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8 **Three-parameter stochastic lognormal diffusion model:**
9 **statistical computation and simulating**
10 **annealing – application to real case**
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19 In this paper, we propose a new study of a stochastic lognormal diffusion process (SLDP), with
20 three parameters, which can be considered as an extension of the bi-parametric lognormal process
21 with the addition of a threshold parameter. From the Kolmogorov equation, we obtain the probability
22 density function and the moments of this process. The statistical inference of the parameter is studied
23 by considering discrete sampling of the sample paths of the model and then using the maximum
24 likelihood (ML) method. The estimation of the threshold parameter requires the solution of a nonlinear
25 equation. To do so, we propose two methods: the classical Newton–Raphson (NR) method and one
26 based on simulated annealing (SA). This methodology is applied to an example with simulated data
27 corresponding to the process with known parameters. From this, we obtain the estimators of the
parameters by both methods (NR and SA). Finally, the methodology studied is applied to a real case
concerning the mean age of males in Spain at the date of their first wedding.

28 *Keywords:* Three-parameter lognormal diffusion process; Discrete sampling; Simulated annealing;
29 Fits and forecast; Mean age of males in Spain at the date of their first wedding
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34 **1. Introduction**
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36 In the context of three-parameter lognormal distributions, we discuss the original study of the
37 three-parameter lognormal diffusion process, which is one-dimensional in the endogenous
38 variable and has three parameters.

39 We seek to obtain a three-parameter univariate lognormal model, which is flexible and
40 broad enough to cover important fields of application that are currently not served by standard
41 models. Moreover, taking possible applications into account, the maximum likelihood (ML)
42 estimation is constructed on the basis of discrete sampling based on the conditioned likelihood
43 derived from the transitions that are the solutions to the corresponding Kolmogorov equations.
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51 The importance of three-parameter lognormal distribution as a probability model has been
52 recognized in a wide range of scientific disciplines, including biology, geology, agricul-
53 tural science, statistics and economics. For example, Wicksell [1] and Guerrieri [2] applied
54 three-parameter distribution in a study of the age distribution of those marrying for the first
55 time, using the direct estimation method for the parameters of Wicksell [1]. In 1957, Aitchison
56 and Brown [3] applied all the methods available for 65 simulated samples. Royston [4] used
57 this process in a study of the concentration of antibodies in blood, and Crawford [5] applied
58 the same method to study the acidity of lakes. Given the importance of three-parameter log-
59 normal distribution, many studies have been aimed at the problems involved in estimating
60 the parameters of this distribution for data samples, particularly concerning the theoretical
61 and computational difficulties that may arise when applying the ML method. In response to
62 these difficulties, a considerable number of estimators and estimation methods have been
63 proposed. Cohen [6] and Harter and Moore [7] obtained local ML estimates, while Hill
64 [8] proposed Bayesian estimators. Calitz [9], on the other hand, used simulation proce-
65 dures to compare likelihoods, percentiles and estimators of the moments. More recently,
66 Giesbrecht and Kempthorne [10] obtained ML estimators for discrete models, considering
67 grouped intervals, and Wingo [11] introduced *penalty and barrier functions* to increase con-
68 vergence when calculating local ML estimators. Cohen and Witten [12], Cohen *et al.* [13]
69 and Crow and Shimizu [14] proposed various modifications for ML estimators and for esti-
70 mators of the moments. Lifson and Bhattacharyya [15] used a regression method to estimate
71 the percentiles. Wingo [11] worked using a computational algorithm to maximize the like-
72 lihood function (as a function of the third parameter). Kappenman [16] estimated the three
73 parameters by using iterative procedures and comparing the results with the likelihood esti-
74 mators. Finally, Royston [4] estimated the *threshold parameter* using the properties of the
75 median of the lognormal distribution, designing a test to compare hypotheses, based on the
76 median.

77 An important theoretical difficulty that must be overcome is that the likelihood function is
78 maximum where the parameters present unacceptable values. In this respect, Hill [8] obtained
79 Bayesian arguments to justify the use of parametric estimators, which correspond to large local
80 maxima. Moreover, Heyde [17] showed that the three-parameter lognormal distribution cannot
81 be determined solely from its moments, as various problems arise concerning the estimation
82 by the method of moments. From a non-Bayesian standpoint, Griffiths [18] showed that the
83 ML method can be considered a reasonably reliable approach to the problem.

