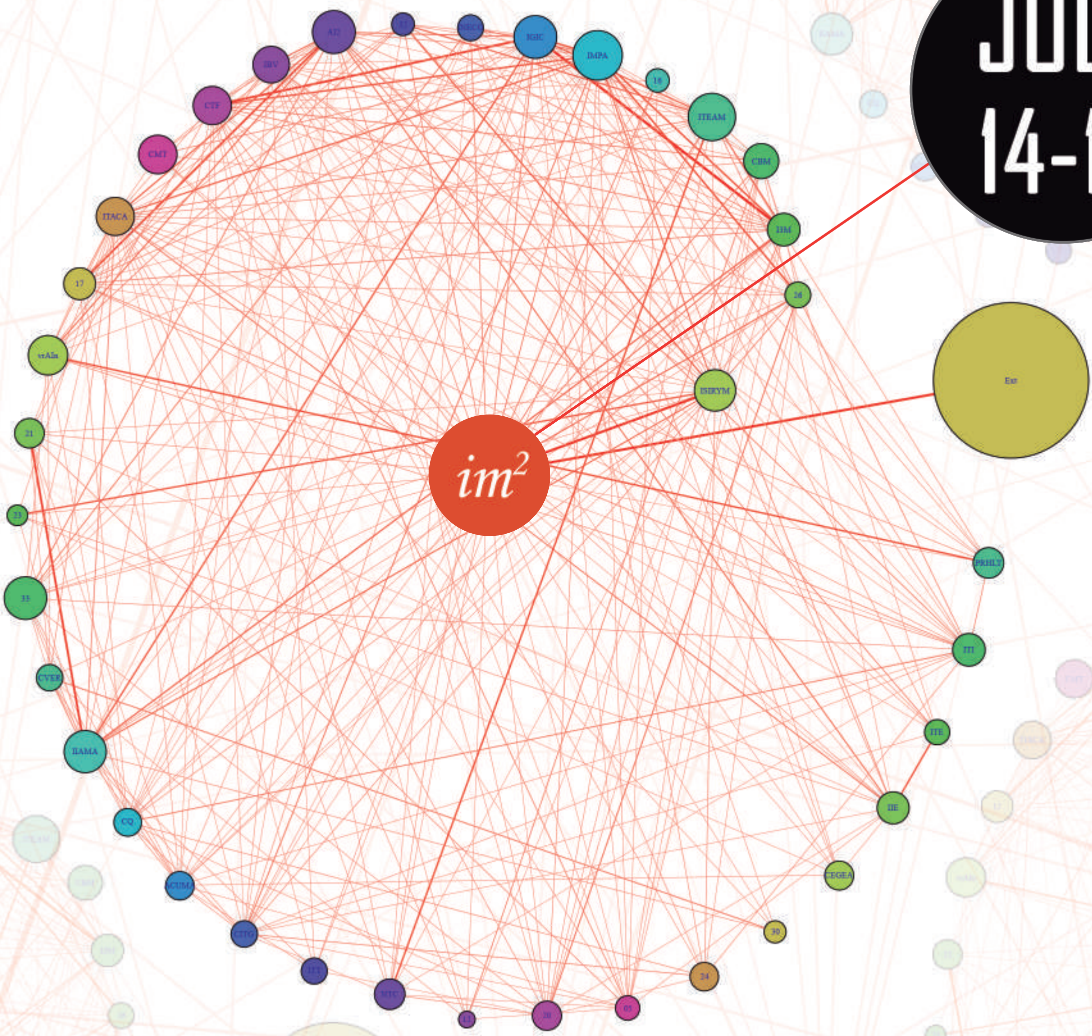
MODELLING FOR ENGINEERING & HUMAN BEHAVIOUR

2021

JULY 14-16



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Modelling for Engineering & Human Behaviour 2021

València, July 14th-16th, 2021

This book includes the extended abstracts of papers presented at XXIII Edition of the Mathematical Modelling Conference Series at the Institute for Multidisciplinary Mathematics *Mathematical Modelling in Engineering & Human Behaviour*.

