

**A LOOK AT THE HYPOTHETICAL PIECEWISE SMOOTH
GENERALIZED SIGMOIDAL GROWTH FUNCTION.
SOME APPLICATIONS. II**

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ABSTRACT: Following the ideas given in [2] in this paper we define a hypothetical piecewise smooth generalized sigmoidal model $Q(q_1(t), q_2(t))$ using the generalized logistic model. We will discuss precise bounds for the Hausdorff distance d between the Heaviside function h_0 and the sigmoid Q . Studies in this paper can also be applied to a random shifted sigmoidal functions. We define also the piecewise cut function associated to the function $Q(t)$. In the present work we discuss the usage of the framework of chemical reaction networks for the construction of new dynamical model. Some numerical examples with real data, using *CAS MATHEMATICA* illustrating our results are given.

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1. THE BASIC PROBLEM

The generalized logistic distribution [1] has been used in the analysis of extreme values. The cumulative distribution function is defined by [1]:

$$M(t; a, b, c) = \frac{1}{\left(1 + e^{\frac{a-t}{b}}\right)^c}. \quad (1)$$

Following the ideas given in [2] the reader can formulate a hypothetical piecewise smooth sigmoidal model using the generalized logistic model:

$$p_1(t) = \frac{B}{\left(1 + Ae^{-\frac{1}{b}(t-a)}\right)^c},$$

where $b > 0$, $c > 0$. It is easy to see that the hypothetical piecewise smooth model is of the form:

$$P(t) := \begin{cases} \frac{B}{\left(1 + Ae^{-\frac{1}{b}(t-a)}\right)^c} := p_1(t), & 0 < t < a \\ \frac{B}{(1+A)^c}, & t = a \\ \frac{B}{\left(1 + Ae^{\frac{-1}{b}(t-a)}\right)^c} := p_2(t), & t > a. \end{cases} \quad (2)$$

The model (2) for fixed values of the parameters $B = 1.7$, $A = 2$, $b = 0.1$, $a = 0.25$, $c = 0.9$ is visualized in Figure 1b; $p_1(t)$ - green for $t \in (0, 1)$ and $p_2(t)$ - red for $t \in (a, 1)$ are visualized in Figure 1a respectively. We will consider the following interesting example.

Example. For the "DataSalmonellae" [3]

$$\begin{aligned} DataSalmonellae := & \{ \{0, 2.83\}, \{2, 2.07\}, \{3, 3.13\}, \{4, 4.49\}, \\ & \{5, 6.46\}, \{6, 4.66\}, \{7, 7.91\}, \{8, 7.80\}, \{9, 9.48\}, \{10, 11.19\}, \\ & \{11, 11.97\}, \{12, 13.12\}, \{13, 14.27\}, \{14, 13.64\}, \{15, 16.34\}, \{26, 17\}, \\ & \{27, 17\}, \{28, 17\} \} \end{aligned}$$

the fitted model $P(p_1(t), p_2(t))$ for $a \approx 15$, $b = 7.06405$, $A = 0.00295489$, $B = 20$, $c = 105.6$ is depicted on Figure 2. We see that the "saturation" to the horizontal asymptote at level $B_1 = \frac{B}{(1+Ae^{-1})^c}$ is reached.

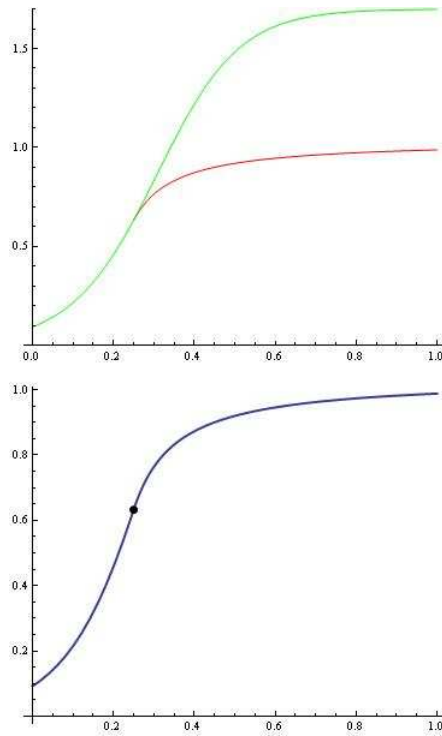


Figure 1: a) For fixed values of the parameters $B = 1.7$, $A = 2$, $b = 0.1$, $a = 0.25$, $c = 0.9$, $p_1(t)$ - (green) for $t \in (0, 1)$ and $p_2(t)$ - red for $t \in (a, 1)$; b) The hypothetical piecewise smooth sigmoidal model $P(p_1(t), p_2(t))$ using the generalized logistic model.