84 The main computational difficulty lies in the fact that the estimation of the parameters
85 complicates the precautions that must be taken (in computational terms) when obtaining the
86 estimators using iterative numerical methods. Many of these methods have been discussed, for
87 example, by Cohen in refs. [6], [12] and [13] and Crow and Shimizu [14], Lambert [19], Harter
88 and Moore [7] and Calitz [9]. If these methods are used without avoiding the region of attraction
89 of infinite ML, then convergence difficulties will be encountered. To avoid such difficulties and
90 to increase the convergence in the estimators of local ML estimators, Wingo [11] introduced
91 frontier function methods with mobile cut-offs.

92 The main objective of this study is to add a threshold parameter to the biparameter stochastic
93 lognormal diffusion process (SLDP), as studied by Gutiérrez *et al.* [20–22]. This work is
94 structured as follows: in section 2, we describe the model using Kolmogorov equations and
95 calculate the probability density function (pdf) and the moments of the model. In section 3,
96 we estimate the parameters of the model by ML method using discrete sampling. In order
97 to estimate the new parameter, we obtain a nonlinear equation, which we propose to solve
98 using NR and SA, reducing the interval of the parameter search by means of Wingo's [11]
99 reparametrization. In section 4, we simulate the trajectory of the process from the exact solution
100 of Itô's stochastic differential equation (SDE) and estimate the parameters by the ML method.

101 In the last section, we apply the model to real data for the mean age of males in Spain at their
102 first wedding.

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105 2. The model and its basic probabilistic characteristics

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108 2.1 The model

109 The one-dimensional lognormal diffusion process with three parameters can be introduced
110 by means of the Kolmogorov backward and forward equation as a Markov process $\{X(t),$
111 $t_0 \leq t \leq T\}$ with values in $]\gamma, +\infty[$, with almost-certainly continuous trajectories and with
112 a distribution function for the process transition that is given by $P(y, t|x, s) = P[X(t) \leq$
113 $y|X(s) = x]$, $x > \gamma$, $y > \gamma$ and $\gamma \in \mathbb{R}$.

114 And by assuming the following conditions:

- 115 • $\lim_{h \rightarrow 0} 1/h \int_{|y-x|>\epsilon} P(dy, t+h|x, t) = 0$,
- 116 • $\lim_{h \rightarrow 0} 1/h \int_{|y-x| \leq \epsilon} (y-x)P(dy, t+h|x, t) = A_1(x, t; \gamma) = \mu(x-\gamma)$,
- 117 • $\lim_{h \rightarrow 0} 1/h \int_{|y-x| \leq \epsilon} (y-x)^2 P(dy, t+h|x, t) = A_2(x, t; \gamma) = \sigma^2(x-\gamma)^2 > 0$,
- 118 • the higher-order infinitesimal moments are null,

119 where $\mu > 0$, $\sigma > 0$, $\mu, \sigma \in \mathbb{R}$, the infinitesimal moments of the process are

$$120 \quad A_1(x, t; \gamma) = \mu(x - \gamma),$$

$$121 \quad A_2(x, t; \gamma) = \sigma^2(x - \gamma)^2,$$

122 and the corresponding Kolmogorov backward and forward equation are

$$123 \quad \frac{\partial p}{\partial s} + \frac{1}{2}\sigma^2(x-\gamma)^2 \frac{\partial^2 p}{\partial x^2} + \mu(x-\gamma) \frac{\partial p}{\partial x} = 0,$$

$$124 \quad -\frac{\partial p}{\partial t} + \frac{1}{2}\sigma^2 \frac{\partial^2 (y-\gamma)^2 p}{\partial y^2} - \mu \frac{\partial (y-\mu)p}{\partial y} = 0,$$

125 where p denotes the transition pdf, $p(y, t|x, s)$, corresponding to the transition distribution
126 function $P(y, t|x, s)$.

127 The common solution to these equations, which can be obtained using Ricciardi's theorem
128 (see [23]), is

$$129 \quad p(y, t|x, s) = \frac{1}{(y-\gamma)\sigma} \frac{1}{\sqrt{2\pi(t-s)}} \exp \left\{ -\frac{1}{2\sigma^2(t-s)} (\ln(y-\gamma) \right.$$

$$130 \quad \left. - \ln(x-\gamma) - a(t-s))^2 \right\}, \quad (1)$$

131 with the initial condition $p(y, s|x, s) = \delta(y-x)$, where $a = \mu - \sigma^2/2$.

132 The distribution of the random variable $X(t)|X(s) = x$ is the one-dimensional three-
133 parameter lognormal distribution

$$134 \quad \Lambda_1 [\gamma + \ln(x-\gamma) + a(t-s); \sigma^2(t-s)],$$

135 $\Lambda_1[\alpha; \beta]$ denotes the one-dimensional three-parameter lognormal distribution with parameters
136 α and β .