I.S.B.N.: 978-84-09-36287-5

November 30th, 2021
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Contents

1

Density-based uncertainty quantification in a generalized Logistic-type model

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1 Introduction

The Logistic equation is a classical and widely used mathematical model which appears in several areas of science such as in ecology, chemistry or artificial neural networks. However, in this contribution the authors consider with the generalized Logistic ordinary differential equation (ODE) model:

$$X'(t) = \alpha(t)\, r X(t) \left(1 - \left(\frac{X(t)}{K}\right)^{\nu}\right),\ t \geq t_0, \quad X(t_0) = X_0. \tag{1}$$

As usual, t is interpreted as the time, the parameter r is the growth rate and K is the carrying capacity. The differential equation is generalized by adding two terms: a positive, monotonically growing function $\alpha(\cdot)$ and a constant positive term ν. The first term, $\alpha(\cdot)$, allows to control the so-called *lag phase*, which is the growth phase in which the population under study has not yet achieved a fully exponential growth. The latter, ν, is a power that controls how fast the carrying capacity K is approached and is termed as *deceleration term*. When $\nu = 1$, the classical logistic differential equation is obtained. And when ν tends to 0, the Gompertz equation is given. The incorporation of both the function $\alpha(\cdot)$ and the power ν allows for more flexible S-shaped curves to model growth phenomena over time. Some examples of application include tumor growth [1–4], bacterial culture growth [5] and diseases such as SARS [6, 7], dengue fever [8], influenza H1N1 [9], Zika [10], Ebola [11], and COVID-19 [12–15].

In order to represent and predict real world dynamics by means of Equation (1), it is necessary to determine the initial state X_0 and the model parameters r, K, ν and $\alpha(\cdot)$ accounting for the underlying uncertainty. Uncertainty may appear due to tolerance errors in measurement devices when performing experiments and by the inherent uncertainty of factors such as the lag phase or the deceleration term, which cannot be directly measured.

Since the objective is to analyze and predict real world behavior, the model is considered with uncertainty at its parameters such as the initial condition, growth rate, etc. The first probability density function (1-PDF) of the solution stochastic process is obtained by numerically solving its related Liouville partial differential equation (PDE) as detailed in the following Section.

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2 Methods

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space. Let $X_0 \in \mathrm{L}^2(\Omega)$, that is, a random variable with finite variance. Let $\mathbf{g} : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ verify a Lipschitz condition in the spatial variables. Consider the following random ODE:

$$\begin{cases} \mathbf{X}'(t,\omega) = \mathbf{g}(\mathbf{X}(t,\omega), t), & t > 0, \\ \mathbf{X}(0,\omega) = \mathbf{X}_0(\omega), & \omega \in \Omega, \end{cases}$$

where the derivative may be interpreted in the path-wise or mean-square sense. It can be shown (see [2,17]) that the 1-PDF of the solution stochastic process $\mathbf{X}(t,\omega)$ verifies the Liouville equation in the weak sense:

$$\begin{cases} \partial_t f(\mathbf{x},t) + \mathrm{Div}_{\mathbf{x}} \left(\mathbf{g}(\mathbf{x},t) f(\mathbf{x},t)\right) = 0, & t > 0, \\ f(\mathbf{x},0) = f_0(\mathbf{x}), & \mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^n. \end{cases}$$

Furthermore, at all points where the first derivatives of $\mathbf{g}$ are also Lipschitz continuous, a more practical form of the equation is obtained just by computing the divergence of the product between $\mathbf{g}$ and f:

$$\begin{cases} \partial_t f(\mathbf{x},t) + \mathbf{g}(\mathbf{x},t) \cdot \nabla_{\mathbf{x}} f(\mathbf{x},t) = -f(\mathbf{x},t)\,\mathrm{Div}_{\mathbf{x}}\,\mathbf{g}(\mathbf{x},t), & t > 0, \\ f(\mathbf{x},0) = f_0(\mathbf{x}), & \mathbf{x} \in \mathcal{D} \subseteq \mathbb{R}^n. \end{cases}$$

In the particular case under study, the flow function and its divergence for the Liouville Equation are, respectively,

$$g(x,t) = \alpha(t)\, r\, x \left(1 - \left(\frac{x}{K}\right)^{\nu}\right), \quad \nabla_x \cdot g(x,t) = \partial_x g(x,t) = \alpha(t)\, r \left(1 - (1+\nu)\left(\frac{x}{K}\right)^{\nu}\right),$$

with $x \in [0, K]$. Despite the various choices available for $\alpha(\cdot)$, the one chosen by [18] will be used:

$$\alpha(t) := \frac{q}{q + \mathrm{e}^{-m\,t}}, \quad t \geq 0, \quad q,\, m > 0.$$

