
<tbody>
<tr>
<td>0.1</td>
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<tr>
<td>+</td>
<td>x</td>
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<tr>
<td>2</td>
<td>2</td>
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</tbody>
</table>

Step 2

<table>
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<th>Memory</th>
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</thead>
<tbody>
<tr>
<td>0.1</td>
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<tr>
<td>+</td>
<td>x</td>
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<tr>
<td>2</td>
<td>2</td>
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</tbody>
</table>

Step 3

<table>
<thead>
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<th>Memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
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</tr>
<tr>
<td>+</td>
<td>x</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

Fig. 2. Example of the decoding algorithm in the PGP (pass from genotype to phenotype).

corresponding level (input, weight, function or pointer), randomly generated. Note that the weights (level 2) are a special case, since they are continuous variables. In this case we use a Gaussian noise to modify each weight when necessary.
3 Experiments and results

3.1 Experiments in UCI classification problems

Several data sets from the well-known repository UC-Irvine Machine Learning Repository (UCI) and a simple artificial data set (named data2D) are used [12]. A description of the sets and their number of input vectors and features are shown in Table 1.

<table>
<thead>
<tr>
<th>Dataset</th>
<th># Input Vectors</th>
<th># Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data2D</td>
<td>105</td>
<td>2</td>
</tr>
<tr>
<td>BreastCancer</td>
<td>683</td>
<td>10</td>
</tr>
<tr>
<td>German</td>
<td>1000</td>
<td>20</td>
</tr>
<tr>
<td>Australian</td>
<td>690</td>
<td>14</td>
</tr>
<tr>
<td>Diabetes</td>
<td>768</td>
<td>8</td>
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<tr>
<td>Ionosphere</td>
<td>351</td>
<td>33</td>
</tr>
</tbody>
</table>

Taking into account the whole set of input vectors, 30 permutations of the original data sets have been randomly generated in order to carry out a cross validation procedure. Thus, we divide each permutation into train and test sets by using the 80% and 20% of the data respectively. Finally, by using the information contained in the training set, we re-scale all features to zero mean and variance one.

Table 2 shows the results obtained by the PGP, compared to different alternative classifiers. The results of the PGP are significant, obtaining excellent classification rates, comparable to the best existing algorithms in the literature.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Classical GP</th>
<th>k-NN (k=20)</th>
<th>MLP</th>
<th>PGP</th>
</tr>
</thead>
<tbody>
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<td>data2D</td>
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<td>0.8619</td>
<td>0.8714</td>
<td>0.8698</td>
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<tr>
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<td>0.9596</td>
</tr>
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<td>0.7247</td>
<td>0.7282</td>
</tr>
<tr>
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<td>0.8582</td>
<td>0.8413</td>
<td>0.8541</td>
</tr>
<tr>
<td>Diabetes</td>
<td>0.6502</td>
<td>0.7444</td>
<td>0.7446</td>
<td>0.7535</td>
</tr>
<tr>
<td>Ionosphere</td>
<td>0.7342</td>
<td>0.8263</td>
<td>0.9056</td>
<td>0.8667</td>
</tr>
</tbody>
</table>
3.2 A year-ahead claims prediction in insurance automobile companies

The second classification problem tackled in this paper consists of classifying the policies of an insurance automobile company according to the prediction of their claims for the next year. For this purpose, we use for a set of risk factors obtained from one database of an important Spanish insurance company. Specifically, a set of 5500 labelled samples is available, each defined by 13 features: vehicle type, use given (private or public), vehicle power, weight, number of places, vehicle age, vehicle type of fuel, driver age, number of years with driver licence, driver gender, region of use (in Spain) and bonus malus (according to driver claim history), and their corresponding label (1 for claim and 0 for no-claim in the next year). The database contains 48.13% labelled as “claims” and 51.87% samples labelled as “no-claim”, so it is almost balanced. The problem consists of classifying the samples in claim/no-claim in the most accurately possible way, based on the known examples of the database. For this, a partition of the whole sample is carried out, in such a way that we have 4400 for training (80%) and 1100 for testing (20%). All the results are calculated in the test set of 1100 samples.

Table 3 shows a comparison of the results achieved by a classical GP and the proposed PGP. Note that the PGP obtains the best result in terms of correct classification rate, outperforming the classical GP approach.

<table>
<thead>
<tr>
<th></th>
<th>Classical GP</th>
<th>PGP</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>62.1%</td>
<td>68.3%</td>
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</tbody>
</table>

4 Conclusions

In this paper we have presented a new model of Genetic Programming, called Pointer Genetic Programming (PGP). The PGP is based on a novel genotype-phenotype mapping, in which the genotype is a matrix, where each row represents a given level of GP components (inputs, weights, functions and pointers). The decoding algorithm to obtain the phenotype (tree graph) is based on offsets (pointers) given in the last row of the encoding matrix. In this paper we have detailed the encoding, the decoding algorithm and several results in different classification problems, where the PGP obtains significant results.

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References

SOME FILTERING TECHNIQUES FOR DATA ASSIMILATION IN A PLANT GROWTH MODEL

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Abstract. Data assimilation techniques have received considerable attention due to their capability to improve prediction and the most important applications concern weather forecasting and hydrology. Among many competing data assimilation approaches, those based on sequential Monte Carlo (SMC) methods, known as “particle filters”, have gained their popularity because they are adaptive to nonlinearity and non-Gaussianity. In this study we test the performance of three filtering techniques to predict biomass production and allocation in a dynamically evolving plant-growth model that can be formalized as a nonlinear state-space model. The first method concerns an extension of a post-regularized particle filter (Musso and Oudjane[19]), called Convolution Particle Filter (CPF) (Campillo and Rossi[3]) and the other two methods concern two extensions of the classic Kalman filter, such as the Unscented Kalman Filter (UKF) and the Ensemble Kalman Filter (EnKF), which are particularly adapted for nonlinear systems. All three filtering techniques deal simultaneously in their state vector fixed model parameters and state variables in a Bayesian way.

In the proposed data assimilation approach, all these algorithms are firstly applied iteratively to a first dataset to calibrate the model parameters. In the following prediction step, the CPF algorithm is carried out based on a new dataset with only few available observations. This assimilation step corresponds to a second calibration based on these early stage data. The final estimations provided by the three algorithms are used as predictive distributions and their performance and limitations are compared and discussed based on real data from the sugar-beet. Our estimation and prediction results suggest that these methods cope well with realistic scenarios with sparse observations.

Keywords: plant growth model, data assimilation, sequential Monte-Carlo methods, Kalman filter, kernel based method, stochastic EM algorithms, sugar-beet.

1 Introduction

The parametrization and the predictive capacity of plant growth models are considered to be complex and critical issues. Indeed, measurements are often limited and unevenly distributed over time and the models are usually built based on simplified assumptions and principles which inevitably lead to imperfectly defined parameters. In order to handle these difficulties, sequential data assimilation techniques, especially the Bayesian filtering methods have received considerable attention, not only for the possibility to reconstruct the system by estimating simultaneously model parameters and state variables but also
for their capability to identify the sources of uncertainties in order to improve prediction accuracy and to reduce the corresponding confidence intervals.

In a Bayesian framework, the filtering methods provide distributional estimates instead of point estimates as most of the frequentist methods do, so while using a historical batch of data to fit the system, the filtering methods could take into account the variation of model parameters over time. This feature corresponds exactly to the need of the prediction problem in the context of plant growth models, since it allows us to evaluate the uncertainty related to the estimated parameters of the model and to assess properly the uncertainties stemming from other sources in order to preserve them during the data assimilation step. However, the most desired feature still remains to be the capacity of predicting nonlinear growth behaviors, for example, occasionally occurred skewness due to sudden or unusual climate changes.

When dealing with linear systems, the most efficient filtering method is the Kalman filter (Kalman[14]). To date, many efforts have been made to develop extensions of the Kalman filter for nonlinear systems. The most well known are the extended Kalman filter (EKF) (Evensen[10]), the unscented Kalman filter (UKF) (Julier and Uhlmann[12], Quach et al.[21]) and the ensemble Kalman filter (EnKF) (Evensen[10]). The EKF simply linearizes locally the model so that the traditional Kalman filter can be applied. However, in the case that the nonlinearity is significant, it may cause divergence and the method proves to be no longer reliable. On the other hand, the UKF adopts deterministic sampling aiming at using a small set of discretely sampled points, known as sigma-points (Julier et al.[13], Wan and Van Der Merwe[22]), to get hold of the information of higher order for both the mean and the covariance matrix. The EnKF relies on normality assumptions in order to improve the accuracy of its estimates with a more important number of samples compared to the UKF. Both latter methods generalize elegantly to nonlinear systems which are free of the linearization required by the EKF.

Another important alternative is the Particle Filter (Gordon et al.[11], Kitagawa[15]), also known as Sequential Importance Sampling. Unlike the Kalman filter based methods, these Monte Carlo filtering methods intend to provide a better approximation of the exact posterior distributions by creating a set of randomly drawn samples with each an associated weight to represent the probability distribution of the hidden states and parameters conditioned on a series of observations. However, their main weakness is the potential degeneracy (Arulampalam et al.[1]) and impoverishment (Gordon et al.[11]). With the purpose of alleviating the undesirable side effect of resampling to improve the parametrization performance when facing restricted datasets, we opted for the Convolution Particle Filter (CPF) proposed by Campillo and Rossi[3] which extends the so-called post-Regularized Particle Filter (post-RPF) (Musso and Oudjane[19], Le Gland and Oudjane[16]).

In this paper, we aim to investigate the performance of the aforementioned filtering methods (UKF, EnKF, CPF) in the context of sequential data assimilation, when scarce observations describing plant growth are only available. We mostly focus on their abilities to provide reliable a priori estimates for data assimilation and prediction purposes. Experimental data are available from three
different years of sugar beet growth, obtained in comparable but different situations. One dataset is used for parameter estimation and the two others are used to test model prediction with data assimilation from early growth stages. The data are fitted with the LNAS model of sugar beet growth (Cournède et al. [9]).

In Section 2, the basic principles of the three filtering methods are recalled and their iterative version for parameter estimation is introduced. Section 3 contains a brief outline of the LNAS model and the experimental datasets, as well as the description of the calibration and assimilation procedures. The results that we obtained based on a real experimental dataset are presented in Section 4, together with a corresponding discussion. Finally, some conclusions are given in Section 5.

## 2 Methods

Plant growth models or crop models are generally deterministic and written in a state-space form. One can easily get their stochastic counterparts by introducing modeling and measurement noises. For both cases, the statistical framework of sequential data assimilation can be used to estimate the time evolving state variables, such as the yield. However, some difficulties arise in their implementation, not only from the presence of uneven and irregular measurement data, but also from sudden or unusual climate changes which occasionally induce skewness difficult to predict.

The proposed approach consists of three steps. In the first place, the least influential model parameters are screened using sensitivity analysis methods (Campolongo et al. [4]) and are thus fixed. Since, in general, no satisfactory distributions are available for the selected and thus most influential parameters, these are calibrated in the second step based on a given experimental dataset.

In this paper, the selected parameters are estimated in three different ways, resulting from three different filtering methods (UKF, EnKF, CPF). To obtain more precise estimates, the filtering process is iterated by taking the posterior distribution of iteration $k$ as prior distribution for iteration $k + 1$ until the convergence of all the estimates is achieved. For a theoretical justification of this approach when normal priors are used for the selected parameters see Chen et al. [8]. The modeling and measurement noises can thereafter be evaluated. Meanwhile, since the final distributions are influenced by the regularization effect and by the empirical estimation of the modeling and measurement noises, they therefore can no longer represent the uncertainty of the estimates. The uncertainty related to the unknown parameters is hence assessed by parametric bootstrap.

During the third assimilation phase, the CPF approach is implemented again with three different prior distributions provided by the three filtering methods used in the second (calibration) step. A new comparable experimental dataset with few measurements is introduced, so that a recalibration can be carried out. The probability density is represented by a great number of samples (particles) which evolve in time. Model parameters and state variables are adjusted and updated based on the available data of early growth stages.
The predictions are then calculated based on the forecasted values of all the particles.

In this section, the general state-space model framework is presented. The three filtering algorithms as well as their iterative version are thereby briefly described in order to provide an outline of the parameter estimation step.

### 2.1 General State-Space Models:

Let a general nonlinear dynamic system be described by the following discrete time equations:

\[
\begin{align*}
X(t + 1) &= f(X(t), \Theta, \eta(t), t) \\
Y(t) &= g(X(t), \Theta, \xi(t), t)
\end{align*}
\]  

(1)

\(X(t)\) represents the system state variable vector at time \(t\), \(f\) operates the propagation of the model states. \(\Theta\) is a vector of parameters of dimension \(p\) and \(\eta(t)\) is the modeling noise, corresponding to model imperfections or uncertainty in the model inputs. \(Y(t)\) is the noisy observation vector of the system which consists of state variables that can be observed experimentally and usually differ from \(X(t)\) (such as biomasses of some plant organs that can be measured while the daily biomass production cannot). \(g\) is the transition operator which links the observations to the system states by adding measurement noises, denoted by \(\xi(t)\). \((\eta(t))_t\) and \((\xi(t))_t\) are considered as sequences of independent and identically distributed random variables. Since experimental observations are usually limited due to high costs, observations are only available at irregular times. Let \((t_1, t_2, ... t_N)\) be the \(N\) measurement time steps. For all \(n \in [1; N]\), we set: \(X_n := X(t_n), Y_n := Y(t_n)\) and \(Y_{1:n} := (Y(t_1), Y(t_2), ..., Y(t_n))\).

The objective of the filtering methods is to estimate jointly the parameters and the hidden states of the dynamic system by processing the data online. An augmented state vector \(X_n^a = (X_n, \Theta_n)\) is thus defined with \(X_n\) the true hidden state at time \(t_n\) and \(\Theta_n\) the vector of unknown parameters. In the following, if \(X\) represents a random variable with values in \(\mathcal{X}\), then for all \(x \in \mathcal{X}\), \(p(x)\) will denote the probability density of \(X\) in \(x\). The first-order hidden Markov model is characterized by the transition density \(p(x_n^a | x_{n-1}^a)\) corresponding to the state equation, the observation density \(p(y_n | x_n^a)\) corresponding to the observation equation and the initial density \(p(x_0^a)\).

### 2.2 Convolution Particle Filter

Particle filter has been regarded as a standard technique for performing recursive nonlinear estimation (Arulampalam et al.[1]). However, since the discrete approximation of the filtering distribution may result in sample impoverishment, a regularization strategy was invented to transform the discrete approximation to a continuous one, this approach is thus named as Post-Regularized Particle Filter (Oudjane and Musso[20]). In the case that the analytic form of the observation density \(p(y_n | x_n)\) is unknown, an observation kernel can similarly be introduced (Campillo and Rossi[3]), the approach is thus called the Convolution Particle Filter.
In the initialization step, the particles are initialized from either informative distributions \( p(x_0^n) \) or non-informative distributions. Uniform weights are assigned to each particle. Only at time steps when the observation is available that the filtering process is carried out with two steps:

**Prediction:** A kernel estimator denoted by \( \hat{p}(x_{n+1}^a, y_{n+1} | y_{0:n}) \) is built. \( M \) particles \( \{\tilde{x}_n^a(i), i = 1, \ldots, M\} \) are sampled from the distribution with conditional density \( \hat{p}(x_{n+1}^a | y_{0:n}) \). The \( M \) particles are integrated forward in time by the evolution model until the next available measurement date to obtain the forecasted states \( \{\tilde{x}_{n+1}^a(i), i = 1, \ldots, M\} \). A weight is assigned to each particle based on the experimental measurements and the forecasted value. The empirical kernel approximation of the probability density of \( (X_{n+1}^a, Y_{n+1}) \) conditional to \( Y_{0:n} \) can thus be deduced using the Parzen-Rosenblatt kernel \( K_{X_M}^X \), with bandwidth parameter \( h_M^X \):

\[
\hat{p}(x_{n+1}^a, y_{n+1} | y_{0:n}) = \frac{1}{M} \sum_{i=1}^{M} K_{X_M}^X \left( x_{n+1}^a - \tilde{x}_{n+1}^a(i) \right) \times p(y_{n+1} | \tilde{x}_{n+1}^a(i)).
\]

**Correction:** The regularization is performed on the weighted samples, therefore the kernel approximation for \( p(x_{n+1}^a | y_{1:n+1}) \) can be expressed under the form:

\[
\hat{p}(x_{n+1}^a | y_{1:n+1}) = \frac{1}{\sum_{i=1}^{M} p(y_{n+1} | \tilde{x}_{n+1}^a(i))} \times \sum_{i=1}^{M} K_{X_M}^X \left( x_{n+1}^a - \tilde{x}_{n+1}^a(i) \right) p(y_{n+1} | \tilde{x}_{n+1}^a(i)).
\]

Where \( p(y_{n+1} | \tilde{x}_{n+1}^a(i)) / \sum_{i=1}^{M} p(y_{n+1} | \tilde{x}_{n+1}^a(i)) \) can be regarded as the normalized weight \( \tilde{w}_{n+1}^{(i)} \) associated to the particle \( \tilde{x}_{n+1}^a(i) \). In the case that the likelihood function cannot be compute, inspired by the Post-Regularized Particle Filter, a convolution kernel is introduced to regularize the likelihood of the observation.

### 2.3 Unscented Kalman Filter

The Unscented Kalman Filter is known as one of the nonlinear extensions of classical Kalman Filter. When \( f_n \) and \( g_n \) are no longer linear, the density \( p(x_{n+1}^a | y_{0:n}) \) doesn’t follow the normal distribution any more. Based on normal assumptions, an approximation is adopted by creating a series of sigma-points for nonlinear systems.

**Prediction:**
\[ d_\eta = \text{dim}(\eta_{n+1}), d_X = \text{dim}(\tilde{x}_n^a), d_{\eta,X} = d_\eta + d_X \]
\[ J_n \text{ and } R_n \text{ are the covariance matrix for } \eta_n \text{ and } \xi_n \text{ respectively} \]
Compute the \(2d_n \cdot x + 1\) sigma-points \(\chi^i_{n+1} \) and their weights \(\omega_i\) according to \(\mathcal{N}(\hat{x}^b_{n+1}, \hat{\Sigma}^{x^b}_{n+1})\), with

\[
\hat{x}^b_{n+1} = (\hat{x}^a_{n+1}, 0_{d_n}) \quad \text{and} \quad \hat{\Sigma}^{x^b}_{n+1} = \begin{pmatrix} \hat{\Sigma}^a_{n+1} & 0_{d_n \cdot d_n} \\ 0_{d_n \cdot d_n} & J_{n+1}^T \end{pmatrix}
\]

We propagate the sigma-points to obtain the expectation at time \(n + 1\):

\[
\hat{x}^a_{n+1|n} = \sum_{i=1}^{2d_n \cdot x + 1} \omega_i \chi^i_{n+1|n} \quad \text{and} \quad \hat{y}_{n+1|n} = \sum_{i=1}^{2d_n \cdot x + 1} \omega_i g_{n+1}(\chi^i_{n+1|n})
\]

The associated covariance matrix:

\[
\hat{\Sigma}^{x^a}_{n+1|n} = \sum_{i=1}^{2d_n \cdot x + 1} \omega_i (\chi^i_{n+1|n} - \hat{x}^a_{n+1|n})^T(\chi^i_{n+1|n} - \hat{x}^a_{n+1|n}), \quad (4)
\]

\[
\hat{\Sigma}^{y}_{n+1|n} = \sum_{i=1}^{2d_n \cdot x + 1} \omega_i (\chi^i_{n+1|n} - \hat{y}_{n+1|n})^T(\chi^i_{n+1|n} - \hat{y}_{n+1|n}). \quad (5)
\]

\[
\hat{\Sigma}^{x^a \cdot y}_{n+1|n} = \sum_{i=1}^{2d_n \cdot x + 1} \omega_i (\chi^i_{n+1|n} - \hat{x}^a_{n+1|n})^T(g_{n+1}(\chi^i_{n+1|n}) - \hat{y}_{n+1|n}). \quad (6)
\]

**Correction:**

Compute the Kalman gain:

\[
K_{n+1} = \hat{\Sigma}^{x^a \cdot y}_{n+1|n} \left(\hat{\Sigma}^{y}_{n+1|n}\right)^{-1}
\]

The corrected estimator and the corresponding covariance matrix at time \(n + 1\):

\[
\hat{x}^a_{n+1|n+1} = \hat{x}^a_{n+1|n} + K_{n+1}(\hat{y}_{n+1|n} - \hat{y}_{n+1|n})^T \quad (7)
\]

\[
\hat{\Sigma}^{x^a}_{n+1|n+1} = \hat{\Sigma}^{x^a}_{n+1|n} - K_{n+1} \hat{\Sigma}^{y}_{n+1|n} K_{n+1}^T. \quad (8)
\]

### 2.4 Ensemble Kalman Filter

The Ensemble Kalman Filter is another extension of Kalman filter designed for nonlinear systems. It’s established based on the Monte-Carlo method coupled with the Kalman formulation.

**Prediction:**

The expectation of \(X^a_{n+1|n}\) given \(Y_{0:n}\) can be obtained with the evolution equation:

\[
\hat{x}^a_{n+1|n} = E[X^a_{n+1|Y_{0:n}}] = E[f^a_{n+1}(X^a_{n}, \eta^a_{n+1})|Y_{0:n}].
\]

The covariance matrix associated to \(X^a_{n+1|n}\) given \(Y_{0:n}\) is:

\[
\hat{\Sigma}^{x^a}_{n+1|n} = E[(X^a_{n+1} - \hat{x}^a_{n+1|n})^T(X^a_{n+1} - \hat{x}^a_{n+1|n})|Y_{0:n}]. \quad (9)
\]
In the same way for \( p(y_{n+1}|y_{0:n}) \), we may obtain the corresponding expectation as following:

\[
\hat{y}_{n+1} = E[Y_{n+1}|Y_{0:n}] = E[g_{n+1}(X^a_{n+1}) + \xi_{n+1}|Y_{0:n}] = E[g_{n+1}(X^a_{n+1})|Y_{0:n}]
\]

and the associate covariance matrix can thus be calculated:

\[
\hat{\Sigma}^y_{n+1|n} = E[(Y_{n+1} - \hat{y}_{n+1|n})^T(Y_{n+1} - \hat{y}_{n+1|n})|Y_{0:n}] = E[(g_{n+1}(X^a_{n+1}) - \hat{g}_{n+1}(X^a_{n+1}) - \hat{\hat{y}}_{n+1|n}|Y_{0:n}) + R_{n+1}.
\]

The cross correlation matrix of \( X^a_{n+1} \) and \( Y_{n+1} \) given \( Y_{0:n} \) is also corrected as follows:

\[
\hat{\Sigma}^{x^a|y}_{n+1|n} = E[(X^a_{n+1} - \hat{x}^{a}_{n+1|n})^T(Y_{n+1} - \hat{y}_{n+1|n})|Y_{0:n}].
\]

Correction:
Computed in the same way as in the UKF approach.

2.5 Iterative Filtering and the Conditional Approach

In the case of off-line estimation with a finite number of observations, in order to determine the prior distributions for data assimilation, an iterative version of filtering (Chen et al.[6], [8]) can hence be applied. At iteration \( k \), the particles \( x^{(i)}_{0} \) are obtained as follows: the initial state vectors \( \tilde{x}^{(i)}_{0} = i = 1, \ldots, M \) are selected in the same way as for the classical filtering process (sampled from \( p(x_0) \)), and the vectors of unknown parameters \( \tilde{\Theta}^{(i)}_0 \) are sampled from the multivariate Gaussian distribution defined by the mean and covariance matrix of \( \tilde{\Theta}^{(i)}_{N} = i = 1, \ldots, M \) at iteration \( k - 1 \). An averaging technique (Cappé et al.[5]) is used to smooth parameter estimates after a small burn-in period.

In order to evaluate the modeling and the observation noises, a conditional maximization approach (Chen et al.[7]) is carried out to estimate the noise related parameters, denoted \( \Theta_2 \). Based on the results of the model parameter (denoted \( \Theta_1 \)) and state variable estimation performed by the iterative filtering processes, the noise parameters are therefore estimated empirically. The model and noise parameter estimation are alternated so as to provide coherent estimates of \( \Theta \).

3 Application

3.1 LNAS Model of Plant Growth

The equations are specifically derived for the sugar beet, per unit surface area, with two kinds of organ compartments taken into account: foliage and root system.

Biomass production: \( Q(t) \) is the biomass production on day \( t \) per unit surface area \( (g.m^{-2}) \) which can be obtained by generalizing the Beer-Lambert
law (Monteith[18]): \( (1 - e^{-\lambda Q_g(t)}) \) represents the fraction of intercepted radiation, with \( \lambda (g^{-1}.m^2) \) a parameter and \( Q_g(t) \) the total mass of green leaves on day \( t \) (in \( g.m^{-2} \)). The biomass production of the whole plant is then deduced by multiplying the total amount of absorbed photosynthetically active radiation per unit surface area (PAR, in \( MJ.m^{-2} \)) and an energetic efficiency \( \mu \) (in \( g \cdot MJ^{-1} \)):

\[
Q(t) = \left( \mu \cdot PAR(t) \left(1 - e^{-\lambda Q_g(t)} \right) \right) \cdot (1 + \eta_Q(t))
\]

with the modeling noise \( \eta_Q \sim \mathcal{N}(0, \sigma_Q^2) \).

**Allocation** for the foliage and root system compartments:

\[
Q_f(t+1) = Q_f(t) + \gamma(t) \cdot Q(t)
\]

\[
Q_r(t+1) = Q_r(t) + (1 - \gamma(t)) \cdot Q(t)
\]

where

\[
\gamma(t) = (\gamma_0 + (\gamma_f - \gamma_0) \cdot G_a(\tau(t))) \cdot (1 + \eta_\gamma(t))
\]

with \( \tau(t) \) the thermal time, which corresponds to the accumulated daily temperature since emergence day, \( G_a \) the cumulative distribution function of a log-normal law parameterized by its median \( \mu_a \) and standard deviation \( s_a \), and the modeling noise (process noise) denoted by \( \eta_\gamma(t) \sim \mathcal{N}(0, \sigma_\gamma^2) \).

**Senescence:** The senescent foliage mass \( Q_s \) is a proportion of the accumulated foliage mass given by the cumulative distribution of a log-normal law of median \( \mu_s \) and standard deviation \( s_s \):

\[
Q_s(t) = G_s(\tau(t) - \tau_{sen})Q_f(t)
\]

with \( \tau_{sen} \) the thermal time at which the senescence process initiates. The green foliage mass \( Q_g \) can then be obtained easily:

\[
Q_g(t) = Q_f(t) - Q_s(t)
\]

**Observations:** The observation variables potentially available from field measurements are:

\[
Y(t) = \begin{pmatrix}
Q_g(t) \cdot (1 + \epsilon_g(t)) \\
Q_r(t) \cdot (1 + \epsilon_r(t))
\end{pmatrix}
\]

with measurement noises: \( \epsilon_g(t) \sim \mathcal{N}(0, \sigma_g^2) \), and \( \epsilon_r(t) \sim \mathcal{N}(0, \sigma_r^2) \).

