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The nonhomogeneous lognormal diffusion process as a general process to model particular types of growth patterns

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Abstract. In the present article, we have considered the nonhomogeneous lognormal diffusion process (also known as the lognormal diffusion process with exogenous factors) as a way to generate stochastic diffusion models associated with a variety of growth curves. To this end, general conditions have been set, and then we have looked into how it applies to curves commonly used in several fields of application, such as the Gompertz, the logistic, the Bertalanffy, and the Richards curves. Since the resulting processes are transformations of the Wiener process, this fact can be used for sample-path simulation purposes, or we may instead discretize the corresponding stochastic differential equation. A function in R is presented to allow for both options. The problem of the maximum likelihood estimation of parameters is treated, and the use of stochastic optimization procedures such as Simulated Annealing or Variable Neighborhood Search is suggested. For the efficient application of these procedures, some strategies are presented in order to bound the associated parametric spaces.

1. INTRODUCTION.

The nonhomogeneous lognormal diffusion process (or lognormal diffusion process with exogenous factors) is defined by a diffusion process $\{X(t); t_0 \leq t \leq T\}$, taking values on $\mathbb{R}^+$, with infinitesimal moments

$$
\begin{aligned}
A_1(x,t) &= h(t)x \\
A_2(x) &= \sigma^2 x^2 ,
\end{aligned}
\tag{1}
$$

where $h(t)$ is a continuous function in $[t_0, T]$ and $\sigma > 0$, and with a lognormal or degenerate initial distribution. This process generalizes the homogeneous version of the process, in which case $h(t) = m$, with $m \in \mathbb{R}$.

The homogeneous lognormal diffusion process has been commonly used in several scientific fields in which the variable under consideration shows an exponential

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trend. For example, in the study of population growth in ecological studies ([3] and [17]) or, in Economics, to model dynamic variables ([4], [15] and [16]), where it is commonly associated with the Black-Scholes model ([2]) and its extensions ([14]).

One of the main reasons to include a function $h(t)$ in the infinitesimal mean of the homogeneous process is that it allows to represent time-dependent external influences on the behavior of the variable under study (endogenous variable) which affect the drift of the process. In some situations, these influences may be expressed in terms of a set of external variables whose behavior is assumed as known, and they must contribute to the description of the evolution of the process as well as to its external control. Concretely, the possibility of there being several external influences to the endogenous variable of the process makes it customary to consider a linear exogenous factor $h(t) = \beta_0 + \sum_{j=1}^{q} \beta_j F_j(t)$, with $\beta_j \in \mathbb{R}$ and F_j time-continuous functions in $[t_0, T]$, $j = 1, \cdots, q$. This case has been widely studied as related to some aspects of inference as well as first-passage times ([6], [7], [9], [12] and [23]) and has been applied to the modeling of time-variables in several fields. For example, Gutiérrez *et al.* ([8], [10]), built a nonhomogeneous lognormal diffusion process to fit Spain's *gross national product* by considering *consumer spending* and *gross domestic fixed capital formation* as exogenous variables. These applications are examples of the endogenous variable itself helping identify the exogenous factors. Nevertheless, there are situations in which external variables to the process that have an influence on the system are not available, or situations in which their functional expressions are unknown. In such a case, Gutiérrez *et al.* [11] suggested approaching the exogenous factors by means of polynomial functions. Here, specifically: $h(t) = \sum_{j=0}^{k} \beta_j^{k)} P_j^{k)}(t)$, where $P_j^{k)}$ is a q-degree polynomial ($P_0^{k)} = 1$) and $\beta_j^{k)}$ are real fixed parameters, $j = 1, \cdots, k$.

On the other hand, considering particular $h(t)$ functions has enabled diffusion processes associated to alternative expressions of already-known growth curves to be defined. Along these lines, we may cite a Gompertz-type process (introduced in [13] and applied to the study of rabbit growth), a generalized von Bertalanffy diffusion process (introduced in [18], with an application to the growth of fish species), a logistic-type process (introduced in [20], with an application to the growth of a microorganism culture) and a Richards-type diffusion process (introduced in [22]).

The goal of the present study is to delve deeper into this second approach, with a general nonhomogeneous lognormal process as the starting point. We will focus on aspects which may affect a general analysis of the process, but also on those which are specific to each particular curve.

Section 2 will present the main characteristics of the nonhomogeneous lognormal process, and Section 3 will deal with the properties that a curve must verify for its behavior pattern to be modeled using a nonhomogeneous lognormal process. In Section 4, a function in R will be used to tackle sample paths simulation in some particular processes. Finally, Section 5 will look into the problem of the maximum likelihood estimation of parameters of nonhomogeneous lognormal processes in general. Given the inherent difficulties of providing general solution strategies for likelihood equations that must contemplate all particular models, the use of stochastic optimization procedures is suggested. For an efficient application of such procedures, the bounding of parametric space is defined for the particular models considered in this paper.

2. THE NONHOMOGENEOUS LOGNORMAL DIFFUSION PROCESS (OR THE LOGNORMAL DIFFUSION PROCESS WITH EXOGENOUS FACTORS)

The nonhomogeneous lognormal diffusion process (or lognormal diffusion process with exogenous factors), with infinitesimal moments given by (1), is the solution to the stochastic differential equation (SDE):

$$\begin{aligned} dX(t) &= h(t)X(t)dt + \sigma X(t)dW(t) \\ X(t_0) &= X_0 \ , \end{aligned} \tag{2}$$

where $W(t)$ is a standard Wiener process independent on X_0, $t \geq t_0$.

Equation (2) can be obtained from the ordinary differential equation

$$\frac{d\,x(t)}{dt} = h(t)x(t) \ , \tag{3}$$

which can be viewed as a generalization of the Malthusian growth model with a time-dependent fertility rate $h(t)$. By replacing in (3) the function $h(t)$ with $h(t) + \Lambda(t)$, where $\Lambda(t)$ is a white noise with variance σ^2, a Langevin equation is obtained, which leads to (2) if rewritten as a SDE.