Now, in order to solve the Liouville Equation with the flow described by the generalized Logistic Equation, the PDE will be considered through the characteristic curves:

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}s} x(s) &= \alpha(s) r\, x(s) \left(1 - \left(\tfrac{x(s)}{K}\right)^{\nu}\right), \quad x(0) = x_0, \\ \tfrac{\mathrm{d}}{\mathrm{d}s} f(x(s),s) &= -f(x(s),s)\, \partial_x g(x(s),s), \quad f(x(0),0) = f_0(x_0), \end{aligned}$$

where x_0 is any point of the initial discretized grid. The 1-PDF along the characteristic curves has a closed form which can be computed by approximating an integral:

$$f(x(s),s) = f_0(x_0) \exp\left(-\int_0^s \partial_x g(x(s),s) \mathrm{d}s\right);$$

Any ODE numerical solver can be employed. The authors have used a 4th order Runge Kutta ODE solver.

Although this formulation may be not be very clarifying, it allows the use of the so-called lagrangian numerical methods, in which initial points in a grid are treated as individual particles whose positions and values change through time. However, not all points of a mesh are going to be updated; a wavelet compression-based adaptive mesh refinement algorithm has been implemented in order to select only those points that contain a higher variability and, therefore, have to be tracked with higher precision.

Another important question is the determination of the initial PDF from the known data at initial time. The initial PDF has been assigned by the use of the so-called Principle of Maximum Entropy (PME or MaxEnt):

$$f_0 = \text{argmax} \left\{ -\int_{\mathcal{D}} f(x) \log(f(x)) \mathrm{d}x \quad : \quad f \in L^1(\mathcal{D}),\, f \geq 0 \,\text{a.e. } \mathcal{D} \subseteq \mathbb{R} \right\}$$

When applied to this case, the constraints are given by the central moments up to any finite order p, which is denoted by $\{\mu_i\}_{i=1}^p$. It can be shown that the general form of the function obtained by applying PME has the following form:

$$f_0(x) = \exp\left(-1 - \sum_{i=0}^{p} \lambda_i x^i \right), \quad x \in \mathcal{D},$$

where the terms $\{\lambda_i\}_{i=1}^p$, called *Lagrange multipliers*, are obtained by solving:

$$\begin{aligned} \textstyle\int_{\mathcal{D}} f(x)\mathrm{d}x \quad &= 1, \\ \textstyle\int_{\mathcal{D}} x\, f(x)\mathrm{d}x \quad &= \mu_1, \\ &\vdots \\ \textstyle\int_{\mathcal{D}} x^p\, f(x)\mathrm{d}x \quad &= \mu_p, \end{aligned}$$

Finally, the inverse problem of determining the parameters r, ν, K, q and m that best represent our real world problem is tackled by making use of the Particle Swarm Optimization algorithm (PSO) (see [19]). This optimization algorithm creates several parameter vectors and evaluates a predefined fitness function for each of these parameter vectors. It then evolves these parameter values according to the fitness function in the same way that a swarm of birds search for food.

3 Results

Only the case of real data is going to be shown due to the fact that it is the most interesting case. The model consists of a biological culture growth experiment (see [20]), in which several samples have been obtained at 28, approximately equidistant, time instants during the first 7 hours, approximately. Tables 1 and 2 show the optimal multipliers and parameter values, respectively, obtained by following the aforementioned techniques.

λ_0	λ_1	λ_2
440.8872	-3112.2887	5434.2539

Table 1: Optimal multipliers

Parameters	q	m	r	ν	K
Example 1	0.8085	0.001	1.1249	1	0.65

Table 2: Optimal Parameters given by PSO procedure.

As it can be seen, the simulation with optimal parameters is able to describe the microbial growth evolution. The time step used for the numerical solution of the characteristic curves is $\Delta t = 0.005$, and the simulation took 0.6 seconds to compute. The computation of the optimal parameters through the PSO algorithm took around 5 minutes. All computations were performed using MATLAB$^{\text{ő}}$ in a laptop with a Ryzen 7 5800H processor.