2. NEW CLASS OF GROWTH FUNCTION GENERATED BY REACTION NETWORKS AND BASED ON "CORRECTING AMENDMENTS OF FRACTIONAL LINEAR FUNCTION-TYPE"

The classical generalized logistic model is of the form:

$$q_1(t) = \frac{B}{(1 + Ae^{-kt})^c} \tag{3}$$

where $A > 0$, $B > 0$; $k > 0$, $c > 0$. For a visualization of the model (3) at fixed values of the parameters k, A, B, c , see Figure 3a. As noted in [2], in the field of Population Dynamics the problem often arises how to construct a modified model at already fixed

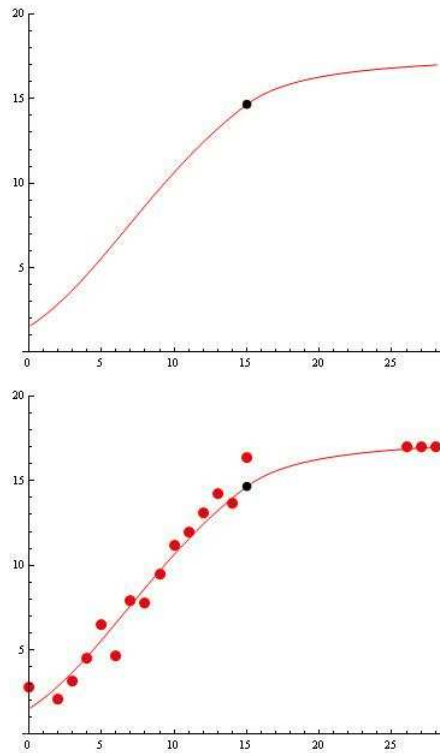


Figure 2: The fitted model $P(p_1(t), p_2(t))$ for "DataSalmonellae".

values of parameters k, A, B, c and a change in the dynamics of the growth process for $t > t_0$, in which saturation to the horizontal asymptote at level $B_1 = \frac{B}{(1+ Ae^{-1})^c}$ is reached. This can be achieved, for example, with the function $g_2(t)$ (for $t > 0$, see Figure 3b)

$$q_2(t) = \frac{B}{\left(1 + Ae^{\frac{-kt}{1+kt}}\right)^c}. \quad (4)$$

The hypothetical piecewise smooth sigmoidal model based on the classical generalized logistic model is of the form

$$Q(t) := \begin{cases} \frac{B}{(1 + Ae^{-kt})^c} := q_1(t), & t < 0 \\ \frac{B}{(1 + A)^c}, & t = 0 \\ \frac{B}{\left(1 + Ae^{\frac{-kt}{1+kt}}\right)^c} := q_2(t), & t > 0. \end{cases} \quad (5)$$

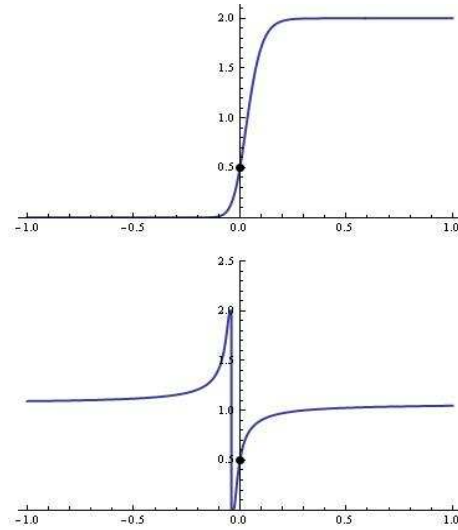


Figure 3: a) The function $q_1(t)$ for fixed $k = 25$, $B = 2$, $A = 1$, $c = 2$ ($q_1(0) = \frac{1}{2}$); b) The function $q_2(t)$ for fixed $k = 25$, $B = 2$, $A = 1$, $c = 2$ ($q_2(0) = \frac{1}{2}$).