### 3.2 Experimental Data

The concerned datasets consist of limited experimental observations furnished by the French institute for Sugar Beet research (ITB, Paris, France) in 2006, 2008 and 2010 with different cultivars and measured in different locations (further experimental protocols details are presented in Lemaire et al.[17]). The 2010 dataset is chosen for calibration simply because it contains more observation points. Dry matter of root and leaves of 50 plants were collected at 14 dates:

\[
O_{2010} = \{54, 68, 76, 83, 90, 98, 104, 110, 118, 125, 132, 139, 145, 160\}.
\]
whilst for the assimilation and prediction step, the two other datasets (2006 and 2008) are used, with observation times given by

\[ O_{2006} = \{54, 59, 66, 88, 114, 142, 198\} , \]
\[ O_{2008} = \{39, 60, 67, 75, 88, 122, 158\} . \]

The final observations contain the mean values (over 50 plants) of the green foliage mass \( Q_g(t) \) and the root compartment mass \( Q_r(t) \) for all the available dates and extrapolated at \( m^2 \).

### 3.3 Three-step analysis for prediction

The prediction process is carried out in three steps as indicated in Fig. 1.

**Parameter Screening by Sensitivity Analysis:** Plant growth models contain frequently a large number of parameters which make parameter estimation from experimental data difficult and with a large amount of uncertainty linked to the estimates. With the purpose of selecting the most influential parameters to be estimated, sensitivity analysis is therefore applied. Those screened as the least influential parameters can be fixed to any values in their domains. This method is called “screening” or “factor fixing” (Campolongo *et al.*[4]).

To this purpose, we use the algorithm proposed by Wu *et al.*[23] to compute Sobol’s indices (first order and total order) of all the functional parameters (not related to modelling or observation noises), by using a generalized least-squares criteria.

As indicated by Fig. 2, we screen the parameters \( s_a, \mu_{sen}, s_{sen} \) and fix them to their mean values of the variation interval, as their total order indexes are all below 0.02 . For the five other parameters, their total order effects suggest that they should be estimated from experimental data.

**Parameter Estimation:** Based on the sensitivity analysis results, the unknown parameter vector for the deterministic part of the model is \( \Theta_1 = (\mu, \lambda, \mu_a, \gamma_0, \gamma_f) \) and the unknown noise parameter vector is \( \Theta_2 = (\sigma_Q, \sigma_{\gamma}, \sigma_g, \sigma_r) \). For the conditional ICPF approach, 150000 particles
Fig. 2. Comparison of the first and total order indexes for $\mu$, $\lambda$, $\gamma_0$, $\gamma_f$, $\mu_a$, $s_a$, $\mu_{sen}$ and $s_{sen}$.

were initialized with the same prior distributions as for the conditional IEnKF and IUKF approach. For the conditional IEnKF approach, an ensemble size of 400 is adopted. For all the three approaches, the conditional estimation process began with the estimation of $\Theta_1$ given $\Theta_2$, then $\Theta_2$ was estimated empirically based on the estimates of the hidden states. The estimation then proceeded with the new value of $\Theta_2$ and iterated. The convergence of both $\Theta_1$ and $\Theta_2$ was claimed by a standard stopping rule based on the relative changes in the estimations during three successive estimations (Booth and Hobert[2]). A parametric bootstrap was also implemented to evaluate the estimates’ uncertainty. Standard deviations and confidence intervals were hence obtained from 100 bootstrap samples. The corresponding results are given in Table 1.

Data Assimilation with CPF: As a first attempt, we propose to use the CPF algorithm to perform the assimilation step. Since in the calibration step, all of the three filtering methods ICPF, IUKF and IEnKF are applied to the LNAS model which allow us to estimate jointly the unknown parameters and the hidden state variables based on a historical batch of data (2010 dataset), the quality of the predictions obtained in the assimilation step is therefore only dependent on the parameter estimation performance of the three algorithms presented in the calibration step.

The parametric bootstrap results provided by the three filtering methods were used as prior information of the CPF method in this assimilation step. 500000 particles were simulated for the prediction purpose. For both the 2006 and 2008 datasets, all but the last two measurements were used to update the parameter and state estimates, that is until day 114 for the 2006 dataset, and until day 88 for the 2008 dataset. The propagation of particles continued without any further correction. The simulated values of the state variables $Q_g$ and $Q_r$ on day 142 and 198 (resp. day 122 and 158 for the 2008 dataset) of all the particles as well as their associated weights were used to build the predictive distributions.
---|---|---|---|---|---|---
\(\mu\) | 3.60 | 0.15 | 3.56 | 0.12 | 3.90 | 0.27
\(\lambda\) | 60.16 | 6.51 | 59.55 | 3.13 | 60.18 | 6.49
\(\gamma_0\) | 0.83 | 0.09 | 0.84 | 0.04 | 0.80 | 0.06
\(\gamma_f\) | 0.206 | 0.058 | 0.194 | 0.053 | 0.216 | 0.048
\(\mu_a\) | 639.39 | 83.28 | 642.33 | 62.40 | 579.98 | 73.75
\(s_a\) | 276.18 | 149.83 | 308.69 | 109.95 | 338.31 | 44.89
\(\sigma_Q\) | 0.040 | 0.004 | 0.042 | 0.008 | 0.040 | -
\(\sigma_\gamma\) | 0.061 | 0.002 | 0.064 | 0.015 | 0.060 | -
\(\sigma_{\gamma f}\) | 0.137 | 0.028 | 0.142 | 0.032 | 0.156 | 0.070
\(\sigma_r\) | 0.166 | 0.027 | 0.165 | 0.024 | 0.193 | 0.092

Table 1. Estimated values and standard deviations for all the parameters of the LNAS model provided by the IEnKF, ICPF and IUKF algorithms. The Log-likelihood, the AIC and the BIC values are also given. *:For the IUKF method, due to numerical problems, the modeling noise parameters \(\sigma_Q\) and \(\sigma_\gamma\) are fixed based on the estimation given by the two other methods.

4 Results and Discussion

As illustrated by Table 2, the best performance in the evaluation of the log-likelihood was achieved by the ICPF algorithm, since it attained the maximum value as compared to the IEnKF and the IUKF algorithms. This obviously holds for the AIC and the BIC as well.

In this study, we chose the CPF as the only algorithm to perform the assimilation step, while we could have adapted the UKF and the EnKF algorithms to perform this step as well. The aim here is to identify the difference of the predictive performance only due to the calibration step (prior information of the assimilation step). The comparison of the three filtering algorithms used in the assimilation step is a part of an ongoing work. Another interesting comparison between the prior information given by the CPF and the ICPF algorithm in the context of data assimilation problems can be found in Chen et al. [7].

Generally speaking the assimilation step has well established its undeniable value as demonstrated by Table 2 compared to the prediction results without assimilation. The estimation relative error was greatly reduced when data assimilation was performed. In the meantime, the standard error related to
the prediction was also significantly decreased in all cases when the second calibration has taken place based on the early growth data.

\begin{table}
\centering
\begin{tabular}{llllll}
\hline
         & IEnKF & RCPF & IUKF  \\
\hline
         & DA   & UA   & DA   & UA   & DA   & UA   \\
\hline
Q_b \(t_{142}\) & Relative error & 4.2\% & 45.8\% & 2.1\% & 44.5\% & 6.1\% & 55.6\% \\
         & Std.   & 56.0 & 163.7 & 56.1 & 128.7 & 62.7 & 165.0 \\
\hline
Q_b \(t_{198}\) & Relative error & 11.2\% & 46.5\% & 7.2\% & 43.4\% & 14.4\% & 58.5\% \\
         & Std.   & 63.1 & 141.2 & 61.5 & 116.8 & 68.3 & 144.2 \\
\hline
Q_r \(t_{142}\) & Relative error & 4.8\% & 29.8\% & 5.7\% & 32.2\% & 6.3\% & 43.1\% \\
         & Std.   & 256.0 & 384.3 & 256.1 & 354.3 & 303.4 & 479.2 \\
\hline
Q_r \(t_{198}\) & Relative error & 2.5\% & 18.6\% & 3.9\% & 20.6\% & 4.8\% & 29.8\% \\
         & Std.   & 420.4 & 553.4 & 419.9 & 522.3 & 503.7 & 693.6 \\
\hline
\end{tabular}
\caption{Comparison of model prediction capacity of estimates provided by three filtering methods (IEnKF, ICPF and IUKF) based on the 2006 dataset with and without assimilation of data at the early growth stage. DA: with data assimilation, UA: uncertainty analysis without data assimilation.}
\end{table}

For green leaf biomass allocation, it has always been the ICPF estimates that led to the best predictions for both years, as indicated by Fig. 6 and Fig. 7. This may be related to its important nonlinearity.

IUKF provided the best 2008 root prediction. A possible explanation lies on the fact that the root biomass allocation is more linear than the green leaf biomass allocation according to Fig. 3 and Fig 4. This may also explain the fact that the prediction based on the IUKF estimates for the green leaf biomass are less accurate compared to the results given by the other two estimates.

However, it is not quite the case for the 2006 root biomass prediction. Although the IEnKF estimates displayed the best performance, we notice that the performance of the three sets of estimates were relatively close, as suggested by Fig. 5.

Therefore in general, the most accurate predictions are those obtained by using the ICPF algorithm in the first calibration step, if we disregard the computation time and the memory requirements.

\begin{table}
\centering
\begin{tabular}{llllll}
\hline
Real Data & 2006 & IEnKF estimates & Std. & ICPF estimates & Std. & IUKF estimates & Std. \\
\hline
         &       & (relative error in %) &       & (relative error in %) &       & (relative error in %) &       \\
\hline
Q_b \(t_{142}\) & 355.2 & 370.2 (4.2\%) & 56.0 & 362.7 (2.1\%) & 56.1 & 376.8 (6.1\%) & 62.7 \\
Q_b \(t_{198}\) & 320.6 & 356.6 (11.2\%) & 63.1 & 348.3 (7.2\%) & 61.5 & 366.8 (14.4\%) & 68.3 \\
Q_r \(t_{142}\) & 1459.2 & 1529.1 (4.8\%) & 256.0 & 1542.7 (5.7\%) & 256.1 & 1551.3 (6.3\%) & 303.4 \\
Q_r \(t_{198}\) & 2400.0 & 2460.6 (2.5\%) & 420.4 & 2493.0 (3.9\%) & 419.9 & 2513.9 (4.8\%) & 503.7 \\
\hline
\end{tabular}
\caption{Comparison of model prediction capacity of estimates provided by three filtering methods (IEnKF, ICPF and IUKF) based on the 2006 dataset with assimilation of data at the early growth stages.}
\end{table}
Fig. 3. Comparison of the predictions of $Q_r$ in 2008 performed with or without data assimilation (Uncertainty Analysis) based on IUKF estimates.

Fig. 4. Comparison of the predictions of $Q_b$ in 2008 performed with or without data assimilation (Uncertainty Analysis) based on ICPF estimates.

Table 4. Comparison of model prediction capacity of estimates provided by three filtering methods (IEnKF, ICPF and IUKF) based on the 2008 dataset with assimilation of data at the early growth stages.

<table>
<thead>
<tr>
<th></th>
<th>Real Data 2008</th>
<th>IEnKF estimates (relative error in %)</th>
<th>Std.</th>
<th>ICPF estimates (relative error in %)</th>
<th>Std.</th>
<th>IUKF estimates (relative error in %)</th>
<th>Std.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Q_b$ ($t_{122}$)</td>
<td>373.5</td>
<td>419.5 (12.3%)</td>
<td>68.9</td>
<td>410.6 (9.9%)</td>
<td>68.1</td>
<td>440.9 (18.1%)</td>
<td>77.4</td>
</tr>
<tr>
<td>$Q_b$ ($t_{135}$)</td>
<td>380.6</td>
<td>433.1 (13.8%)</td>
<td>80.5</td>
<td>418.9 (10.1%)</td>
<td>77.8</td>
<td>461.1 (21.2%)</td>
<td>88.4</td>
</tr>
<tr>
<td>$Q_r$ ($t_{122}$)</td>
<td>1559.1</td>
<td>1460.5 (6.3%)</td>
<td>248.5</td>
<td>1466.7 (5.9%)</td>
<td>246.7</td>
<td>1508.8 (3.2%)</td>
<td>298.3</td>
</tr>
<tr>
<td>$Q_r$ ($t_{135}$)</td>
<td>2327.7</td>
<td>2125.6 (8.7%)</td>
<td>367.1</td>
<td>2137.6 (8.2%)</td>
<td>363.2</td>
<td>2213.7 (4.9%)</td>
<td>444.4</td>
</tr>
</tbody>
</table>

Considering the time-consuming problem related to an iterative use of the particle filtering methods, it might be interesting to be less strict on the model parameter estimation and loosen the convergence criterion so as to reduce the
Fig. 5. Comparison of the predictions of $Q_r$ in 2006 performed with data assimilation based on IEnKF, IUKF and ICPF estimates.

Fig. 6. Comparison of the predictions of $Q_g$ in 2006 performed with data assimilation based on IEnKF, IUKF and ICPF estimates.

iteration numbers. Given the fact that the parameters will be further adjusted in the assimilation step, the importance of the first calibration step might be over evaluated. We pinpoint also the fact that only two datasets were used for the prediction purposes and having available more datasets would increase the statistical significance of our results.

On the other hand, it is noteworthy that the noise related parameters have played a crucial role in the uncertainty assessment of the predictions. According to our tests, the prediction results are very sensitive to the level of observation noises. Since the level of noise parameter evaluated on one year cannot represent the corresponding level in another year or in a different location, applying the same level of noises in the assimilation step with a different dataset
is debatable. Further studies are hence needed to address the influence of the observation noise level to the prediction quality.

5 Conclusion

Overall, the proposed three-step sequential data assimilation approach allows us to address properly various sources of uncertainties and to obtain satisfactory prediction results. The filtering methods allow us to consider that certain model parameters are time-variant and the procedure used in this study preserve the flexibility to investigate the possible time-variant parameters.

Regarding the three filtering methods, the use of ICPF as a first calibration step provided globally the most accurate predictions and the smallest standard deviations, nonetheless, the IEnKF approach despite the normality assumption led to prediction results which are slightly worse, and sometimes even better than those obtained with the ICPF algorithm. By taking into account the fact that the former is far less time consuming than the latter algorithm during the calibration step, the results suggest that the use of IEnKF in the calibration step could be preferable, unless the nonlinearity is remarkable or cannot be easily evaluated, or more precise parameter estimation results are desired. In these cases the ICPF approach is more suitable.

References


Scan Statistics for Monitoring Data Modeled by a Negative Binomial Distribution

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Abstract. In this article we investigate the performance of approximations and inequalities for the distribution of scan statistics for independent and identically distributed observations from geometric and negative binomial distributions. The use of scan statistics is discussed for prospective and retrospective type experiments. These scan statistics can be also used in a sequential type experiments for monitoring data, modeled by a geometric or a negative binomial distribution, for detecting a local change in the waiting time for a specified event (batch of events). Potential applications include: business, ecology, criminology, entomology, quality control and sampling schemes. Numerical results are presented to evaluate the performance of the approximations discussed in this article. Extensions to variable window scan statistics, multiple scan statistics and two dimensional data are mentioned as well.

Keywords: Approximations, Inequalities, Moving sum, Sequential monitoring, Waiting time.

1 Introduction

Approximations and inequalities for the distribution of scan statistics for a sequence of independent and identically distributed (iid) observations from a binomial or Poisson distribution have been investigated in Chen and Glaz [5] and [6], Glaz and Naus [9], Glaz et al. ([10], Chapter 13), Glaz and Zhang [12], Haiman [14] and Karwe and Naus [17].

The geometric and negative binomial models for a sequence of iid integer valued data have been extensively discussed in the scientific literature, including business (Chatfield [3] and Chattfield et al. [4]), criminology (Nelson [18]), ecology (White and Bennetts [22]), entomology (Anscombe [1] and [2]), quality control (Hirano and Aki [15], Kaminsky et al. [16] and Weiss [20]) and sampling (Wise [21]). In this article, we also introduce a scan statistic for monitoring and detection of a local change in the parameter of a geometric or a negative binomial model.

The article is organized as follows. In Section 2, we derive approximations and inequalities for the distribution of a scan statistic. In Section 3, we present a scan statistic for a sequential monitoring type experiment. In Section 4, we discuss briefly a scan statistic in retrospective type investigations. In Section 5, for selected values of the parameters of the geometric and negative binomial models, we evaluate the accuracy of the approximations and inequalities derived in Section 2 and 3. Concluding remarks are presented in Section 6.
2 Approximations and Inequalities for the Distribution of a Scan Statistic

Let \( X_1, X_2, \ldots, X_N \) be iid observations from a negative binomial distribution with parameters \( 0 < p < 1, r \geq 0 \) an integer, and a probability function given by:

\[
P(X_i = x_i) = \binom{r + x_i - 1}{x_i} p^r (1 - p)^{x_i},
\]

where \( x_i, 1 \leq i \leq N, \) are non-negative integers. If \( r = 1, \) the negative binomial distribution reduces to the geometric distribution, with probability function:

\[
P(X_i = x_i) = p(1 - p)^{x_i},
\]

where \( x_i, 1 \leq i \leq N, \) are non-negative integers. It is well known that if \( X_1, X_2, \ldots, X_r \) are iid random variables from a geometric distribution with parameter \( 0 < p < 1, \) then \( \sum_{i=1}^{r} X_i \) has a negative binomial distribution with probability function given in Equation (1).

For integers \( 2 \leq m < N, \) a scan statistic with a scanning window of length \( m \) is defined as follows:

\[
S_{m,N} = \max \{ X_i + \cdots + X_{i+m-1}; 1 \leq i \leq N - m + 1 \}.
\]

We are interested in accurate approximations and inequalities for tail probabilities

\[
P(k; m, N) = P(S_{m,N} \geq k),
\]

where \( k \geq 2. \) For \( m \leq j \leq N, \) let

\[
q_j = 1 - P(k; m, j).
\]

When the size of the observed sample is clearly understood, we will abbreviate \( S_{m,N} \) to \( S_m. \)

For \( N \geq 3m, \) it follows from Glaz and Naus [9] and Glaz et al. ([10], Chapter 13.3) that a lower and upper bound for \( q_N = 1 - P(k; m, N) \) is given by:

\[
q_N \geq \frac{q_{3m}}{1 + \frac{q_{2m-1} - q_{2m}}{q_{3m-1}}} N^{-3m}
\]

and

\[
q_N \leq q_{3m} [1 - (q_{2m-1} - q_{2m})] N^{-3m},
\]

respectively.

For \( N = Lm + \nu, L \geq 3 \) and \( 1 \leq \nu \leq m - 1, \) the following approximation for \( q_N \) follows from Chen and Glaz ([6], Chapter 7.2.2):

\[
q_N \approx q_{3m} \left( \frac{q_{3m}}{q_{2m}} \right)^{L-3} \left( \frac{q_{2m+\nu}}{q_{2m}} \right).
\]
For, $N = Lm, L \geq 3$, the approximation (8) reduces to:

$$q_N \approx q_{3m} \left( \frac{q_{3m}}{q_{2m}} \right)^{L-3}.$$  \hfill (9)

Haiman ([13] and [14]) derived accurate approximations for $q_N$ for a sequence of $N$ iid discrete random variables. A nice feature of these approximations is that a sharp error bound can be easily evaluated. For the problem at hand, for any $k$ and $N \geq 3m$, such that $1 - q_{2m} \leq 0.025$ and $3.3N[1 - q_{2m}]^2(N/m - 1) \leq 1$, the following approximation for $q_N$ is obtained from Haiman ([14], Corollary 2 and Eq. 2.2):

$$q_N \approx \frac{2q_{2m} - q_{3m}}{[1 + q_{2m} - q_{3m} + 2(q_{2m} - q_{3m})^2]^{N/m-1}},$$  \hfill (10)

with an error bound of approximately

$$3.3[1 - q_{2m}]^2(N/m - 1).$$  \hfill (11)

In Section 5, for selected values of the parameters of the negative binomial model, we evaluate the accuracy of the bounds and approximations for $q_N$ given in (6), (7), (9) and (10), respectively, via an algorithm in Karwe and Naus [17] and a simulation, whenever the algorithm in Karwe and Naus [17] is computationally not feasible. We also evaluate the error bound given in Equation (11).

A variable window scan statistic, based on minimum $p$-values of fixed window scan statistics, can be developed using an approach of Glaz and Zhang [12]. We will not discuss this further in this article.

### 3 A Scan Statistic in Sequential Experiments

Let $X_1, X_2, \cdots, X_j$, be a sequence of iid negative binomial random variables with probability function given in Equation (1). The random variable $X_j$ measures the number of events or signals that have been observed at the end of the $j^{th}$ time interval or at the location. Define

$$W_{k,m} = \inf \left\{ j \geq 1; \sum_{i=\max(1,j-m+1)}^{j} X_i \geq k \right\},$$  \hfill (12)

as the waiting time for detecting at least $k$ events or signals in $m$ consecutive time intervals or locations. Denote by $E(W_{k,m})$ the mean waiting time or recurrence time for observing at least $k$ events or signals in $m$ consecutive time intervals or locations. Accurate approximations and inequalities for the distribution of $W_{k,m}$ and $E(W_{k,m})$ and are of importance in applications.

It follows from (3) and (12) that

$$P(W_{k,m} > N) = P(S_{m,N} \leq k - 1).$$  \hfill (13)
Therefore, accurate approximations and inequalities for scan statistic probabilities in Section 2, will yield accurate approximations for $P(W_{k,m} > N)$ and

$$E(W_{k,m}) = \sum_{N=0}^{\infty} P(W_{k,m} > N).$$ (14)

It follows from Chen and Glaz ([6], Section 7.2.2) that:

$$\sum_{j=0}^{2m-1} q_j + q_{2m} \left[ 1 + \frac{q_{2m-1}q_{2m}}{q_{2m-1} - q_{2m}} \right] \leq E(W_{k,m}) \leq \sum_{j=0}^{2m-1} q_j + \frac{q_{2m}}{q_{2m-1} - q_{2m}},$$ (15)

$$\sum_{j=0}^{3m-1} q_j + q_{3m} \left[ 1 + q_{3m-1}/(q_{2m-1} - q_{2m}) \right] \leq E(W_{k,m}) \leq \sum_{j=0}^{3m-1} q_j + \frac{q_{3m}}{q_{2m-1} - q_{2m}},$$ (16)

and for $N = Lm + \nu, L \geq 3$ and $1 \leq \nu \leq m - 1$,

$$E(W_{k,m}) \approx \sum_{j=0}^{2m} q_j + \frac{q_{2m}}{q_{2m} - q_{3m}} \sum_{\nu=1}^{m} q_{2m+\nu}.$$ (17)

In Section 5, for selected values of the parameters we present numerical results for approximations and inequalities in this section.

4 A Conditional Scan Statistic in Retrospective Investigations

In retrospective type experiments the total number of observed events in a random sample $X_1, X_2, ..., X_N$ is known. In that case the conditional distribution of $X_1, X_2, ..., X_N$ given $\sum_{i=1}^{N} X_i = n$ has to be considered. For the negative binomial model in Section 2, it follows that:

$$P\left(X_1 = x_1, X_2 = x_2, ..., X_N = x_N \mid \sum_{i=1}^{N} X_i = n\right)$$

$$= \frac{\prod_{i=1}^{N-1} \binom{r+x_i-1}{r-1} p^r q^{x_i} \binom{r+n-\sum_{i=1}^{N-1} x_i-1}{r-1} p^r q^{n-\sum_{i=1}^{N-1} x_i} \binom{N+r+n-1}{N-1} p^r q^n}{\binom{N+r+n-1}{N-1} p^r q^n}$$

$$= \frac{\prod_{i=1}^{N-1} \binom{r+x_i-1}{r-1} \binom{r+n-\sum_{i=1}^{N-1} x_i-1}{r-1}}{\binom{N+r+n-1}{N-1}}$$

$$= \frac{\prod_{i=1}^{N-1} \binom{r+x_i-1}{r-1} \binom{r+n-\sum_{i=1}^{N-1} x_i-1}{n-\sum_{i=1}^{N-1} x_i}}{\binom{N+r+n-1}{N-1}}.$$ (18)
is a multivariate hypergeometric probability function. For the geometric model $r = 1$, in which case:

$$P\left( X_1 = x_1, X_2 = x_2, \ldots, X_N = x_N \mid \sum_{i=1}^{N} X_i = n \right) = \frac{1}{\binom{N+n-1}{n}},$$

(19)

is a discrete uniform probability function. For these conditional negative binomial and geometric models a scan statistic can be formulated and implemented via algorithms that have been investigated in Chen and Glaz [5]. We will not discuss this further in this article. Moreover, a variable window scan statistic, based on minimum p-values of fixed window scan statistics, can be developed using an approach of Glaz and Zhang [12].

5 Numerical Results

In Tables 1-2 of this section, for limited values of the parameters, approximations and bounds discussed in Section 2, are derived for the geometric and negative binomial models, via simulation with 10,000 trials and the algorithms in Karwe and Naus [17]. In Table 3, approximations and bounds for the expected stopping time are evaluated via simulation with 10,000 trials and the algorithms in Karwe and Naus [17]. Based on these numerical results one can conclude that in most cases the approximations and bound are quite accurate. For small value of $p$ and large $k$, the computing is quite intensive and in some cases the approximations are not accurate. For example, In Table 1, for $m = 5$, $p = .10$, and $k = 130$, the upper bound is .0775, while the simulated value is .0806. More accurate algorithms are needed.

6 Concluding Remarks

In this article, we have focused on fixed window scan statistics for geometric and negative binomial data in one dimension. When the length of the scanning window is unknown, a variable window scan statistic based on minimum p-values of fixed window scan statistics can be employed (Glaz and Zhang [12]). It is also of interest to extend the results in this article to multiple scan statistics that are closely related to r-scan statistics (Dembo and Karlin [8], Glaz et al. [11] and Su and Wallenstein [19]). Extensions to scan statistics for two dimensional data (Glaz et al. [10], Chapter 16, and Chen and Glaz [7]), for geometric and negative binomial models, are also of interest in the area of spatial statistics.
### Table 1. Approximations and Bounds for $P(S_{m,N} \geq k)$ for a Geometric Model

<table>
<thead>
<tr>
<th>$m$</th>
<th>$p$</th>
<th>$k$</th>
<th>Eq. (7)</th>
<th>Eq. (9)</th>
<th>Eq. (10)</th>
<th>Eq. (6)</th>
<th>Eq. (11)</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.01</td>
<td>1200</td>
<td>0.2434</td>
<td>0.2571</td>
<td>0.2547</td>
<td>0.2497</td>
<td>0.0398</td>
<td>0.2774</td>
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<tr>
<td></td>
<td></td>
<td>1250</td>
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<td>0.2214</td>
<td>0.0241</td>
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<td></td>
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<td>1300</td>
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<td>0.1630</td>
<td>0.1627</td>
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<td>0.1514</td>
</tr>
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<td>0.05</td>
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<td>0.5946</td>
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### Table 2. Approximations and Bounds for $P(S_{m,N} \geq k)$ for a Negative Binomial Model

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Table 3. Approximations and Bounds for $E(W_{k,m})$ for Geometric and Negative Binomial Models

References


Prediction for Count Time Series

Vasiliki Christou and Konstantinos Fokianos

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Abstract. We study inference and diagnostics for count time series regression models which include a feedback mechanism. In particular, we are interested in negative binomial processes for count time series. We study probabilistic properties and quasi likelihood estimation for this class of processes. The resulting estimators are consistent and asymptotically normally distributed. The key observation in developing the theory is a mean parameterized form of the negative binomial distribution. In addition, we provide probabilistic forecasts based on the assumption of negative binomial or Poisson distribution and we propose the use of probability integral transformation histogram (PIT), marginal calibration plot and scoring rules to assess the predictive performance and rank the competing forecast models.