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151 Alternatively, the above-defined process can be considered as the solution of the following
152 Itô's SDE

$$153 \quad dX(t) = \mu(X(t) - \gamma)dt + \sigma(X(t) - \gamma)dW(t), \quad X(t_0) = x_0, \quad (2)$$

154 where $W(t)$ represents the Wiener process with independent increments $W(t) - W(s)$
155 distributed according to $\mathcal{N}(0, t - s)$ for $t > s$.

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2.2 Moments of the process

The different moments of the process are obtained from the following expression,

$$E[(X(t) - \gamma)^k | X(s) = x_s] = (x_s - \gamma)^k \exp \left\{ \left(ka + \frac{1}{2} k^2 \sigma^2 \right) (t - s) \right\}.$$

Then the conditioned trend function of the process is

$$E[X(t) | X(s) = x_s] = \gamma + (x_s - \gamma) \exp\{\mu(t - s)\}. \quad (3)$$

Taking into account the initial condition $P[X(t_0) = x_0] = 1$, the trend function is given by

$$E[X(t)] = \gamma + (x_0 - \gamma) \exp\{\mu(t - t_0)\}. \quad (4)$$

The covariance function has the following form

$$\text{Cov}[X(t)X(s)] = (x_0 - \gamma)^2 \exp\{\mu((t - t_0) + (s - t_0))\} [\exp\{\sigma^2((t \wedge s) - t_0)\} - 1],$$

with $t \wedge s = \min(t, s)$.

3. Estimation of the parameters

3.1 Maximum likelihood estimation

We shall now estimate the parameters of the model using the ML method. Let us consider a discrete sampling of the process

$$\{X(t_1) = x_1, X(t_2) = x_2, \dots, X(t_n) = x_n\}$$

for the instants t_1, \dots, t_n , with the initial condition $P[X(t_1) = x_1] = 1$. The associated ML function is thus

$$\mathbb{L}(x_1, \dots, x_n; a, \sigma^2, \gamma) = \prod_{i=2}^n P(x_i, t_i | x_{i-1}, t_{i-1}).$$

This function tends to infinity when γ tends to $x_{(1)}$, where $x_{(1)} = \inf_{0 \leq j \leq n} (x_j)$.

By using equation (1), the log-likelihood function is then

$$\begin{aligned} \ln[\mathbb{L}(x_1, \dots, x_n; a, \sigma^2, \gamma)] &= -\frac{n-1}{2} \ln(2\pi\sigma^2) \sum_{i=2}^n \ln(x_i - \gamma) - \frac{1}{2} \sum_{i=2}^n \ln(t_i - t_{i-1}) \\ &\quad - \frac{1}{2\sigma^2} \sum_{i=2}^n \frac{1}{(t_i - t_{i-1})} [\ln(x_i - \gamma) - \ln(x_{i-1} - \gamma) \\ &\quad - a(t_i - t_{i-1})]^2. \end{aligned} \quad (5)$$

From equation (5), differentiating with respect to each of the parameters and setting the results equal to zero, we obtain the likelihood equations for a , σ^2 and γ . By performing some

201 calculations, we obtain the following expressions for the estimators \hat{a} , $\hat{\sigma}^2$ and $\hat{\gamma}$,

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$$\hat{a} = \frac{[\ln(x_n - \hat{\gamma}) - \ln(x_1 - \hat{\gamma})]}{t_n - t_1}, \quad (6)$$

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$$\hat{\sigma}^2 = \frac{1}{n-1} \sum_{i=2}^n \frac{[\ln(x_i - \hat{\gamma}) - \ln(x_{i-1} - \hat{\gamma}) - \hat{a}(t_i - t_{i-1})]^2}{t_i - t_{i-1}}, \quad (7)$$

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$$\lambda(\hat{\gamma}) = \hat{\sigma}^2 \sum_{i=2}^n \frac{1}{(x_i - \hat{\gamma})} - \sum_{i=2}^n \frac{(x_i - x_{i-1})[\ln(x_i - \hat{\gamma}) - \ln(x_{i-1} - \hat{\gamma})]}{(x_i - \hat{\gamma})(x_{i-1} - \hat{\gamma})(t_i - t_{i-1})}$$

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$$+ \hat{a} \frac{x_n - x_1}{(x_n - \hat{\gamma})(x_1 - \hat{\gamma})}, \quad (8)$$

212 where $\lambda(\hat{\gamma}) = 0$ and $\gamma < x_{(1)}$.