Equation (2) verifies the conditions of the existence and the uniqueness theorem for SDEs (see Arnold [1]), being its solution

$$X(t) = X_0 \, \exp\left(\int_{t_0}^{t} h(u)\, du - \frac{\sigma^2}{2}(t - t_0) + \sigma(W(t) - W(t_0)) \right) \quad , \quad t \geq t_0 \ . \tag{4}$$

In order to calculate the finite-dimensional distributions of this process, the distribution of X_0 must be fixed. Here, we have considered a degenerate distribution at t_0, that is $P[X(t_0) = x_0] = 1$, or lognormal $\Lambda_1(\mu_0, \sigma_0^2)$ [1]. In such a case, all finite-dimensional distributions are lognormal. Concretely, $\forall n \in \mathbb{N}$ and $t_1 < t_2 < \cdots < t_n$, we have

$$(X(t_1), \cdots, X(t_n))^T \ \sim \ \Lambda_n(\mu, \Sigma) \ ,$$

where the components of vector $\mu = (\mu_1, \cdots, \mu_n)^T$ and the matrix $\Sigma = (\sigma_{ij}),\ i, j = 1, \cdots, n$, are

$$\mu_i = E[X_0] + \int_{t_0}^{t_i} h(u)\, du - \frac{\sigma^2}{2}(t_i - t_0) \quad , \quad i = 1, \cdots, n$$

and

$$\sigma_{ij} = \mathrm{Var}[X_0] + \sigma_0^2(t_i - t_0) \quad , \quad i, j = 1, \cdots, n \ .$$

In particular, from the bidimensional distribution $(X(s), X(t))^T,\ s < t$, the transition distribution of the process is

$$X(t)|X(s) = x_s \sim \Lambda_1 \left(\ln x_s + \int_s^t h(u)\, du - \frac{\sigma^2}{2}(t - s), \sigma^2(t - s) \right) \ , \ s < t \ . \tag{5}$$

Once the finite dimensional distribution has been calculated, the main characteristics of the process can be obtained. We will now describe some of these characteristics, focusing on the most commonly-employed practical applications (in particular

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[1] Note that the former case is a particular case of the second, with $\mu_0 = \log x_0$ and $\sigma_0^2 = 0$.

for fitting and forecasting purposes): the n-th moment, the mode and quantile functions (as well as their conditional versions). Their expressions can be formulated jointly for the two aforementioned initial distributions from the following function:

$$G^{\lambda}(t|y,\tau) = M(t|y,\tau)^{\lambda_1} \exp\left(\lambda_2 \left(\lambda_3 \sigma_0^2 + \sigma^2(t-\tau)\right)^{\lambda_4}\right) ,$$

with $\lambda = (\lambda_1, \lambda_2, \lambda_3, \lambda_4)^T$ and where

$$M(t|y,\tau) = \exp\left(\int_{\tau}^{t} h(u)\,du + y - \frac{\sigma^2(t-\tau)}{2}\right) .$$

Table 1 summarizes the different functions according to the values of λ, τ and y. In particular, the mean function of the process and the one conditioned on an initial value x_0 are

Function	Expression	y	τ	λ
n-th moment	$E[X(t)^n]$	μ_0	t_0	$(n, n^2/2, 1, 1)^T$
n-th conditional moment	$E[X(t)^n \vert X(s) = x_s]$	$\ln x_s$	s	$(n, n^2/2, 0, 1)^T$
mode	$\mathrm{Mode}[X(t)]$	μ_0	t_0	$(1, -1, 1, 1)^T$
conditional mode	$\mathrm{Mode}[X(t) \vert X(s) = x_s]$	$\ln x_s$	s	$(1, -1, 0, 1)^T$
α-quantile	$C_\alpha[X(t)]$	μ_0	t_0	$(1, z_\alpha, 1, 1/2)^T$
α-conditional quantile	$C_\alpha[X(t) \vert X(s) = x_s]$	$\ln x_s$	s	$(1, z_\alpha, 0, 1/2)^T$

Table 1. Values of λ, τ and y used to obtain the n-th moment, the mode and quantile functions from $G^{\lambda}(t|y,\tau)$. Here z_α denotes the α-quantile of a standard normal distribution.

$$m(t) = E[X(t)] = \exp\left(\mu_0 + \frac{\sigma_0^2}{2} + \int_{t_0}^{t} h(u)\,du\right)$$
$$m(t|t_0) = E[X(t)|X(t_0) = x_0] = x_0 \exp\left(\int_{t_0}^{t} h(u)\,du\right)$$

and verify the ordinary differential equation (3), that is

$$m'(t) = m(t)h(t) \quad , \quad m'(t|t_0) = m(t|t_0)h(t) .$$

This last property makes the diffusion process defined by (2) able to model several behavior patterns (concretely those showing a behavior fitting $m(t)$). Furthermore, function $m(t|t_0)$ allows to consider situations in which the properties of the mean function may depend on the initial value.

In the next section we present a broad family of growth curves verifying (3), for which it is possible to define particular nonhomogeneous lognormal diffusion processes modeling behavior patterns associated with each curve. Moreover, the mean function of each process matches the corresponding curve.

3. Several growth curves whose behavior pattern can be modeled by a nonhomogeneous lognormal diffusion process

Condition (2) includes a wide range of curves, but we will focus on some positive, bounded and sigmoidal growth curves which have proven to be useful in several fields of application (Economics, Biology, Medicine, etc.). In general, let $f_\theta(t)$ be a positive function defined over $[t_0, +\infty)$, verifying that:

a) it is continuous, bounded and differentiable;
b) its functional form depends on a parameter $\theta = (\theta_1, \cdots, \theta_k)^T$, being Θ the associated parameter space;
c) $f_\theta(t) = k(\theta) g_\theta(t)$ with $\lim_{t\to+\infty} g_\theta(t) = 1$;
d) $f'_\theta(t) = f_\theta(t) h_\theta(t)$, with $h_\theta(t)$ being continuous and bounded at $[t_0, +\infty)$;
e) f_θ has at least one inflection point.