Keywords: Diagnostics, Prediction, Quasi-maximum likelihood estimation.

1 Introduction

We study inference and diagnostics for count time series regression models which include a feedback mechanism. Despite the fact that the Poisson distribution is the most common distribution that is used to model count time series, we claim that in some cases a better approach is provided by the negative binomial distribution suitably reparameterized. Figure 1 shows the Probability Integral Transformation (PIT) histograms, see Czado et al. [3], for breech births data in a hospital of South Africa. These plots are constructed histograms that examine the adequacy of the predictive distribution. Inverse U-shaped histograms point to overdispersed predictive distribution while uniform histograms demonstrate the suitability of the hypothesized model. The figure shows that the Poisson assumption fails to model these data and a better approach is provided by the negative binomial distribution.

We propose estimation of the regression parameters based on quasi-likelihood function obtained from the Poisson distribution. It turns out, that the correct mean specification yields consistent estimates. In the case of negative binomial distribution the additional parameter is estimated consistently by two standard methods of moments estimators. In this approach, we avoid complicated likelihood functions and still provide inference and diagnostics for this larger class of processes.

In addition, we provide probabilistic forecasts based on the assumption of negative binomial or Poisson distribution and we consider tools for the evaluation of the predictive performance and the assessment of the assumed distributional assumption. We strive to maximize the sharpness of the predictive distribution subject to calibration. We propose the use of a nonrandomized
version of the probability integral transformation histogram to assess the probabilistic calibration, while for the assessment of the marginal calibration we consider the use of the marginal calibration plot. Addressing sharpness can be made via scoring rules, that is negatively oriented penalties that the forecaster wishes to minimize. The diagnostic approach is illustrated by an evaluation and ranking of the two competing forecasters for breech births data in a hospital of South Africa.

2 Autoregressive modeling, inference and prediction

Assume that \( \{Y_t, t \geq 1\} \) is a count time series and let \( \{\lambda_t, t \geq 1\} \) be an unobserved sequence of mean processes. Denote by \( F^Y_t,\lambda \) the history of the response process up to and including time \( t \). We suppose that the conditional distribution of \( Y_t \mid F^Y_{t-1} \) is either the Poisson or the negative binomial. The negative binomial distribution is suitably reparameterized to have the same mean as the Poisson distribution, i.e. \( \lambda_t \). We consider the linear model

\[
\lambda_t = d + a\lambda_{t-1} + bY_{t-1}
\]

and the non linear model

\[
\lambda_t = \frac{d}{(1 + \lambda_{t-1})^\gamma} + a\lambda_{t-1} + bY_{t-1},
\]

where parameters \( d, a, b, \gamma \) are assumed to be positive.

We suggest to use the Poisson based score estimating function for estimating the unknown parameters of the model. This methodology avoids complicated likelihood function and it ensures that the regression parameters are estimated consistently. In addition, it can be shown that the estimators are asymptotically normally distributed. For more details see Christou and Fokianos[1], Fokianos[4] and Fokianos et al.[5]. For the case of the negative binomial distribution, the additional parameter \( \nu \) is estimated consistently by the method of moments. Once the consistent estimators are obtained, and because of the fact that \( E(Y_t \mid F^Y_{t-1}) = \lambda_t \), we predict \( Y_t \) by \( \hat{\lambda}_t \). Regardless the chosen response distribution, \( \hat{\lambda}_t \) is identical for both cases. Following Gneiting et al.[6], we take the point of view that predictions should be probabilistic in nature. In addition, they should strive to maximize the sharpness of the predictive distribution subject to calibration. Calibration refers to the statistical consistency between the predictive distribution and the observations, and it is a joint property of the forecasts and the values that utilize. The notion of sharpness refers to the concentration of the predictive distribution and is a property of the forecasts only. It follows that if the predictive distribution is more concentrated, then the forecasts obtained are sharper. Therefore, this will yield better predictions subject to calibration.

The key tool in assessing probabilistic calibration is the nonrandomized Probability Integral Transformation (PIT) histogram as discussed by Czado et al.[3]. U-shaped histograms point at underdispersed predictive distributions,
hump or inverse U-shaped histograms indicate overdispersion and uniformity of histograms hints well calibrated predictive distributions.

To assess marginal calibration we construct the marginal calibration plot. If the marginal calibration hypothesis is true, then we expect minor fluctuations about 0. Major excursions from zero hint that the forecaster lacks marginal calibration. Addressing sharpness is accomplished via scoring rules, which help us to rank the competing forecast models. They are negatively oriented penalties that the forecaster wishes to minimize.

Details for the construction and the application of the above diagnostics can be found in Christou and Fokianos[2], Czado et al.[3] and Gneiting et al.[6].

3 Case study

We consider a count time series corresponds to the number of monthly breech births data in Edendale hospital of South Africa from February 1977 to January 1986. The size of the collection is 108. We fit the linear and the non linear model and employing the quasi likelihood methodology, we obtain the quasi maximum likelihood estimators. Substituting these estimators to the expression of \( \lambda_t \) we estimate the mean process. After obtaining \( \hat{\lambda}_t \), we construct the PIT histograms of Figure 1, the marginal calibration plots of Figure 2 and the various scoring rules of Table 1. The results indicate that the negative binomial distribution outperforms the Poisson.

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Table 1. Scoring rules calculated for the breech births data after fitting the linear model and the non linear model for \( \gamma = 0.5 \). Bold face numbers in each column indicate the minimum value obtained between the two forecasters.

4 Conclusions

Reparameterizing the negative binomial process so that it has the same mean value as the Poisson, allow for consistent estimation using the quasi likelihood inference based on the Poisson distribution. The variance of the negative binomial process is larger than the corresponding variance of the Poisson. This takes into account overdispersion which is a phenomenon observed repeatedly in count dependent data. So, for overdispersed count data the negative binomial assumption outperforms the Poisson assumption and improves considerably the fit. In addition, forecast based on the negative binomial distribution seems to be superior to the corresponding prediction from Poisson.
**Fig. 1.** PIT histograms applied to the number of breech births in Edendale hospital from February 1977 to January 1986. From top to bottom: PIT histograms for the linear model and the non linear model for $\gamma = 0.5$. Left Plots: The conditional distribution is Poisson. Right Plots: The conditional distribution is negative binomial.

**References**

Fig. 2. Left Plot: Marginal calibration plot for the breech births data if we fit the linear model. Right Plot: Marginal calibration plot for the births data if we fit the non-linear model for $\gamma = 0.5$. Solid line corresponds to the negative binomial prediction, while dashed line is for the Poisson forecast.
A strong optimality result for anisotropic self–similar textures

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Abstract. In [13,14], we proposed a method to characterize jointly self-similarity and anisotropy properties of a large class of self–similar Gaussian random fields. We provide here a mathematical analysis of our approach, proving that the sharpest way of measuring smoothness is related to these anisotropies and thus to the geometry of these fields.

Keywords: Operator scaling Gaussian random field, anisotropy, sample paths properties, anisotropic Besov spaces.

1 Introduction and motivations

In numerous modern applications (geography [10], biomedical imagery (see [3] for example), geophysics [15], art investigation [1], . . . ), the data available for analysis consist of images of homogeneous textures, that need to be characterized. For such images, a key issue consists first in describing, within a suitable framework, the anisotropy of the texture, and then in defining regularity anisotropy parameters that can actually and efficiently be measured via numerical procedures and further involved into e.g., classification schemes.

Furthermore, in many cases the analyzed textures display at the same time self–similarity and anisotropy properties. This is for example such the case in medical imaging (osteoporosis, muscular tissues, mammographies,...), cf. e.g. [4,5], hydrology [12], fracture surfaces analysis [9], . . . .

In [13,14], we proposed a method for studying jointly self-similarity and anisotropy in images by focusing on a specific classic class of Gaussian anisotropic selfsimilar processes. We consider $\ell^p$ norms of hyperbolic wavelets coefficients which permits the use of different dilation factors along the horizontal and vertical axis. We prove empirically that these $\ell^p$ norms are maximal for a specific ratio of the horizontal and vertical axis, directly related to the anisotropy of the model.

In [2], we proved that there is a close relationship between $\ell^p$ norms of the hyperbolic wavelet coefficients of a function and its norm in a convenient class of anisotropic functional spaces : the anisotropic Besov spaces. The consistence properties of the estimators introduced in [13,14] can then be reformulated using sample paths properties of the model in anisotropic Besov spaces. The aim of this paper is to provide mathematical foundations of the empirical results.
of \cite{13,14}. Here, we prove what we call a strong optimality result, namely that the critical exponent of the model in anisotropic Besov spaces is maximal when the parameters of the analyzing space fit these of the analyzed textures, which is the exact transcription into a mathematical way of the empirical results of \cite{13,14}.

The paper is organized as follows. In Section 2, we first present the studied self–similar anisotropic model. Thereafter in Section 3, we recall some basic facts about anisotropic Besov spaces. In Section 4 we then state our main result. The proofs are postponed in Section 5.

In what follows, we denote \( \mathcal{E}^+ \) the collection of \( 2 \times 2 \) matrices whose eigenvalues have positive real parts.

## 2 Presentation of the studied model

In \cite{13,14}, we choosed to investigate the properties of a large class of anisotropic Gaussian self–similar fields, introduced in \cite{4,5}, referred as Operator Scaling Gaussian Random Field, in short OSGRF.

For any matrix \( E_0 \) belonging in \( \mathcal{E}^+ \) such that \( \text{Tr}(E_0) = 2 \) and any \( H_0 \in (0, \min_{\lambda \in \text{Sp}(E_0)} \text{Re}(\lambda)) \), this class can be defined using the following harmonizable representation:

\[
X_{\rho, E_0, H_0}(\mathbf{x}) = \int_{\mathbb{R}^2} (e^{i\langle \xi, \mathbf{x} \rangle} - 1)\rho(\xi)^{-1(H_0+1)}d\hat{W}(\xi),
\]

where \( \mathbf{x} = (x_1, x_2), \xi = (\xi_1, \xi_2) \) and \( d\hat{W}(\xi) \) stands for a 2D Wiener measure. Here \( \rho \) is an \( E_0 \)-homogeneous continuous positive function, that satisfies the following homogeneity relationship \( \rho(\alpha E_0 \xi) = \alpha f(\xi) \) on \( \mathbb{R}^2 \). We also assume that \( \int (1 + |\xi|^2)\rho(\xi)^{-2(H_0+1)}d\xi < +\infty \) which ensures the existence of the Gaussian field \( X \) (see \cite{5}).

With this construction, the OSGRF \( X_{\rho, E_0, H_0} \) has stationary increments. Further it satisfies an anisotropic version of the scaling property with parameter \( H_0 \) (where \( \equiv \) denotes equality for all finite dimensional distributions):

\[
\forall a > 0, \{X_{\rho(aE_0, \mathbf{x})}\} \equiv \{a^{H_0}X_{\rho, E_0}(\mathbf{x})\}. \tag{2}
\]

(As usual \( a^{E_0} = \exp(E_0 \log(a)) = \sum_k (\log a)^k E_0^k / k! \).

Constructions of \( E_0 \)-homogeneous continuous positive function have been proposed in [5] via an integral formula (Theorem 2.11). An alternative construction, more fitted for numerical simulations, can be found in [6].

Let us now give a concrete example of OSGRF. Consider the case where \( E_0 = \left( \begin{array}{cc} \alpha_0 & 0 \\ 0 & 2 - \alpha_0 \end{array} \right) \) with \( \alpha_0 \in (0, 2) \) and set

\[
\rho(\xi_1, \xi_2) = |\xi_1|^{1/\alpha_0} + |\xi_2|^{1/(2-\alpha_0)}.
\]

The function \( \rho \) is obviously an \( E_0 \) homogeneous positive continuous function. For any \( H_0 \in \min(\alpha_0, 2 - \alpha_0) \), the associated Gaussian field will be

\[
X_{\rho, E_0, H_0}(x_1, x_2) = \int_{\mathbb{R}^2} \frac{e^{i\langle \xi, \mathbf{x} \rangle} - 1}{(|\xi_1|^{1/\alpha_0} + |\xi_2|^{1/(2-\alpha_0)})^{H_0+1}}d\hat{W}(\xi),
\]
The scaling property satisfied by this field is then
\[ \forall a > 0, \{ X_{\rho, E_0, H_0}(a^{\alpha_0}x_1, a^{2-\alpha_0}x_2) \} \overset{d}{=} \{ a^{H_0} X_{\rho, E_0, H_0}(x_1, x_2) \}. \]

3 Anisotropic concepts of smoothness

Our main goal here is to study the sample paths properties of this class of Gaussian fields in suitable anisotropic functional spaces. This approach is quite natural (see [11]) since the studied model is anisotropic. To this end, suitable concepts of anisotropic smoothness are needed. The aim of this section is to give some background about the appropriate anisotropic functional spaces: Anisotropic Besov spaces. These spaces generalize classical (isotropic) Besov spaces and have been studied in parallel with them. Let \( D \) a diagonalizable matrix of \( E^+ \) with eigenvalues \( \lambda_1, \lambda_2 \) and associated eigenvalues \( (e_1, e_2) \).

**Definition 1.** Let \((p, q) \in [1, +\infty]^2, s > 0 \) and \( \beta \in \mathbb{R} \). For any \( f \in L^p(\mathbb{R}^2) \) set
\[
\| f \|_{B^s_{p,q,|\log|^\beta}(\mathbb{R}^2, D)} = \sum_{\ell=1}^{\infty} \left( \int_0^1 \|(\Delta_{e_\ell} f)(x)\|_{L^p} t^{-sq/\alpha_\ell-1} \log(t)^{-\beta q/\alpha_\ell} dt \right)^{1/q}.
\]
By definition
\[
B^s_{p,q,|\log|^\beta}(\mathbb{R}^2, D) = \{ f \in L^p(\mathbb{R}^2), \| f \|_{B^s_{p,q,|\log|^\beta}(\mathbb{R}^2, D)} < +\infty \}.
\]
The matrix \( D \) is called the anisotropy of the Besov space \( B^s_{p,q,|\log|^\beta}(\mathbb{R}^2, D) \).

**Remark 1.** It is well-known that there exists a strong relationship between \( \ell^p \) norms and classical wavelet coefficients (see [16,17]). In [13,14], our estimators are based on hyperbolic wavelet analysis. In [2], we proved that \( \ell^p \) norms of hyperbolic wavelet coefficients of a functions are related to its norms in anisotropic Besov spaces. It is the reason why the natural mathematical framework to relate anisotropy and self-similar properties of the model to its sample paths properties is this of anisotropic Besov spaces.

**Remark 2.** Let \( D \) a diagonalizable matrix of \( E^+ \). For any \( a > 0, \lambda D \) is also a diagonalizable matrix of \( E^+ \) with eigenvalues \( a\lambda_1, a\lambda_2 \) and same eigenvectors as \( D \). Hence for any \( s > 0, B^s_{p,q}(\mathbb{R}^2, \lambda D) = B^s_{p,q}(\mathbb{R}^2, D) \).

Using Remark 2, we deduce that without loss of generality, we can assume in the sequel that \( \text{Tr}(D) = 2 \). We then define
\[ \mathcal{E}^+_2 = \{ E \in \mathcal{E}^+, \text{Tr}(E) = 2 \}. \]
As it is the case for isotropic spaces, anisotropic Hölder spaces \( C^\alpha(\mathbb{R}^2, E) \) can be defined as particular anisotropic Besov spaces.
Definition 2. Let \( s > 0, \beta \in \mathbb{R} \). The anisotropic Hölder spaces \( \mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, D) \) are defined by

\[
\mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, E) = B^s_{\infty, \infty, \log|\beta|}(\mathbb{R}^2, E).
\]

Hence, a bounded function \( f \) belongs to \( \mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, E) \) if and only if for any \( r \in (0, 1), \Theta \in S^E_0(\cdot, |E|) \) and \( x \in \mathbb{R}^d \), one has

\[
|f(x + r^E\Theta) - f(x)| \leq C_0 r^s |\log(r)|^\beta,
\]

for some \( C_0 > 0 \), that is if and only if its restriction \( f_\Theta \) along any parametric curve of the form

\[
r > 0 \mapsto r^E\Theta,
\]

with \( \Theta \in S^E_0(\cdot, |E|) \) is in the usual Hölder space \( \mathcal{C}^s_{\log|\beta|}(\mathbb{R}) \) and \( \|f_\Theta\|_{\mathcal{C}^s_{\log|\beta|}(\mathbb{R})} \) does not depend on \( \Theta \). Roughly speaking, the anisotropic “directional” regularity in any anisotropic “direction” has to be larger than \( s \). In other words, we replace straight lines of isotropic setting by curves with parametric equation \( r > 0 \mapsto r^E\Theta \) adapted to anisotropic setting.

To state our optimality results we need a local version of anisotropic Besov spaces:

Definition 3. Let \( D \in \mathcal{E}^+ \) be a fixed diagonalizable anisotropy, \( 1 \leq p, q \leq \infty, \beta \in \mathbb{R}, 0 < s < \infty \) and \( f \in L^{p,loc}_0(\mathbb{R}^2) \).

The function \( f \) belongs to \( B^s_{p,q,\log|\beta|,loc}(\mathbb{R}^2, E) \) if for any \( \varphi \in \mathcal{D}(\mathbb{R}^d) \), the function \( \varphi f \) belongs to \( B^s_{p,q,\log|\beta|}(\mathbb{R}^2, D) \).

The anisotropic local critical exponent in anisotropic Besov spaces \( B^s_{p,q}(\mathbb{R}^2, E) \) of \( f \in L^{p,loc}_0(\mathbb{R}^2) \) is then defined by

\[
\alpha_{f,loc}(E, p, q) = \sup \{ s, f \in B^s_{p,q,loc}(\mathbb{R}^2, E) \}.
\]

4 Statement of our main result

In what follows, we are given \( E_0 \in \mathcal{E}^+_2 \) and \( \rho_{E_0} \) an \( E_0 \)-homogeneous continuous positive function, \( H_0 \in (0, \min_{\lambda \in \mathcal{S}(E_0)} \text{Re}(\lambda)) \).

Our results will be based on a comparison between the topology related to \( \rho_{E_0} \) involved in the construction of the Gaussian field \( \{X_{\rho_{E_0}, E_0, H_0}(x)\}_{x \in \mathbb{R}^d} \) defined by equation (1) and this of the analyzing spaces \( B^s_{p,q}(\mathbb{R}^2, D) \). To be able to compare these two topologies, we also assume that \( D \in \mathcal{E}^+_2 \).

We characterize in some sense an anisotropy \( E_0 \) and an Hurst index of the field \( \{X_{\rho_{E_0}, H_0}(x)\}_{x \in \mathbb{R}^d} \), which is interesting when analyzing anisotropic self–similar textures. Combining the results of this paper and these of [2], our approach can thus be turned in an effective algorithm for the estimation of the anisotropy of self similar textures (see [13,14]). In the case where \( q = \infty \), Theorem 1 is the exact mathematical reformulation of equation (9) stated in [14], on which are based the definition of the estimators of the anisotropy and smoothness of the model. Our main result in then both a mathematical justification and an extension of the results empirically proved in [13,14]:

\[
\text{Definition 2. Let } s > 0, \beta \in \mathbb{R}. \text{ The anisotropic Hölder spaces } \mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, D) \text{ are defined by } \\
\mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, E) = B^s_{\infty, \infty, \log|\beta|}(\mathbb{R}^2, E). \\
\text{Hence, a bounded function } f \text{ belongs to } \mathcal{C}^s_{\log|\beta|}(\mathbb{R}^2, E) \text{ if and only if for any } r \in (0, 1), \Theta \in S^E_0(\cdot, |E|) \text{ and } x \in \mathbb{R}^d, \text{ one has } \\
|f(x + r^E\Theta) - f(x)| \leq C_0 r^s |\log(r)|^\beta, \\
\text{for some } C_0 > 0, \text{ that is if and only if its restriction } f_\Theta \text{ along any parametric curve of the form } \\
r > 0 \mapsto r^E\Theta, \\
\text{with } \Theta \in S^E_0(\cdot, |E|) \text{ is in the usual Hölder space } \mathcal{C}^s_{\log|\beta|}(\mathbb{R}) \text{ and } \|f_\Theta\|_{\mathcal{C}^s_{\log|\beta|}(\mathbb{R})} \text{ does not depend on } \Theta. \text{ Roughly speaking, the anisotropic “directional” regularity in any anisotropic “direction” has to be larger than } s. \text{ In other words, we replace straight lines of isotropic setting by curves with parametric equation } r > 0 \mapsto r^E\Theta \text{ adapted to anisotropic setting.} \\
\text{To state our optimality results we need a local version of anisotropic Besov spaces:} \\
\text{Definition 3. Let } D \in \mathcal{E}^+ \text{ be a fixed diagonalizable anisotropy, } 1 \leq p, q \leq \infty, \beta \in \mathbb{R}, 0 < s < \infty \text{ and } f \in L^{p,loc}_0(\mathbb{R}^2). \\
\text{The function } f \text{ belongs to } B^s_{p,q,\log|\beta|,loc}(\mathbb{R}^2, E) \text{ if for any } \varphi \in \mathcal{D}(\mathbb{R}^d), \text{ the function } \varphi f \text{ belongs to } B^s_{p,q,\log|\beta|}(\mathbb{R}^2, D). \\
\text{The anisotropic local critical exponent in anisotropic Besov spaces } B^s_{p,q}(\mathbb{R}^2, E) \text{ of } f \in L^{p,loc}_0(\mathbb{R}^2) \text{ is then defined by } \\
\alpha_{f,loc}(E, p, q) = \sup \{ s, f \in B^s_{p,q,loc}(\mathbb{R}^2, E) \}. \\
\text{4 Statement of our main result} \\
\text{In what follows, we are given } E_0 \in \mathcal{E}^+_2 \text{ and } \rho_{E_0} \text{ an } E_0 \text{-homogeneous continuous positive function, } H_0 \in (0, \min_{\lambda \in \mathcal{S}(E_0)} \text{Re}(\lambda)). \\
\text{Our results will be based on a comparison between the topology related to } \rho_{E_0} \text{ involved in the construction of the Gaussian field } \{X_{\rho_{E_0}, E_0, H_0}(x)\}_{x \in \mathbb{R}^d} \text{ defined by equation (1) and this of the analyzing spaces } B^s_{p,q}(\mathbb{R}^2, D). \text{ To be able to compare these two topologies, we also assume that } D \in \mathcal{E}^+_2. \\
\text{We characterize in some sense an anisotropy } E_0 \text{ and an Hurst index of the field } \{X_{\rho_{E_0}, H_0}(x)\}_{x \in \mathbb{R}^d}, \text{ which is interesting when analyzing anisotropic self–similar textures. Combining the results of this paper and these of [2], our approach can thus be turned in an effective algorithm for the estimation of the anisotropy of self similar textures (see [13,14]). In the case where } q = \infty, \text{ Theorem 1 is the exact mathematical reformulation of equation (9) stated in [14], on which are based the definition of the estimators of the anisotropy and smoothness of the model. Our main result in then both a mathematical justification and an extension of the results empirically proved in [13,14]:}
where $\rho_{E_0}, \rho_{D_0}$ are respectively two $E_0$- and $D_0$-homogeneous continuous positive functions and $\{X_{\rho_{E_0}, H_0}(x)\}_{x \in \mathbb{R}^d}, \{X_{\rho_{D_0}, H_0}(x)\}_{x \in \mathbb{R}^d}$ the associated Gaussian fields by (1). One can then investigate the sample paths properties of $\{X_{\rho_{E_0}, H_0}(x)\}_{x \in \mathbb{R}^d}$ instead of this of $\{X_{\rho_{E_0}, H_0}(x)\}_{x \in \mathbb{R}^d}$.

Hence from now, we then assume that $E_0$ equals its diagonalizable real part, namely that $E_0 = D_0$. Even if $D$ and $D_0$ are both diagonalizable since these matrices are not commuting we cannot assume that $D_0$ and $D$ are both diagonal.

Let $\varphi \in D(\mathbb{R}^d)$. As above, one may assume $\text{supp}(\varphi) \subset K = B_{D_0}(0, 1)$. Denote $\lambda_1^0 \leq \lambda_2^0$ (resp $\lambda_1 \leq \lambda_2$) the two eigenvalues of $D_0$ (resp. $D$) and $e_1^0, e_2^0$ (resp $e_1, e_2$) some associated eigenvectors. We exclude the two cases $\lambda_1^0 = \lambda_2^0$, $\lambda_1 = \lambda_2$ corresponding to the cases $D_0 = Id, D = Id$ which can be deduced from Theorem 4.1 of [8]. Hence the inequalities between the eigenvalues are strict.

Let us fix $p \in [1, +\infty]$. By assumption $[H_0/\lambda_1^0] = [H_0/\lambda_2^0] = 1$. The proof of Proposition 5.5 of [8] provides us with the following equalities

$$H_0 = \sup \{\beta, \int_0^1 \|\varphi(x+t e_1^0) - (\varphi(x))(p, t^{\beta p/\lambda_1^0 - 1} dt < +\infty \}
\sup \{\beta, \int_0^1 \|\varphi(x+t e_2^0) - (\varphi(x))(p, t^{\beta p/\lambda_2^0 - 1} dt < +\infty \}.$$ (3)
Define now the two followings indices

\[ \alpha_1(p) = \sup\{\beta, \int_0^1 \| (\varphi X)(x + t e_1) - (\varphi X)(x) \|_{L^p} t^{-\beta p/\lambda_1 - 1} dt < +\infty \} , \]

\[ \alpha_2(p) = \sup\{\beta, \int_0^1 \| (\varphi X)(x + t e_2) - (\varphi X)(x) \|_{L^p} t^{-\beta p/\lambda_2 - 1} dt < +\infty \} . \]

Thereafter set \( \alpha(p) = \min(\alpha_1(p), \alpha_2(p)) \). Assume that for some \( p \in [1, +\infty] \) one has \( \alpha(p) > H_0 \), that is \( \varphi X \in B_{p, p}^{\alpha(p)}(\mathbb{R}^2, D) \) with \( \alpha(p) > H_0 \).

We first need the following lemma:

**Lemma 1.** Only five cases are possible:

1. \( \frac{H_0}{\lambda_1} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) \leq \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) . \)

2. \( \frac{H_0}{\lambda_1} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) > \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) > \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) . \)

3. \( \frac{H_0}{\lambda_1} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) > \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) . \)

4. \( \frac{H_0}{\lambda_1} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) > \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) = \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) . \)

5. \( \max\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) > \frac{H_0}{\lambda_1'} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) > \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) = \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) . \)

**Proof of Lemma 1.** The only point to prove is that the case

\( \max\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) = \frac{H_0}{H_0} = \max\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) > \min\left( \frac{\alpha_1(p)}{\lambda_1}, \frac{\alpha_2(p)}{\lambda_2} \right) = \frac{H_0}{\lambda_2'} = \min\left( \frac{H_0}{\lambda_1'}, \frac{H_0}{\lambda_2'} \right) . \)

is impossible. Suppose that this relationship holds. Then one has

\( \left( \frac{\alpha_1(p)}{\lambda_1} = \frac{H_0}{\lambda_1'} \text{ and } \frac{\alpha_2(p)}{\lambda_2} = \frac{H_0}{\lambda_2'} \right) \) or \( \left( \frac{\alpha_2(p)}{\lambda_2} = \frac{H_0}{\lambda_2'} \text{ and } \frac{\alpha_1(p)}{\lambda_1} = \frac{H_0}{\lambda_1'} \right) . \)

Since \( \min(\alpha_1(p), \alpha_2(p)) > H_0 \), it implies that

\( \left( \frac{H_0}{\lambda_1} < \frac{H_0}{\lambda_1'} \text{ and } \frac{H_0}{\lambda_2} < \frac{H_0}{\lambda_2'} \right) \) or \( \left( \frac{H_0}{\lambda_2} < \frac{H_0}{\lambda_2'} \text{ and } \frac{H_0}{\lambda_1} < \frac{H_0}{\lambda_1'} \right) . \)
that is

\[ \{ \lambda_1 > \lambda_0^0 \text{ and } \lambda_2 > \lambda_0^0 \} \text{ or } \{ \lambda_2 > \lambda_0^0 \text{ and } \lambda_1 > \lambda_0^0 \} . \]

Since \( \lambda_0^0 + \lambda_0^0 = \lambda_1 + \lambda_2 = 2 \), it yields to a contradiction.