216 3.2 Reparametrization of the process, according to Wingo

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218 Estimating the third parameter that is to be introduced into the three-parameter lognormal
219 distribution is well known to be problematic.

220 The main theoretical difficulty is that the likelihood function reaches global maxima at
221 points where the parameters present unacceptable values and where the global maximum
222 value of the likelihood function is $+\infty$.

223 The main computational difficulty encountered is that the iterative numerical methods used
224 for ML estimation must be employed with great care, as these methods do not avoid the region
225 of attraction of infinite ML, and so problems of convergence arise. In other words, when
226 we seek to find a solution to the equation (8) by means of a numerical approach, and as the
227 initial estimate of γ is not close enough to the solution, this method will converge toward
228 the degenerate solution $\gamma = -\infty$. Thus, we require an algorithm that is both computationally
229 efficient and definitely convergent. In an attempt to resolve this problem, Wingo [11], for the
230 case of three-parameter lognormal distribution, proposed a computational algorithm based on
231 the reparametrization of the likelihood function, using a parametric transform, to reduce the
232 interval of the real slope on which many finite local maxima of the log-likelihood function
233 are located. This function is globally maximized by means of numerical methods within the
234 reduced interval that has been found. The upper part of the search interval can be chosen
235 depending on the precision of the data that are observed.

236 Let us now describe the algorithm used by Wingo and consider the same reparametrization
237 for the case of the one-dimensional lognormal diffusion process with three parameters.

238 Consider the following transform

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$$\gamma(\theta) = x_1 - \exp(-\theta), \quad] - \infty, +\infty[, \quad (9)$$

241 where x_1 is the minimum of the values in the sample.

242 It can be shown that $\gamma \rightarrow x_1$ when $\theta \rightarrow +\infty$ and that $\gamma \rightarrow -\infty$ when $\theta \rightarrow -\infty$, and
243 substituting in equation (5), we obtain $\ln[\mathbb{L}(x_1, \dots, x_n; a, \sigma^2, \gamma(\theta))]$, denoted by $\mathbb{L}^*(a, \sigma^2, \theta)$.

244 The computational algorithm is straightforward.

- 245
246 • Globally maximize $\mathbb{L}^*(a, \sigma^2, \theta)$ in a compact interval on the real slope to obtain a global
247 maximum $\hat{\theta}$.
- 248 • The local ML estimator, $\hat{\gamma}$, is then calculated by means of

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$$\hat{\gamma}(\theta) = x_1 - \exp(-\hat{\theta}). \quad (10)$$

- The remaining ML estimators are calculated by substituting the value $\hat{\gamma}$ in the equations (6) and (7).

The transform (9) can be seen, approximately, as a compression of the range of values over which the conditioned log-likelihood function must be maximized to find $\hat{\gamma}$. Obviously, this compression is computationally advantageous; it can be shown that maximizing equation (5) over γ may require up to 10 more evaluations of the objective function than when it is maximized over θ .

In the numerical data presented in ref. [11], the search interval chosen for θ was $[-10, 10]$. This choice of search range for θ has the advantage of being wide enough to cover the area in which the real value of the threshold parameter γ may be found, yet small enough as to exclude the infinite maximum of the log-likelihood function given in $\theta = +\infty$. This interval corresponds approximately to $[-20.000; x_1 - \epsilon]$ in γ -space, where $\epsilon \simeq 4 \times 10^{-5}$, a choice that may be useful for most of the samples likely to be found in practice.

Sometimes, it is useful to express the right-hand side of the search interval for θ as a function of the precision of the data. For example, if each of the observations x_i is fitted to three decimal places and the log-likelihood function has to be maximized over the interval $[-20.000, x_1 - \epsilon]$ of γ , then $\epsilon < 10^{-3}$ cannot be chosen, as the probability of the finite maximum of the log-likelihood function for γ belonging to the interval $x_1 - \epsilon < \gamma < x_1$ for $\epsilon < 10^{-3}$ is extremely remote. To reflect the precision of the data, we could choose $\epsilon < 10^{-d}$ or $\epsilon = |x_1| \times 10^{-10}$, where $d \geq 1$ is the number of decimal places of precision in the data. The corresponding upper limit of the search interval for θ could be $\theta = -\ln(10^{-d})$ or $\theta = -\ln(|x_1| \times 10^{-10})$.