In addition, we will consider the interesting problem of approximating the Heaviside step function

$$h_0(t) = \begin{cases} 0, & \text{if } t < 0, \\ [0, B_1], & \text{if } t = 0, \\ B_1, & \text{if } t > 0, \end{cases}$$

with the new class of growth functions $Q(t)$ with respect to the Hausdorff distance [4]. Evidently,

$$q'_1(0) = q'_2(0).$$

For the H-distances - d_1 and d_2 using $q_1(t)$ and $q_2(t)$ we have

$$q_1(-d_1) = d_1 \tag{6}$$

and

$$q_2(d_2) = B_1 - d_2. \tag{7}$$

For example, for fixed $k = 25$, $B = 2$, $A = 1$, $c = 2$ we find $d_1 = 0.0618051$ and $d_2 = 0.134238$. For $k = 60$ we have $d_1 = 0.0321596$ and $d_2 = 0.0905275$ (see, Figure 4). Evidently, for the H-distance d between the Heaviside step function h_0 and the sigmoidal function Q is fulfilled:

$$d = \max\{d_1, d_2\}. \tag{8}$$

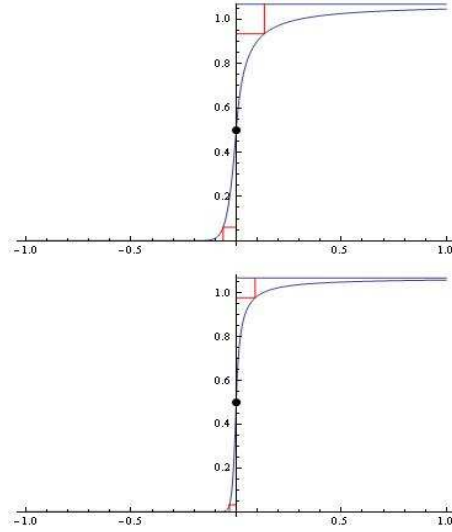


Figure 4: The function $Q(t)$ for fixed $B = 2$, $A = 1$, $c = 2$: a) $k = 25$; b) $k = 60$ (Asymptote at level $B_1 = \frac{B}{(1+Ae^{-1})^c}$ is ≈ 1.06889).

The following is valid

Theorem C. Let

$$\frac{B}{(1+A)^c} = \frac{1}{2}, \quad B_1 = \frac{B}{(1+Ae^{-1})^c}, \quad M = 1 + \frac{ck}{2} \left(1 - \frac{1}{(2B)^{\frac{1}{c}}} \right), \quad 0 < d < \frac{1}{2}$$

For sufficiently large values of k , for the "saturation" - d we have

$$d \approx \frac{\ln(C_1 M)}{C_1 M} \quad (9)$$

where C_1 is positive constant.

Sketch of the proof. Insofar as the proof is based on a technique proposed in [7], we will only note that from (8) it is easy to see that $d(= d_2)$ is the only positive root of the nonlinear equation:

$$F(d) := q_2(d) - B_1 + d = 0. \quad (10)$$

Evidently, the function

$$H(d) := B_1 + \frac{1}{2} + \left(1 + \frac{ck}{2} \left(1 - \frac{1}{(2B)^{\frac{1}{c}}} \right) \right) d = B_1 + \frac{1}{2} + Md \quad (11)$$

approximates $F(d)$ with $d \rightarrow 0$ as $\mathcal{O}(d^2)$ (see, for example Figure 5).

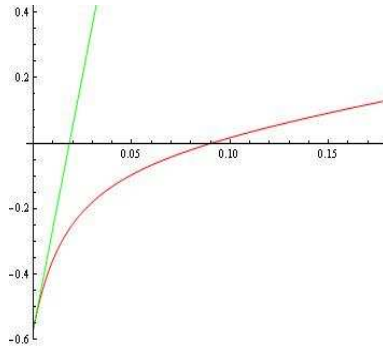


Figure 5: The functions $F(d)$ (red) and $H(d)$ (green) for fixed $k = 60$, $A = 1$, $B = 2$, $c = 2$; Hausdorff distance $d = 0.0905275$.

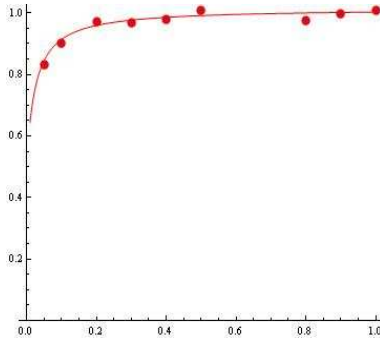


Figure 6: The fitted model for "DataFailure".

We will explicitly note that the sigmoidal function $g_2(t)$ gives very good results in approximating data sets in the fields of debugging theory and the spread of computer viruses. Naturally, the researchers working in these areas, knowing the saturation height B_1 of the experimental data, can easily determine the other parameters of the proposed new model. We will illustrate what has been said with an appropriate example.

Example. For the

$$DataFailure := \{\{0.05, 0.83\}, \{0.1, 0.9\}, \{0.2, 0.971\}, \{0.3, 0.966\}, \\ \{0.4, 0.98\}, \{0.5, 1.01\}, \{0.8, 0.976\}, \{0.9, 0.999\}, \{1, 1.01\}\}$$

the fitted model for $B = 2.11$, $c = 1.252$, $k = 45.3$, $B_1 = 1.01508$ is depicted on Fig. 6.