We now deal successively with the five cases of Lemma 1. Let us first assume that point (1) of Lemma 1 holds.

Let \( s \in (H_0/\lambda_0^0, \min(\alpha_1(p)/\lambda_1, \alpha_2(p)/\lambda_2, 1)) \). Then, by definition of \( s \) one has

\[ \int_0^1 \| (\varphi X)(x + te_1) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt < +\infty , \]

and

\[ \int_0^1 \| (\varphi X)(x + te_2) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt < +\infty . \]

The, using the finite difference characterization of classical Besov spaces, one deduces that \( \varphi X \in B_{p,p}^s(\mathbb{R}^2) \). Since, by Proposition 5.6 of [8], \( B_{p,p}^s(\mathbb{R}^2) \hookrightarrow B_{p,p}^{\lambda_0^0}(\mathbb{R}^2, D_0) \) and \( s > H_0/\lambda_0^0 \) it yields to a contradiction.

Now suppose that point (2) of Lemma 1 holds. Assume that \( \min(\alpha_1(p)/\lambda_1, \alpha_2(p)/\lambda_2) = \alpha_1(p)/\lambda_1 \). The other case will be similar. Observe that that if \( e_1^0 = ae_1 \) for some \( a \in \mathbb{R} \), one then has

\[ H_0/\lambda_0^0 = \sup \{ s, \int_0^1 \| (\varphi X)(x + te_1) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt < +\infty \} = \alpha_1(p)/\lambda_1 , \]

which is impossible since by assumption \( H_0/\lambda_0^0 > \alpha_1(p)/\lambda_1 \).

Then the family \( (e_1, e_1^0) \) is necessarily a basis of \( \mathbb{R}^2 \). Hence

\[ e_2^0 = ae_1 + be_1^0 , \]

for some \( (a, b) \in \mathbb{R}^2 \). By (3), for any \( \varepsilon > 0 \) one has a.s.

\[ \int_0^1 \| (\varphi X)(x + te_2^0) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt < +\infty . \]

Further, the triangular inequality and equation (4) implies that

\[ \int_0^1 \| (\varphi X)(x + te_2^0) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt \leq 2 \int_0^1 \| (\varphi X)(x + t(ae_1 + be_1^0)) - (\varphi X)(x + tbe_1^0) \|_{p, t^{-s p - 1}} dt + \int_0^1 \| (\varphi X)(x + tbe_1^0) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt . \]

Set now \( y = x + tbe_1^0 \) and remark that

\[ \| (\varphi X)(x + t(ae_1 + be_1^0)) - (\varphi X)(x + tbe_1^0) \|_{p, t^{-s p - 1}} = |(\varphi X)(y + tae_1) - (\varphi X)(y)\|_{p, t^{-s p - 1}} \]

In addition, \( H_0/\lambda_0^0 < \alpha_1/\lambda_1 < H_0/\lambda_0^0 \). Since

\[ H_0/\lambda_0^0 = \sup \{ s, \int_0^1 \| (\varphi X)(x + te_1) - (\varphi X)(x) \|_{p, t^{-s p - 1}} dt < +\infty \} , \]

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and by definition of $\alpha_1(p)$, one deduces that for any $\varepsilon > 0$ sufficiently small
\[
\int_0^1 \| (\varphi X)(y+tae_1) - (\varphi X)(y) \|^p_{L^p} t^{- \frac{\alpha_1(p)_L}{\alpha_1}} - 1 \, dt \leq \int_0^1 \| (\varphi X)(y+tae_1) - (\varphi X)(y) \|^p_{L^p} t^{- \frac{\alpha_1(p)_L}{\alpha_1}} - 1 \, dt ,
\]
and
\[
\int_0^1 \| (\varphi X)(x+tbe_0) - (\varphi X)(x) \|^p_{L^p} t^{- \frac{\alpha_1(p)_L}{\alpha_1}} - 1 \, dt \leq \int_0^1 \| (\varphi X)(x+tbe_0) - (\varphi X)(x) \|^p_{L^p} t^{- \frac{\alpha_1(p)_L}{\alpha_1}} - 1 \, dt ,
\]
are finite. Combining this information with Equations (6), (5), implies a contradiction. The proof of Theorem 1 in the three other cases of Lemma 1 is exactly similar.

References

The Impact of a Pandemic Influenza on Mortality, Temporary Disability and Hospitalization Risks for Protection Insurance, and Hedging Strategies

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Abstract. As far as Protection Insurance is concerned, the emergence of an influenza pandemic could lead to an excess of claims in the insured population. A pandemic would obviously have a significant impact on Death risk, but could also affect the risk of Temporary Disability and Hospitalisation. The aim of this article is to determine how to model the effects of a pandemic event on mortality risk, and to analyse how a pandemic may affect the risk of Temporary Disability and Hospitalisation.

Knowing that a pandemic could cause bankruptcy in the worst scenarios, an insurance company should consider buying adequate coverage. The last part of this article is devoted to the search for a solution to hedge against a pandemic event. This overview is not limited to standardized products sold by reinsurers, but more elaborate and exotic offers are described, with their advantages and drawbacks.

Keywords: Pandemic Risk, Influenza, Protection Insurance, Mortality Risk, Temporary Disability, Hospitalization, Hedging Strategies, Reinsurance, Securitization
1 Introduction

An influenza pandemic is defined as a global outbreak of the disease due to viruses with new antigenic subtypes. In the last decade, some influenza viruses could have caused a pandemic but the catastrophe has been hopefully avoided. For example, the H5N1 virus in 2005 has severely contaminated birds but only a few human cases have been suspected. The virus might have evolved, by mutation or genetic assortment, into a virus capable of human-to-human transmission. Should this happened, this virus would have been a major threat to human health. Another example is the virus H1N1 in 2009. This virus has spread very fast around the world, but has hopefully killed a few people. If a genetic combination of the viruses H1N1 and H5N1 had taken place, a major pandemic could have happened.

As far as Protection Insurance is concerned, an influenza pandemic could lead to high levels of Death, Temporary Disability and Hospitalisation among insured people, and this could potentially lead the insurance company to bankruptcy. To avoid this, the insurance company can buy a strategic coverage.

This paper is structured in two parts. The objective of the first part is to build a model to assess mortality risk for Protection Business, and to discuss about possible extensions to Temporary Disability and Hospitalisation. The second part aims at describing different coverages and to determine if one of them is better than the other.

2 Modelling Mortality Risk for Protection Business, and Possible Extension to Temporary Disability and Hospitalisation

In order to modelDeath risk for Protection business (Creditor Insurance and Individual Protection), it is possible to describe mortality risk as a trend, on which catastrophic shocks events are added. In fact, as explained in Juillard et al. (2008), such a model should integrate two components in order to consider all the volatility of mortality:
- The uncertainty of the trend of mortality: it encompasses risk tendency and the risk of oscillations around these tendencies;
- Extreme shocks of mortality, such as pandemics.

This section will describe a model that respects this split of mortality risk in two parts. For more details on it, the reader can refer to Corlosquet-Habart et al. (2011), Corlosquet-Habart et al. (2012).
Concerning the trend of mortality, it can be modeled differently depending on available data of the insurance company, and of the segmentation level chosen. If the company has individual data, a prospective stochastic mortality table can be implemented (mortality risk is monitored by the probability to die). If the company has aggregated or partial data, a stochastic loss ratio model can be implemented (mortality risk is monitored by actuarial loss ratio, which represents the claims charge divided by the risk premium of the portfolio).

Concerning pandemic shock, it can be included by a frequency x cost approach. Frequency is usually modelled by a Bernoulli distribution with a parameter $p$. Cost can be modelled by an exponential distribution with mean $\varepsilon$, as explained in Juillard et al. (2008). In fact, $\varepsilon$ represents the average cost of a pandemic event (in term of mortality rate) and can be calculated by an epidemiological model. To sum up, the “pandemic shock” component is given by:

$$\text{Mortality}(t)_{\text{pandemic shock}} = B_r(p) \cdot \text{Exp}(\varepsilon).$$

To estimate the average cost of a pandemic, the most efficient models are compartmental models. The population is divided into compartments, which correspond to a few key characteristics of the disease. The dynamic of influenza can be represented by four compartments using a SEIR model:

- Individuals who are susceptible to the disease (noted S).
- Individuals who are exposed (noted E). They are in latent phase, which is the period of time during which the individual has been infected but is not yet infectious himself.
- Individuals who are infected (noted I).
- Individuals who have recovered and are immune, or who are dead (noted R).

From the initial conditions (namely the number of individuals in each class), the rate of occurrence of new cases and deaths caused by disease, compartmental models determine the number of individuals in each class at each moment. The SEIR original model, which includes transportation, was created by Baroyan et al. (1969). Epstein et al. (2007) have extended the model by adding travel restrictions and vaccination. The topic of calibration of such model for insurance companies to meet Solvency II expectations has been studied in Habart (2010), and Corlosquet-Habart et al. (2011).

The model consists of a system of difference equations in discrete time domain, describing the disease dynamics within each city and air travel by individuals from one city to another. Key elements of the model are the following:

- Individuals are assumed to be well-mixed, therefore contacts between Susceptible and Infectious persons are uniformly distributed.
- The number of random contacts between individuals follows a Poisson distribution.
- Random travel between cities is implemented as a series of draws from binomial distributions.
- Two strategies of intervention are implemented in order to limit the spread of the virus: travel restriction and vaccination.
- The seasonality of influenza is taken into account.

Therefore, the model integrates 8 equations:

\[
\hat{N}S_i(t+1) = NS_i(t) + \Omega[N\tilde{S}_i(t)] + v \cdot (S_i(t) + \Omega[S_i(t)])
\]

\[
E_i(0,t+1) = \frac{s f(l_i,t) \cdot \lambda \cdot (S_i(t) + \Omega[S_i(t)])}{T_i(t) - D_i(t) + \alpha[T_i(t) - D_i(t)]} \sum_{\tau=0}^{\tau_1} I_i(\tau,t)
\]

\[
\tilde{S}_i(t+1) = S_i(t) + \Omega[S_i(t)] - E_i(0,t+1) - v \cdot (S_i(t) + \Omega[S_i(t)])
\]

\[
E_i(\tau+1,t+1) = (1 - \gamma(\tau)) \cdot (E_i(\tau,t) + \Omega[E_i(\tau,t)]) \quad \text{for } \tau = 0,1,\ldots,\tau_1 - 1
\]

\[
I_i(\tau+1,t+1) = \left[\gamma(\tau) \cdot (E_i(\tau,t) + \Omega[E_i(\tau,t)]) + (1 - \delta(\tau)) \cdot I_i(\tau,t)\right] \quad \text{for } \tau = 0,1,\ldots,\tau_1
\]

\[
I_i(\tau+1,t+1) = \left[(1 - \delta(\tau)) \cdot I_i(\tau,t)\right] \quad \text{for } \tau = \tau_1 + 1, \tau_1 + 2, \ldots, \tau_2 - 1
\]

\[
R_i(t+1) = R_i(t) + \Omega[R_i(t)] + (1 - d) \sum_{\tau=0}^{\tau_1} \delta(\tau) \cdot I_i(\tau,t)
\]

\[
D_i(t+1) = D_i(t) + d \sum_{\tau=0}^{\tau_1} \delta(\tau) \cdot I_i(\tau,t)
\]

\[
T_i(t+1) = NS_i(t+1) + S_i(+1) + \sum_{\tau=0}^{\tau_1} E_i(\tau,t+1) + \sum_{\tau=0}^{\tau_1} I_i(\tau,t+1) + R_i(t+1) + D_i(t+1)
\]

where \( \gamma(t) \) is the probability that an individual becomes Infectious on day \( \tau + 1 \), given that that person was still in the Exposed state on day \( \tau \), and \( \delta(\tau) \) is the probability that an individual is Recovered or Dead on day \( \tau + 1 \), given that that person was still in the Infectious state on day \( \tau \).

Therefore, the SEIR model gives the number of dead people in each city at the end of the projection period of one year (\( t_{\text{end}} \)). The mortality shock is consequently the following:

\[
\text{Mortality Shock}_{i}(t_{\text{end}}) = \frac{D_i(t_{\text{end}})}{T_i(t_{\text{end}})}
\]
The limits of the model are the following.
- The difficulty to calibrate the parameters because there were only a few pandemics in the past.
- The uncertainty of the prevention measures that would be implemented against the pandemic (vaccines, antivirals).

Despite these limitations, the SEIR model is efficient for Death Risk. Nevertheless, is it necessary to take into account Temporary Disability and Hospitalization, and if so, is it possible to extend the SEIR model to these risks?

The average duration of influenza is recorded about a week (the minimum duration is a few days and the maximum period is 2 weeks). Only a minority of people may develop serious complications after influenza (for seasonal flu, it represents between 5% and 20% of the population). It concerns seniors over 65 years, young children, people with medical conditions (such as asthma, diabetes, heart disease or overweight) or pregnant women. These types of people do little or no part of policyholders, given medical screening and age limits for subscription.

Concerning Temporary Disability, contracts include a waiting period during which insured people is not paid if a claim occurs. The duration of the waiting period depends on insurance companies and on countries, but it is usually more than two weeks. Thus, it appears that waiting periods enable insurance companies to cover against the excess risk on Temporary Disability. A pandemic would have little or no impact on this risk. Therefore it does not seem necessary to model Temporary Disability risk.

Concerning Hospitalization, the observed duration for the H1N1 pandemic was 4 days, and the average waiting period for this risk is superior to 5 days. Given the low impact of a pandemic on this risk, it does not seem necessary to model it.

To conclude, a model SEIR to take into account Death Risk seems to be sufficient to correctly calculate the impact of a pandemic for Protection Business.
3 Looking for the Best Hedging Strategy

If a pandemic occurs, the cost for an insurance company would be substantial and could even lead it to bankruptcy. It is therefore strongly advised to buy a hedging strategy. The following table sums up the different coverage solutions sold by the current market of reinsurance, their advantages and drawbacks.

<table>
<thead>
<tr>
<th>Coverage solution</th>
<th>Advantages</th>
<th>Drawbacks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual Stop Loss (for death risk)</td>
<td>Traditional coverage</td>
<td>The duration is too short (renewal is not possible if a pandemic is declared)</td>
</tr>
<tr>
<td>Bi/Triennial Stop Loss (for death risk)</td>
<td>Partial coverage of the portfolio after the year of subscription</td>
<td>More expensive than an annual Stop Loss, with a smaller capacity</td>
</tr>
<tr>
<td>Pandemic Stop Loss (with a trigger based on the WHO alerts)</td>
<td>Less expensive than an annual Stop Loss</td>
<td>The definition of the trigger can be difficult</td>
</tr>
<tr>
<td></td>
<td></td>
<td>This coverage is based on an internal model</td>
</tr>
<tr>
<td>Annual Stop Loss with a renewal option</td>
<td>Discretionary choice to renew</td>
<td>A little more expensive than an annual Stop Loss</td>
</tr>
<tr>
<td></td>
<td>The price is capped</td>
<td></td>
</tr>
<tr>
<td>Frequency Stop</td>
<td>Simplicity of management, modeling, parameterization</td>
<td>Same disadvantage as the Stop Loss for the duration of the coverage</td>
</tr>
<tr>
<td>Cashless Value Protection</td>
<td>Perfectly adapted to creditor insurance</td>
<td>Applicable only to portfolios with a duration greater than one year</td>
</tr>
<tr>
<td>Securitization</td>
<td>Suited for large capacity</td>
<td>High costs</td>
</tr>
</tbody>
</table>

Table 1: Coverage solutions sold by the current market (Source: Guy Carpenter (2012)).

From the above solutions, Frequency Stop seems to be the solution that is the most adapted to Protection insurance. For example, let us consider the portfolio of an insurance company, which has a Loss Ratio of 50%. The Loss Ratio is simply the claims charge divided by the risk premium. Let us consider that this level of Loss Ratio corresponds to 25 000 deaths with a capital superior to 10 k€. The coverage is triggered if the Loss Ratio is between 70% and 100%. For example, if the Loss Ratio increases from 50% to 70%, which corresponds to a number of deaths that increases from 25 000 to 35 000, then reinsurers will support 10k€ per claim slice. The total capacity is set to 250M€, for a period of 3 years. This coverage is efficient in terms of cost, available capacity and is easy to implement.
Conclusion

To put it in a nutshell, the occurrence of a pandemic event would have dramatic consequences for an insurance company. Death risk is obviously of paramount importance and it can be assessed using a SEIR model. The greatest limit of such a model is the calibration of parameters because of the lack of reliable existing data. Other risks for Protection Business, particularly Temporary Disability and Hospitalization, would have no or little impact because contracts have a waiting period, which is generally superior to average observed duration of the flu.

Given the cost of a pandemic for Death risk, it is advised to buy a cover strategy. Under current market conditions, Frequency stop seems to be the solution that is the most adapted to Protection insurance.

References


Undergraduate Students’ Career in Italy: a non Homogeneous Markov Approach with Fuzzy States

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Abstract. The Italian university administrative organisation does not allow to relate students career accumulation of credits to their academic years of registration clearly, as it is instead the case in the majority of the European Higher Education (HE) systems. For instance, two freshmen might belong to different progression levels according to the actual number of exams they passed; nonetheless, regardless of the amount of exams they succeeded in the two past syllabuses, both these two freshmen at the end of their first academic year are equally permitted to register at their second academic year and therefore show an identical administrative situation. With reference to the aforementioned HE system, in this paper we apply the theory of non homogeneous Markov systems with fuzzy states, in order to describe the actual students’ educational progress in two different faculties of the university of Milano-Bicocca. The levels of students career progression will be related to the academic years using a stochastic model that assumes the progress levels as fuzzy states [Symeonaki, Kalamatianou, 2011] with a membership function related both to the exam’s final grade and to the time needed to pass the exam in comparison with the schedule provided in the syllabus. Moreover, the membership function that relates each fuzzy state to the administrative situation will be analysed, so as to derive further insight in students’ progression, with particular focus on the possibility of obtaining a function of undergraduates’ difficulty in passing the various exams.

Keywords: Progression of students carriers, Non Homogeneous Markov system, fuzzy states, membership function, exams difficulty.

1 Introduction

A comprehensive analysis of the efficacy of higher education (HE) asks for a thorough consideration of all costs, both direct and indirect, to be balanced against the future benefits of a better educated, capable population and employable workforce. Undergraduates’s completion of their curricular paths and the attainment of their degree implies not only their personal success, but a successful attainment of the HE system as a whole and of society at large. Symmetrically, university dropouts may appear, at first sight, as an individual failure but in truth the induced losses extend their effect as a dispersion of
talents and abilities. Addressing the topic of HE dropouts in the Italian university requires a clear understanding of the undergraduates’ degree of freedom in answering to the curricular requirements. As a matter of fact, in the Italian HE system the administrative registration to the subsequent academic years does not correspond to a unique situation in terms of accumulated formative credits. In fact, unlike several other countries in the European Union, in Italy registering to the subsequent year is admissible to all students at the end of a certain academic year, regardless of the number of exams passed not only in the current year, but also in all the previous ones. Therefore, dropouts can be originate from several behavioural patterns in terms of curricular developments. In addition, it should be underline how HE students’ credit balance might be due, on the one side, to the difficulty in complying with specific curricular requirements, on the other side to the development of optimal strategies in coping with the requirements themselves. Hereafter the focus is addressed to the actual credits balances associated with dropouts, in terms both of the number and of the type for passed examinations. The administrative registration to a certain academic year, can be conceived as a fuzzy state, where several curricular conditions coexists. As a matter of fact, no overlapping would take place when students pass all the exams, stated in the a specific yearly syllabus, right during that academic year and no registration to the next year would be allowed unless all credits are gained. The academic dynamics between two fuzzy states can be modelled in terms of all the observed states related to students’ registered administratively to that specific year [1].

2 Fuzzy states in a Markov chains approach

Until recently, Markov chains methods have been widely applied to career evolutionary paths, ranging from the labour force to the education population. Their traditional applications are conceived in their fundamental form, where states are mutually exclusive and can be clearly identified and each state is influenced only by the previous one, a dynamic that can be expressed as the future being determined by the present, with no memory of the past. Markov chains belong to the family of stochastic processes, i.e. to a family of aleatory variables:

\[ X \{ X_t, t \in T \} \]  

dependent on a parameter \( t \) that belongs to the set \( T \). If the set \( T \) of values that the parameter \( t \) can assume consists of an interval of at most countable elements, then the stochastic process \( X_t \) is discrete and we have that \( t \geq 0 \). The state space \( \langle S \rangle \) represents the set of values that the stochastic process can assume. When discrete, it is named discrete stochastic process. In Markov chains \( T \) is generally represented by the set of natural numbers \( N \) and it stands for the observational time points. Markov chain models have been successfully applied to various HE setting [2][3]. However, as previously discussed, the clarity of identification of states can fail in some HE systems, giving place to fuzzy states, when two sorts of situations essentially occur. In the first place, when it is impossible to measure precisely the states of the system and thus the states
used to model the system are intrinsically not distinct. In the second kind of situations, the actual states can be exactly measured and observed, but their number is so large that decisions are not associated with the exact states of the system. In these two sorts of situations, decisions are associated with non mutually exclusive states which can be defined as fuzzy sets on the original non-fuzzy state space of the system, where the system has a large number of states. The recognition of fuzzy states in HE has been applied at an earlier stage to time series[4],[5],[6]. Recent theoretical development have allowed the introduction of fuzzy states in Markov chains [7], with highly effective applications to educational situations where students access consecutive years with no restraints on credits and where the interest focuses on patterns and strategies of these accesses. It is the case of the Italian HE systems, where the registration to the next academic year, as previously described, leaves behind a wide spectrum of situations in terms of the amount and the composition of formative credits. In these scenery, two extreme situations may occur, one the one side with a student acquiring no credits at all or, on the other side, when she/he attains all the credits in her/his curricular syllabus/es. The optimal condition of having accomplished all due requirements can be identified in terms of successful strategies, potentially in a wide behavioural spectrum [8]. Furthermore, the relation of every combination of credits and exams to the fuzzy state can be quantified and associated to dropouts. The fuzzy space state is,

$$F_r() : S[0; 1]$$

(2)

where the expression above is said the membership function $\mu_{F_r}(j)$ and it quantifies the relative compositional quota of each observable state with respect to the fuzzy state under scrutiny. Besides, $F = \{F_1, F_2, ..F_N\}$ is assumed to define a fuzzy partition on $S$ so that:

$$\sum_{r=1}^{N} \mu_{F_r}() = 1$$

(3)

In case the time-event of interest be the dropout, it needs to be highlighted that it is an absorbing state, in the sense that, once experimented, it is impossible to leave for any other state.

3 Students’ administrative versus formative condition: the membership function.

It has been shown how, even if administratively belonging to the same academic year, two students cannot be considered in the same career position, that is to say in the same state, when the number of acquired formative credits differ. Therefore, fuzzy states play a relevant role and their number can
be extremely relevant, due to the several conditions, in terms of total credits attained with different combinations of exams considered either in the last or the previous years syllabus. Each actual condition in terms of the combination of the amount of gained credits and the exams passes needs to be referred to the administrative year of registration by means of an explicit quantification of intensity, in order to specify analytically the membership function in equation (2). With respect to the to sth student, his record of passed examinations are considered. With respect to each passed exam, \( i = 1, 2, ..., l + 1 \), the index \( md_i \) [9] is computed, in order to evaluate its relative difficulty compared with the whole student’s accomplishment, apart from the exam under consideration:

\[
md_i = \frac{\sum_{s=1}^{n} y_{si} - \sum_{k=1}^{l} y_{sk}}{n}
\]

being \( y_{si} \) the grade the student obtained at that examination, \( l \) is the total number of exams the student has passed in the same administrative year, excluding the \( i^{th} \) one under scrutiny, \( n \) the number of students that successfully passed the exam \( l^{th} \) in the year considered. Therefore the index in equation 4 relies on the individual difference between the specified mark and the average mark in all other passed exams in the same academic year and it estimates the relative difficulty of examinations in different subjects.

Then, from this index, the membership function \( \mu_{F_r} \) for the fuzzy sets \( F_r \) is estimated [Symeonaki and Kalamatianou, 2011]:

\[
\mu_{F_r} = 1 + \frac{\sum md_i}{m_1}
\]

where \( \sum md_i \) refers to the exams neither taken nor passed in the year of enrollment and \( m_1 \) is the total number of examinations included in the syllabus for that year and it quantifies the relative compositional quota of each observable state with respect to the fuzzy state under scrutiny. The index in (5) has been adjusted for the Italian situation as follows:

\[
\mu_{F_r} = 1 + \frac{\sum md_i \cdot fc_i}{m_1}
\]

The membership function in (6) weighs the missing exams for their formative credits, \( fc_i \) and then divides this product by the maximum difference in grades, where 33 and are the highest and the lowest pass marks respectively. For an undergraduate university programme, three fuzzy states \( F_r \) represent the levels of progress due to the enrollment to each academic year, whilst for each year dropout and graduation are considered. Then for each curricular year, the probability for a student to belong to the fuzzy state has been derived by means of the following expression:

\[
P[Y^I(t - 1) = F_r] = \sum_{j=1}^{k} P[Y(t - 1) = j] \cdot \mu_{F_r}(j).
\]
where \( Y(t) \) and \( Y^f(t) \) represent respectively the state and fuzzy state of a student in the system \( S \) at time \( t \). In case the time-event of interest be the dropout, it needs to be highlighted that it is an absorbing state, in the sense that, once experimented, it is impossible to leave for any other state.

