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A NOTE ON A HYPOTHETICAL PIECEWISE SMOOTH SIGMOIDAL GROWTH FUNCTION: REACTION NETWORK ANALYSIS, APPLICATIONS

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ABSTRACT: Typically, the researcher is faced with the following dilemma when analyzing and approximating data (in practice - grouped data): How, in a fixed model in the field of Growth Theory with parameters: A_i, $i = 0, 1, \dots n$ (for which there is a theoretical, substantiated justification for good modeling of the studied dynamic model), to obtain an adequate analytical continuation when the dynamics of the observed model changes at $t > t_1$, whereby a lower (respectively higher) asymptotic saturation is achieved from what the basic model offers, but with the same fixed parameters: $A_i, i = 0, 1, \dots n$. In attacking this topical issue (related to data approximation and modeling in the field of Population Dynamics and Debugging Theory, etc.), research has been conducted related to:

- the possibility for smooth stitching of sigmoidal functions with fractionally rational argument;
- providing researchers (who are not necessarily specialists - mathematicians and computer scientists) with reliable software tools for statistical analysis of specific data;
- the possibility to describe the mentioned "analytical extensions" in terms of the reaction-kinetic mechanisms - as solutions of reaction systems from differential equations.

AMS Subject Classification: 41A46
Key Words: hypothetical piecewise smooth sigmoidal growth function, Hausdorff distance, reaction network

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1. THE BASIC PROBLEM

Verhulst model [1] makes an extensive use of the sigmoidal function:

$$s_1(t) = \frac{B}{1 + Ae^{-kt}}. \tag{1}$$

Studying "Canteloup growth", Pearl et al. [2]–[3] empirically found that one should generalized the logistic map in order to reproduce better the data. Rather than the mere logistic, they propose a form like $y(t) = \frac{r}{1+e^{a_0+a_1t+a_2t^2+\ldots}}$, where y, is the number of seedlings of the canteloups. An extensive overview on the topic can be found in [4], see also [5]–[12]).

For a visualization of the model (1) at fixed values of the parameters k, A, B, see Figure 1. In the field of Population Dynamics the problem often arises how to construct a modified model at already fixed values of parameters k, A, B and a change in the dynamics of the growth process for $t > t_0$, in which saturation to the horizontal asymptote at level $B_1 = \frac{B}{1+Ae^{-1}}$ is reached. This can be achieved, for example, with the function $s_2(t)$ (for $t > 0$, see Figure 2)

$$s_2(t) = \frac{B}{1 + Ae^{-\frac{kt}{1+kt}}}. \tag{2}$$

Definition 1. This leads us to think of the following hypothetical piecewise smooth sigmoidal growth function

$$S(t) := \begin{cases} \dfrac{B}{1 + Ae^{-kt}} := s_1(t), & t < 0 \\ 0.5, & t = 0 \\ \dfrac{B}{1 + Ae^{-\frac{kt}{1+kt}}} := s_2(t), & t > 0. \end{cases} \tag{3}$$

Evidently, from (3) we have $s_1'(0) = s_2'(0)$.

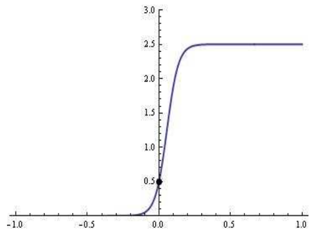

Figure 1: The sigmoidal function $s_1(t)$ for fixed $k = 25$, $B = 2.5$, $A = 4$, $(s_1(0) = \frac{1}{2})$.

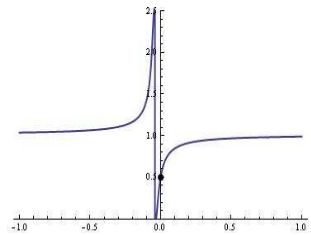

Figure 2: The function $s_2(t)$ for fixed $k = 25$, $B = 2.5$, $A = 4$, $(s_2(0) = \frac{1}{2})$.