A look at the cut function associated to the function $Q(t)$.

Let

$$\begin{aligned} k_1 &= \frac{kABc}{(1+A)^{c+1}} = q'_2(0) = q'_1(0); \quad B_1 = \frac{B}{(1+Ae^{-1})^c}; \\ t_0 &= -\frac{0.5}{k_1}; \quad t_1 = \frac{B_1-0.5}{k_1}. \end{aligned} \quad (12)$$

Define the following piecewise cut function associated to the function $Q(t)$ (5):

$$C_1(t) := \begin{cases} 0, & t < t_0 \\ k_1 t + \frac{1}{2} := L_1(t), & -t_0 \leq t \leq t_1 \\ B_1, & t > t_1. \end{cases} \quad (13)$$

This function can find a variety of applications in mathematics and engineering. Of interest is the problem of approximating the cut function $C_1(t)$ by function $Q(t)$ with respect to the uniform distance (or Hausdorff distance).

The following is valid

Proposition. The function $Q(t)$ approximates the cut function $C_1(t)$ in uniform metric with an error

$$\rho(C_1, Q) = f_1(A, B, c) \quad (14)$$

that does not depend on the reaction rate k of the model growth function.

The proof is trivial. Evidently,

$$\begin{aligned} \rho(C_1, Q) &= \max\{\rho(C_1, q_2(t_1)), \rho(C_1, q_1(t_0))\} = \rho(C_1, q_2(t_1)) \\ &= B_1 - q_2(t_1) = B_1 - \frac{B}{1+Ae^{-\frac{kt_1}{1+kt_1}}} \end{aligned}$$

Further,

$$kt_1 = \frac{k}{k_1} \left(B_1 - \frac{1}{2} \right) = \frac{(1+A)^{c+1}}{ABc} \left(B_1 - \frac{1}{2} \right).$$

This completes the proof of the proposition.

By contrast, it turns out that the Hausdorff distance (H-distance) depends on the slope k and tends to zero when increasing the slope.

Consider the logistic growth–decay pair generated by the following reaction network (in canonical form) involving two reacting species Y, X :



wherein $\lambda(t)$ is the "rate function".

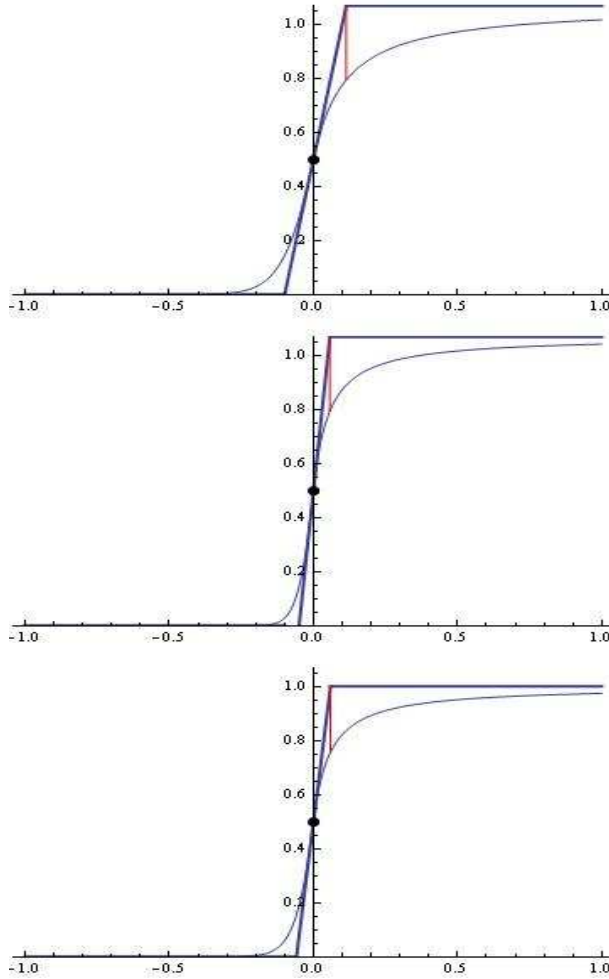


Figure 7: The functions $C_1(t)$ and $Q(t)$ for a) $c = 2$, $B = 2$, $A = 1$, $k = 10$; The uniform distance: $\rho = 0.275088$; b) $c = 2$, $B = 2$, $A = 1$, $k = 20$; The uniform distance: $\rho = 0.275088$; c) $c = 1.28$, $B = 2$, $A = 1.95363$, $k = 20$; The uniform distance: $\rho = 0.243214$.