In our preliminary data analysis, membership functions and transition probabilities have been estimated in the R environment, developing an original \textit{ad hoc} code \cite{10}. We examined two undergraduate courses in two different former faculties, Psychological Sciences and Techniques, Faculty of Psychology and Marketing on the one side, Corporate Communications and Global Markets, Faculty of Economics on the other side, with respect to the cohort enrolling in autumn 2005. Only enrollments that start their credit attainment anew have been taken into account, their cohorts accounting to 573 and 576 for students at the Faculty of Economics and Psychology respectively. Undergraduates’ career was followed up to five year after matriculation, so as to allow for observing graduation. As far as the estimation of the membership function is concerned, results show an extremely wide range of membership function estimates as expected, the more in the psychology program with contemplates a slightly wider range of examinations that students can freely decide to undertake. For illustrative purposes, three different conditions are considered with reference to the end of the fist, second and third academic year respectively, just before the enrollment to the subsequent year. Membership functions are referred to the pertaining level of progression, the fuzzy state that indicates the optimal condition of having accomplished all the requirements stated in the yearly syllabus. This is the case of condition A1 in Table 1, related to 12 students matriculated in Psychology in 2005 that passed all examinations in the syllabus at the end of the administrative year. Condition B1 shows the condition of students who accomplished almost all their requirements: their quota of belonging to the the second level of progression equals 0.8201, whereas the complementary to one value, 0.1790, indicates that slightly less than 20% were still to pass. Condition C1 concerns 92 students that do not renew their enrollment for the subsequent year, by the end of the matriculation year and even if administratively entitled to it. Condition A2 implies that 7 students, on the verge of subscribing to the third academic year, still are due to pass approximately 11% of the examinations in their second year syllabus, while all previous university requirements had been fulfilled, the related membership function value equal to 0. On the contrary, condition B2 shows how 14.8% of first year and 32.61% of second year examinations are still to pass, whilst only around half of requirements of the pertaining level of progression have been satisfied. The highest the value that links the completed year of enrollment to the level of progression, e.g. the end of first year with respect to second level of progression an the alike, the higher is the membership function and then the more favourable is the students’ condition. Dropout is clearly an absorbent state, as well as graduation. The Italian HE system has undergone recently a deep evolution in the normative framework concerning HE, that has involved also the organisational structure of undergraduate and graduate programs. Our adjustment of the membership function for the domestic setting, applied to our case, reflects a conservative stance, with no penalties linked to the time lag for
unmet requirements. In other words, the membership function for the due level of progression assumes the very same value in case the examinations to pass belong either to the immediately preceding syllabus or to two academic years earlier. Further developments will consider also the effects of the inclusion of penalties on the understanding of the various students\' strategic approaches to HE requirements.

4 Not finished yet, already at next step: fuzzy states in academic accomplishment

In the Italian undergraduate academic curricular system, the completion of each year requires the acquisition of a definite amount of credits, 60 as a general rule, per academic year. As aforementioned, however, the administrative registration to the following year does not ask for the full attainment of the credits of the previous year. Besides, during each year a student can opt for transferring to a different undergraduate course within the same faculty, or in a different faculty in the same university or in a different university altogether. All the previously listed events represent transitory states. On the contrary, a dropout is an absorbent state, as well as graduation as the attainment of the whole amount of 180 credits of an undergraduate course. It needs to be underlined how students show two strategies of abandonment. In the first place, they are entitled to a written declaration of willingness to withdraw from university. In the second place, they may simply skip next academic year registration. The former option is far less practiced, whereas the second behaviour is the most recurrent.

The first undergraduate course under scrutiny, Marketing, Corporate Communications and Global Markets, shows a pattern of relative adherence to the curricular requirements (see Table 2), with some constraints in the range of choices within the pertaining academic year, giving place to a relevant dropout rate. Relative results in Table 2 show how, at the end of the first curricular year (first raw in the table, label First), similarly to students in Psychology, the probability of failing to adhere to the first year syllabus regards 30.9 out of 100 enrolled students, instead the probability of successfully acquiring all the 60 credits is lower, as it involves 40% enrolled students, due to a higher
dropout probability. At the end of second curricular year, the correspondent fuzzy state scores a higher probability, showing how a large amount of students failed to adhere to the first and second year syllabus altogether. With respect to Psychological Sciences and Techniques undergraduates in Table 3, the situation appears far more fragmented than the other undergraduate program, due to the higher number of examinations left to the undergraduates’ free choice. To this regard, Table 3 shows how, at the end of first curricular year (first raw in the table, label ‘First’), the probability of failing to adhere to the first year syllabus, that is to stay behind the first level of progression with an attainment of 60 formative credits, regards 30.3% enrolled students, whereas the probability of successfully acquiring all the 60 credits involves 50.7% enrolled students. Clearly, no graduations take place. Similarly, the situation at the end of the second academic year, that is the instant preceding the registration to the third curricular year, is depicted in the second raw of Table 3. Still in contrast with the previous undergraduate program, these scattered formative conditions co-exists with a milder dropout rate. In line with applications to other national contexts, our preliminary results underline how the introduction of fuzzy states in the theoretical frame of Markov chains leads to a meaningful new insight in the dynamics of HE population. In truth, this theoretical approach, when confronted with real settings, allows a comprehensive inclusion of a reality that can be extremely fragmented, even scattered in some cases, and it proves apt to frame it in interpretative guidelines that can sustain challenge for university

<table>
<thead>
<tr>
<th>Level of progression</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>graduation</th>
<th>dropout</th>
</tr>
</thead>
<tbody>
<tr>
<td>First</td>
<td>0.309</td>
<td>0.400</td>
<td>0.000</td>
<td>0.000</td>
<td>0.291</td>
</tr>
<tr>
<td>Second</td>
<td>0.203</td>
<td>0.367</td>
<td>0.249</td>
<td>0.000</td>
<td>0.189</td>
</tr>
<tr>
<td>Third</td>
<td>0.197</td>
<td>0.320</td>
<td>0.0910</td>
<td>0.300</td>
<td>0.093</td>
</tr>
<tr>
<td>First out of programme</td>
<td>0.160</td>
<td>0.221</td>
<td>0.072</td>
<td>0.481</td>
<td>0.067</td>
</tr>
<tr>
<td>Second out of programme</td>
<td>0.055</td>
<td>0.093</td>
<td>0.067</td>
<td>0.491</td>
<td>0.295</td>
</tr>
</tbody>
</table>

Table 2. Undergraduate course in Marketing, Corporate Communications and Global Markets: probabilities of meeting the examination program scheduled in the year of enrollment

<table>
<thead>
<tr>
<th>Level of progression</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
<th>graduation</th>
<th>dropout</th>
</tr>
</thead>
<tbody>
<tr>
<td>First</td>
<td>0.303</td>
<td>0.507</td>
<td>0.000</td>
<td>0.000</td>
<td>0.190</td>
</tr>
<tr>
<td>Second</td>
<td>0.219</td>
<td>0.288</td>
<td>0.414</td>
<td>0.000</td>
<td>0.079</td>
</tr>
<tr>
<td>Third</td>
<td>0.142</td>
<td>0.177</td>
<td>0.120</td>
<td>0.512</td>
<td>0.067</td>
</tr>
<tr>
<td>First out of programme</td>
<td>0.285</td>
<td>0.199</td>
<td>0.058</td>
<td>0.378</td>
<td>0.081</td>
</tr>
<tr>
<td>Second out of programme</td>
<td>0.192</td>
<td>0.172</td>
<td>0.063</td>
<td>0.243</td>
<td>0.330</td>
</tr>
</tbody>
</table>

Table 3. Undergraduate course in Psychological and Technical Sciences: probabilities of meeting the examination program scheduled in the year of enrollment
governance to make better informed policy decisions that can streamline the
degree completion process in every step of its development.

References

1. G. Betti, B. Chelli and R. Cambini. A statistical model for the dynamics between
two fuzzy states: theory and an application to poverty analysis, *Metron - Inter-
2. J. Gani. Formulae for projecting enrolments and degrees awarded in universities,
3. S. Massa and S.S. Puliafito. *An Application of Data Mining to the Problem of the
University Students’ Dropout Using Markov Chains*, Principles of Data Min-
ing and Knowledge Discovery Lecture Notes in Computer Science, 1704, 51-60
(1999)
4. Q. Song and B. Chissom. Forecasting enrollments with fuzzy time series part I,
*Fuzzy sets and system*, 54, (1993)
5. Q. Song and B. Chissom, Forecasting enrollments with fuzzy time series part II,
*Fuzzy sets and system*, 62, (1994)
6. M. Sah and Y. Degtiarev, *Forecasting enrollment model based on first order fuzzy
time series*, Proceedings of world academy of science, engineering and technology,
vol.1, 2005.
7. M. Symeonaki and A. Kalamatianou *Markov system with fuzzy states for describing
students’ educational progress in Greek universities*, World Statistics Congress
(ISI), Dublin, (2011)
8. M. Symeonaki and G.B. Stamoub. Theory of Markov systems with fuzzy states,
9. A. Kelly. The relative standards of subject examinations, *Research Intelligence* 2,
34-38 (1975)
10. M. Mazzeni *Le catene di markov con stati fuzzy: un’ applicazione al caso delle
carriere universitarie*, Final Dissertation, Master Degree In Economics, University
of Milano-Bicocca, Milan, Italy, (2011)
How high is it possible to extend the retirement age? Life expectancy vs. healthy life expectancy?

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Abstract. The European Commission has declared 2012 The European year for active aging and solidarity between generations. This issue calls each society to analyze the process of population aging and it’s social and economic consequences. Currently active aging can be the key to solve the demographic trends, because Europe is the continent with the slowest population growth. Current demographic trends are connected with low fertility rate, increasing number of seniors and increasing life expectancy. These unfavorable demographic changes have a socio-economic impact on society and this situation calls each society to deal with quality of life of older people and with their economic activity in the labor market. Submitted study follows the question of increasing the retirement age as a possible way for growing economic activity of the post-productive population. We ask whether increasing the retirement age is beneficial or not. Extending life expectancy may have a positive effect on the productivity of seniors and their life satisfaction in case seniors live and work in good health without diseases. The aim of this work is to characterize the evolution of population aging and compare life expectancy and healthy life expectancy in the Czech Republic and in selected European countries. Another aim is reflecting the retirement age and highlighting its likely future development – how far is it possible to extend the retirement age?

Keywords: aging of population, retirement age, healthy life expectancy.

1 Introduction

Current demographic trends show that population aging in Europe means an unstoppable process for the following decades. From social and cultural aspect we talk about the positive development of civilization. Seniors live longer, compared with the pre-war period. Thanks to advanced medicine and technologies, many of them are able to work and satisfy their needs. However, population aging has significant consequences in the area of public resources. Extending life expectancy creates pressure on the need of large financial resources from public budgets, particularly in the area of pension security and health system.
In EU countries we see the extending retirement age. In this connection we should answer the question about growing proportion of the elderly and their potential usefulness. Seniors represent a significant part of the total market demand of consumer goods and services. What is more, they are able and willing to work and are important for the labor market because they can pass on their acquired knowledge and experience to the next generations. Ability, willingness and need of the elderly to work is connected with satisfying their needs. All around Europe, we daily talk about modernization and reform of the pension systems (e.g. increasing the retirement age) that is necessary for sustainability of the pension systems. The purpose of this study is to analyze current demographic processes and their expected effect on the number of old people. We present calculations of the increasing retirement age in current demographic environment. Calculations are directed in following areas: dependency rate of older people, growing life expectancy forecasts and retirement age forecasts.

2 Basic data

To judge whether the increase in retirement age is significant in terms of human life and health we use the comparison of the human life expectancy, healthy life expectancy and the current retirement age.

Life expectancy (LE) represents number of years that an average person lived with presumption, if structure of mortality remained at the same level as in the year. It is a hypothetical figure. This indicator is most often used as the life expectancy at birth, which is the average life span of just born children. If the person overcomes the risk of death in infancy and childhood, his life expectancy will increase. Therefore, we are working besides the life expectancy at birth with the life expectancy at age of 65, which is the most common age of retirement. (ČSÚ [2])

The indicator of healthy life expectancy (HLE) represents the average number of remaining years of life that a person of specific age lives in good health, i.e. without any health limitation. It attempts to characterize not only the quantity (expressed in number of lived years), but also the quality of life, with its division of the part lived in good health and the part of lived in the disease (with physical limitations). This indicator is measured subjectively, based on the question whether the respondent was in last six months somehow limited in his activities because of health problems, with three possible answers: very limited, limited and unlimited. Therefore, it needs to be heedful at interpretation of results and in particular in international comparison. Although the data come from surveys harmonized across the EU, the respondent’s answers may be influenced by various social or cultural influences. The Healthy life expectancy we present at birth and also at the age of 65, separate for men and women. (ÚZIS [10])

The retirement age (RA) is gradually increasing not only in the Czech Republic. It increases by two months for men and about 4 months for women every year since 1996. Now the retirement age in the Czech Republic depends on the year of birth and number of children. For simplicity, at present we expect
to age of 62 for men and age of 58 for women with two children. According to the current legislation, the rising of retirement age should stop at age of 67 for both men and women born by 1977. For people born after 1977, the retirement age will determined by the age of 67 with addition of the number of calendar months, which corresponds to double of difference between the year of birth and year of 1977. (CSSZ [4])

For comparison with the situation in the Czech Republic we chose five European countries. We chose Slovakia (as our closest neighbors), Romania, Sweden, the Netherlands and Spain, which are representatives of countries from different parts of Europe (north, south, west and east). For all European countries would be difficult to harmonize the data, because some countries do not publish a healthy life span.

3 Results – Is it possible to extend the retirement age?

In this part of the paper we reflect on increasing the retirement age, if it is beneficial or not. Extending life expectancy may have a positive effect on the productivity of seniors and their life satisfaction in case seniors live and work in good health without diseases. We characterize the evolution of population aging and compare life expectancy and healthy life expectancy in the Czech Republic and in selected European countries.

With comparison of life expectancy and healthy life expectancy at birth we obtain some information about the part of life lived in good health.

![Fig. 1. Life expectancy and healthy life expectancy at birth and at age of 65 in 2001 and 2011](image)

In figure 1 we can see how life expectancy varies by sex, whereas healthy life expectancy does not. Life expectancy of born women was 81.1 years in 2011, born men lived only 74.8 years on average in 2011. Compared to 2001, we can see in the figure the increase in life expectancy at birth by 2.5 years for women and 2.7 years for men. Healthy life expectancy at birth hasn’t changed between 2001 and 2011. Born men had healthy life expectancy about
62 years in 2001 and also in 2011, born women are the same, their healthy life expectancy was 63 years in both compared years. The comparison of life expectancy and healthy life expectancy in age of 65 is better. Life expectancy for men aged 65 was 14 years in 2001 and it increased to 15.6 years until 2011. Healthy life expectancy of men aged 65 did not increase in the reference period even decreased from the value of 9.5 to 8.4 years. Women aged 65 had the life expectancy 17.3 years in 2001 and 19.2 years in 2011, in good health they spent 8.4 years in 2001 and 8.7 years in 2011. Life expectancy of men and women in the Czech Republic is rising, while the healthy life expectancy has not changed, for men it has even slightly decreased.

In the figure below there is the difference in the life expectancy among regions; the aging of population along with current economic situation affects some European countries more than others. This figure shows comparison of life expectancy at age 65 years, healthy life expectancy at 65 years and the retirement age in some chosen European countries in 2011. Life expectancies at age 65 are increased by a constant 65.

![Fig. 2. The comparison of life expectancy at age of 65, healthy life expectancy at age of 65 and retirement age in several European countries in 2011](image)

The retirement age is still a matter for national legislation in the Member States, it is not harmonized. The retirement age is different; currently it is set usually between 60 to 65 years (ČSSZ [3]). It is interesting to compare the healthy life expectancy and retirement age in some European countries. The set retirement age is lower than healthy life expectancy in all chosen countries. Noticeable difference is in Sweden, where the age of retirement is lower than the healthy life expectancy at age of 65 about 14 years for men and 16 years for women. It is evident that it is possible in all selected countries continue to increase the retirement age within the pension reforms due to alleviation the impact of aging population. If the healthy life expectancy at retirement age is lower, it would not be effective to increase the age of retirement.

In connection with the retirement age is also interesting to look at the rates of economic activity around the age of retirement in European countries.
Many Europeans don’t want and can’t work to the retirement age established by state, so with the increasing age of retirement grows the number of people benefiting from opportunities to take early retirement. Although early pension is less than classic retirement pension, the popularity of early retirement in Europe is rising. People create during their economically active life their own savings, which are higher for many of them than the state retirement pension and they go into early retirement.

The economic activity rates of men at the age of 55 to 59 exceed 80%, except for Spain and Romania (see figure 3). At the same age, there are around 60% economically active women in chosen European countries; the exception is Romania again, where the economic activity rate of women is only 60%. On the other hand, the highest economic activity rate at the age of 55 to 59 is in Sweden, where are 83% economically active women. At the age of 60 to 64 years, which is a transition group between working life and retirement, there isn’t economically active nor half of population. The exception is Sweden again, where the level of economic activity remains high in both sexes until the end of their working life. View of Romania is interesting, because it has approximately the same level of economic activity rates at the age of 60 to 64 and of 65 to 69 years contrary of the other countries. Very few people are economically active around retirement age in all countries. At the age of 65 to 69 years there are economically active only about 20% people, the lowest level of economic activity have women in Slovakia – only 3%.

4 Discussion – How can we measure active aging?

Population aging is aglobal phenomenon, which needs to be analyzed, finding possible solutions and develop an effective plan for the future challenges of population aging.

The key for active and healthy aging can be the process of lifelong learning and volunteering. Education of the elderly and voluntary work of older people
should be encouraged at national and regional levels, as well as at EU level. In this way we can prolong their working life and support activities in retirement age. We remind that active aging is the key problem and key objective for Europe’s next years and that’s why it is important for local and regional authorities to be involved in making necessary strategies. We believe that supporting active aging and solidarity between generations will bring economic benefits in the EU and also at the national and local level.

Active aging is creating opportunities for older people to stay healthy and stay at work and contribute to the wealth of society.

Active aging:

• gives older people the opportunity to fully participate in society,
• supports job opportunities for seniors,
• enables older people to actively participate in voluntary work (usually as family caregivers),
• enables to live independently due to the modified infrastructure, housing and transport.

In the context of the European Year for Active Aging and Solidarity between Generations (2012) a construction of an appropriate index was needed. Active aging can be measured by Active Aging Index (AAI) which measures the potential of the elderly for active and healthy aging across countries. It measures the level of independent living, participation in paid employment, social activities and capacity for active aging of the elderly. That means that the Active Aging Index consists of these four domains that create the Overall Active Aging Index.

In figures 4, 5, 6 below we can see contribution of domains to the overall index. We considered both men and women together.

Figure 4 informs us about participation of population aged 55+ in society including voluntary activities, care to children and grandchildren, care to older adults and political participation. The main goal of this domain is to describe
the unpaid activities of older people like voluntary activities, care or political activities. As we see, the main activity of the elderly is taking care for their children or grandchildren. In Netherland, the proportion of those who do voluntary activities, is 34%. By volunteering, they feel beneficial while helping others.

Figure 5 represents some chosen indicators for the domain independent, healthy and secure living. Parts of this domain are physical exercise, physical safety, independent living possibility, lifelong learning, access to health care and no material deprivation or risk of poverty. Indicator of access to health care is very important for older people because healthcare is essential to their active, independent and healthy lives. As we can see in this figure, this indicator obtains in each of the countries and moves between 20% and 30%.

From figure 6 we see the capacity for active aging. The most important indicators are Remaining Life Expectancy (RLE) and Healthy Life Years (HLY). HLY measures years spent without activity limitation. In modern society, information and communication technologies (ICT) are an unthinkable part of our everyday lives. Using ICT measures how older people stay in touch with their environment. For old people meeting their relatives, friends means staying fit and vital, fulfilling their active life.

The contribution of four mentioned domains to the overall active aging index in selected EU countries is presented in the figure below.

For example, the relative contribution of the domain capacity for active aging to the AAI is the highest in Spain (34,5%). Country with the highest relative contribution of the domain independent, healthy and secure living is Slovakia (24,2%). When looking at social participation, the contribution of this domain to the overall index is the highest in Netherlands (20,1%) and the lowest in Romania (14,6%). Finally, Romania is the country with the highest contribution of the domain employment to the overall index (35,5%). On the other hand, Spain is quite behind from the same domain (25,1%).
5 Conclusion

The aim of this paper was the reflection on increasing retirement age in connection with the problem population aging. We compared the life expectancy and healthy life expectancy in the Czech Republic and a few selected European countries with reference to retirement age. The purpose was decision on whether extending of life expectancy has a positive effect or there are only rising years lived in diseases and the question of benefits of increasing retirement age.

A comparison of the healthy life expectancy at age of 65 years to retirement age in particular European countries has shown the possibility of increasing the retirement age, because it is still the time spent in good health. The healthy life expectancy at the age of 65 is higher than retirement age about 10 years on average, the life expectancy at age of 65 even more about 20 years. The data on economic activity rates by sex and age shows that only a small percentage of people are economically active before retirement age. The reason for this situation is the ability to take early retirement. Some people in this age have
already enough saved up and have a little motivation to remain in the workforce longer than necessary.

Many of the seniors have health problems or limitations in daily activities and these products may help them to satisfy their specific needs. Developing a range of products and services oriented on the needs of seniors represents the growth potential of the EU countries. Particular attention should be given to the existing institutions for seniors, especially emphasizing their high price that means for most of the seniors a big problem. What is more, there are not enough nursing homes – it would be necessary to extend these institutions.

It is important to realize that population aging doesn’t mean exclusion. For people in the third age money isn’t the factor which means unconditional happiness. What they really want is an important and useful role not only in the family, but also in the society they live in. Old age is not equal to lack of action – seniors can be active participants in our society – in case the society really wants and needs them to be.

References

Multiple Population Projections by Lee Carter Models

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Abstract. The academic literature in longevity field has recently focused on models for detecting multiple population trends ([9],[17],[20], etc.). In particular increasing interest has been shown about “related” population dynamics or “parent” populations characterized by similar socio-economic conditions and eventually also by geographical proximity. These studies suggest dependence across multiple populations and common long run relationships between countries (for instance see [13]). In order to investigate cross-country longevity common trends, we adopt a multiple population approach. The algorithm we propose retains the parametric structure of the Lee Carter model, extending the basic framework to include some cross dependence in the error term. As far as time dependence is concerned, we allow for all idiosyncratic components (both in the common stochastic trend and in the error term) to follow a linear process, thus considering a highly flexible specification for the serial dependence structure of our data. We also relax the assumption of normality, which is typical of early studies on mortality [14] and on factor models (see e.g. the textbook by [1]). The empirical results show that the Multiple Lee Carter Approach works well in presence of dependence.

Keywords: Serial and Cross-sectional Correlation, Factor Models, Vector Auto-Regression, Sieve Bootstrap, Lee Carter model

1 Introduction

In the last few years, in the actuarial literature, has been demonstrated the improvement of the mortality projections for individual countries by taking into account the patterns in a larger group [15]. Thus, it has been highlighted that investigating long-run equilibrium relationships might provide valuable information about the factors driving changes in mortality, in particular across ages and across countries. This aspect has contributed to the growth of the interest in studying cross-country longevity common trends. For this reason, we
have observed a development of country and age-based longevity risk models ([13], [17],[20]). The existence of dependence in mortality data involves the interactions between age and time. In fact, the mortality experience of countries in the industrialized world over the course of the twentieth century would suggest a substantial age-time interaction: two dominant trends affect different age groups at different times. In order to study cross-country longevity common trends, it is essential to consider tools to quantify, compare and model the strength of dependence. Therefore it is necessary to take into account either the dependence for adjacent age groups, or the dependence structure across time in a single population setting: a sort of intra-dependence structure [9]. At the same time, it is important to consider the dependence across multiple populations, what we call inter-dependence, for capturing common long run relationships between countries.

In this contribution, we keep on taking into account the issue of cross-sectional and time dependence, by proposing an algorithm based on the Lee Carter framework [14], but relaxing the assumption of normality, which is typical of early studies on mortality and on factor models (see e.g. [1]).

We also consider a bootstrap procedure for dependent data, thus preserving both the historical parametric structure and the intra-group error correlation structure. In particular, we apply a sieve bootstrap algorithm [5] to the Vector AutoRegression (VAR henceforth) model containing the estimated common factors (both stationary and no stationary). However, in a previous paper [8] we stated that in our context we cannot apply a standard sieve bootstrap algorithm, since, when resampling the estimated common factors, a generated regressors problem arises. In this order of ideas, our paper bases on Trapani [22], which develops the full blown theory to apply sieve bootstrap to the context of no stationary panel factor series, developing selection rules for the order of the VAR and showing the superior performance of sieve bootstrap compared to first-order asymptotic. In particular, the paper is structured as follows: Section 2 deeps the scheme of multiple alignment of different populations. In section 3, we propose a flexible approach of the Multiple Lee Carter Panel Sieve. Concluding Remarks are presented in Section 4.

2 The Multiple Alignment

The representation of multiple populations founds on similar mortality behaviours typical for people which share analogous living conditions. Studying mortality experience for a group of populations with similar mortality behaviours might improve the stability of mortality modelling [23] and allow for solving the problem of small population. Indeed some authors propose the replication of the data by mixing appropriately the mortality data from neighbouring countries [18]. To handle the joint development across different populations of mortality rates a new framework needs to introduce cross
sectional dependence for adjacent age groups, across countries and serial/time dependence.
The first step is characterized by the correct alignment of the data related to the countries under consideration. The alternatives are several like pairwise alignment, alignment by age, by time or by clusters or neural networks.
In this paper the common trends are represented by the separately fitted parameters $k_i$ of the Lee Carter model in its Poisson version [19] on the $M$ different populations composed by the same ages $x = a, a + 1, \ldots, a + N$ and years $t = b, b + 1, \ldots, b + T$, where $a$ respectively represents the first age and $b$ the first time.
The multiple panel data is obtained by collecting by rows the $M$ time series of $k_i$ in a matrix we use for performing the algorithm explained in Section 3.

3 Multiple Lee Carter Panel Sieve: a flexible approach

D’Amato et al. 2012 [9] develops the idea of first fitting Lee Carter parametric model, because of its well known properties [11] and then re-sampling a particular class of the residuals, the so-called centred residuals, according to the sieve scheme, through an autoregressive approximation for generating bootstrap replications of the data. In particular, they make use of the main statistical tool of the Lee Carter method, the least-square estimation, based on the hypothesis of homoskedastic errors. However, as it is shown by the empirical evidence, the validness of this assumption has been rejected. The Poisson log-bilinear model allows for overcoming the problems associated with the OLS method in the fitting procedure. Because the number of deaths is a counting random variable, according to Brillinger [3], the Poisson assumption appears to be plausible. It has been argued that the number of deaths when the central exposed-to-risk is given may be assumed to follow Poisson distribution and the promising estimates may be obtained by fitting the Poisson regression (see [19]):

$$D_{x,t} \approx \text{Poisson}(E_{x,t}, \mu_{x,t}) \text{ with } \mu_{x,t} = \exp(a_x + b_x k_t)$$

(3)

where the parameters are still subjected to the constraints $\sum_t k_t = 0$ and $\sum_x b_x = 1$ and force of mortality is thus assumed to have the log-bilinear form:

$$\ln(\mu_{x,t}) = a_x + k_t b_x.$$ 

Recently the Poisson version of the Lee-Carter model has been deepened and applied in actuarial literature. Some essential improvements have been introduced by [4]. They estimate parameters by Poisson log-bilinear regression and [19] describes the model in the GLM terms. In the light of this
consideration, we exploit the Poisson version of the Lee Carter model in the Panel Sieve bootstrap, as an extension of the model shown in [8] and present the following bootstrapping algorithm:

Step 1. Estimation of the parameters and residuals of the Poisson Lee Carter:

(1.1) Estimate the $\beta_s$ and $k_t$ in (2) through the Poisson version of the Lee Carter model.

\[
\hat{\beta}_s = \sum_{y} \hat{y}_{s,t} \cdot \hat{k}_t - \hat{\beta}_s \cdot \hat{k}_t
\]

(1.2) Generate the residuals $\hat{u}_{s,t} = y_{s,t} - \hat{\beta}_s \cdot \hat{k}_t$ and define

\[
\hat{\xi}_{s,t} = \left[ \hat{\Delta k}_t, \hat{u}_{s,t} \right].
\]

Step 2. Estimation of the autoregressive processes

(2.1) Estimate $A_{q,j}$ and $\gamma_{q,j}$ by applying OLS to (5) – after replacing $u_{s,t}$ and $\Delta k_t$ with their estimated counterparts.

\[
\hat{A}_{q,j} = \sum_{j=1}^{qK} \hat{A}_{q,j} \cdot \hat{\Delta k}_{t-j}, \quad \text{and}
\]

\[
\hat{e}_{s,t,q} = \hat{u}_{s,t} - \sum_{j=1}^{qK} \hat{\gamma}_{q,j} \cdot \hat{u}_{s,t-j}, \quad \text{and define}
\]

\[
\hat{e}_{s,t,q} = \left[ \hat{\xi}_{s,t}, \hat{\Delta k}_t, \hat{e}_{s,t,q} \right],
\]

center the residuals around their mean, defining them $\hat{\xi}_{s,t,q}$.

