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Logistic probability function: an analysis and modification from the perspective of reaction network theory

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Abstract. In this work we study some characteristics of growth functions of the logistic type. The standard logistic function and the 2-logistic growth function are solutions of ordinary differential equations derived from the perspective of reaction network theory. These solutions are compared in terms of their shape. We are interested in the new 2-logistic probability distribution and its characteristics. Using the tools of reaction network theory and numerical methods we derive some properties of this distribution.

1. Introduction

The logistic distribution is a continuous probability distribution that has become highly relevant in many fields. Often used to describe growth processes, it has roots in the work by Verhulst [1], from which the alternative name "Verhulst model" derives. This distribution serves as the foundation for the logistic function, which is frequently employed to characterize phenomena that exhibit a sigmoidal behavior pattern. Such patterns can be observed in scenarios like population growth or the spread of diseases, making the logistic distribution a versatile and valuable tool in various disciplines. It has also found application in statistical analysis and machine learning, where it has proved suitable for modeling the underlying probability of binary outcome events.

Details on the logistic distribution can be found in the monograph of Balakrishnan [2] and also in Johnson, Kotz and Balakrishnan [3]. The standard logistic distribution is an exponential mixture of extreme value distributions [4]. The shape of the logistic distribution is similar to the shape of the normal distribution. It has heavier tails than the normal distribution and this unique property is usually used for the purposes of the data analysis.

The standard logistic distribution has important uses in describing growth phenomena [5]. This fact has attracted many applications in the modeling of physicochemical processes, weight gain data and etc. Growth models are often used in modeling of various dynamical processes in biology, ecology, epidemiology, social and economic sciences, engineering and natural sciences, demography and also in many others scientific fields. They are frequently formulated in the terms of a system of ODEs (see [6] for a recent example).

Reaction network theory provides a powerful toolkit for formalizing models of growth phenomena. Both the logistic (Verhulst) and the Gompertz models can be derived in a reaction-theoretic framework, as shown in [7]. In this paper we show how the logistic growth model, as derived from a reaction network, can be modified to obtain a version of the logistic distribution. Moreover, we show how a reaction-theoretic formulation naturally suggests a generalization of the logistic model that we call the 2-logistic model. This generalization, as well as the associated probability distribution derived from it, is studied analytically and numerically.

2. The logistic growth model

The logistic growth function can be obtained as a solution of the following differential equation:

$$x' = k_L x \left(1 - \frac{x}{K_L}\right),$$

where k_L and K_L are positive parameters, respectively called (intrinsic) *reaction rate* and *carrying capacity.*

For our purposes it is more convenient to rewrite this differential equation in the form

$$x' = kx(c - x),$$

with $k := k_L/K_L$ and $c := K_L$.

The solution of this equation is a sigmoidal growth function $x = x(t), t \in R$. The related decay function is implicitly involved in the right-hand side of the differential equation as $c - x$, where $c > 0$. Usually $c = 1$.

The logistic growth model can be obtained from the following reaction network:

$$S + X \xrightarrow{k} 2X. \tag{1}$$

Under the assumption of homogeneity and mass action kinetics, the network (1) induces the following system of ordinary differential equations:

$$s' = -ksx,\ x' = +ksx \tag{2}$$

with the initial conditions

$$s(0) = s_0 > 0,\ x(0) = x_0 > 0$$

The system (2) satisfies a conservation relation, which is given by:

$$s' +\ x' = 0 \quad \Rightarrow \quad s + x = c = const$$

In addition, the dynamical system implies that:

$$s' = -ks(c - s),\ x' = kx(c - x),\ c = s_0 + x_0.$$

The solution of the dynamical system for $x(t)$ is given by the following equation:

$$x(t) = \frac{cx_0}{x_0 + (c - x_0)e^{-ckt}} \tag{3}$$

3. The logistic distribution

Using the expression of solution (3) for $c = 1$ as the cumulative distribution function (CDF), we can define a probability distribution which is based on the logistic model. This has the potential drawback that the CDF has a discontinuity at 0. One approach to circumventing this problem would be to set $x_0 = \epsilon > 0$ and $c = 1 + \epsilon$.

Then the CDF can be defined as

$$F_L(t) := x(t) - \epsilon$$

and the associated probability density function is

$$f_L(t) = F'(t).$$

This is a version of the classical logistic distribution.

Illustrative shapes of the CDF of the obtained logistic distribution are presented in Figures 1 and 2. Depending on the combination of parameter values, one can arrive at CDFs with or without inflection points.