By applying this transform to our process, the log-likelihood function would then be

$$\begin{aligned} \mathbb{L}^*(a, \sigma^2, \theta) = & -\frac{n-1}{2} \ln(2\pi\sigma^2) - \sum_{i=2}^n \ln(x_i - [x_1 - \exp(-\theta)]) \\ & - \frac{1}{2} \sum_{i=2}^n \ln(t_i - t_{i-1}) - \sum_{i=2}^n \frac{1}{2\sigma^2(t_i - t_{i-1})} [\ln(x_i - [x_1 - \exp(-\theta)]) \\ & - \ln(x_{i-1} - [x_1 - \exp(-\theta)]) - a(t_i - t_{i-1})]^2. \end{aligned} \quad (11)$$

By differentiating equation (11) with respect to θ and setting the result equal to zero, we obtain the following expression that provides an estimator for θ . By substituting this expression in the other likelihood equations, we obtain the estimators for the remaining parameters, as described above.

$$\begin{aligned} \hat{a} \left(\frac{1}{(x_n - \hat{\gamma}(\theta))} - \frac{1}{(x_1 - \hat{\gamma}(\theta))} \right) = & \sum_{i=2}^n \frac{e^{-\theta} \hat{\sigma}^2}{(x_i - \hat{\gamma}(\theta))} \\ & - \sum_{i=2}^n \frac{(x_i - x_{i-1}) [\ln(x_i - \hat{\gamma}(\theta)) \ln(x_{i-1} - \hat{\gamma}(\theta))]}{(x_i - \hat{\gamma}(\theta))(x_{i-1} - \hat{\gamma}(\theta))(t_i - t_{i-1})}. \end{aligned} \quad (12)$$

3.3 Simulated annealing optimization method

The *simulated annealing* (SA) or *simulated overheating* method is a technique that has attracted considerable attention in large-scale optimization problems. It originated in the study by Metropolis *et al.* [24] aimed at minimizing a function on a very large finite set, although it could also be applied to optimization on a continuous set (see [25]). Various authors, such as

301 Kirkpatrick *et al.* [26], have demonstrated the utility of this method for finding global solutions
 302 to combinatory optimization problems.

303 The problem we address is

$$304 \max_{\theta \in \Theta} h(\theta) \quad (13)$$

305
 306 or equivalently

$$307 \min_{\theta \in \Theta} -h(\theta). \quad (14)$$

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 309 The fundamental idea of the method is that a change of scale, called the temperature, allows
 310 faster movements over the surface of the function h to be maximized, the negative of which is
 311 termed energy (see [27, 28]). The optimum state, therefore, is achieved if T decreases slowly
 312 and well under control. The change in the partial scale avoids the attraction of local maxima.

313 To simulate the evolution of a physical system, we introduce the iterative method known as
 314 *the Metropolis acceptance rule*, which induces a change in the current state of the system in
 315 the following terms:

- 316 • If the system energy S decreases, the modification is accepted.
- 317 • If the energy increases by ΔS , the modification may be accepted with a probability of
 318 $\exp\{-\Delta S/T\}$, where T is the temperature and Δ the increase in h .

319
 320 The implementation of the SA algorithm is remarkably easy. The following elements must
 321 be provided:

- 322 (i) a representation of possible solutions,
- 323 (ii) a generator of random changes in solutions,
- 324 (iii) a means of evaluating the problem functions,
- 325 (iv) an annealing schedule (an initial temperature and rules for lowering it as the search
 326 progresses).

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 328 In practice, the temperature parameter decreases by levels, generating a succession of states,
 329 enabling the system to approximate the equilibrium for each level. The algorithm stops for a
 330 small value of T , such that virtually no new generation is accepted. Thus, what is chosen as
 331 the solution to the problem is the state that optimizes the objective function among the states
 332 of the succession that is generated.

333 Various studies have shown that the asymptotic convergence of SA is guaranteed, but in
 334 practice it is necessary to implement the algorithm within a finite time. To do so, we define a
 335 finite succession of truncated Markov chains, associated with decreasing temperature values.

336 The basic structure of SA algorithm is presented in table 1. The following notations are
 337 used:

- 338 θ = the current solution,
- 339 θ^* = the best solution,
- 340 θ_n = neighboring solution,
- 341 $h(\theta)$ = the value of objective function at solution θ ,
- 342 n = repetition counter,
- 343 T_0 = initial temperature,
- 344 T_f = final temperature,
- 345 L = number of repetition allowed at each temperature level,
- 346 p = probability of accepting θ_n when it is not better than θ .

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 348 The algorithm starts with an initial solution for the problem. As we can see in table 1, SA
 349 has two cycles, inner and outer. In the inner cycle, SA is repeated while $n < L$, a neighboring
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Table 1. SA algorithm for minimization problem.