Step 3. (bootstrap) for $b=1,...,\mathcal{T}$ iterations

(3.1) (resampling)

(3.1.a) Draw (with replacement) $T$ values from $\{\hat{e}_{s,t,q}\}_{i=1}^{T}$ to obtain the bootstrap sample $\{\hat{e}_{s,t,b}\}_{b=1}^{T}$, where we define

\[
\hat{e}_{s,t,b} = \left[ \hat{\xi}_{s,t,b}, \hat{\Delta k}_{t,b}, \hat{e}_{s,t,b} \right].
\]

(3.2) (generation of the bootstrap sample)

(3.2.a) Generate recursively the pseudo sample

\[
\hat{\xi}_{s,t,b} = \left[ \hat{\Delta k}_{t,b}, \hat{u}_{s,t,b} \right] \quad \text{as} \quad \hat{\Delta k}_{t,b} = \sum_{j=1}^{qK} \hat{A}_{q,j} \cdot \hat{\Delta k}_{t-j,b} + \hat{e}_{s,t,b}
\]

and

\[
\hat{u}_{s,t,b} = \sum_{j=1}^{qK} \hat{\gamma}_{q,j} \cdot \hat{u}_{s,t-j,b} + \hat{e}_{s,t,b}, \quad \text{using as initialisation}
\]

\[
\left\{ \hat{\xi}_{s,t,b}, ..., \hat{\xi}_{s,t,b} \right\} = \left\{ \hat{\xi}_{s,t}, ..., \hat{\xi}_{s,t} \right\}.
\]
(3.2.b) Generate $k_{t,b}$ as $k_{t,b} = k_{0,b} + \sum_{j=1}^{T} \Delta k_{j,b}$, with initialisation $k_{0,b} = k_0$.

(3.2.c) Generate the pseudo sample \( \{ y_{st,b} \}_{s=1}^{r} \) as

\[
y_{st,b} = \hat{\beta}_x k_{t,b} + u_{st,b}.
\]

The advancement of the research consists into use a more accurate fitting procedure of the mortality data, based on the Poisson version of the Lee Carter model. In this way, the bootstrap algorithm successively applied to the parameter $K_t$ offers more appropriate estimates of the mortality. We highlight that this improvement has been made possible thanks to the flexibility of the procedure developed in [8].

4 Concluding Remarks

The actuarial literature reveals an increasing interest about modeling multiple populations characterized by similar socio-economic and living conditions. The problem which arises from simultaneously considering different countries is strictly related to the dependence analysis. The dependence structure emerges for adjacent age groups, across age and time and also across the different populations. From a methodological point of view, we retain the parametric structure of the Lee Carter model in its Poisson version, extending this basic framework to include some cross dependence in the error term on the basis of a tailor-made bootstrap algorithm which we explain in details in section 3. Further researches will be oriented to consider the flexibility of the framework in the context of other models.

References


Towards Dynamic Bayes Networks to model Time Series from the WatSan4Dev subset

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Abstract

Water assumes a similar key role if considering human/society development: water supply heavy burden and lack of sanitation slows down the economy, social improvement and population well-being. However, millions of people lack access to drinkable water (894 million) and/or basic sanitation (2.5 billion). A current research of the Joint Research Centre – European Commission, has developed a coherent database (WatSan4Dev) to identify the most influential variables on Water Supply and Sanitation (WSS) services in developing countries. The WatSan4Dev dataset is constituted of official indicators provided by international agencies. The 25 variables selected are organized into five thematic areas (water resources, human activity pressure on water resources, country environmental concern, human development and official development aid) for 101 developing countries.

The objective of this work is to develop Dynamic Bayesian Networks (DBNs) to model time series from the WatSan4Dev subset. Three temporal points (2000, 2004 and 2007) are used to create two different DBNs (one for water supply and another for sanitation) based on six composite variables. The BNs set links between the three time slices to create a unique network. The error rates of the query variables (WSS) were below 11%, allowing using the networks to run and analyze different scenarios. This tool is useful to orient and support decision/strategy making related to WSS and beyond, to human development. Methods and progresses made towards dynamic model (DBNs) are presented.

Keywords: Water Supply and Sanitation services, Bayesian networks, time series, sustainable development, Millennium Development Goals

1 Introduction

On the World Water Day 2013 the UN highlighted the reality that “the fulfilment of basic human needs, our environment, socio-economic development and poverty reduction are all heavily dependent on water”. Rapidly increasing urbanisation, pollution and climate change are threatening this resource, while at the same time demand water is increasing. More water than ever is needed for the food production, energy and industrial and domestic uses of an ever-increasing global population. 25 variables selected from the WatSan4dev database (Dondeynaz et al, 2012) are used and organized into five thematic areas (water resources, human activity pressure on water resources, country

http://www.unwater.org/statistics_san.html

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This paper looks at extending the Bayesian Networks (BNs) modelling of this subset (preliminary done for 2004) to the time period 2000-2007 (Fig.4). The retrospective modelling approach is adopted to integrate past records and simulate variables status to reach user-defined targets. Running simulations allow the analysis of impacts and sensibility of the different variables involved in the water sector. The paper focuses on the development of the methodological approach. The data recorded at three temporal points, 2000, 2004 and 2007, have been retained. Therefore, section 2 summarises the review of the data series for the different years (2000, 2004, 2007), while section 3 provides details on DBNs methodology. Section 4 describes the DBNs model build and their performance using a retrospective approach.

2 Data review

The variable selection builds on the prior work performed for 2004 and is fully described in Dondeynaz et al (2013). Table 1 describes variables selected, their classification in pillars and the missing data rates. These pillars were defined according to the first six components of the Principal Component Analysis (PCA, namely Human Development Poverty (HDP), Activity Pressure (AP) and Country Environmental Concern (CEC), Water Resource (WR) and Official Development Assistance Composite indicator (ODA CI). The period spans three temporal points: 2000, 2004, and 2007. Prior to 2000, data present high levels of missing data for developing countries, even for demographic and socio-economic variables. Environmental variables are scarce with only the datasets for 2004 showing acceptable missing data rates— in particular the water withdrawal variables for 2000 and 2007 presented missing data rates of above 70% when collected. Water resources are considered to have been constant over this 10 year period. The AP and CEC pillars were the most affected by missing values (total withdrawals, water withdrawals for industries and municipal purposes) and by the absence of variables (water use intensity in agriculture and participation in international environmental agreements). The continuous updating of water demand data (withdrawal indicators) could address the high rate of missing data in the near future.
Proceedings, 15th Applied Stochastic Models and Data Analysis (ASMDA2013) 
International Conference, Mataró (Barcelona), Spain 25 - 28 June 2013

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**Table 1:** Overview of data series availability and percentage of missing data for 2000, 2004 and 2007

### 3 Dynamic Bayesian Networks: Methodology and Application

#### 3.1 Dynamic Bayesian Networks

Dynamic Bayesian Networks (DBNs) or Temporal Bayesian Networks are probabilistic graphical models oriented to model time series data structures. Although the theoretical origins of those statistical techniques could be tracked to the late 1980s (i.e. Dean and Kanazawa, 1988 and 1989; Cooper et al., 1989), these directed acyclic models are relatively less common than their static counterparts (Nagarajan, Scutari & Lèbre, 2013).
Considering three variables $Y_n$, $Y_i$, $Y_j$, the intra-slice edges i.e. $Y_n \rightarrow Y_i$ and inter-slice edges i.e. $Y_i \rightarrow Y_{i+1}$ or $Y_i \rightarrow Y_{i-1}$, the DBNs proceed as follow:

Fig.1: Dynamic Bayesian networks structure and organisation (adapted from Nicholoson and Krob, 2004)

DBNs can be described as a probability function for the sequence of $T$ hidden-state variables $X = \{x_1, \ldots, x_T\}$ and the sequence of $T$ observables variables $Y = \{y_1, \ldots, y_T\}$, where $T$ is the time boundary for the event being investigated (Mihajlovic and Petkovic). It can be expressed as

$$B_r(x, y) = \prod_{t=1}^{T} P_r(x_t | x_{t-1}) \prod_{t=1}^{T} P_r(y_t | x_t) P_i(x_0)$$

where three sets of parameters need to be defined:

- Transition state of the probability distribution functions $P_r(x_t | x_{t-1})$ that specifies time dependencies between states or times slices.
- Observation of the probability distribution functions $P_r(y_t | x_t)$ that specifies dependencies of observation nodes as they relate to other nodes at time slice $t$.
- Initial state distribution $P_i(x_0)$ that outlines the initial probability distribution at the beginning of the process.

DBNs are useful when modelling time-dependent and dynamic problems, like those found in meteorological forecasts and population growth forecasts and the areas of robotics and speech recognition (i.e. Zweig, 1998). Zweig (1998) summarises the advantages of using DBNs in modelling temporal processes as follows: 1) the DBNs handle non-linear behaviour through the use of a “tabular representation of conditional probabilities”; 2) the interpretation process is facilitated by the fact that each variable represents a specific concept; 3) the maximum factorisation of the joint distribution favours both statistical and computational efficiency; 4) the DBNs can handle a large number of variables that could then be included in the graph structure; and 5) the DBNs have “precise and well-understood probabilistic semantics”.

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3.2 Structuring the models
Each time slice is modelled according to a structure based on preliminary multivariate analysis which is identical for three temporal points (Dondeynaz et al, 2013). Indeed, the PCA confirms that variables organised themselves similarly over that period (Fig.3). The different directions of relationships are set in this paper with a particular focus on the conditional link between CEC, AP and WSS. The WR indicator is removed, having proven to have little influence on WSS and to be a constant over the different years (Dondeynaz et al, 2013). Figure 2 presents the model’ structure (nodes and links) used for each time slice. The links are set according to the correlations observed (in PCA).

![Fig.2: Principal component analysis including 2000, 2004 and 2007, where F1 is the green axis, F2 the red axis and F3 the size of the dots. The three first components explain 65.23% of the total variability.](image)

3.3 Input data processing
The variables were grouped and computed using two composite indicators—Human development and Poverty (HDP) and Official Development Assistance Composite Indicator (ODA CI)—and multivariate analyses for each year:

- HDP includes income (Gdp per cap), the proportion of urban population (Urban pop), the girls’ attendance at primary school (School G/B), the school enrolment rate for both sexes (School enrol), the women economic
participation rate (women eco), the proportion of the population living in slums (% slums), the prevalence of malaria (Malaria), the child mortality rate under five years (Child Mortal-5) and the governance effectiveness index (WGI GE).

- ODA CI is computed using the amount of Official development Aid (ODA), the specific amount of ODA dedicated to WSS (ODA WSS) and the political stability and absence of violence index (WGI PSAV).

Each variable is normalised with the appropriate standard method. Urban Pop, School Enrol, Women eco, WGI-GE and WGI PSAV are by virtue of their nature already normalised. The proportion of irrigation in agricultural areas (% irrigation) and the voice and accountability index (WGI VA) are included as a single variable like the Water supply and Sanitation variables. As the Bayesian Networks method deals with non-normal distribution, these variables are kept in their original format.

The variables are discretised in three categories (High, Mid and Low) with common limits for the three years (Table 2). WSS variables are categorised according to the MDG targets (88% of worldwide population having access to improved WS and 75% to basic sanitation – UN., 2012).

4 Description of the temporal models for WS and S (Fig.4)

The performance for the WS model exceeds 87% of correct classification, with a better estimation for the low categories than the high categories and the 2004 and 2007 years (Table 3). The statistical performance is estimated by estimating the Error Rate, Logarithmic Loss (LL), Quadratic Loss (QL) and Spherical Payoff (SP) coefficients. The main parameters that influence the 2007 WS variable are the previous state of WS (2004), HDP in 2007, Irrigation (2000 to 2007) and WS in 2000. The previous states of HDP and WGI VA are of medium importance. The external financial flow (ODA CI) has the least influence (Table 3).

The performance level of the S model reaches at least 90%, with better estimations for 2007 and 2004 and the Low category. The sensitivity analysis is similar to the one from the WS model. The first six variables provided are, in order, S in 2004, HDP in 2007, Irrigation (2000 to 2007) and S in 2000. The ODA CI and WGI VA levels in 2000 come last. The main divergence with the WS model resides in the fact that ODA CI variable ranks slightly higher than WGI VA, in contrast to the WS sensitivity analysis.
Table 3: Performance parameters of WS and S models with results of the 2007 sensitivity analyses for WS and S

WS Model | Low | CL | SS | S Model | Low | CL | SS
---|---|---|---|---|---|---|---
WS, 2004 | 1.82% | 0.02 | 0.02 | S, 2004 | 1.59% | 0.02 | 0.02
WS, 2003 | 1.84% | 0.02 | 0.02 | S, 2003 | 1.59% | 0.02 | 0.02

| Low | CL | SS | rank |
---|---|---|---
WS, 2004 | 1.82% | 0.02 | 1 | S, 2004 | 1.59% | 0.02 | 1
WS, 2003 | 1.84% | 0.02 | 1 | S, 2003 | 1.59% | 0.02 | 1

*nodes for 2000 are in yellow, nodes for 2004 are in red and nodes for 2007 are in green

Fig. 3: DAG of W model and initial probabilities (same structure is used for Sanitation)

This type of model offers the advantage of being able to learn from the past by integrating past records. The analysis of initial probabilities provides a detailed and direct overview of trends on the period. This tool also allows a running
retrospective simulation setting a user-defined target: for instance, 100% of the selected countries have reached the 88% of access to improved WS (MDG target). The high category for WS 2007 is set to 100% and the simulated probabilities are recomputed by the model and then, are compared with the initial state (IS). The difference provides an estimation of efforts/impacts that would be necessary to reach the target.

5. Conclusions
These retrospective models are supporting tools that facilitate our understanding of multiple variables trends that occurred over the 2000-2007 period. Bayesian networks allow computing the initial state (IS) so as to describe the probabilistic distribution of each variable for each time slice. When modifying one or several parameters, the initial probabilities are recomputed to provide an estimation of the variables according to new conditions set. Their statistical performance was good, with classification error rates of below 12%, and therefore the models fit the data well. WS and S are sensitive in a similar way, as the six first variables involved in the WSS changes are identical. The S model is slightly more sensitive to ODA CI, while WS is slightly more sensitive to WGI VA. This similarity may be due to the scale (101 countries) and synthetic nature of the indexes, which may mask potential divergences in detail (either within a country or within sub-indicators).

Beyond the quantitative and probabilistic analysis of the dataset, the models allow running retrospective scenarios, modifying parameters of variables. As example, the achievement in 2007 of the MDG targets for WSS (88% WS and 75% S) could be simulated for our countries; the model re-computing the estimation of previous variables probabilistic states/distributions.

For simulation, the number of temporal points included in such a model is crucial to how well it can identify mid-long term trends. The limited time period implies high probability changes to achieve the targets set in simulations. These estimated probabilities are therefore difficult to implement in reality. The extension of the observation period would reinforce the progressivity of the changes needed and provide achievable estimations.

The retrospective approach appears to be a robust approach. The development of a predictive/forecasting approach could complement this work in an interesting way. The development of this complementary approach requires further research.

References
Modeling of mortality of the Czech and Spanish populations

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Abstract. Mortality is recently very important topic, not only for demographers. It is due to its connection with a discussed topic of population aging. Based on the analysis of population mortality in European countries, it is clear that there is a gradual improvement in mortality. This development is due to the increasing level of medical care, and also the growing interest of people in a healthy lifestyle. This leads to a gradual lengthening of life expectancy at exact age x and thus to improve mortality rates. This development means that more and more people live to the highest ages. Previously, there was no need to pay close attention to the oldest-old mortality, because the highest ages lingered only a small number of people. Recently, the situation is changed. More and more people live to the highest ages. Still, however, that the oldest-old mortality is different from the mortality of younger persons. For this reason, it is necessary to model mortality of oldest persons. Previously, was the most used Gompertz-Makeham function. The development means that it is necessary to look for new models. Among the most popular are logistic models. In this paper we will analyze the mortality of Czech and Spanish population. The selected logistic models (Thatcher and Kannisto) will be applied on disposable data about mortality. The results will be compared with previously most common Gompertz-Makeham model. The aim is to determine which of these models the best describe mortality in both countries. The second aim is to determine if there are any changes during the reporting period. In the last part we will compare mortality trend in both countries.

Keywords: mortality, Gompertz-Makeham function, Kannisto and Thatcher model.

1 Introduction

Mortality has been very interesting topic for a long time for demographers. The Gompertz-Makeham (or modified Gompertz-Makeham) function was the most frequented model in the previous years. Now the situation is a little bit different. People live longer. It means changes in the mortality of the oldest persons. This is the reason why it is so important to create new model. Logistic models are the most preferable in these days. On the other hand it is very important to know that for different population is good to use different model.
2 Methodology

The life expectancy is very frequent indicator for analysing of mortality. We can find it in the mortality tables. The life expectancy means how long can somebody live (in average) [5], if the mortality rates are the same for the whole life of somebody. The calculation of the mortality tables consists of several parts. The first one is the calculation of the specific mortality rates:

$$m_{t,x} := \frac{M_{t,x}}{S_{t,x}}. \tag{1}$$

Where $M_{t,x}$ is the number of deaths at exact age $x$ and in the year $t$, $S_{t,x}$ is the mean number of living people. It is very important to realize that we can have problems with calculation of the specific mortality rates at the highest ages. The reason is small number of deaths at the highest ages. That is why we need to use some of the existing models used for extrapolating mortality curves (for example the Gompertz-Makeham, Kannisto or Thatcher model). These models will be used for extrapolating specific mortality rates. For own calculation we have to use the extrapolated specific mortality rates. The other parts include calculations which we need for calculation of the life expectancy. In this paper we will present the Thatcher and Kannisto model [2], [6], [1]. The results will be compared with the mortality tables without extrapolation and with the Gompertz-Makeham model [3], [4].

**Thatcher model:**

$$\mu_x := \frac{z}{1 + z} + \gamma. \tag{2}$$

Where $\mu_x$ is the intensity of mortality at the exact age $x$, $z$, $\gamma$ are parameters of the model and $x$ is age.

**Kannisto model:**

$$\mu_x := \frac{\exp(\theta_0 + \theta_1 \cdot (x - 80))}{1 + \exp(\theta_0 + \theta_1 \cdot (x - 80))}. \tag{3}$$

Where $\mu_x$ is the intensity of mortality at the exact age $x$, $\theta_0$, $\theta_1$ are parameters of the model and $x$ is age.

**Gompertz-Makeham function:**

$$\mu_x := a + b \cdot c^x. \tag{4}$$

Where $\mu_x$ is the intensity of mortality at exact age $x$, $a$, $b$, and $c$ are parameters of the model. Assumption for the Gompertz-Makeham function is the constant increase of the intensity of mortality with the increasing age. The last step includes calculation of complete life tables. We use it for an algorithm for calculation of complete life tables.
3 Mortality

In this part we will present the results for the Czech and Spanish populations. The results will be presented separately for men and women and for selected ages. The attention is focused on the period from 1970 to 2010. Data was taken from Eurostat database and Human mortality database.

<table>
<thead>
<tr>
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<th>0</th>
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<th>20</th>
<th>50</th>
<th>65</th>
<th>80</th>
<th>85</th>
<th>90</th>
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<td>54.9</td>
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<td>3.2</td>
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Table 1. Life expectancy - Czech Republic - men

If we compare the results obtained from the mortality tables without extrapolation with the selected models, we can see that the life expectancy from life tables without extrapolation is the highest one (this is true for every single age). On the other hand the Kannisto model is very optimistic. It gives us the highest life expectancy from selected models. It is not true for the Gompertz-Makeham model. It is the most pessimistic among the selected models. Values of the life expectancy according to the Gompertz-Makeham model are the lowest ones.

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<tr>
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<td>5.8</td>
<td>4.0</td>
<td>2.8</td>
<td>1.9</td>
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Table 2. Life expectancy - Czech Republic - women

From the results for Czech women we can see a little bit different situation from the Czech men. The life expectancy for women in the Czech Republic is higher than for the Czech men (it corresponds with the original assumption: women live longer in average than men). The other results are similar. If we focus on the selected models we can see that for example Kannisto model gives the highest values for the life expectancy.
If we look at the results for Spanish men we can see similar situation. For example the Gompertz-Makeham function is the most pessimistic one and the Kannisto model is the most optimistic model.

The situation for Spanish women is similar like for Czech women. The life expectancy is higher then for the Spanish men. The Kannisto model gives the highest values from the selected models for every single age.
In the figure 1 we can see that the life expectancy for the Czech men is increasing for the whole reporting period. It means that population of the Czech men will be older and older. If we look at the results more carefully, we can see that the life expectancy from the life tables without extrapolation is not the highest one for the whole period. Even at the beginning of the reporting period is the lowest one. On the other hand Kannisto model gives the highest values of it for the whole period.

![Life expectancy at exact age x - women - Czech Republic - 1970 - 2010](image)

**Fig. 2.** Czech Republic - women

The results for the Czech women are similar. The obtained values are higher (it is according to the original assumption). The values are increasing for the whole reporting period. It means that the population of the Czech women is getting older. The highest values gives the Kannisto model. Very similar results we can obtain from Thatcher model (it is true at the end of the period).
The results for the Spanish men mean that they are getting older (the values of the life expectancy are increasing). There is not so clear which model is the most optimistic one. If we compare the results we can see that we have very similar results for the Gompertz-Makeham and for the Kannisto model. The situation begins to change approximately from the year 2000. During this part of reporting period the Kannisto model gives the highest values of the life expectancy.
The situation for the Spanish women is very similar. The life expectancy is increasing for the whole period. If we look at the results more carefully we can see that the highest values of the life expectancy gives the Thatcher model. Very similar vaues we can obtain from the Gompertz-Makeham model. It is very interesting that the Kannisto model gives the lowest values. But it is very important to know that the value of life expectancy is dependent on selected model [4].

4 Conclusion

For the Czech and Spanish population it is true that they are getting older (the life expectancy is increasing). If we compare the results for the Czech and the Spanish population, we find out that the mortality is better in the Spain. The life expectancy is 3 years higher (at the beginning of the reporting period) and 4 years higher at the end of the period. The situation is similar for women but the differences are not so big. The life expectancy is approximately 3 years higher for Spanish women. When we study the results according to every single model, we can see that the Kannisto model is very optimistic. The Gompertz-Makeham model is very pessimistic (the values of the life expectancy are the lowest one). This conclusion is not true for the Spanish women. Here the Kannisto model is the most pessimistic one and the Gompertz-Makeham model is the most optimistic according to values of the life expectancy. At the end we can say that populations in both countries are getting older. The best model for describing the development of mortality is the Kannisto model. Different situation is for Spanish women. But it is very important to know that the suitability of every single model is dependent on the disposable data.

References

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Robust Interpolation of Periodically Correlated Random Processes

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Abstract. The problem of the mean square optimal estimation of the functional $A_N = \int_{0}^{(N+1)T} a(t)\zeta(t)dt$ depending on the unknown values of periodically correlated stochastic process $\zeta(t)$ from observations of the process $\zeta(t)$ for $t \in R \setminus [0, (N+1)T]$ is considered. Formulas for calculating the spectral characteristic and the mean square error of the optimal linear estimation of the functional are proposed in the case where spectral densities are exactly known. Formulas that determine the least favorable spectral densities and the minimax (robust) spectral characteristics of optimal estimates of the functional are proposed for some rather general classes of admissible spectral densities.

Keywords: Periodically correlated process, optimal linear estimate, mean square error, least favorable spectral density, minimax spectral characteristic.

1 Introduction

Methods of investigation of the problem of estimation of the unknown values of stationary stochastic processes (extrapolation, interpolation and filtering problems) are developed in the works of A.N. Kolmogorov [1], N. Wiener [2], A.M. Yaglom [3,4]. These methods are based on the assumption that spectral densities of processes are exactly known. In the case where complete information on the spectral densities is impossible, but a set of admissible densities is given, the minimax approach to estimation problem is applied. That is we find the estimate that minimizes the mean square error for all spectral densities from a given class simultaneously. Ulf Grenander [5] was the first who applied the minimax estimation method to the extrapolation problem for stationary processes. M.P. Moklyachuk [6], M.P. Moklyachuk and A.Yu. Masyutka [7] investigated the extrapolation, interpolation and filtering problems for stationary processes and sequences.

In the paper by E.G. Gladyshev [8] investigation of periodically correlated processes was started. The analysis of properties of correlation function and representation of periodically correlated processes is presented. The connection between periodically correlated processes and stationary processes is proposed by A. Makagon [9], [10].

In this paper we study the problem of the mean square optimal linear estimation of the functional $A_N = \int_{0}^{(N+1)T} a(t)\zeta(t)dt$ which depends on the unknown values of a periodically correlated stochastic process $\zeta(t)$. The estimation is based on observations of the process $\zeta(t)$ for $t \in R \setminus [0, (N+1)T]$. We
obtain formulas for calculation the mean square error and the spectral characteristic of the optimal linear estimate of $A_N\zeta$. The least favorable spectral density and the minimax (robust) spectral characteristic of the optimal linear estimate of $A_N\zeta$ are found in the case when the spectral density is not known, but the class of admissible densities is given.

2 Periodically correlated processes and generated vector stationary sequences

Definition 1. Mean square continuous stochastic process $\zeta: R \to H = L_2(\Omega, \mathcal{F}, P)$, $\mathbb{E}\xi(t) = 0$, is called periodically correlated (PC) with period $T$, if its correlation function $K(t + u, u) = \mathbb{E}\zeta(t + u)\zeta(u)$ for all $t, u \in R$ and some fixed $T > 0$ is such that

$$K(t + u, u) = \mathbb{E}\zeta(t + u)\zeta(u) = \mathbb{E}\zeta(t + u + T)\zeta(u + T) = K(t + u + T, u + T).$$

Let $\zeta(t), t \in R$ be a periodically correlated process. We construct the sequence of stochastic functions

$$\{\zeta_j(u) = \zeta(u + jT), u \in [0, T], j \in Z\}. \tag{1}$$

The sequence (1) forms the $L_2([0, T]; H)$-valued stationary stochastic sequence $\{\zeta_j, j \in Z\}$ with the correlation function $B(l, j) = \langle \zeta_i, \zeta_j \rangle_H$, that is

$$B(l, j) = \int_0^T \mathbb{E}[\zeta(u + lT)\zeta(u + jT)]du = \int_0^T K(u + (l - j)T, u)du = B(l - j).$$

Let us define in the space $L_2([0, T]; R)$ the orthonormal basis

$$\{\tilde{e}_k = \frac{1}{\sqrt{T}}e^{2\pi i(-1)^k[\frac{u}{T}]}, k = 1, 2, 3, \ldots\}, \quad \langle \tilde{e}_j, \tilde{e}_k \rangle = \delta_{kj}.$$ 

The stationary sequence $\{\zeta_j, j \in Z\}$ in this case can be represented in the form

$$\zeta_j = \sum_{k=1}^\infty \zeta_{kj}\tilde{e}_k, \quad \zeta_{kj} = \langle \zeta_j, \tilde{e}_k \rangle = \frac{1}{\sqrt{T}}\int_0^T \zeta_j(v)e^{-2\pi i(-1)^k[\frac{v}{T}]}dv. \tag{2}$$

Components $\zeta_{kj}$ are such that $[11] \mathbb{E}\zeta_{kj} = 0, \quad \|\zeta_j\|_H^2 = \sum_{k=1}^\infty E|\zeta_{kj}|^2 \leq P_1, \quad \mathbb{E}\zeta_{ki}\zeta_{nj} = \langle R(l - j)e_k, e_n \rangle$, where $\{e_k, k = 1, 2, \ldots\}$ is the basis in the space $\ell_2$. The correlation function $R(j)$ of the stationary sequence $\{\zeta_j, j \in Z\}$ is a correlation operator function in $\ell_2$. The correlation operator $R(0) = R$ is kernel operator and its kernel norm satisfies the following restriction $\|\zeta_j\|_H^2 = \sum_{k=1}^\infty \langle R(e_k, e_k) \leq P$.