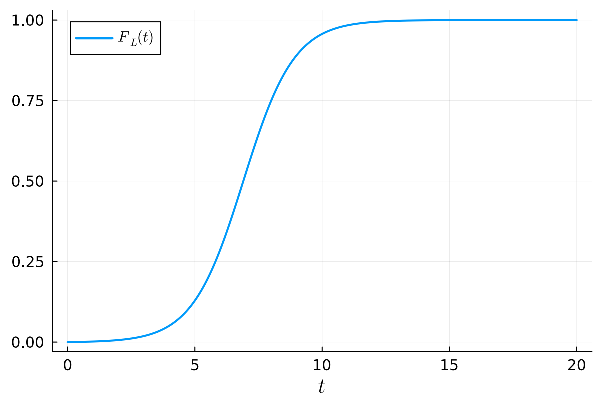

Figure 1. The logistic cumulative distribution function, $\epsilon = 0.001,\ k = 1.0$

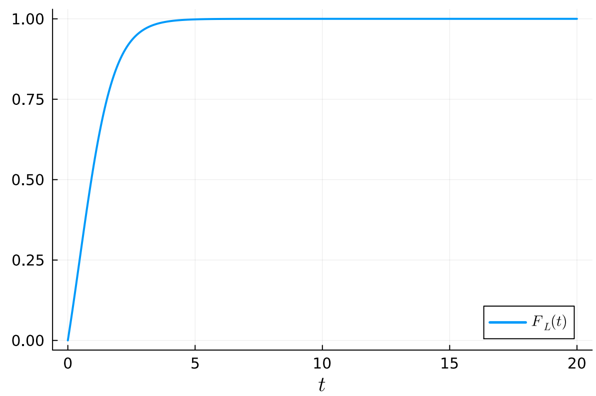

Figure 2. The logistic cumulative distribution function, $\epsilon = 0.5,\ k = 1.0$

4. The 2-logistic growth-decay model

The reaction network derivation of the logistic model suggests natural avenues of generalization of this approach by varying the number of reactants. One possibility is to require a higher number of representatives of species S to enter as reactants in order to trigger a transformation. In the particular case of requiring the presence of two representatives instead of one, we obtain a model that we refer to as the 2-logistic model.

To derive the 2-logistic growth-decay model, we consider the following reaction network:

$$2S + X \xrightarrow{k_1} 3X. \tag{4}$$

The dynamical system induced (assuming homogeneity and mass actions kinetics) by the reaction network (4) is:

$$s' = -2k_1 x s^2, \quad x' = +2k_1 x s^2 \tag{5}$$

and we can define $k = 2k_1$ to simplify notation.

The initial conditions required to define an initial-value problem are given by

$$s(0) = s_0 > 0, \ x(0) = x_0 > 0.$$

The system (5) satisfies the conservation relation: $s(t) + x(t) = c$

Hence for $x(t)$ we have

$$x' = kx\,(c - x)^2$$

5. The 2-logistic distribution

Similarly to the classical logistic distribution, setting $c = 1$ results in a CDF with a discontinuity at 0. We can again set $x_0 = \epsilon > 0$ and $c = 1 + \epsilon$, and define the CDF as

$$F_{2L}(t) := x(t) - \epsilon,$$

with the probability density function given by $f_{2L}(t) = F'(t)$. In this way the 2-logistic distribution is obtained.

The 2-logistic cumulative distribution function for different parameter values is presented in Figures 3 and 4. The figures suggest substantial flexibility in terms of the shapes obtainable in this framework.

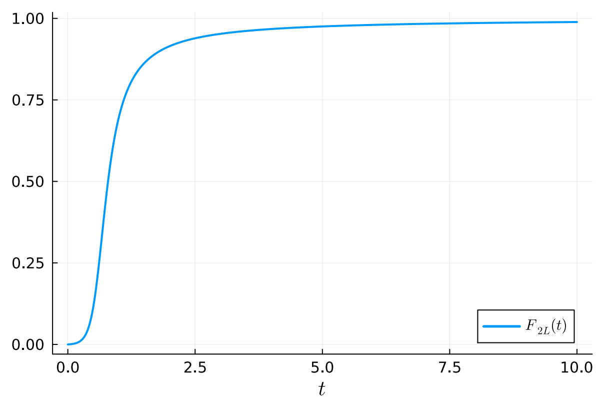

Figure 3. The 2-logistic cumulative distribution function, $\epsilon = 0.001, \ k = 5.0$

Figure 5 shows that the 2-logistic CDF possesses a monotonicity property with respect to the parameter k.

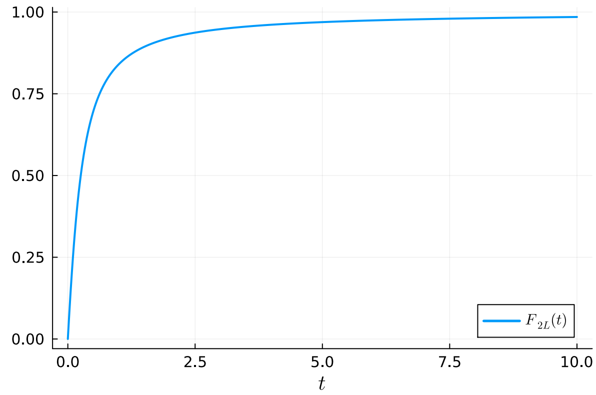

Figure 4. The 2-logistic cumulative distribution function, $\epsilon = 0.7,\ k = 2.0$