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Initialize the SA control parameter ( $T_0, L$ )
Select an initial solution,  $\theta_0$ 
Set  $T = T_0$ ; Set  $\theta = \theta_0$ ; Set  $\theta^* = \theta_0$ ; Calculate  $h(\theta_0)$ ;
While the stop criterion is not reached do:
  Set  $n = 1$ 
  While  $n < L$  do:
    Generate solution  $\theta_n$  in the neighborhood of  $\theta_0$ ; Calculate  $\Delta = h(\theta_n) - h(\theta)$ ;
    If  $\Delta \leq 0$ 
       $\theta = \theta_n$ 
    else
      generate a random number,  $r \in (0, 1)$ 
      if ( $r \leq p = e^{-\Delta/T}$ );
         $\theta = \theta_n$ ;  $n = n + 1$ ;
      end
    end
    if ( $h(\theta) < h(\theta^*)$ )
       $\theta^* = \theta$ ;
    end
  end
  reduce the temperature  $T$ ;
end

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solution θ_n of the current solution, θ is generated. If $\Delta \leq 0$ (θ_n is better than θ), then the generated solution replaces the current solution, otherwise the solution is accepted with the criterion probability $p = e^{-\Delta/T}$. The value of the temperature, T , decreases in each iteration of the outer cycle of the algorithm. The performance of SA depends on the definition of the several control parameters:

- (i) The initial temperature should be high enough that, in the first iteration of the algorithm, the probability of accepting a worse solution is, at least, 80%.
- (ii) We shall now determine all the initial values required by the algorithm and the temperature reduction rate. In the particular case in question, it is determined by means of the following expression:

$$T_i = \frac{T_0}{i + 1},$$

where T_0 is the initial temperature fixed. This rate ensures that the cooling is slow enough for the optimum value to be reached.

- (iii) The stopping criterion defines when the system has reached a desired energy level.

3.4 Application of the simulated annealing optimization method

The function to be minimized in the case in question is

$$\begin{aligned}
 -\ln[L(x_1, \dots, x_n; a, \sigma^2, \gamma)] &= \frac{n-1}{2} \ln(2\pi\sigma^2) + \sum_{i=2}^n \ln(x_i - \gamma) + \frac{1}{2} \sum_{i=2}^n \ln(t_i - t_{i-1}) \\
 &+ \frac{1}{2\sigma^2} \sum_{i=2}^n \frac{1}{(t_i - t_{i-1})} [\ln(x_i - \gamma) - \ln(x_{i-1} - \gamma) \\
 &- a(t_i - t_{i-1})]^2
 \end{aligned} \tag{15}$$

401 By applying the reparametrization proposed by Wingo [11] to the above function, we obtain

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$$\begin{aligned}
 -\ln[L(x_1, \dots, x_n; a, \sigma^2, \theta)] &= \frac{n-1}{2} \ln(2\pi\sigma^2) + \sum_{i=2}^n \ln(x_i - [x_1 - \exp(-\theta)]) \\
 &+ \frac{1}{2} \sum_{i=2}^n \ln(t_i - t_{i-1}) + \sum_{i=2}^n \frac{1}{2\sigma^2(t_i - t_{i-1})} \\
 &\times [\ln(x_i - [x_1 - \exp(-\theta)]) - \ln(x_{i-1} - [x_1 - \exp(-\theta)]) \\
 &- a(t_i - t_{i-1})]^2,
 \end{aligned}$$

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where x_1 is the minimum of the sample values.

There now arises the problem of deciding upon the new neighbor, *i.e.* how we are to choose a new value for the parameters. To do this, we generate the value of a distribution uniform, which is added to the previous value of the parameter, provided that always the new value is located within an appropriate range of possible values for the parameters. To ensure this, we must decide as to which range is acceptable for each parameter. In the present case, various graphic procedures are used, based on likelihood equations, so that we may bound the possible optimum values of the parameters.

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4. Simulation studies

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The stochastic differential equation (2) has a single continuous solution in the interval $[t_0, T]$, which corresponds to the three-parameter lognormal diffusion process, the explicit expression of which can be obtained by means of Itô's formula, applied to the transform $\ln(X(t) - \gamma)$, and which has the following form

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$$X(t) = \gamma + (x_0 - \gamma) \exp \left\{ \left(\mu - \frac{\sigma^2}{2} \right) (t - t_0) + \sigma (W(t) - W(t_0)) \right\}. \quad (16)$$

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From this explicit solution, we can obtain the simulated trajectories of the process by discretizing the time interval $[t_0, T]$, with the initial condition $W(t_0) = 0$. The Wiener process is obtained as the sum of the distributions $\mathcal{N}(0, h)$, where $h = t_i - t_{i-1}$.