Please note that condition d) enables us to consider a nonhomogeneous lognormal diffusion process of the type (4), whose mean is function $f_\theta(t)$. To this end, we have but to consider

$$h_\theta(t) = \frac{f'_\theta(t)}{f_\theta(t)} = \frac{g'_\theta(t)}{g_\theta(t)} .$$

Let us observe that $\lim_{t\to+\infty} f_\theta(t) = k(\theta)$, regardless of the values previously taken by the curve. In certain occasions this property will not be verified, with the limit value depending on some feature of the curve as its initial value. For instance, the evolution of the weight of individuals of the same animal or vegetal species may exhibit a similar behavior, but the limit value for each individual may depend on its weight at birth (see Gutiérrez et al. [13]; Román and Torres, [21]). This requires a reparametrization of the original curve. For the purposes of the present study, we will consider the case of the value of the limit value depending on the initial value (a similar reasoning can be applied if it is dependent on any other value taken by the curve). Thus, if $f_\theta(t_0) = x_0 = k(\theta) g_\theta(t_0)$, we may say that

$$f_\theta(t) = x_0 \, \frac{g_\theta(t)}{g_\theta(t_0)} .$$

As for other features of the curve, growth intervals will depend on the sign of $h_\theta(t)$, whereas time instants at which the inflections are reached are those which solve the equation $h^2_\theta(t) + h'_\theta(t) = 0$.

The present paper will focus solely on curves presenting a single inflection point. We will specifically deal with Gompertz, Bertalanffy, logistic, and Richards curves. Table 2 summarizes all the features already mentioned. Alongside with the name of the curve, a reference is included to the article describing its modelization through a nonhomogeneous lognormal diffusion process (the notation of the parameters used in each article has been maintained). In addition to functions g_θ and h_θ, limit values ($k(\theta)$), inflection time (t_I), and value of the curve at this time are displayed. The last column shows the condition affecting the parameters so that the inflection time can be visualized (i.e. happens at an instant after t_0). The notation of the parameters used in each article has also been maintained here.

4. SIMULATION OF SAMPLE PATHS

The simulation of sample paths for a particular nonhomogeneous lognormal process can be approached, among others, in the following ways:

- by applying (4) from the simulated sample paths of a standard Wiener process;
- by solving the SDE (2) using numerical methods.

To consider the mentioned approaches, we have created a function in R (GeneralLognormalSimulation) whose code is shown in Appendix 1.

The arguments of this function are:

N_Sp Number of sample paths to be simulated.

n Data number in each sample path (regardless of the initial value).

r Simulation step.

t0 Initial time.

x0 Initial distribution (value of x_0 for a degenerate distribution of vector of parameters (μ_0, σ_0) for the case of a lognormal distribution $\Lambda(\mu_0, \sigma_0^2)$).

s Value of σ in the infinitesimal variance.

method A choice between "TransfW" (if the transformation to the Wiener is used to perform the simulation) and "sde" (if the SDE is solved). In the second case, the package Sim.DiffProc [5] is used, in its default settings for the simulation of the SDE (Itô type) and the numerical method used (Euler).

The function interactively asks the particular process to be simulated to choose between GT (GompertzType), Be (Bertalanffy), LT (LogisticType), RT (RichardsType), or An (Another). In the first case, the function interactively asks the parameter values included in the infinitesimal mean. In the second case, the expression of the function $h(t)$ is required in order to define the process, as well as a named list with the names and values of the parameters included therein.

The value of the function is a matrix (if method="TransfW") or a 'ts' object (if method="sde") containing the time instants and the simulated sample paths.

4.1. **Example 1: simulation of a Gompertz-type process.** To simulate 10 sample paths with 101 data points each (from 0 to 10, with step 0.1) for a particular Gompertz-type process with $m = 1$, $\beta = 0.5$, $\sigma = 0.01$ and degenerate initial distribution at 1 (using the transformation to Wiener), we can use the following code:

```
R> Res<-GeneralLognormalSimulation(N_Sp=10,n=100,r=0.1,t0=0,x0=1,s=0.01,
+                             method="TransfW")
```

that requests

```
R> Process to be simulated (you can choose GT (GompertzType),
+  Be (Bertalanffy), LT (LogisticType), RT (RichardsType) or An (Another))=
```

After introducing

```
GT
```

requests

```
R> Value of m?
```

(we introduce 1)

```
R> Value of beta?
```

(we introduce 0.5)

The simulated sample paths are shown in Figure 1.

4.2. **Example 2: Simulation of a Bertalanffy process.** To simulate 100 sample paths with 301 data points each (from 0 to 30, with step 0.1) for a particular Bertalanffy process with $b = 2$, $c = 0.8$, $k = 0.2$, $\sigma = 0.01$ and a $\Lambda(3, 0.2^2)$ as initial distribution (using the transformation to Wiener), we can use the following code:

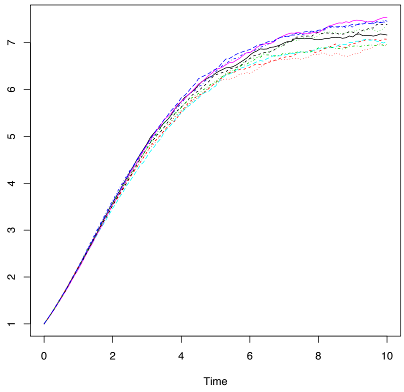

FIGURE 1. Simulated sample paths of a Gompertz-type process.

```
R> Res<-GeneralLognormalSimulation(N_Sp=100,n=300,r=0.1,t0=0,x0=c(3,0.2),
+                                s=0.01, method="TransfW")
```

that requests

```
R> Process to be simulated (you can choose GT (GompertzType),
+ Be (Bertalanffy), LT (LogisticType), RT (RichardsType) or
+ An (Another))=
```

After introducing

```
Be
```

requests

```
R> Value of b?
```

(we introduce 2)

```
R> Value of c?
```

(we introduce 0.8)

```
R> Value of k?
```

(we introduce 0.2)

The simulated sample paths are shown in Figure 2.

4.3. **Example 3: simulation of a logistic-type process.** To simulate 50 sample paths with 501 data points each (from 0 to 50, with step 0.1) for a particular logistic-type process with $b = 200$, $c = 0.25$, $\sigma = 0.01$ and degenerate initial distribution at 5 (using the discretization of the corresponding SDE), we can use the following code:

```
Res<-GeneralLognormalSimulation(N_Sp=50,n=500,r=0.1,t0=0,x0=5,s=0.01,
+                           method="sde")
```

that requests

```
R> Process to be simulated (you can choose GT (GompertzType),
+ Be (Bertalanffy), LT (LogisticType), RT (RichardsType) or An (Another)) =
```

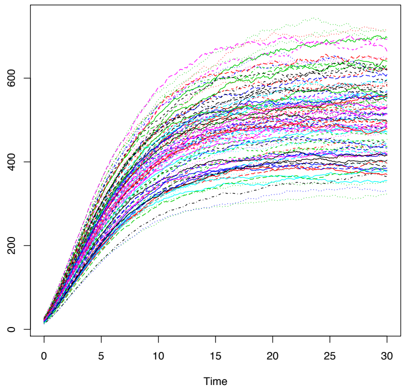

Figure 2. Simulated sample paths of a Bertalanffy process.