The symbol $2X$ in (15) is an abbreviation for $X + X$. We discuss the usage of the framework of chemical reaction networks for the construction of new dynamical model. Reaction network (15) induces the following differential system

$$\begin{cases} \frac{dy(t)}{dt} = -\lambda(t)y(t)x(t) \\ \frac{dx(t)}{dt} = \lambda(t)y(t)x(t) \end{cases} \quad (16)$$

with $y(0) = y_0$; $x(0) = x_0$.

The above example illustrates the process of translation of a chemical reaction networks into systems of ordinary differential equations. Let

$$\lambda(t) = \frac{kc}{B^{\frac{1}{c}}(1+kt)^2}.$$

Hence, the new model can be written for the growth function in the form:

$$\begin{aligned} x'(t) &= \frac{kc}{B^{\frac{1}{c}}(1+kt)^2} x(t) (B^{\frac{1}{c}} - (x(t))^{\frac{1}{c}}) \\ x(0) &= \frac{B}{(1+A)^c}. \end{aligned} \tag{17}$$

Some computational examples using *CAS Mathematica* are given in Figures 8–9.

Obviously, the function $x(t)$ coincides with the second component $q_2(t)$ of the defined and studied in this article hypothetical piecewise smooth sigmoidal growth function $Q(q_1(t), q_2(t))$. The new model has been applied to simulate biological growth data sets coming from various fields of science. We develop some dynamic programming modules implemented within the programming environment CAS Wolfram Mathematica and Wolfram Cloud Open Access.

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```

k = Input["k"]; (* 10 *)
Print["k = ", k];
B = Input["B"]; (* 3 *)
Print["B = ", B];
c = Input["c"]; (* 0.5 *)
Print["c = ", c];
K = Input["K"]; (* 9 *)
Print["K = ", K];
x0 = Input["Input initial condition - x[0]"]; (* 0.5 *)
Print["Initial condition x0 = ", x0];
y0 = Input["Input initial condition - y[0]"]; (* 0.51 *)
Print["Initial condition y0 = ", y0];
t0 = Input["Input t0"];
Print["t0 = ", t0];
t1 = Input["Input t1"];
Print["t1 = ", t1];
Print["The solution of the system of differential equations"];
NDSolve[{x'[t] == (k*c/K) / (1+k*t)^2 * x[t] * (K-x[t]^2), x[0] == x0,
  y'[t] == -(k*c/K) / (1+k*t)^2 * y[t] * (K-y[t]^2), y[0] == y0}, {x, y}, {t, t0, t1}];
Plot[Evaluate[{x[t], y[t]} /. First[%]], {t, t0, t1}, AxesOrigin -> {0, 0}]

k = 10
B = 3
c = 0.5
K = 9
Initial condition x0 = 0.5
Initial condition y0 = 0.51
t0 = 0
t1 = 10
The solution of the system of differential equations

```

Figure 8: Module in the software environment *CAS Mathematica* for solving and visualizing the solution of system of the differential equations (16) (for $k = 10$, $c = 0.5$, $B = 3$, $A = 35$, $x_0 = 0.5$).

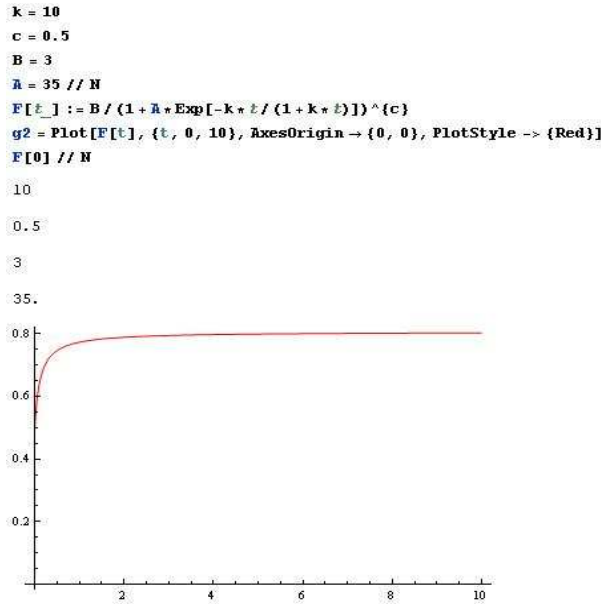


Figure 9: The component $q_2(t)$ of the function $Q(q_1(t), q_2(t))$ for $k = 10$, $c = 0.5$, $B = 3$, $A = 35$.

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