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From this simulated process sample, we estimate the parameters by ML, first using the Newton–Raphson (NR) nonlinear approach to approximate the value of $\hat{\gamma}$. Secondly, we discuss the problems that occur in estimating the parameters of the three-parameter lognormal diffusion process. We propose SA optimization to the estimation of the parameters, by which some of the above-discussed problems may be overcome.

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The process is reparametrized, as described in section 3.2, in order to perform a compression of the range of values over which the conditioned log-likelihood function must be maximized to find $\hat{\gamma}$.

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The parameters of the process are estimated by applying the method to the simulated data set described previously, which enable us to test the effectiveness of the method.

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Table 2 shows the values used in the simulation and the results obtained by estimating the parameters, using the methods described above, implemented using the Mathematica packages by considering $h = 1$, $n = 25$ and an initial value $x_0 = 1.22139$.

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These results clearly show that the SA algorithm is a good estimation method and that it enables us to eliminate many of the difficulties encountered with ML estimation.

Table 2. Starting values used in the simulation and estimation of the parameters.

	γ	μ	σ
Simulation	1	0.2	0.00010
Estimation NR	1.00006	0.200006	0.00008
Estimation SA	1.00483	0.214715	0.00091

5. Application to real data

5.1 Description of the methodology

We studied the evolution of a basic demographic indicator, that of the weddings taking place in a society and, specifically, the time-dependent stochastic variable:

$$Y(t) = \text{mean age of males in Spain at the date of their first wedding.}$$

The following steps were performed in the statistical methodology:

- Values were observed for the period 1982–2001 for the estimation of the parameters, reserving the values observed for the years 2002 and 2003 for comparison with the corresponding prediction by the model. The values observed correspond to observations over time intervals equal to 1 year. The source for the data was the Spanish National Institute of Statistics (INE).
- The estimations of the parameters were calculated by ML, using the expressions obtained in equations (6)–(8). The expression (8) was approximated numerically using the NR and SA methods.

Table 3. Observed values, MLCTF estimated trends for NR and SA and predicted value.

Years	Observed $Y(t)$	MLCTF-NR	MLCTF-SA
1982	26.70	26.7000	26.7000
1983	26.76	26.8303	26.7939
1984	26.90	26.8929	26.8556
1985	27.03	27.0389	26.9996
1986	27.15	27.1745	27.1333
1987	27.23	27.2997	27.2567
1988	27.39	27.3832	27.3389
1989	27.56	27.5501	27.5035
1990	27.81	27.7275	27.6783
1991	28.09	27.9883	27.9354
1992	28.35	28.2804	28.2233
1993	28.66	28.5517	28.4907
1994	28.92	28.8751	28.8095
1995	29.16	29.1464	29.0769
1996	29.46	29.3968	29.3237
1997	29.69	29.7097	29.6322
1998	29.85	29.9497	29.8687
1999	30.01	30.1166	30.0333
2000	30.16	30.2836	30.1978
2001	30.41	30.4400	30.3521
<i>Prediction</i>			
2002	30.63	30.7009	30.6092
2003	30.89	30.9304	30.8354

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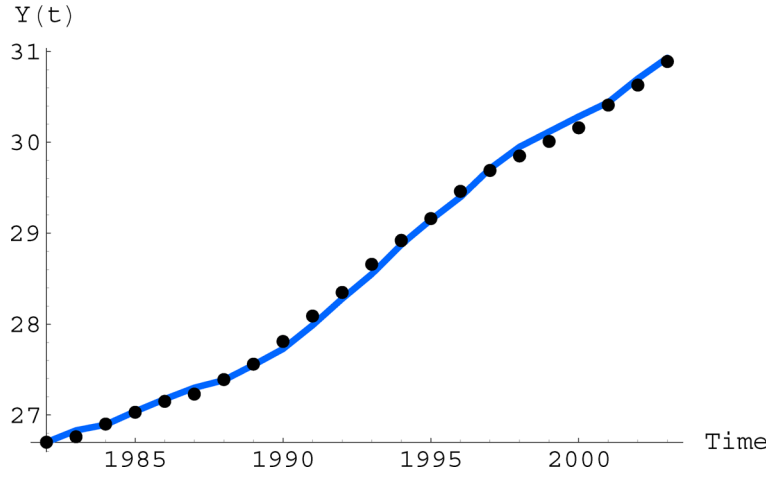


Figure 1. Fit and prediction based on MLCTF-NR.