After introducing

```
LT
```

requests

```
R> Value of b?
```

(we introduce 200)

```
R> Value of c?
```

(we introduce 0.25)

The R code `plot(Res,plot.type="single", ylab=" ")` produces the Figure 3.

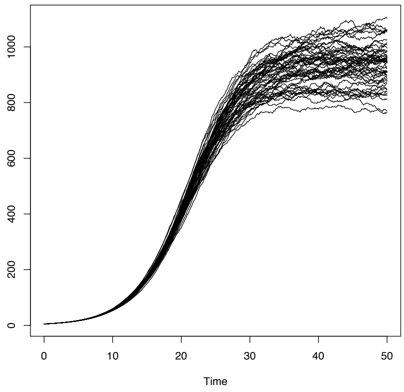

Figure 3. Simulated sample paths of a logistic-type process.

4.4. **Example 4: simulation of a Richards-type process.** To simulate 25 sample paths with 401 data points each (from 0 to 40, with step 0.1) for a particular Richards-type process with $b = 20$, $c = 0.7$, $q = 0.85$, $\sigma = 0.01$ and a $\Lambda(1, 0.2^2)$ as initial distribution (using the discretization of the corresponding SDE), we can use the following code:

```
Res<-GeneralLognormalSimulation(N_Sp=25,n=400,r=0.1,t0=0,x0=c(1,0.2),s=0.01,
+                               method="sde")
```

that requests

```
R> Process to be simulated (you can choose GT (GompertzType),
+  Be (Bertalanffy), LT (LogisticType), RT (RichardsType) or An (Another)) =
```

After introducing

```
RT
```

requests

```
R> Value of b?
```

(we introduce 20)

```
R> Value of c?
```

(we introduce 0.7)

```
R> Value of q?
```

(we introduce 0.85)

The simulated sample paths are shown in Figure 4.

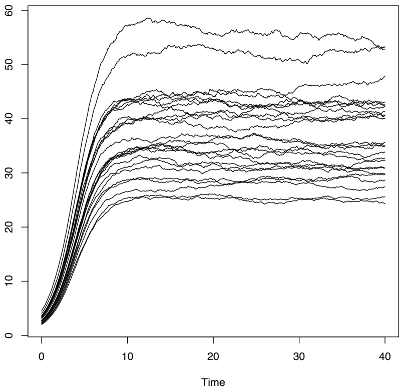

FIGURE 4. Simulated sample paths of a Richards-type process.

5. ESTIMATION OF THE PARAMETERS OF THE MODEL

As mentioned above, for each function $f_\theta(t)$ considered in the previous section, we can build a nonhomogeneous lognormal diffusion process such that its mean and conditioned mean functions exhibit a behavior pattern associated with the function. This makes the process here described appropriate to model phenomena exhibiting such behavior. These functions will allow, for instance, to predict the evolution of the variable under study, once estimated. These functions (as well as the rest included in Table 1) are parametric functions of the model, so for their maximum likelihood (ML) estimation we must only carry out that of their parameters. This will be the goal of this section.

Let us consider a discrete sampling of the process, based on d sample paths, for times t_{ij}, $(i = 1, \cdots, d,\ j = 1, \cdots, n_i)$ with $t_{i1} = t_1$, $i = 1, \cdots, d$. That is, we will observe variables $X(t_{ij})$ whose values $\mathbf{x} = \{x_{ij}\}_{i=1,\cdots,d;j=1,\cdots,n_i}$ make up the sample for the inferential study.

The likelihood function depends on the choice of the initial distribution. If $f(x, t|y, s)$ is the transition probability density function (p.d.f.) of the process, when $P[X(t_1) = x_1] = 1$ the likelihood function is

$$L_{\mathbf{x}}(\theta, \sigma^2) = \prod_{i=1}^{d} \prod_{j=2}^{n_i} f(x_{ij}, t_{ij}|x_{i,j-1}, t_{i,j-1}) \ ,$$

whereas if $X(t_1) \sim \Lambda(\mu, \delta^2)$, then

$$L_{\mathbf{x}}(\mu, \delta^2, \theta, \sigma^2) = \prod_{i=1}^{d} f_{X(t_1)}(x_{i1}) \prod_{j=2}^{n_i} f(x_{ij}, t_{ij}|x_{i,j-1}, t_{i,j-1}) \ .$$

In the second case there are two additional parameters that must be included in the estimation procedure. Nevertheless, the estimation of μ and δ^2 depends only on the initial values of each sample path, and does not influence that of the rest of parameters. Hence, the ML estimates of θ and σ^2 are the same in both cases. From now on, we will consider the case when the initial distribution is lognormal. From (5), the transition p.d.f. of the process can be written as

$$f(x, t|y, s) = \frac{1}{x\sqrt{2\pi\sigma^2(t-s)}} \cdot$$

$$\cdot \exp\left(-\frac{1}{2} \frac{\left[\ln\frac{x}{y} - \ln\frac{f_\theta(t)}{f_\theta(s)} + \frac{\sigma^2}{2}(t-s) \right]^2}{(t-s)\sigma^2} \right) \quad , \quad t < s \ ,$$

so, denoting $n = \sum_{i=1}^{d} n_i$, the log-likelihood function of the sample is

$$\ln L_{\mathbf{x}}(\mu, \delta^2, \theta, \sigma^2) = -\frac{n}{2}\ \ln(2\pi) - \frac{d}{2}\ \ln\delta^2 - \frac{n-d}{2}\ \ln\sigma^2 - \sum_{i=1}^{d} \ln x_{i1} -$$