The stationary sequence $\{\zeta_j, j \in Z\}$ has the spectral density function $f(\lambda)$ that is positive operator valued function of variable $\lambda \in [-\pi, \pi]$ in $\ell_2$, if its correlation function $R(j)$ can be represented in the form

$$\langle R(j)e_k, e_n \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ij\lambda}\langle f(\lambda)e_k, e_n \rangle d\lambda, \quad k, n = 1, 2, \ldots.$$
Spectral density $f(\lambda)$ a.e. on $[-\pi, \pi]$ is a kernel operator with integrable kernel norm

$$
\sum_{k=1}^{\infty} \frac{1}{2\pi} \int_{-\pi}^{\pi} \langle f(\lambda)e_k, e_k \rangle d\lambda = \sum_{k=1}^{\infty} \langle Re_k, e_k \rangle = \| \zeta_j \|^2_H \leq P.
$$

3 The classical approach to interpolation of periodically correlated processes

Consider the problem of the mean square optimal linear estimation of the functional

$$
AN\zeta = \int_{0}^{(N+1)T} a(t)\zeta(t) dt
$$

depending on the unknown values of PC stochastic process $\zeta(t)$ from the class $Y$ of the mean square continuous PC processes $\zeta(t)$. The estimation is based on observations of the process $\zeta(t)$ for $t < 0$. The function $a(t), t \in R$, satisfies the condition

$$
\int_{0}^{(N+1)T} |a(t)| dt < \infty.
$$

The functional $AN\zeta$ can be represented as

$$
AN\zeta = \sum_{j=0}^{N} \int_{0}^{T} a_j(u)\zeta_j(u) du,
$$

$$
a(u + jT) = a_j(u), \quad \zeta(u + jT) = \zeta_j(u), \quad u \in [0,T).
$$

Taking into account the decomposition (2) of the stationary sequence $\{\zeta_j, j \in Z\}$, the functional $AN\zeta$ can be represented in the following form

$$
AN\zeta = \sum_{j=0}^{N} \sum_{k=1}^{\infty} \int_{0}^{T} a_{kj} \zeta_j(u) du,
$$

$$
\zeta_j = (\zeta_{kj}, k = 1, 2, \ldots),
$$

$$
a_j = (a_{kj}, k = 1, 2, \ldots) = (a_{1j}, a_{3j}, a_{2j}, \ldots, a_{2k+1,j}, a_{2k,j}, \ldots)^T,
$$

$$
a_{kj} = (a_j, \bar{e}_k) = \frac{1}{\sqrt{T}} \int_{0}^{T} a_j(v)e^{-2\pi i((-1)^k)v/T} dv.
$$

Assume that coefficients $\{a_j, j = 0, 1, \ldots, N\}$ satisfy conditions

$$
\|a_j\| < \infty, \quad \|a_j\|^2 = \sum_{k=1}^{\infty} |a_{kj}|^2, \quad j = 0, 1, \ldots, N.
$$

Note, that under condition (3) the functional $AN\zeta$ has finite second moment.

Suppose that the spectral density $f(\lambda)$ of stationary sequence $\{\zeta_j, j \in Z\}$ satisfy the minimality condition

$$
\int_{-\pi}^{\pi} Tr[(f(\lambda))^{-1}] d\lambda < \infty.
$$
Condition (4) is necessary and sufficient in order that the error-free interpolation of unknown values of the sequence \( \{ \zeta_j, j \in Z \} \) is impossible [12]. Denote by \( L_2(f) \) the Hilbert space of complex valued vector functions \( b(\lambda) = \{ b_k(\lambda) \}_{k=1}^{\infty} \) that satisfy condition

\[
\int_{-\pi}^{\pi} b^\top(\lambda)f(\lambda)b(\lambda)d\lambda = \int_{-\pi}^{\pi} \sum_{k,n=1}^{\infty} b_k(\lambda)b_n(\lambda)(f(\lambda)e_k, e_n)d\lambda < \infty.
\]

Denote by \( L^N_2(f) \) the subspace of \( L_2(f) \) generated by the functions \( e^{ij\lambda}\delta_k, \delta_k = \{ \delta_{kn} \}_{k=1}^{\infty}, k = 1, 2, \ldots; j \in Z \setminus \{ 0, 1, \ldots, N \} \), where \( \delta_{kk} = 1, \delta_{kn} = 0 \) for \( k \neq n \). Every linear estimate \( \hat{A}_N\zeta \) of the functional \( A_N\zeta \) from observations of the sequence \( \{ \zeta_j, j \in Z \} \) for \( j \in Z \setminus \{ 0, 1, \ldots, N \} \) is of the form

\[
\hat{A}_N\zeta = \int_{-\pi}^{\pi} h^\top(\ell \lambda)Z(d\lambda) = \int_{-\pi}^{\pi} \sum_{k=1}^{\infty} h_k(\ell \lambda)Z_k(d\lambda),
\]

where \( Z(\Delta) = \{ Z_k(\Delta) \}_{k=1}^{\infty} \) is orthogonal stochastic measure of the sequence \( \{ \zeta_j, j \in Z \} \), \( h(\ell \lambda) = \{ h_k(\ell \lambda) \}_{k=1}^{\infty} \) is the spectral characteristic of the estimate \( \hat{A}_N\zeta \), \( h(\ell \lambda) \in L^N_2(f) \).

The mean square error \( \Delta(h; f) \) of the linear estimate \( \hat{A}_N\zeta \) is defined as follows

\[
\Delta(h; f) = E|A_N\zeta - \hat{A}_N\zeta|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[ A_N(e^{ij\lambda}) - h(e^{ij\lambda}) \right]\top f(\lambda)[A_N(e^{ij\lambda}) - h(e^{ij\lambda})]d\lambda,
\]

\[
A_N(e^{ij\lambda}) = \sum_{j=0}^{N} a_j e^{ij\lambda}.
\]

The spectral characteristic \( h(f) \) of the optimal linear estimate \( \hat{A}_N\zeta \) minimizes the value of the mean square error

\[
\Delta(f) = \Delta(h(f); f) = \min_{h \in L^N_2(f)} \Delta(h; f) = \min_{\hat{A}_N\zeta} E|A_N\zeta - \hat{A}_N\zeta|^2.
\]

The optimal linear estimate \( \hat{A}_N\zeta \) is a solution of the optimization problem (6). The classical Kolmogorov’s projection method [1] allows us to find the value of the mean square error \( \Delta(f) \) and the spectral characteristic \( h(f) \) of the optimal linear estimate of the functional \( A_N\zeta \) under the condition that the spectral density \( f(\lambda) \) of the sequence \( \{ \zeta_j, j \in Z \} \) is known. In this case

\[
h^\top(f) = A_N^\top(e^{ij\lambda}) - C_N^\top(e^{ij\lambda})[f(\lambda)]^{-1},
\]

\[
\Delta(f) = \langle c_N, a_N \rangle,
\]

where \( C_N(e^{ij\lambda}) = \sum_{j=0}^{N} c_j e^{ij\lambda}, a_N = \{ a_j \}_{j=0}^{N}, c_N = \{ c_j \}_{j=0}^{N} = B_N^{-1}a_N, \langle a, b \rangle \) is the scalar product in \( \ell_2 \), the matrix \( B_N = \{ B_N(j, l) \}_{j,l=0}^{N} \) is determined by elements:

\[
B_N(j, l) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left[ (f(\lambda))^{-1} \right]\top e^{i(l-j)\lambda}d\lambda, \quad j, l = 0, 1, \ldots, N.
\]

The following theorem holds true.
Theorem 1. Let \( \{\zeta(t), t \in R\} \) be a periodically correlated process such that the stationary sequence \( \{\zeta_j, j \in Z\} \), constructed by relation (1), has the spectral density \( f(\lambda) \) that satisfies the minimality condition (4). Suppose that coefficients \( \{a_j, j = 0, 1, \ldots, N\} \), that define the functional \( A_N\zeta \), satisfy condition (3). Then the spectral characteristic \( h(f) \) and the mean square error \( \Delta(f) \) of the optimal linear estimate of the functional \( A_N\zeta \) from observations of the process \( \zeta(t) \) for \( t \in R\setminus[0,(N+1)T] \) are given by formulas (7) and (8). The optimal estimate \( A_N\zeta \) of the functional \( A_N\zeta \) is calculated by formula (5).

4 Minimax (robust) approach to the interpolation problem

Formulas (7), (8) for calculating the spectral characteristic and the mean square error of the optimal linear estimate of the functional \( A_N\zeta \) can be applied in the case where the spectral density \( f(\lambda) \) of the stationary sequence \( \{\zeta_j, j \in Z\} \), constructed with the help of relation (1), is known. If the spectral density is not known exactly, but a set of admissible densities \( D \) is given, then the minimax approach to estimation of functional of unknown values is applied. In this case we find the estimate which minimizes the mean square error for all spectral densities from the given set simultaneously.

Definition 2. For a given class of spectral densities \( D \) the spectral density \( f^0(\lambda) \in D \) is called the least favorable in \( D \) for the optimal linear estimate of the functional \( A_N\zeta \) if

\[
\Delta(f^0) = \Delta(h(f^0); f^0) = \max_{f \in D} \Delta(h(f); f).
\]

Definition 3. For a given class of spectral densities \( D \) the spectral characteristic \( h^0(\lambda) \) of the optimal linear estimate of the functional \( A_N\zeta \) is called minimax (robust) if

\[
h^0(\lambda) \in H_D = \bigcap_{f \in D} \mathbb{L}^2_{-}(f), \quad \min_{h \in H_D, f \in D} \max_{f \in D} \Delta(h; f) = \max_{f \in D} \Delta(h^0; f).
\]

Lemma 1. Let \( f^0(\lambda) \) satisfy the minimality condition (4). The spectral density \( f^0(\lambda) \in D \) is the least favorable in the class \( D \) for the optimal linear estimate of the functional \( A_N\zeta \) from observations of the process \( \zeta(t) \) for \( t \in R\setminus[0,(N+1)T] \), if the Fourier coefficients of function \( (f^0(\lambda))^{-1} \) form the matrix \( \mathbf{B}_N^0 \) which determines solution of the conditional extremum problem

\[
\max_{f \in D} \langle \mathbf{B}_N^{-1} a_N, a_N \rangle = \langle (\mathbf{B}_N^0)^{-1} a_N, a_N \rangle.
\]

The minimax spectral characteristic \( h^0 = h(f^0) \) of the optimal linear estimate of the functional \( A_N\zeta \) is given by formulas (7) if \( h(f^0) \in H_D \).

The least favorable spectral density \( f^0(\lambda) \in D \) and the minimax spectral characteristic \( h^0 = h(f^0) \) form a saddle point of the function \( \Delta(h; f) \) on the set \( H_D \times D \). The saddle point inequalities

\[
\Delta(h^0; f) \leq \Delta(h^0; f^0) \leq \Delta(h; f^0), \forall h \in H_D, \forall f \in D.
\]
hold if $h^0 = h(f^0)$, $h(f^0) \in H_D$ and $f^0(\lambda)$ is a solution of the conditional extremum problem

$$
\Delta(h(f^0); f) \to \sup, \quad f(\lambda) \in D, \quad (9)
$$

$$
\Delta(h(f^0); f) = \frac{1}{2\pi} \int_{-\pi}^{\pi} (C_N^0(e^{i\lambda}))^{\top} (f^0(\lambda))^{-1} f(\lambda)(f^0(\lambda))^{-1} (C_N^0(e^{i\lambda}))d\lambda.
$$

**Lemma 2.** Let $f^0(\lambda)$ satisfy the minimality condition (4) and gives solution of the conditional extremum problem (9). Then $f^0(\lambda) \in D$ is the least favorable spectral density for the optimal linear estimate of the functional $A_N \zeta$ from observations of the process $\zeta(t)$ for $t \in R \setminus [0, (N + 1)T]$. The spectral characteristic $h^0 = h(f^0)$ of the optimal linear estimate of the functional $A_N \zeta$, calculated by formulas (7), is the minimax spectral characteristic if $h(f^0) \in H_D$.

The conditional extremum problem (9) is equivalent to the unconditional extremum problem

$$
\Delta_D(f) = -\Delta(h(f^0); f) + \delta(f|D) \to \inf, \quad (f)
$$

where $\delta(f|D)$ is the indicator function of the set $D$. Solution $f^0(\lambda)$ of this extremum problem is determined by the condition $0 \in \partial \Delta_D(f^0)$ [13], which is necessary and sufficient for the point $(f^0)$ belongs to set of minimums of convex functional; $\partial \Delta_D(f^0)$ is the subdifferential of the convex functional $\Delta_D(f, g)$ at point $(f) = (f^0)$.

## 5 Least favorable spectral densities in the class $D_M^-\bar{\Delta}$

Consider the minimax estimation problem of the functional $A_N \zeta$ from observations $\zeta(t)$ for $t \in R \setminus [0, (N + 1)T]$ under the condition that the spectral density $f(\lambda)$ of stationary sequence $\{\zeta_j, j \in Z\}$, constructed with the help of relation (1), belongs to the class

$$
D_M^- = \left\{ f(\lambda) \frac{1}{2\pi} \int_{-\pi}^{\pi} f^{-1}(\lambda) \cos(m \lambda) d\lambda = P(m), m = 0, 1, \ldots, M \right\},
$$

where the sequence of matrices $P(m) = \{p_{kn}(m)\}_{k,n=1}^{\infty}$, $m = 0, 1, \ldots, M$, is such that $P(m) = P^*(-m)$ and the matrix function $\sum_{m=-M}^{M} P(m)e^{im\lambda}$ is positive definite and has nonzero determinant. With the help of Lagrange multipliers method we can find that solution $f^0(\lambda)$ of the conditional extremum problem (9) satisfies the relation

$$
[(f^0(\lambda))^{-1}]^{\top} C_N^0(e^{i\lambda}) (C_N^0(e^{i\lambda}))^* [(f^0(\lambda))^{-1}]^{\top} =
$$

$$
= [(f^0(\lambda))^{-1}]^{\top} \left( \sum_{m=0}^{M} \alpha_m e^{im\lambda} \right) \left( \sum_{m=0}^{M} \alpha_m e^{im\lambda} \right)^* [(f^0(\lambda))^{-1}]^{\top}, \quad (10)
$$

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\( \alpha_m, m = 0, 1, \ldots, M, \) are Lagrange multipliers. The equality (10) holds if

\[
\sum_{j=0}^{N} c_j e^{ij\lambda} = \sum_{m=0}^{M} \alpha_m e^{im\lambda}.
\]

Let \( M \geq N. \) Then the Fourier coefficients of the function \( (f^0(\lambda))^{-1} \) determine the matrix \( B_N^0 \) and the extremum problem (9) is degenerated. Put \( \alpha_{N+1} = \ldots = \alpha_M = 0 \) and find \( \alpha_0, \alpha_1, \ldots, \alpha_N \) from the equation \( B_N^0 \alpha_N^0 = \alpha_N, \) where \( \alpha_N^0 = (\alpha_0, \ldots, \alpha_N)^T. \) Then the least favorable spectral density \( f^0(\lambda) \) satisfy the relation [14]

\[
f^0(\lambda) = \left( \sum_{m=-M}^{M} P(m)e^{im\lambda} \right)^{-1} = \left( \left( \sum_{j=0}^{M} A_j e^{-ij\lambda} \right) \left( \sum_{j=0}^{M} A_j e^{-ij\lambda} \right)^* \right)^{-1},
\]

and is the spectral density of the vector autoregressive stochastic sequence

\[
\sum_{j=0}^{M} A_j \xi_{t-j} = \varepsilon_t.
\]

Let \( M < N. \) Then matrix \( B_N \) is determined by the Fourier coefficients of the function \( (f(\lambda))^{-1}. \) Among them \( P(m), m = 0, \ldots, M, \) are known and \( P(m), m = M + 1, \ldots, N, \) are unknown. The unknown \( \alpha_m, m = 0, \ldots, M, \) and \( P(m), m = M + 1, \ldots, N, \) can be found from the equation \( B_N \alpha_N^M = \alpha_N, \) where \( \alpha_N^M = (\alpha_0, \ldots, \alpha_M, 0, \ldots, 0)^T. \) If the sequence \( P(m), m = 0, \ldots, N, \) is such that the matrix function \( \sum_{m=-N}^{N} P(m)e^{im\lambda} \) is positive definite and has nonzero determinant, then the least favorable spectral density [14]

\[
f^0(\lambda) = \left( \sum_{m=-N}^{N} P(m)e^{im\lambda} \right)^{-1} = \left( \left( \sum_{j=0}^{N} A_j e^{-ij\lambda} \right) \left( \sum_{j=0}^{N} A_j e^{-ij\lambda} \right)^* \right)^{-1}.
\]

is the spectral density of the vector autoregressive stochastic sequence

\[
\sum_{j=0}^{N} A_j \xi_{t-j} = \varepsilon_t.
\]

**Theorem 2.** The spectral density (11) of the vector autoregressive stochastic sequence (12) of order \( M, \) which is determined by matrices \( P(m), m = 0, 1, \ldots, M, \) is the least favorable in the class \( D_M \) for the optimal linear estimate of the functional \( A_N \xi \) if \( M \geq N. \) In the case where \( M < N \) and solutions \( P(m), m = M + 1, \ldots, N, \) of the equation \( B_N \alpha_N^M = \alpha_N \) with coefficients \( P(m), m = 0, \ldots, M, \) form a positive definite matrix function \( \sum_{m=-N}^{N} P(m)e^{im\lambda} \) with nonzero determinant, the spectral density (13) of the vector autoregressive stochastic sequence (14) of order \( N \) is the least favorable in the class \( D_M. \) The minimax spectral characteristic \( h(f^0) \) is given by formula (7).
6 Conclusions

We propose formulas for calculating the mean square error and the spectral characteristic of the optimal linear estimate of the functional $A_N \zeta$ depending on the unknown values of periodically correlated stochastic process $\zeta(t)$ from observations of the process $\zeta(t)$ for $t \in \mathbb{R} \setminus [0, (N + 1)T]$. The problem is considered under conditions of spectral certainty and spectral uncertainty.

References

On option pricing in illiquid markets with jumps

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Abstract. One of the shortcomings of the Black and Scholes model on option pricing is the assumption that trading of the underlying asset does not affect the price of that asset. This assumption can be fulfilled only in perfectly liquid markets. Since most markets are illiquid, this assumption might be too restrictive. Thus, taking into account the price impact in option pricing is an important issue. This issue has been dealt with, to some extent, for illiquid markets by assuming a continuous process, mainly based on the Brownian motion. However, the recent financial crisis and its effects on the global stock markets have propagated the urgent need for more realistic models where the stochastic process describing the price trajectories involves random jumps. Nonetheless, works related to markets with jumps are scant compared to the continuous ones. In addition, these previous studies do not deal with illiquid markets. The contribution of this paper is to tackle the pricing problem for options in illiquid markets with jumps as well as the hedging strategy within this context, which is the first of its kind to the best knowledge.

Keywords: Options pricing, Illiquid markets, Jump diffusion, Incomplete markets.

1 Introduction

Financial derivatives are important tools for dealing with financial risk. An option is an example of such derivatives, which gives the right but not the obligation, to engage in a future transaction on some underlying financial asset. For instance, a European call option on an asset with the price \((S_t)_{t\in[0,T]}\) is a contract between two agents (buyer and seller), which gives the holder the right to buy the asset at a pre-specified future time \(T\) (the expiration date) for an amount \(K\) (called the strike). The buyer of the option is not obliged to exercise the option. When the contract is issued they buyer of the option needs to pay a certain amount of money called the premium. The payoff for this option is defined as \(h(S_T) = \max(S_T - K, 0) = (S_T - K)_{+}\). The writer of the option receives a premium that is invested in the combination of the risky and risk free assets. The pricing problem is then to determine the premium, i.e. the price that the seller should charge for this option.

The pricing problem has been solved in the pioneer work of Black and Scholes\cite{Black1973}. One of the shortcomings of the Black and Scholes model is the assumption that an option trader cannot affect the underlying asset price. However, it
is well-known that in a market with imperfect liquidity, trading does affect the underlying asset price (see, for example, Chan and Lakonishok[1], Keim and Madhavan[6], and Sharpe et al.[10]).

In Liu and Yong[7], the authors study the effect of the replication of a European option on the underlying asset price. They obtain a generalization of the Black Scholes pricing P.D.E. as the following:

\[
\frac{\partial v}{\partial t}(S,t) + \frac{\sigma^2 S^2}{2} \frac{\partial^2 v}{\partial S^2}(S,t) + \frac{\sigma^2 S^2}{2} \left(1 - \lambda(S,t)\right) \frac{\partial^2 v}{\partial S^2}(S,t) + r \frac{\partial v}{\partial S}(S,t) - rt v(S,t) = 0,
\]

for \((S,t) \in [0, +\infty[ \times [0, T]\) (1)

\[
v(S,T) = f(S), \quad 0 < S < \infty,
\]

where \(\lambda(S,t)\) is the price impact function of the trader. The classical BlackScholes P.D.E. is a special case of (2) when \(\lambda(S,t) = 0\).

There are also several other papers that have studied the financial markets with jumps (among others, Merton[8], Dritschel and Protter[3], El-Khatib and Privault[4]) and El-Khatib and Al-Mdallal[5]. However, none of the previous studies based on the jump-diffusion approach deals with illiquid markets, to the best knowledge. This paper is extends the model of Liu and Yong[7] by including a jump-diffusion structure in the underlying option pricing model. This appears to be an important issue because the model that is suggested in this paper allows for the possibility to account for sudden and random significant changes in the market that might not be captured by the existing models in the literature such as the continuous model suggested by Liu and Yong[7]. Hence, the approach that is developed in this paper is expected to be more useful in financial risk management, especially in the cases in which the financial markets are under stress.

The disposition of the rest of the paper is the following. Section 2 introduces the jump-diffusion model for an illiquid market. Section 3 deals with the pricing problem of an option within the context of a jump-diffusion model along with the proof for the suggested solution. Section 4 concludes the paper.

2 A jump-diffusion model for illiquid markets

We start with presenting some necessary denotations. Let \((N_t)_{t \in [0,T]}\) be a Poisson process with deterministic intensity \(\rho\). Let also \( M_t = N_t - pt \) be its associated compensated process. The process \((B_t)_{t \in [0,T]}\) denotes a Brownian motion. The probability space of interest is \((\Omega, F, \mathbb{P})\) with \((N_t)_{t \in [0,T]}\) and \((B_t)_{t \in [0,T]}\) being independent. Let \((\mathcal{F}_t)_{t \in [0,T]}\) signify the filtration generated by \((N_t)_{t \in [0,T]}\) and \((B_t)_{t \in [0,T]}\). The market is assumed to have two assets: a risky asset \((S_t)_{t \in [0,T]}\) and a risk-free denoted by \((A_t)_{t \in [0,T]}\). The maturity is \(T\), the strike is \(K\) and the payoff is \(h(S_T) = (S_T - K)^+ \equiv \max\{S_T - K, 0\}\). As in Liu and Yong[7], the return on the risk free asset indirectly depends on \(S_t\) and the option trader’s trading in the stock market has a direct impact on the
stock price. This price impact, which an investor can cause by trading on an asset, functions in such way that it increases the price when buying the asset and it decreases the price when selling the asset. The price of the risk-free asset is given by

$$dA_t = r(t, S_t)A_t dt, \quad t \in [0, T],$$

where $r > 0$ denotes the interest rate. The price of the risky asset is generated by the following stochastic differential equation:

$$dS_t = \mu(t, S_t) dt + \sigma(t, S_t)(dW_t + a dM_t) + \lambda(t, S_t) d\theta_t, \quad t \in [0, T], \quad S_0 = x > 0,$$

where $\mu$ and $\sigma$ represent the expected return and volatility, respectively, the term $a$ is a real constant and $\lambda(S, t)$ denotes the price impact factor created by the trader via selling or buying the underlying asset. $\theta_t$ is the number of shares that the trader has in the stock at time $t$. Hence, $\lambda(S, t) d\theta_t$, captures the price impact of trading. Before dealing with the pricing of a European option in a jump-diffusion illiquid market, we need to observe the following remark.

Remark 1. The parameter $a$ in (4) determines the direction of the jumps$^1$. In fact the following can be stated:

- If $a < 0$ the jumps are pushing the stock price down, i.e. the stock price is decreasing at each jump.
- If $a = 0$ then there are no jumps and therefore model (4) is reduced to the model in Liu and Yong[7].
- If $a > 0$ the jumps are pushing the stock, i.e. the stock price is increasing at each jump.

3 Pricing of a European option in jump-diffusion illiquid market

Let $(V_t)_{t \in [0,T]}$ be the wealth process for the trader. Let also $(\psi_t)_{t \in [0,T]}$ denote the number of shares invested in the risk-free asset. Then, the value of the portfolio is given by

$$V_t = \psi_t A_t + \theta_t S_t, \quad t \in [0, T].$$

Assume that the number of shares of the risky asset satisfies the following condition:

$$d\theta_t = \eta_t dt + \zeta_t (dW_t + b dM_t), \quad t \in [0, T].$$

Let us consider a European call option with the payoff defined as $h(S_T) := (S_T - K)^+$. In order to replicate the option for a perfect hedge, we search for a strategy $(\psi_t, \theta_t)_{t \in [0,T]}$ which, at the expiration date of the option, leads to having a value of the underlying wealth to be equal to the payoff, that is $V_T = h(S_T)$. Then we can state the following corollary.

$^1$ it affects also the jumps size.
Let \( \text{Lemma 1.} \)

We need Itô formula which is given by the following lemma (see Protter[9]).