- The ML conditional trend function of the process (MLCTF) can be obtained using Zehna’s theorem (see [29]), replacing the parameter with the estimators in equation (3). Thus, we obtain two MLCTF, the first when $\hat{\gamma}$ is obtained by NR, which we denote as MLCTF-NR, and the second when $\hat{\gamma}$ is obtained by SA, which is denoted as MLCTF-SA. These two functions are used to fit and predict.

5.2 Fitting the model using ML

The expression (8) is approximated numerically using NR and we thus obtain the following ML estimates $\hat{\gamma} = 23.6911$, $\hat{\mu} = 0.042381$ and $\hat{\sigma} = 0.0140717$.

After estimating the parameters for the variable considered using SA, the results achieved are as follows: $\hat{\gamma} = 23.3911$, $\hat{\mu} = 0.027979$, $\hat{\sigma} = 0.0007018$.

Table 3 shows the observed values of the variable and those of the estimated ML conditioned trend functions using NR and SA.

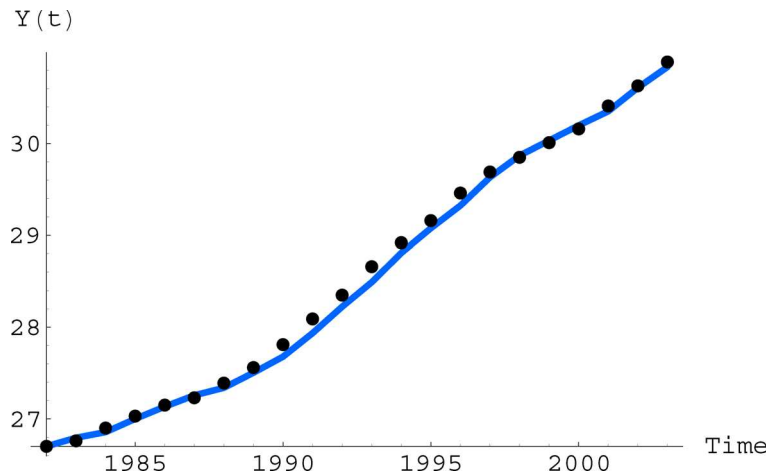


Figure 2. Fit and prediction based on MLCTF-SA.

Figure 1 shows the fit and the prediction for $Y(t)$ using the MLCTF-NR. Figure 2 shows the fit and the prediction for $Y(t)$ using the MLCTF-SA.

6. Conclusions

The fundamental goal of this study is to introduce and examine a stochastic three-parameter lognormal diffusion process. To do this, we determine the basic probabilistic results (section 2) and inferential results, in particular estimation based on discrete sampling of the process using ML (section 3). The problems that arise in applying ML estimation with a threshold parameter are addressed via an extension of Wingo's reparametrization technique in the case of a three-parameter lognormal distribution to the process proposed in this study. The main conclusion reached, from a computational standpoint is that when this reparametrization method is used, calculating the estimator of the threshold parameter of the process using numerical methods based on the reparametrized equation (12) and obtaining it by the alternative SA methodology produce similar results, regarding both simulated and real data.

The tables 4 and 5 show the results obtained using the two estimation methods described; table 4 shows the process parameters from the simulation of $X(t)$ and table 5 shows those estimated from the observed data of process $Y(t)$.

The small discrepancies observed between the two methods could be reduced by adjusting the precision and number of iterations when using the SA algorithm.

We calculated a global descriptive measure of the discrepancy between the adjusted values and those observed, using the sampling variance; in the case of NR estimation, the value was 0.003, and for estimation by the SA method it was 0.004, thus confirming the similarity of the two methodologies.

Although the proposed method is still being refined, the results obtained lead us to believe that it constitutes a good alternative to existing methods, as both its theoretical basis and its implementation or adaptation to any type of problem are much more straightforward. Moreover, most existing methods depend to a large extent on the initial solution. With the proposed method, however, if the Markov chain lengths produced are long enough, there is no such dependence, although this fact does mean that more time must be applied in searching for the solution.

Table 4. Estimation of the parameters for the set of simulated data.

	$\hat{\gamma}$	$\hat{\mu}$	$\hat{\sigma}$
Estimation NR	1.00006	0.200006	0.00008
Estimation SA	1.00483	0.214715	0.00091

Table 5. Estimation of the parameters for the observed $Y(t)$.

	$\hat{\gamma}$	$\hat{\mu}$	$\hat{\sigma}$
Estimation NR	23.6911	0.042381	0.0140717
Estimation SA	23.3911	0.027979	0.0007018

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