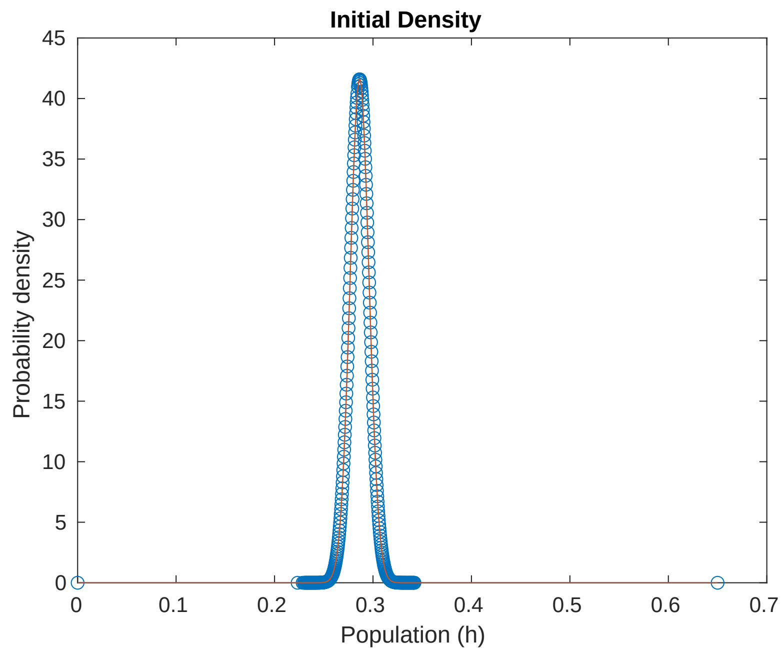

Figure 1: Inital PDF obtained by PME, with the multipliers shown in Table 1. The inital grid is 4096 points. Adapted grid is obtained consisting of only 353 points.

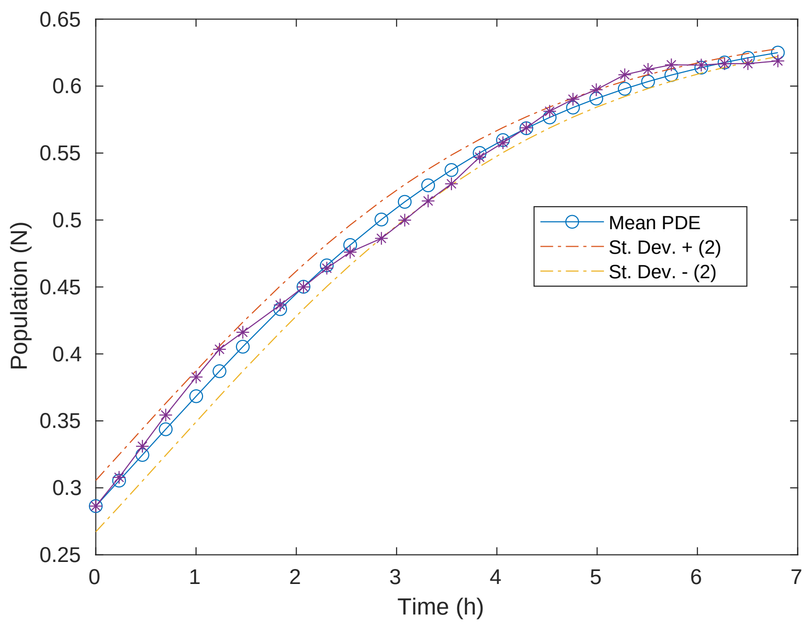

Figure 2: Mean and 2-standard deviations confidence interval with optimal parameters obtained by PSO, as in Table 2.

4 Conclusions

The random generalized Logistic equation has been studied through the time evolution of its first probability density function, obtained as the solution of the related Liouville partial differential equation. Several techniques, such as wavelet compression-based adaptive mesh refinement, the principle of maximum entropy or the particle swarm optimization algorithm have been employed in order to fine-tune the parameter values for a correct representation of a real world biological culture growth experiment. The case of where, not only the initial condition of the equation, but also its coefficients are considered as random variables is currently under study. Furthermore, this same point of view can be applied to model consisting of 2 or more differential equations, both coupled or uncoupled. Last but not least, the authors are also studying the computation of the probability of events, by using the approximated probability density function, as well as the computation of confidence intervals.

Acknowledgments

This work has been supported by the Spanish Agencia Estatal de Investigación (AEI) and Fondo Europeo de Desarrollo Regional (FEDER UE) grant ID2020-115270GB-I00.