The above system is called FBSDE (forward-backward stochastic differential equations) system. In order to derive the P.D.E. for the European option price, we need Itô formula which is given by (4). We replicate the European option by searching a wealth \( V_t \) such that

\[
V_T = h(S_T).
\]

Our aim in this paper is to price the European option with payoff \( h(S_T) \) where \( S_T \) is given by (4). We replicate the European option by searching a wealth \( (V_t)_{t \in [0,T]} \) which leads to the terminal value \( V_T = h(S_T) \). Thus, as in Liu and Yong[7], we need to solve the following system of stochastic differential equations.

\[
\begin{align*}
    d\theta_t &= \eta_t dt + \zeta_t (dW_t + b M_t), \\
    dS_t &= \left( \mu(t, S_t) + \lambda(t, S_t) \right) dt + \left( \sigma(t, S_t) + \lambda(t, S_t) \right) \theta_t dt + \theta_t \left( a \sigma(t, S_t) + b \lambda(t, S_t) \right) dM_t, \\
    dV_t &= \left( \mu(t, S_t) + \lambda(t, S_t) \right) dt + \left( \sigma(t, S_t) + \lambda(t, S_t) \right) \theta_t dt + \theta_t \left( a \sigma(t, S_t) + b \lambda(t, S_t) \right) dM_t, \\
    \theta_0 &> 0, \quad S_0 > 0, \quad V_T = h(S_T).
\end{align*}
\]

The above system is called FBSDE (forward-backward stochastic differential equations) system. In order to derive the P.D.E. for the European option price, we need Itô formula which is given by the following lemma (see Protter[9]).

\text{Lemma 1.} Let \( g, l, \) and \( k \) be three adapted processes such that

\[
\int_0^t |g_s| ds < \infty, \quad \int_0^t |l_s|^2 ds < \infty, \quad \text{and} \quad \int_0^t \rho |k_s| ds < \infty.
\]

Let \( X = (X_t)_{t \in [0,T]} \) be the process defined by

\[
dX_t = g_t dt + l_t dW_t + k_t dM_t.
\]

For any function \( G \in C^{1,2}([0,T] \times \mathbb{R}) \), we have

\[
G(t, X_t) = G(0, X_0) + \int_0^t \left( \partial_s G(s, X_s) + (g_s - k_s \rho) \partial_x G(s, X_s) \right) ds.
\]
Equation (9) can be written in the following format:

\[
G(t, X_t) = G(0, X_0) + \int_0^t \left[ \partial_s G(s, X_s) + (g_s - k_s \rho) \partial_x G(s, X_s) + \rho G(s, X_s - k_s) - G(s, X_s - ) \right] ds \\
+ \int_0^t \left[ G(s, X_s - + k_s) - G(s, X_s - ) \right] dM_s \\
+ \int_0^t \partial_s G(s, X_s - ) dW_s.
\] (10)

The next proposition provides the P.D.E. for the price of the European option in the jump-diffusion illiquid market presented in section 2.

**Proposition 1.** Let \( f(t, S_t) \) denote the price of the European option at time \( t \in [0, T] \) for the model presented in section 2. Then the corresponding P.D.E. for the underlying option price is given by

\[
r(t, S_t) V_t + [\mu(t, S_t) - r(t, S_t) + \lambda(t, S_t) \eta_t] \theta_t S_t = \\
\partial_t f(t, S_t) + (\mu(t, S_t) + \lambda(t, S_t) \eta_t - \rho(a \sigma(t, S_t) + b \lambda(t, S_t) \zeta_t)) S_t \partial_S f(t, S_t) \\
+ \frac{1}{2} \sigma^2(t, S_t) + \lambda(t, S_t) \zeta_t^2 S_t^2 \partial_S^2 f(t, S_t) + \rho(f(t, S_t - (1 + a \sigma(t, S_t) \\
+ b \lambda(t, S_t) \zeta_t)) - f(t, S_t - ))),
\]

with the terminal condition \( f(T, S_T) = h(S_T) \). Moreover, the market is incomplete and there is no strategy leading to the terminal wealth \( V_T = h(S_T) := f(T, S_T) \). However, the number of shares \( \theta \) that minimizes the variance is given by

\[
\theta_t = \frac{(\sigma + \lambda \zeta)^2 S^2 \partial_S f + \rho S(a \sigma + b \lambda \zeta) \left(f(t, S_t - (1 + a \sigma + b \lambda \zeta)) - f\right)}{(\sigma + \lambda \zeta)^2 S^2 + \rho S^2(a \sigma + b \lambda \zeta)^2}.
\]

**Proof.** Let \((\theta, S, V)\) be an adapted solution of the FBSDE (8) and assume that there exists a smooth function \( f \in C^{3,1}([0, T], [0, \infty]) \) such that \( f(t, S_t) \) represents the price of the European option at time \( t \in [0, T] \). Since the price of the option at maturity is equal to the payoff, then \( f(T, S_T) = h(S_T) \). Now, using Itô formula (10) we obtain

\[
df(t, S_t) = \left\{ (\mu(t, S_t) + \lambda(t, S_t) \eta_t - \rho(a \sigma(t, S_t) + b \lambda(t, S_t) \zeta_t)) S_t \partial_S f(t, S_t) \\
+ \frac{1}{2} \sigma^2(t, S_t) + \lambda(t, S_t) \zeta_t^2 S_t^2 \partial_S^2 f(t, S_t) + \partial_t f(t, S_t) \\
+ \rho(f(t, S_t - (1 + a \sigma(t, S_t) + b \lambda(t, S_t) \zeta_t)) - f(t, S_t - ))) \right\} dt \\
+ \left[ \sigma(t, S_t) + \lambda(t, S_t) \zeta_t \right] S_t \partial_S f(t, S_t) dW_t \\
+ \left[ f(t, S_t - (1 + a \sigma(t, S_t) + b \lambda(t, S_t) \zeta_t)) - f(t, S_t - ) \right] dM_t.
\] (11)
By comparing equations (7) and (11) one can deduce that it is impossible to find a strategy \((\eta_t, \zeta_t)_{t \in [0,T]}\) that results in the terminal wealth \(V_T = h(S_T) := f(T, S_T)\). Thus, we put the term belonging to \(dt\) equations (7) and (11) equal to each other, which gives the P.D.E. of the option price and then we minimize the distance between the wealth \(V_T\) and the price \(f(T, S_T) = h(S_T)\) over the number of shares of the underlying asset, i.e. \(\theta_t\). The P.D.E. of the option price in this case is

\[
\begin{align*}
\frac{\partial}{\partial t}f(t, S_t) + \frac{\sigma(t, S_t)}{2}S_t^2\frac{\partial^2}{\partial S^2}f(t, S_t) + (\mu(t, S_t) - r(t, S_t))S_t\frac{\partial}{\partial S}f(t, S_t) + \frac{\rho}{2}(f(t, S_t) - f(t, S_t^-)) - \theta_t S_t f(t, S_t) = \\
\bigg[\frac{\lambda(t, S_t)S_t}{\sigma(t, S_t)}\bigg]^2S_t^2\frac{\partial^2}{\partial S^2}f(t, S_t) + \rho(f(t, S_t^-) - f(t, S_t^-)),
\end{align*}
\]

(12)

with the terminal condition

\[
f(T, S_T) = h(S_T).
\]

To find the number of shares \(\theta_t\) invested in \(S_t\) we need to solve the following problem:

\[
\text{Minimize}_\theta E[\Pi^2(\theta)],
\]

(13)

where \(\Pi(\theta) := (h(S_T) - V_T)\). By using (7), (11) and (12) we have

\[
E[\Pi^2(\theta)] = E \left[ \left( \int_0^T \left( [\sigma(t, S_t) + \lambda(t, S_t)\zeta_t]S_t(\partial_S f(t, S_t) - \theta_t) \right) dW_t \right)^2 \right] + E \left[ \left( \int_0^T \left( f(t, S_t^-) - f(t, S_t^-) - \theta_t S_t (a\sigma(t, S_t) + b\lambda(t, S_t)\zeta_t) \right) dM_t \right)^2 \right] + E \left[ \left( \int_0^T \left( f(t, S_t^-) - f(t, S_t^-) - \theta_t S_t (a\sigma(t, S_t) + b\lambda(t, S_t)\zeta_t) \right)^2 dt \right) \right]
\]

where

\[
l(x) = (\sigma + \lambda\zeta)^2S^2(\partial_S f - x)^2 + \rho(f(t, S_t^-) - f(t, S_t^-) - \theta_t S_t (a\sigma(t, S_t) + b\lambda(t, S_t)\zeta_t))^2 dt,
\]

The minimum is obtained at \(l'(x) = 0\), which yield the following result:

\[
2(\sigma + \lambda\zeta)^2S^2(\partial_S f - x) - 2S(a\sigma + b\lambda\zeta)\rho(f(t, S_t^-) - f(t, S_t^-) - \theta_t S_t (a\sigma(t, S_t) + b\lambda(t, S_t)\zeta_t)) - f - xS(a\sigma + b\lambda\zeta) = 0,
\]

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and

\[ \theta_t = \frac{(\sigma + \lambda \zeta)^2 S^2 \partial S f + \rho S (a \sigma + b \lambda \zeta) (f(t, S_t - (1 + a \sigma + b \lambda \zeta)) - f)}{(\sigma + \lambda \zeta)^2 S^2 + \rho S^2 (a \sigma + b \lambda \zeta)^2}, \]

which ends the proof.

It is worth mentioning that in the case where there are no jumps, i.e. when \( a = b = 0 \), then \( \theta = \partial S f \) and the P.D.E. in the previous proposition is reduced to the P.D.E. that is obtained in Liu and Yong\cite{7}, assuming there are no dividends.

4 Conclusion

Option pricing is an integral part of modern risk management in increasingly globalized financial markets. The classical Black and Scholes model is regularly used for this purpose. However, one of the main pillars that makes this model operational is the underlying assumption that the markets are perfectly liquid. This assumption is, nonetheless, not fulfilled in reality since perfectly liquid markets do not exist. In our opinion the question should not be whether the markets are illiquid or not, the question should be about the degree of illiquidity.

Thus, taking into account the fact that markets are illiquid can improve on the precision of the underlying option pricing.

This paper is the first attempt, to our best knowledge, that extends the existing literature on option pricing by introducing a jump-diffusion model for illiquid markets. This seems to be a more realistic approach to deal with a market that is incomplete. A solution for the option pricing within this context is provided along with the underlying proof. The suggested solution might be useful to investors in order to determine the optimal value of an option in a market that is characterized by illiquidity.

References

Variations of PageRank with application to linguistic data

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Abstract. In this paper we will give some alternative formulations of PageRank originally used by Google to rank home pages in a search query. By looking at PageRank from a probabilistic perspective using Markov chains we will see how to fix some of the limitations in the original definition of PageRank to make it usable for comparison not only within a system, but also between systems.

Last we will take a short look at an application of PageRank to linguistic data for identification of "important" terms in a corpus of biomedical texts. We show how the method can be applied for this kind of data as well as highlighting some of the limitations of the method and future work.

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1 Background

PageRank can be seen as the stationary distribution of a Markov chain described by a random walk on a directed graph with the following rules: In every step with probability \( c \) we either follow any edge out of the current vertex with equal probability \( 1/n \) where \( n \) is the number of edges going out of the current vertex. With probability \( (1 - c) \) we instead pick a new vertex at random with no consideration of current vertex [5]. We do not allow any vertex to link to itself and special care needs to be taken of vertices with no outgoing edges (dangling nodes), usually by letting them link to all vertices instead. PageRank in its original form can be seen below [1].

Definition 1. PageRank \( R^{(1)} \) for the vertices \( V \) in a directed graph \( G \) is defined as the right eigenvector with eigenvalue one to the matrix

\[
M = c(A + gu^\top) + (1 - c)ue^\top
\]

where \( 0 < c < 1 \), \( A \) is the adjacency matrix of \( G \) with non-zero elements \( a_{ij} = 1/n_i \) where \( n_i \) is the number of non-zero elements on row \( i \), \( u \) is a non-negative column-vector of length \( |V| \) with \( ||u||_1 = 1 \), \( e \) is a column-vector of
length $|V|$ with elements $e_i = 1$, $g$ is a column-vector of length $|V|$ with elements $g_i = 1$ if $v_i$ is a dangling node, and $g_i = 0$ otherwise. $R^{(1)}$ is normalized such that $||R^{(1)}||_1 = 1$ where $||x||_1 = \sum_i |x_i|$ is the $L^1$-norm.

If we consider the random walk on a graph then $u$ is a probability distribution of where to go whenever we start over in a new random vertex either with probability $(1 - c)$ in every step or whenever we end up in a dangling node. $u$ often have elements equal to $1/|V|$ but changes can be made to decrease or increase the influence of certain vertices. It’s easy to see that $M$ is a column stochastic irreducible matrix thus we have a guarantee that $R^{(1)}$ exist and is a positive vector from Perron-Frobenius for non-negative irreducible matrices [3].

While $M$ generally is not sparse, $A$ often is a very large and sparse matrix and as such the Power method is often used to calculate PageRank by iterating

$$R_{n+1}^{(1)} = MR_n^{(1)} = cA^\top R_n^{(1)} + d_n u$$

$$d_n = 1 - \sum_i cA^\top R_n^{(1)}$$

where we use that the part not depending on $A$ in the multiplication is proportional to $u$, $(c(gu^\top)^\top + (1 - c)ue^\top)R^{(1)} \propto u$ and $||R^{(1)}||_1 = 1$.

Since $R^{(1)}$ is normalized to some constant (even if that constant is the number of vertices) we cannot reliably compare PageRank between different graphs, this since dangling nodes are assumed to link to all vertices. If the graphs are big with a similar structure this is unlikely to cause a problem, however for small graph’s it can make a large difference.

We would also like to allow vertices to have a weightsum of links out less than one, for example to differentiate between a clique and one with no edges.

## 2 PageRank from a probability perspective

We will look at PageRank as a Random walk on a graph and define a slightly different variation of PageRank.

**Definition 2.** Consider a random walk on a graph described by $cA$. We walk to a new vertex from our current with probability $0 < c < 1$ and stop with probability $1 - c$. Using a constant weight vector $u$ with all elements equal we define PageRank $R^{(2)}$ for a single vertex as

$$R_j^{(2)} = \left( \sum_{e_i \in S, e_i \neq e_j} P(e_i \rightarrow e_j) + 1 \right) \left( \sum_{k=0}^{\infty} (P(e_j \rightarrow e_j))^k \right)$$

(2)

where $P(e_i \rightarrow e_j)$ is the probability to hit node $e_j$ starting in node $e_i$. This can be seen as the expected number of visits to $e_j$ if we do multiple random walks, starting in every vertex once.
Note that we use $A$ and not $M$ which is modified for dangling nodes nor do we normalize PageRank to some constant. This means that we can now compare PageRank between different graphs without problem, neither do we need to consider dangling nodes as if linking to all vertices. The weight sum of edges out of a vertex can now be anything between zero and one as well.

**Theorem 1.** PageRank $R^{(2)}$ is proportional to $R^{(1)}$ ($R^{(2)} \propto R^{(1)}$).

**Proof.** $(cA^T)^k_{ij}$ is the probability to be in node $e_i$ starting in node $e_j$ after $k$ steps. Multiplying with the one vector $e$ therefor gives the sum of all the probabilities to be in node $e_i$ after $k$ steps starting in every node once (constant $u$). The expected total number of visits is the sum of all probabilities to be in node $e_i$ for every step starting in every node:

$$R^{(2)}_j = \left( \sum_{k=0}^{\infty} (cA^T)^k \right) e_j \tag{3}$$

$\sum_{k=0}^{\infty} (cA^T)^k$ is the Neumann series of $(I - cA^T)^{-1}$ which is guaranteed to converge since $cA^T$ is non-negative and have column sum < 1. This gives:

$$R^{(2)} = \left( \sum_{k=0}^{\infty} (cA^T)^k \right) e = (1 - cA^T)^{-1} e = (1 - cA^T)^{-1} n u \tag{4}$$

where we use that $u$ is constant and $n$ is the number of vertices. Then

$$R^{(1)} = MR^{(1)} \Leftrightarrow (cA^T - I)R^{(1)} = -(cu^T + (1 - c)ue^T)R^{(1)} \tag{5}$$

Since every column of $u g^T$ is either equal to $u$ or zero and all columns equal to $u$ for $ue^T$ we can see that $-(cu^T + (1 - c)ue^T)R^{(1)}$ will be proportional to $u$. This can be written as:

$$(1 - cA^T)R^{(1)} = ku \Leftrightarrow R^{(1)} = (1 - cA^T)^{-1} ku \propto (1 - cA^T)^{-1} nu = R^{(2)} \tag{6}$$

We note that although we made the assumption $u$ constant, it is quite easy to show a similar relation for other $u$ as well by defining $R^{(2)}$ slightly differently.

**2.1 Relation between normalized and non normalized PageRank**

Since we know that they are proportional it’s easy to get from the non-normalized PageRank $R^{(2)}$ to the normalized PageRank $R^{(1)}$ by simply dividing by $||R^{(2)}||_1$:

$$R^{(1)} = \frac{R^{(2)}}{||R^{(2)}||_1} \tag{7}$$

But we do not yet have any way to go from $R^{(1)}$ to $R^{(2)}$. For this we formulate the following:
Theorem 2. The relation between normalized PageRank $R^{(1)}$ and non-normalized PageRank $R^{(2)}$ can be written:

$$R^{(2)} = \frac{nR^{(1)}}{d}$$

where $n$ is the number of nodes and $d = 1 - \sum cA^\top R^{(1)}$ is the value gained from the last step in the power method.

Proof. If we let $S_a$ be the dangling nodes in our system we can rewrite

$$d = 1 - \sum cA^\top R^{(1)} = (1 - c) + c \sum_{a \in S_a} R^{(2)}_a$$

If there’s no dangling nodes then

$$\sum R^{(2)} = n \sum_{k=0}^{\infty} c^k = \frac{n}{1 - c}$$

The loss from a dangling node $a$ can be seen as the PageRank $R^{(2)}_a$ (expected visits to $a$) times the sum of probability going from there if there were no dangling nodes present, this gives

$$\sum R^{(2)} = \frac{n - \sum_{a \in S_a} R^{(2)}_a}{1 - c}$$

where $S_a$ contains all the dangling nodes in our system. By (7) (9) and (11)

$$R^{(1)} = \frac{R^{(2)}(1 - c)}{n - \sum_{a \in S_a} R^{(2)}_a}$$

$$d = (1 - c) + \frac{\sum_{a \in S_a} R^{(2)}_a}{n - \sum_{a \in S_a} R^{(2)}_a} \rightarrow \sum_{a \in S_a} R^{(2)}_a = n - \frac{(1 - c)n}{d}$$

$$R^{(2)} = \frac{(n - \sum_{a \in S_a} R^{(2)}_a)R^{(1)}}{1 - c} = \frac{n(1 - c)R^{(1)}}{d(1 - c)} = \frac{nR^{(1)}}{d}$$

We now have the possibility of comparing the PageRank of different disjoint system immediately by storing the results in $P^{(2)}$ instead. It’s however important to note one restriction: while we can weight vertices differently within a system, we cannot weight systems differently since the weight vector of every subsystem is normalized (and later weighted depending on number of nodes $n$ and its $d$—value). This means that as the weight for one vertex in a subsystem is lowered, other vertices in the same subsystem effectively gets a higher weight compared to those in other systems.

We look at a large system $S$ composed of multiple systems $S_1, S_2, \ldots, S_N$ where we want to use a global weight vector $V$ rather than one for each subsystem. If $v_i$ is the part of $V$ corresponding to nodes in system $S_i$, then as
we normalize $v_i$ and calculate $P^{(2)}$ we would get the correct internal weighting between nodes in $S_i$. In order to get the correct weighting compared to other subsystems we therefore only need to find the correct weight for the subsystem itself. Summation over $v_i$ gives the relative weight of subsystem $S_i$. This gives a slightly new definition:

**Definition 3.** $R_{S_i}^{(3)}$ for system $S_i \in S$ is defined as:

$$R_{S_i}^{(3)} = \frac{R_{S_i}^{(1)}||v_i||_1}{d_i}$$

(15)

where $v_i$ is the part of the global weight vector $V$ belonging to the nodes in system $S_i$. [9]

We note that $||V||_1 \neq 1$ but can now be any non-negative vector. If we also choose $V$ such that we define a "default" weight rather than a total sum of weights, we see that as we change one subsystem the rank of other subsystems never change. For example we could use the default weight 1 and change individual weight from there. If $V$ is the one-vector we easily find that $R^{(2)} = R^{(3)}$. Now that we have this version of PageRank we can compute and make changes to individual subsystems $S_i$ without the need to re-compute PageRank of any other subsystems, while still being able to compare PageRank between subsystems making the method very suitable for continuous updates and parallel computations.

3 Using PageRank to find annotated terms in a text corpus

Regarding the low coverage of the existing terminologies to identify terms in corpus [4,7,17], approaches have been proposed to automatically extract terms from texts, i.e. noun phrases referring to linguistic entities in a specialized domain (e.g. medicine, biology, law, electric power plant, etc.) for text corpora (see [6]). Usually, proposed approaches are based on linguistic rules or collocations. However, even if the extracted terms are useful for terminology building, document indexing or text mining, the quality of the results, especially the precision, is not sufficient. The various strategies of term extraction have difficulties to identify relevant terms among the huge amount of term candidates: terms and irrelevant extracted noun phrases could have similar linguistic characteristics. To tackle this problem, several statistical measures based on term or word frequency, but also lexical or contextual clues have been proposed [8,15] without proposing convicting methods for filtering or ranking the extracted terms: a single measures is not sufficient to rank the terms correctly and we assume that relations shared by terms have to take into account to achieve this aim. In that respect, we focus here on the term ranking by exploiting graph structure and PageRank. PageRank also gives lots of customization options in personalization vector $V$, constant $c$, and how we choose to weight the edges in the graph making it suitable for a machine learning approach.
3.1 Description of data

Our working data is based on the Genia corpus\(^1\) [14]. This text corpus consists of 1999 abstracts issued from Medline portal\(^2\). The abstracts concern the transcription factors in human blood cells (abstracts indexed by the MeSH terms: human, blood cell and transcription factor). The corpus contains 18,545 sentences and 436,967 words. Each abstract is also annotated with terms referring to physical biological entities (organisms, proteins, cells, genes) as well as biologically meaningful terms (e.g. molecular functions). Thus, 96,582 terms are annotated in the abstracts (see Figure 1).

To address potential mechanisms by which estrogens suppress erythropoiesis, we have examined their effects on GATA-1, an erythroid transcription factor that participates in the regulation of the majority of erythroid cell-specific genes and is necessary for full maturation of erythrocytes.

Fig. 1. Excerpt of the Genia corpus: sentence annotated with terms.

We consider this term annotation as our Gold Standard: the list of terms extracted and ranked by our term extraction approach is compared to this reference. In that respect, for the experiment, we randomly split the corpus in two parts: the training set includes 60% of the corpus (1,200 abstracts) while the remaining part of the corpus (799 abstracts) will be the test set. A preprocessing of the text corpora is performed with the Ogmios platform [11]: texts are segmented in words and sentences, and part-of-speech categories and lemma are associated to the words thanks to the TreeTagger [18].

In our experiment, the list of terms have been extracted with linguistic rules [2]. Parsing patterns taking into account the morpho-syntactic variation, are recursively applied to the text and provide noun phrases which seems to be relevant in the targeted domain (see Figure 2).

Additional information is also associated to the extracted terms:

- Syntactic dependencies between term components are computed according to assigned Part-of-Speech tags and shallow parsing rules. Each term is considered as a syntactic binary tree composed of two elements describing the syntactic role of the component in the term: the head component is the main word of the term, and the expansion component modifies the main word. Each component is also considered as a multi-word or a single-word term. For instance, full maturation is the head component of the term analyzed in Figure 3. As several terms can share components, the list of terms can be view as a syntactic network or a graph.

\(^1\) version 3.02, available at http://www.nactem.ac.uk/genia/genia-corpus/
event-corpus
\(^2\) http://www.ncbi.nlm.nih.gov/pubmed
• Statistical measures are provided with each term: term frequency, number of documents where appears a term, C-Value [10,16], TF-IDF, measures based on syntactic and contextual clues [8], etc.

To address potential mechanisms by which estrogens suppress erythropoiesis, we have examined their effects on GATA-1, an erythroid transcription factor that participates in the regulation of the majority of erythroid cell-specific genes and is necessary for full maturation of erythrocytes.

Fig. 2. Excerpt of the Genia corpus: terms automatically extracted.

Fig. 3. Parsing tree of the term full maturation of erythrocytes

3.2 Method

The first thing to consider is how to create a sub-stochastic matrix given a tree such as in Figure 3 for use in our method. We have two different relations "head" and "modifier" which we could choose to weight differently, since they are also directed "A is a "head" of B" we could choose to give different weights depending on direction as well. This gives four different types of edges (to head, from head, to modifier, from modifier), we give every type of edge a non-negative weight which is then used to create our system matrix $A$ by normalizing every row such that they have sum one.

The next point is choosing constant $0 < c < 1$; for a very low $c$ PageRank is mainly decided by the personalization vector $V$ and the immediate neighbors of a vertex in the graph. For a large $c$ the personalization vector $V$ have little effect on the ranking; instead some specific graph structures give a greatly inflated rank (such as two vertices linking only to each other). As $c$ get close to 1 there are also problems with stability and convergence [13][12]. As with the edge weights it’s hard to say what $c$ constitutes an optimal value, initially we choose to start with $c = 0.85$ (as used by Google initially).

Last we need to choose $V$, here a lot of variation can be done such as weighting the terms depending on frequency or similar measurements or by weighting depending on type of vertex. Since we have a tree-structure for our graphs it might be worth it to weight depending on level in the tree or if it can
be divided in "head" and "modifier" or not. Initially we tried using \( V \) with a uniform weight and weights equal to the frequency of corresponding terms.

### 3.3 Initial results

We compare the results to using only the frequency measurement with PageRank using a couple of different parameter values.

![Fig. 4. Precision using frequency or constant \( V = e \) with different values of freq. with \( c = 0.85 \) and different edge weights \( W \) equal.](Fig. 5. Precision using frequency \( V = \) freq. with \( c = 0 \). where \( W = \{ \text{th, tm, fh, fm} \} \))

Where \( \text{th} \) and \( \text{tm} \) is the weight of edges pointing at a head or modifier respectively and \( \text{fh} \) and \( \text{fm} \) are the edges pointing from a head or modifier respectively. From Figure 4 we can see that we have similar results when using PageRank as when using frequency. Using frequency seem to have a slightly better precision initially, but then drops off faster than the PageRank variations. From changing \( c \) we cannot see any major changes, lowering it does seem to even out the curve slightly. We see that both frequency and PageRank to have a very high precision for the first couple of terms but then rapidly fall. Using the frequency by itself or as weights \( V \) seem to give the best results.

In Figure 5 we can see that the result differ significantly depending on how we choose to create our system matrix. We see that we get a better result if we have a higher chance to go down the tree (\( \text{th, tm} \) high) rather than the opposite, and that the head (\( \text{th, fh} \) high) seems to be more important than the modifier.

### 4 Conclusions and future work

We have seen from our initial studies on our training data that we can expect to get a slight improvement compared to using only the frequency. Changes in \( V \) have some effect and can likely be tuned further by looking at other measures or weighting depending on type of vertex. The main thing influencing the result however seem to be how the system matrix is created. Not only the weights \( \{ \text{th, tm, fh, fm} \} \), it’s also possible let \( c \) depend on vertex properties such as it’s depth in the tree. While both frequency and PageRank seem to give similar
results, it’s not clear if they find the same annotated terms or not. While we can expect to find some improvement using PageRank, how large and if the same parameter values can then be used on another text corpus remains to be seen. The next step is in using a machine learning approach to try and optimize parameters for the model and try it on our test data, if this is successful we can then see if it proves useful for another text corpus. One limitation in creating the system matrix is the normalization of rows, while we could potentially have a row sum less than one, we cannot have one larger than one and still guarantee convergence. This is something we would like to look at in the future.

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References