$$-\frac{1}{2\delta^2} \sum_{i=1}^{d} [\ln x_{i1} - \mu]^2 - \sum_{i=1}^{d}\sum_{j=2}^{n_i} \ln x_{ij} - \frac{1}{2} \sum_{i=1}^{d}\sum_{j=2}^{n_i} \ln(t_{ij} - t_{i,j-1}) -$$

$$-\frac{1}{2\,\sigma^2} \sum_{i=1}^{d}\sum_{j=2}^{n_i} \frac{\left[\ln\left(\frac{x_{ij}}{x_{i,j-1}}\right) - \ln\frac{f_\theta(t_{ij})}{f_\theta(t_{i,j-1})} + \frac{\sigma^2}{2}\,(t_{ij} - t_{i,j-1}) \right]^2}{t_{ij} - t_{i,j-1}} \ , \tag{6}$$

from which the ML estimates of μ and δ^2 are

$$\widehat{\mu} = \frac{1}{d} \sum_{i=1}^{d} \ln x_{i1} \quad \text{and} \quad \widehat{\delta}^2 = \frac{1}{d} \sum_{i=1}^{d} (\ln x_{i1} - \widehat{\mu})^2 \ .$$

However, estimating the rest of parameters has some difficulties. Normally, the resulting systems of equations are exceedingly complex and do not have an explicit solution. Therefore, numerical procedures must be employed to find their approximate solutions. In addition, it is impossible to carry out a general study of the systems of equations in order to check the conditions of convergence of the numerical method we have chosen, since the systems are dependent on sample data and may therefore present an unforeseeable behavior. Moreover, we must also select an initial solution. For this last question, some procedures have been proposed for the Bertalanffy case ([18]) and for the logistic one ([20]).

One alternative would be using stochastic optimization procedures like Simulated Annealing (SA) or Variable Neighborhood Search (VNS). These algorithms are designed to solve problems of the type $\min_{\omega\in\Omega} z(\omega)$, and are often more appropriate than classical numerical methods, since they impose fewer restrictions on the space of solutions Ω and on the analytical properties of the function z to be optimized. In [19], SA is used in the context of the Gompertz-type diffusion, whereas in [22] a hybrid VNS-SA procedure is developed for the Richards case.

In our case, once we have found the estimates of μ and δ^2, the problem is maximizing function $\ln L_{\mathbf{x}}(\widehat{\mu}, \widehat{\delta}^2, \theta, \sigma^2)$. Since the previous algorithms are usually formulated for minimization problems, from (6) the target function we will consider is

$$\widetilde{L}_{\mathbf{x}}(\theta,\sigma^2) = \frac{n-d}{2}\,\ln\sigma^2 + \tag{7}$$

$$+\frac{1}{2\sigma^2}\sum_{i=1}^{d}\sum_{j=2}^{n_i}\frac{\left[\ln\left(\dfrac{x_{ij}}{x_{i,j-1}}\right)-\ln\dfrac{f_\theta(t_{ij})}{f_\theta(t_{i,j-1})}+\dfrac{\sigma^2}{2}(t_{ij}-t_{i,j-1})\right]^2}{t_{ij}-t_{i,j-1}}\,.$$

Using metaheuristic optimization algorithms, such as SA or VNS, raises some questions. One of the fundamental problems for the application of these methods is the space of solutions. For (7) this space is $\Omega = \Theta \times \mathbb{R}^+$ (see Θ in Table 2 for each case). This space is continuous and unbounded, which could lead to unnecessary calculation and long algorithm-running times. To avoid this, some strategies are suggested for bounding the space of solutions. In [19] and [22] some procedures have been presented for the Gompertz-type and Richards-type diffusion processes. In the following section we will summarize these ideas and extend them to the Bertalanffy diffusion process. The main idea is to combine the sample data and some of the characteristics of each curve (see Table 2).

5.1. **Bounding the parametric space.** When the parameter σ assumes high values, the sample paths have great variability around the mean of the process. Thus, excessive variability in available sample paths would lead to an inadvisable model. Some simulations performed for several values of σ have led us to consider that $0 < \sigma < 0.1$.

As for the rest of parameter in each of the cases, given the nature of the curves under analysis, the first step would be to carry out their reparametrization. This produces a new parametric space Θ^*, which is often smaller in size than the original. Table 3 displays the reparametrizations performed on the curves of Table 2, and adapts the previous expressions to the new situation.

From the information collected in Table 3, we may devise some strategies to refine the bounding performed on Θ^*. To this end, it may be useful to use the expression of the limit value, the time of inflection, the value of the curve at this time, and the conditions that must be verified for the time of inflection to be visualized. Naturally, these same values will provide information to help in this matter. Taking the above into consideration, and for the curves mentioned before, we suggest the following bounds for Θ^*.

5.1.1. *Gompertz-type process.* In this case, $\theta^* = (a, \alpha)^T$ and $\Theta^* = \mathbb{R}^+ \times (0,1)$, which is why we must only bound the parametric space associated to a.

Since the theoretical limit value associated to a sample path starting at an initial value x_0 is $x_0 e^{a\alpha^{t_0}}$, if the considered sample paths for inference display bounds $k_i,\ i = 1, \cdots, d$, then $e^{\widehat{a}\widehat{\alpha}^{t_1}}$ would be comprised between $\min(k_i/x_{i1})$ and $\max(k_i/x_{i1})$. This enables us to bound the solution space of a when $t_1 = 0$. In that case, we have

$$(\ln(\min(k_i/x_{i1})), \ln(\max(k_i/x_{i1})))\ ,$$

whereas for $t_1 \neq 0$, and for each $\alpha_0 \in (0,1)$, we will consider

$$\left(\frac{\ln(\min(k_i/x_{i1}))}{\alpha_0^{t_1}}\ ,\ \frac{\ln(\max(k_i/x_{i1}))}{\alpha_0^{t_1}} \right)\ .$$

5.1.2. *Bertalanffy process.* In this case, $\theta^* = (\eta, \alpha, b)^T$ and $\Theta^* = \mathbb{R}^+ \times (0,1) \times [1, +\infty)$, where we must point out that parameter b can be either known or unknown. The Bertalanffy curve is the one most commonly used by fishery biologists to study and interpret the growth of fish, such as in fish population dynamics and in the effects of fishery regulations on the catch. In this context, the value $b = 1$ is used when the variable under study is the length. When focusing on weight, and taking into account the existing relation between weight and length, the value $b = 3$ is associated with *isometric* growth, whereas the case $b \neq 3$ is linked with *allometric* growth.