Definition 2. [13]. The Hausdorff distance (the H–distance) $\rho(f, g)$ between two interval functions f, g on $\Omega \subseteq \mathbb{R}$, is the distance between their completed graphs $F(f)$ and $F(g)$ considered as closed subsets of $\Omega \times \mathbb{R}$. More precisely,

$$\rho(f, g) = \max\{ \sup_{A \in F(f)} \inf_{B \in F(g)} ||A - B||, \sup_{B \in F(g)} \inf_{A \in F(f)} ||A - B||\},$$

wherein $||.||$ is any norm in $\mathbb{R}^2$, e. g. the maximum norm $||(t, x)|| = \max\{|t|, |x|\}$; hence the distance between the points $A = (t_A, x_A)$, $B = (t_B, x_B)$ in $\mathbb{R}^2$ is $||A - B|| = \max(|t_A - t_B|, |x_A - x_B|)$.

Definition 3. The modified Heaviside step–function is defined by:

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

In this article we will discuss some features of this new family. More precise bounds for the H–distance d between the Heaviside step function h_0 and the sigmoid Verhulst function $s_0 = 1/(1 + e^{-kt})$ can be found in [5]:

Theorem A. For the H–distance [13] $d = \rho(h_0, s_0)$ between the Heaviside step function h_0 and the sigmoid Verhulst function s_0 the following inequalities hold for

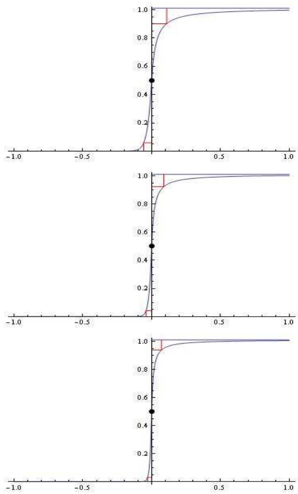

Figure 3: The function $S(t)$ for fixed $B = 2.5$, $A = 4$: a) $k = 40$; b) $k = 65$; c) $k = 100$ (Asymptote at level $B_1 = \frac{B}{1+Ae^{-1}}$ is 1.01152).

$k \geq 2$:

$$\begin{aligned} d_l = \frac{\ln(k+1)}{k+1} - \frac{\ln\ln(k+1)}{(k+1)\left(1+\frac{1}{\ln(k+1)}\right)} < d < \\ < \frac{\ln(k+1)}{k+1} + \frac{\ln\ln(k+1)}{(k+1)\left(\frac{\ln\ln(k+1)}{1-\ln(k+1)}-1\right)} = d_r. \end{aligned} \tag{4}$$

In addition, we will consider the interesting problem of approximating the Heaviside step function with the new class of growth functions $S(t)$ with respect to the Hausdorff distance. In the present work we discuss the usage of the framework of chemical reaction networks for the construction of new dynamical model.

2. MAIN RESULTS

2.1. THE H–DISTANCE BETWEEN FUNCTION H_0 AND THE SIGMOIDAL FUNCTION $S(T)$

For the H–distances - d_1 and d_2 using $s_1(t)$ and $s_2(t)$ we have

$$s_1(-d_1) = d_1 \tag{5}$$

and

$$s_2(d_2) = B_1 - d_2. \tag{6}$$

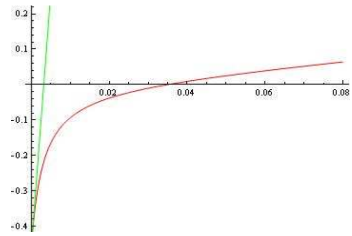

Figure 4: The functions $F(d)$ (red) and $H(d)$ (green) for fixed $k = 380$, $A = 3$, $B = 2$; Hausdorff distance $d = 0.0348992$.

For example, for fixed $k = 40$, $B = 2.5$, $A = 4$ we find $d_1 = 0.0585878$ and $d_2 = 0.109602$. For $k = 65$ we have $d_1 = 0.0414756$ and $d_2 = 0.0881121$ and for $k = 100$ we find $d_1 = 0.0301832$ and $d_2 = 0.0722739$ (see, Figure 3). Evidently, for the H–distance $d = \rho(h_0, S)$ between the Heaviside step function h_0 and the sigmoidal function S is fulfilled:

$$d = \max\{d_1, d_2\}. \tag{7}$$

The following is valid

Theorem B. Let

$$\frac{B}{1+A} = \frac{1}{2},\ B_1 = \frac{B}{1+Ae^{-1}},\ M = 1 + \frac{Ak}{2(1+A)},\ 0 < d < \frac{1}{2}$$