References

[1] Marusic M, Bajzer Z, Vuk-Pavlovic S., Freyer JP. Tumor growth in vivo and as multicellular spheroids compared by mathematical models. Bulletin of Mathematical Biology, 56, 617–631, 1994.

[2] Spratt JS, Meyer JS, Spratt JA. Rates of growth of human neoplasms: Part II. Journal of Surgical Oncology, 61(1), 68–83, 1996.

[3] Birch CP. A new generalized logistic sigmoid growth equation compared with the Richards growth equation. Annals of Botany, 83(6), 713–723, 1999.

[4] Sachs RK, Hlatky LR, Hahnfeldt P. Simple ODE models of tumor growth and anti-angiogenic or radiation treatment. Mathematical and Computer Modelling, 33(12–13), 1297–1305, 2001.

[5] Ram, X.; Dellus-Gur, E.; Bibi, M.; Karkare, K.; Obolski, U.; Feldman, M.W.; Cooper, T.F.; Berman, J.; Hadany, L. *Predicting microbial growth in a mixed culture from growth curve data.* Proc. Natl. Acad. Sci. USA2019,116, 14698–14707.

[6] Hsieh XH, Lee JX, Chang HL. SARS epidemiology modeling. Emerging infectious diseases. 2004; 10(6):1165.

[7] Hsieh XH. Richards model: a simple procedure for real-time prediction of outbreak severity. In: Modeling and Dynamics of Infectious Diseases. World Scientific; 2009. pp. 216–236.

[8] Hsieh XH, Ma S. Intervention measures, turning point, and reproduction number for dengue, Singapore, 2005. The American Journal of Tropical Medicine and Hygiene. 2009; 80(1):66–71.

[9] Hsieh XH. Pandemic influenza A (H1N1) during winter influenza season in the southern hemisphere. Influenza and Other Respiratory Viruses. 2010; 4(4), 187–197

[10] Chowell G, Hincapie-Palacio D, Ospina JF, Pell B, Tariq A, Dahal S, Moghadas SM, Smirnova A, Simonsen L, Viboud C. Using phenomenological models to characterize transmissibility and forecast patterns and final burden of Zika epidemics. PLoS Currents. 2016; 8.

[11] Pell B, Kuang X, Viboud C, Chowell G. Using phenomenological models for forecasting the 2015 Ebola challenge. Epidemics. 2018; 22, 62–70.

[12] Pelinovsky E, Kurkin A, Kurkina O, Kokoulina M, Epifanova A. Logistic equation and COVID-19. Chaos, Solitons & Fractals. 2020; 140: 110241.

[13] Wu K, Darcet D, Wang Q, Sornette D. Generalized logistic growth modeling of the COVID-19 outbreak: comparing the dynamics in the 29 provinces in China and in the rest of the world. Nonlinear dynamics. 2020; 101(3): 1561–1581.

[14] Aviv-Sharon E, Aharoni A. Generalized logistic growth modeling of the COVID-19 pandemic in Asia. Infectious Disease Modelling. 2020; 5: 502-509.

[15] Lee SX, Lei B, Mallick B. Estimation of COVID-19 spread curves integrating global data and borrowing information. PloS One. 2020; 15(7): e0236860.

[16] Soong TT. Random Differential Equations in Science and Engineering. New York: Academic Press; 1973.

[17] Santambrogio, Filippo. Optimal Transport for Applied Mathematicians. Calculus of Variations, PDEs and Modeling; 2015.

[18] Baranyi, József & Roberts, Terry, *A Dynamic Approach to Predicting Bacterial-Growth in Food*. International journal of food microbiology. 23. 277-94. 10.1016/0168-1605(94)90157-0; 1994.

[19] Khemka, Namrata & Jacob, Christian. Exploratory Toolkit for Evolutionary and Swarm-Based Optimization. The Mathematica Journal. 11. 10.3888/tmj.11.3-5; 2008.

[20] Ram, Yoav & Dellus-Gur, Eynat & Bibi, Maayan & Karkare, Kedar & Obolski, Uri & Feldman, Marcus & Cooper, Tim & Berman, Judith & Hadany, Lilach. (2019). Predicting microbial growth in a mixed culture from growth curve data. Proceedings of the National Academy of Sciences. 116. 201902217. 10.1073/pnas.1902217116.