Note that α is bounded, but there does not seem to exist an upper bound for b and η. Nevertheless, the curve presents an inflection point at $t_I = \ln(\eta/b)/\ln(\alpha)$, which is higher than t_0 (i.e. the inflection can be visualized) if and only if $\eta < b\alpha^{t_0}$. In real-life applications, it is logical that the inflection can be seen, which is why we may consider the previous restriction to be true at the initial time of observation, t_1 (or a somewhat less refined bounding like $0 < \eta < b$). Thus, there only remains to bound b. For a known b we may further refine the bounds for η and α, according to the properties of the curve (see Table 3). In the case of b being unknown we will set a large initial interval which we will then strive to reduce. We will now proceed to discuss both cases in more detail. From the properties of the Bertalanffy curve, we may deduce that $\eta = b\alpha^{t_I}$, whereas

$$\alpha = \left(b \left(1 - \left(\frac{x_0}{k} \right)^{1/b} \right) \right)^{1/(t_0 - t_I)}\ ,$$

being k the limit value of the curve. This leads us to consider the following functions:

- $g(t,b) = \left(b \left(1 - \left(\frac{x_0}{k} \right)^{1/q} \right) \right)^{1/(t_0 - t)}$, $b \geq 1$, $t \in I = [t_1^*, t_2^*]$, being I an interval containing the time instant at which the inflection takes place;
- $h(t, \alpha, b) = b\alpha^t$, $b \geq 1$, $t \in I$, $\alpha \in [\alpha_1, \alpha_2] \subset (0,1)$.

Function g is continuous, and since the curve is a increasing function, from the value of $f_\theta(t_I)$ we deduce that $0 < g(t,b) < 1$, $\forall(t,b)$.

For a known b, function g is strictly increasing and reaches its minimum at t_1^* and its maximum at t_2^*. For b unknown, restricting the domain of definition of b to an interval $[b_1, b_2]$ (containing the true value of b), one can verify that the function increases when any of both arguments is fixed. In addition, there are no local extrema, and therefore its minimum value is reached at (t_1^*, b_1) and its maximum at (t_2^*, b_2).

On the other hand, function h is continuous too and, for a known b, we can prove that there are no local extrema, that h is decreasing in t for a fixed α, and that h is increasing in α for a fixed t. Therefore, h reaches its minimum at (b, α_1, t_2^*) and its maximum at (b, α_2, t_1^*). For an unknown b, restricting again the range of b as in the previous case, the function has no local extrema. An analysis similar to the above (just varying each of the arguments) leads us to conclude that the minimum of the function is reached at (b_1, α_1, t_2^*), and the maximum at (b_2, α_2, t_1^*). On the basis of these considerations, we propose the following strategy in order to bound parametric space Θ^*:

- For b being known.
  Since $(1-(1/b))^b$ is the quotient between the value of the curve at t_I and the limit value, we may approximate t_I by taking the first time instant at which the mean of the sample paths exceeds $k^*(1-(1/b))^b$, where k^* is the limit value of the mean of the sample paths. This procedure may be applied when such limit value is known, albeit only approximately. For this purpose, the latest value of the mean is usually employed. Once this value is found, call it t_I^*, we consider interval $[t_1^*, t_2^*]$, where t_1^* is the time value previous to t_I^* and $t_2^* = t_I^*$. From such interval, two intervals for α and η are found, specifically $[g(t_1^*, b), g(t_2^*, b)]$ and $[h(b, \alpha_1, t_2^*), h(b, \alpha_2, t_1^*)]$.
- For b being unknown.
  In this case, since the time of the inflection is contained within the observed time interval, we suggest the interpolation of a function S (usually a natural cubic spline) to the mean of the sample paths, and then finding the time instant t_I^* at which the maximum of its derivative is reached. Let $[t_{I-1}^*, t_{I+1}^*]$ be the interval determined by the observation time instants before and after t_I^*.
  Taking into account once again that $f_\theta(t_I) = k(\theta)(1-(1/b))^b$, we consider a fine partition of the previous interval and select t_2^* as the time instant previous to the first one verifying $S(t)/k^* > e^{-1}$, where k^* is defined as in the previous case. Thus, we will consider interval $[t_1^*, t_2^*]$ with $t_1^* = t_{I-1}^*$. Subsequently, we calculate a first interval $[b_1^*, b_2^*]$ for b from the solutions to equations

$$S(t_i^*) = k^* \left(1 - \frac{1}{b}\right)^b \quad , \quad i = 1, 2 \, .$$

This last interval, however, may be exceedingly large, since function $(1-(1/b))^b$ increases very slowly and small variations in $S(t_i^*)/k^*$ may lead to very large values of b. For this reason, we suggest a procedure to improve the selection made for b, based on the procedure used to find a range of values for the parameter of the Box-Cox transformation in linear models. To this end, if we call $L^*(b) = \operatorname{Sup}_{\eta,\alpha,\sigma^2} \ln L_{\mathbf{x}}(\mu, \delta^2, \eta, \alpha, b, \sigma^2)$, and consider

$L^*(\widehat{b}) = \mathrm{Sup}_{\eta,\alpha,b,\sigma^2} \ln L_{\mathbf{x}}(\mu,\delta^2,\eta,\alpha,b,\sigma^2)$, then $2\left(L^*(\widehat{b}) - L^*(b)\right) \rightsquigarrow \chi^2_1$, from which

$$P\left[L^*(b) \geq L^*(\widehat{b}) - \frac{1}{2}\chi^2_{1,\alpha}\right] = 1-\alpha\ ,$$

being $\chi^2_{1,\alpha}$ the $(1-\alpha)$-th percentile of a χ^2 distribution with one degree of freedom. Splitting $L^*(b)$ with ordinate $L^*(\widehat{b}) - (1/2)\chi^2_{1,\alpha}$ we find two values for b which determine the interval we will consider.

For practical matters, this procedure is performed by considering a grid of values between b_1^* and b_2^* and calculating $L^*(b)$ using the method for the estimation of parameters for the case of b being known. This yields a set of values l_i^*. The ordinate used to determine the values of b will be $\max_i\{l_i^*\} - (1/2)\chi^2_{1,\alpha}$.