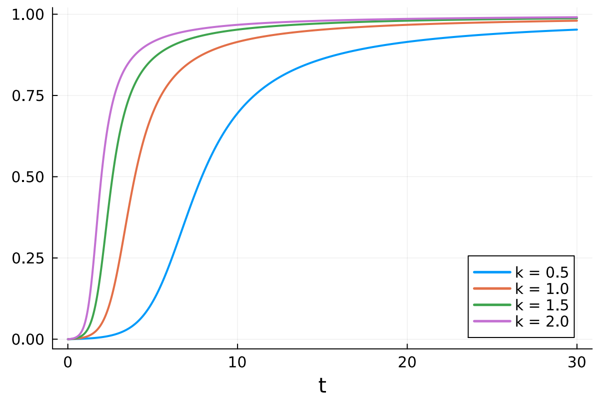

Figure 5. The 2-logistic cumulative distribution function for different values of k, with $\epsilon = 0.001$

To illustrate how the classical logistic and the 2-logistic CDFs differ, Figure 6 compares the shapes of instances of the two CDFs for common values of the parameters ϵ and k. As evidenced by the figure, while the two distributions are derived from common principles and seem to share the “same” parameters, their behavior can differ substantially.

The 2-logistic distribution can be partially characterized by its moments. In order to understand how the latter depend on the parameters of the distribution, we compute and plot the mean and the standard deviation of the 2-logistic distribution for different combinations of values of ϵ and k. Figure 7 demonstrates that the mean is a decreasing function of both ϵ and k, and illustrates the form of the dependence. A similar observation holds with respect to the standard deviation, as shown in Figure 8.

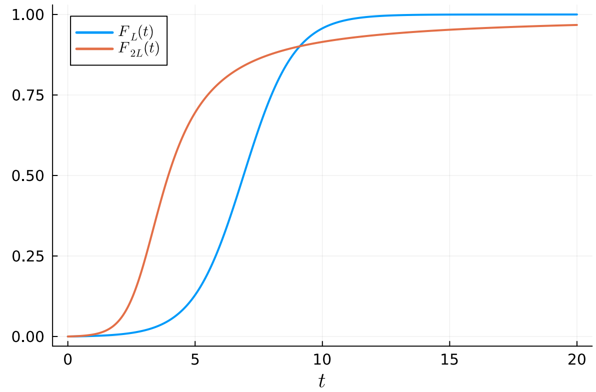

Figure 6. The logistic vs. 2-logistic cumulative distribution functions, common $\epsilon = 0.001,\ k = 1.0$

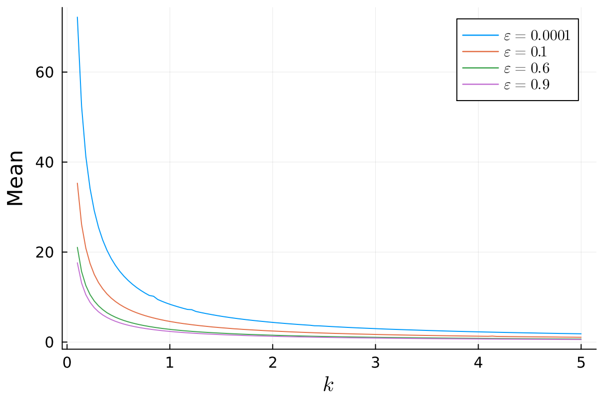

Figure 7. Mean of the 2-logistic distribution for different values of ϵ and k

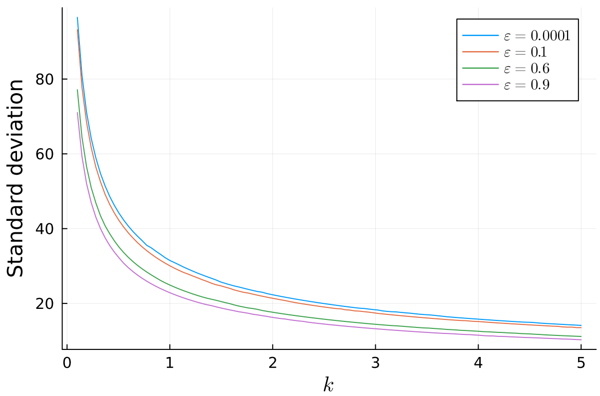

Figure 8. Standard deviation of the 2-logistic distribution for different values of ϵ and k

6. Conclusions

In the present work we formulated a mathematical model which is a modification of the classical logistic (Verhulst) model. We call this model the 2-logistic model. We show how we can derive probability distributions from the classical and the 2-logistic growth-decay models and graphically illustrate some of their properties.

A natural extension of this work would be to delve deeper into the statistical properties of the 2-logistic distribution and, in particular, develop methods for estimating its parameters. Both classical and Bayesian approaches are of interest, especially given the latter's ability to constrain parameter values by means of appropriate priors.

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