From the interval thus found, $[b_1, b_2]$, two intervals are determined for α and η, specifically $[g(t_1^*, b_1), g(t_2^*, b_2)]$ and $[h(b_1,\alpha_1,t_2^*), h(b_2,\alpha_2,t_1^*)]$.

In the evaluation of the function g, it will be taken $t_0 = t_1$ (the initial time of the sample paths), $x_0 = exp(\widehat{\mu_1} + \widehat{\sigma_1}^2/2)$ (the mean of the estimated initial distribution) and $k = k*$.

5.1.3. *Richards-type and logistic-type processes.* For the Richards-type process, $\theta^* = (\eta,\alpha,q)^T$ and $\Theta^* = \mathbb{R}^+ \times (0,1) \times \mathbb{R}^+$, whereas for the logistic-type process, $\theta^* = (\eta,\alpha)^T$ and $\Theta^* = \mathbb{R}^+ \times (0,1)$.

The procedure discussed before for the Bertalanffy curve is also valid for the Richards case by considering

$$g(t,q) = \left(q\left(\left(\frac{k}{x_0}\right)^{1/q} - 1\right)\right)^{1/(t_0-t)} \quad , \quad q>0,\ t \in I = [t_1^*, t_2^*]$$

and the properties verified by this curve and summarized in Table 3. Obviously, the logistic case follows from the procedure for the Richards curve by considering $q = 1$.

APPENDIX

Code of the GeneralLognormalSimulation function

```
GeneralLognormalSimulation<-function(N_Sp,n,r,t0,x0,s,method = c("TransfW",
"sde")){method<-match.arg(method)
process<-PROCESS()
h<-switch(process, An=HFunction(), GT="m*exp(-beta*t)",
Be="b*c*k/(exp(k*t)-c)", LT="b*c/(b+exp(c*t))", RT="b*c*q/(b+exp(c*t))")
env<-switch(process, An=ENV(), GT=ENVGompertzType(), Be=ENVBertalanffy(),
          LT=ENVLogisticType(), RT=ENVRichardsType())
exprh <- as.expression(eval(substitute(substitute(e, env),
list(e = parse(text = h)[[1]]))))
if (length(x0)>1) Initial<-rlnorm(N_Sp,x0[1],x0[2])
else Initial<-rep(x0, N_Sp)
if (method=="TransfW"){
   Win<-WienerSimulation(N_Sp,n,r)
   h.t <- function(t) NULL
   body(h.t)<-parse(text=exprh)
   NHLog1<-array(0,c(n+1,N_Sp))
```

```
    Time<-seq(t0,length=n+1,by=r)
    AA<-sapply(Time, function(u,l,h) integrate(h,l,u)$value, h=h.t,
    l=t0)-(s^2)*(Time-t0)
    for(i in 1:N_Sp) {NHLog1[,i]<-Initial[i]*exp(t(AA)+s*Win[,i])}
    NHLog<- cbind(Time,NHLog1)}
else {exprd<-parse(text=paste(exprh, "*", expression(x)))
      exprs<-as.expression(eval(substitute(expression(a * x),
      list(a = s))))
      NHLog<- snssde1d(N=n,M=N_Sp,x0=Initial,t0=t0,Dt=r,drif=exprd,
      diffusion=exprs)$X}
invisible(NHLog)}
```

Note: The Sim.DiffProc package must be previously loaded.

Code of the functions used by GeneralLognormalSimulation function

To simulate sample paths of a standard Wiener process

```
WienerSimulation<-function(N_Sp,n,r){
Wiener<-rbind(rep(0,N_Sp), apply(array(rnorm(N_Sp*n,0,sqrt(r)),
dim=c(n,N_Sp)),2,cumsum))
invisible(Wiener)}
```

To request the name of the particular diffusion process to be simulated

```
PROCESS <- function(){
vector<-c("GT","Be","LT","RT","An")
p <- readline("Process to be simulated (you can choose between
GT (GompertzType),
Be (Bertalanffy), LT (LogisticType), RT (RichardsType) or An (Another)) = ")
while(!is.element(p,vector))
p <- readline("The name entered is incorrect.
Process to be simulated (you can choose
between GT (GompertzType), Be (Bertalanffy), LT (LogisticType),
RT (RichardsType)
or An (Another)) = ")
p}
```

To request the values of parameters of a Gompertz-type diffusion process

```
ENVGompertzType<-function(){
Value_m <- readline("Value of m? ")
m1<-as.numeric(Value_m)
Value_beta<- readline("Value of beta? ")
beta1<-as.numeric(Value_beta)
E = list(m=m1, beta=beta1)}
```

To request the values of parameters of a Bertalanffy diffusion process

```
ENVBertalanffy<-function(){
Value_b <- readline("Value of b? ")
b1<-as.numeric(Value_b)
Value_c<- readline("Value of c? ")
c1<-as.numeric(Value_c)
Value_k<- readline("Value of k? ")
```

```
k1<-as.numeric(Value_k)
E = list(b=b1, c=c1, k=k1)}
```

To request the values of parameters of a logistic-type diffusion process

```
ENVLogisticType<-function(){
Value_b <- readline("Value of b? ")
b1<-as.numeric(Value_b)
Value_c<- readline("Value of c? ")
c1<-as.numeric(Value_c)
E = list(b=b1, c=c1)}
```

To request the values of parameters of a Richards-type diffusion process

```
ENVRichardsType<-function(){
Value_b <- readline("Value of b? ")
b1<-as.numeric(Value_b)
Value_c<- readline("Value of c? ")
c1<-as.numeric(Value_c)
Value_q<- readline("Value of q? ")
q1<-as.numeric(Value_q)
E = list(b=b1, c=c1, q=q1)}
```

To request the expression of the h function and the values of parameters of another particular diffusion process

```
HFunction<-function(){H<-readline("Expression of the function h(t)?
(unquoted)")
H}

ENV<-function(){E<-readline("Parameters of the process to be simulated,
 in the form: list(Name of parameter1= Value1,
Name of parameter2 = value2, ...)  ")
eval(parse(text=E))}
```

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Curve	$f_\theta(t)$	θ, Θ	$g_\theta(t)$
Gompertz [13]	$x_0 \exp\left(\frac{m}{\beta}\left(e^{-\beta\, t_0} - e^{-\beta\, t}\right)\right)$ $t \geq t_0$	$\theta = (m, \beta)^T$ $\Theta = \mathbb{R}^+ \times \mathbb{R}^+$	$\exp\left(-\frac{m}{\beta} e^{-\beta\, t}\right)$
Bertalanffy [18]	$x_0 \left(\frac{1 - ce^{-k\, t}}{1 - ce^{-k\, t_0}}\right)^b$ $t \geq t_0 > \ln c/k$	$\theta = (c, k, b)^T$ $\Theta = \mathbb{R}^+ \times \mathbb{R}^+ \times [1, +\infty)$	$(1 - ce^{-k\, t})^b$
Logistic [20]	$x_0 \, \frac{1 + be^{-c\, t_0}}{1 + be^{-c\, t}}$ $t \geq t_0 > -\ln b/c$	$\theta = (b, c)^T$ $\Theta = \mathbb{R}^+ \times \mathbb{R}^+$	$1 + be^{-c\, t}$
Richards [22]	$x_0 \left(\frac{1 + be^{-c\, t_0}}{1 + be^{-c\, t}}\right)^q$ $t \geq t_0 > -\ln b/c$	$\theta = (b, c, q)^T$ $\Theta = \mathbb{R}^+ \times \mathbb{R}^+ \times \mathbb{R}^+$	$(1 + be^{-c\, t})^{-q}$

Curve	$h_\theta(t)$	$k(\theta)$	t_I	$f_\theta(t_I)$	$t_I > t_0$
Gompertz [13]	$me^{-\beta\, t}$	$x_0 \exp\left(\frac{m}{\beta} e^{-\beta\, t_0}\right)$	$\frac{\ln(m/\beta)}{\beta}$	$\frac{k(\theta)}{e}$	$m > \beta\, e^{\beta\, t_0}$
Bertalanffy [18]	$\frac{bck}{e^{kt} - c}$	$\frac{x_0}{(1 - ce^{-k\, t_0})^b}$	$\frac{\ln(bc)}{k}$	$k(\theta)\left(1 - \frac{1}{b}\right)^b$	$b > \frac{e^{k\, t_0}}{c}$
Logistic [20]	$\frac{bc}{b + e^{ct}}$	$x_0(1 + be^{-c\, t_0})$	$\frac{\ln(b)}{c}$	$\frac{k(\theta)}{2}$	$b > e^{c\, t_0}$
Richards [22]	$\frac{bcq}{b + e^{ct}}$	$x_0(1 + be^{-c\, t_0})^q$	$\frac{\ln(bq)}{c}$	$k(\theta)\left(\frac{q}{1 + q}\right)^q$	$b > \frac{e^{c\, t_0}}{q}$

Table 2. Description of the the characteristics defining several growth curves.

Curve	Repar.	$f_\theta(t)$	θ^*, Θ^*	$g_\theta(t)$
Gompertz	$\alpha = e^{-\beta}$ $a = -m/\ln\alpha$	$x_0 \exp\left(a\left(\alpha^{t_0} - \alpha^t\right)\right)$	$\theta^* = (a, \alpha)^T$ $\Theta^* = \mathbb{R}^+ \times (0,1)$	$\exp\left(-a\,\alpha^t\right)$
Bertalanffy	$\alpha = e^{-k}$ $\eta = 1/c$	$x_0 \left(\dfrac{\eta - \alpha^t}{\eta - \alpha^{t_0}}\right)^b$	$\theta^* = (\eta, \alpha, b)^T$ $\Theta^* = \mathbb{R}^+ \times (0,1) \times [1, +\infty)$	$\left(1 - \dfrac{\alpha^t}{\eta}\right)^b$
Logistic	$\alpha = e^{-c}$ $\eta = 1/b$	$x_0\, \dfrac{\eta + \alpha^{t_0}}{\eta + \alpha^t}$	$\theta^* = (\eta, \alpha)^T$ $\Theta^* = \mathbb{R}^+ \times (0,1)$	$\dfrac{\eta}{\eta + \alpha^t}$
Richards	$\alpha = e^{-c}$ $\eta = 1/b$	$x_0 \left(\dfrac{\eta + \alpha^{t_0}}{\eta + \alpha^t}\right)^q$	$\theta^* = (\eta, \alpha, q)^T$ $\Theta^* = \mathbb{R}^+ \times (0,1) \times \mathbb{R}^+$	$\left(\dfrac{\eta}{\eta + \alpha^t}\right)^q$

Curve	$h_\theta(t)$	$k(\theta^*)$	t_I	$f_\theta(t_I)$	$t_I > t_0$
Gompertz	$-a\alpha^t \ln\alpha$	$x_0 \exp\left(a\,\alpha^{t_0}\right)$	$-\dfrac{\ln a}{\ln\alpha}$	$\dfrac{k(\theta^*)}{e}$	$a > -\alpha^{t_0}$
Bertalanffy	$-\dfrac{b\alpha^t \ln\alpha}{\eta - \alpha^t}$	$\dfrac{x_0}{\left(1 - \dfrac{\alpha^{t_0}}{\eta}\right)^b}$	$\dfrac{\ln(\eta/b)}{\ln\alpha}$	$k(\theta^*)\left(1 - \dfrac{1}{b}\right)^b$	$\eta < b\alpha^{t_0} < b$
Logistic	$-\dfrac{\alpha^t \ln\alpha}{\eta + \alpha^t}$	$x_0\left(1 + \dfrac{\alpha^{t_0}}{\eta}\right)$	$\dfrac{\ln\eta}{\ln\alpha}$	$\dfrac{k(\theta^*)}{2}$	$\eta < \alpha^{t_0} < 1$
Richards	$-\dfrac{q\alpha^t \ln\alpha}{\eta + \alpha^t}$	$x_0\left(1 + \dfrac{\alpha^{t_0}}{\eta}\right)^q$	$\dfrac{\ln(\eta/q)}{\ln\alpha}$	$k(\theta^*)\left(\dfrac{q}{1+q}\right)^q$	$\eta < \alpha^{t_0} < q$

TABLE 3. Reparametrization of the growth curves in Table 2.