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

$$d \approx \frac{\ln((A-B)M)}{(A-B)M} := d^*. \tag{8}$$

Sketch of the proof. Insofar as the proof is based on a technique proposed in [5], we will only note that from (6) it is easy to see that $d(= d_2)$ is the only positive root of the nonlinear equation:

$$F(d) := s_2(d) - B_1 + d = 0. \tag{9}$$

Evidently, the function

$$H(d) := \frac{1}{2} - \frac{(1+A)e}{2(A+e)} + \left(1 + \frac{Ak}{2(1+A)}\right) d = L + Md \tag{10}$$

approximates $F(d)$ with $d \to 0$ as $\mathcal{O}(d^2)$ (see, for example Fig. 4). After a precise analysis we get the estimate (8).

Some computational examples using relations (6) and (8) are presented in Table 1.

k	A	B	d *computed by* (6)	d^* *computed by* (8)
10	6	3.5	0.219981	0.195342
20	5	3	0.158088	0.15679
40	4	2.5	0.109602	0.127007
65	4	2.5	0.0881121	0.0913902
76	4	2.5	0.082034	0.0817892
300	3	2	0.0390928	0.0416899
350	3	2	0.0363068	0.0369353
380	3	2	0.0348992	0.0346086

Table 1: Bounds for d computed by (6) and (8) for various values of k, A and B.

Remarks.

1. We will explicitly note that the estimate (8) may be useful for users due to the fact that the adaptation of this model in an arbitrary Computer Algebraic Calculation System presupposes the knowledge of an appropriate initial approximation for the root of the nonlinear equation (6), and, moreover, it is necessary double precision operation. **2.** To construct the function $s_2(t)$, we used a substantial "fractional linear correction". The reader can formulate some hypothetical piecewise smooth sigmoidal models using other "fractional rational corrections". **3.** Studies in this article can also be applied to a random shifted sigmoidal functions.

Definition 4. Define the following hypothetical piecewise smooth shifted sigmoidal growth function

$$S^*(t) := \begin{cases} \dfrac{B}{1+Ae^{-k(t-r)}} := s_1^*(t), \ \ 0<t<r \\ 0.5, \ \ t=r \\ \dfrac{B}{1+Ae^{-\frac{k(t-r)}{1+k(t-r)}}} := s_2^*(t), \ \ t>r. \end{cases} \tag{11}$$

Evidently, from (11) we have ${s_1^*}'(r) = {s_2^*}'(r)$.

Definition 5. The shifted Heaviside function is defined by:

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

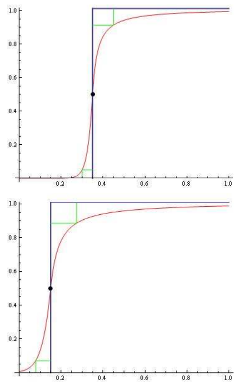

Figure 5: The function $S^*(t)$ for fixed $B = 2.5$, $A = 4$: a) $k = 50$, $r = 0.35$; H-distance $d = 0.0992155$; b) $k = 30$, $r = 0.15$; H-distance $d = 0.124346$.

For example, for fixed $k = 50$, $B = 2.5$, $A = 4$, $r = 0.35$ we find for the H-distance $d = 0.0992155$ and for $k = 30$, $B = 2.5$, $A = 4$, $r = 0.15$ we have $d = 0.124346$ (see, Figure 5).

2.2. A LOOK AT THE CUT FUNCTION ASSOCIATED TO THE FUNCTION S(T)

Let

$$k_1 = \frac{kAB}{(1+A)^2} = s_2'(0) = s_1'(0); \;\; B_1 = \frac{B}{1+Ae^{-1}}; \qquad (12)$$

$$t_0 = -\frac{0.5}{k_1}; \; t_1 = \frac{B_1 - 0.5}{k_1}.$$

Define the following piecewise cut function associated to the function $S(t)$ (3):

$$C(t) := \begin{cases} 0, \;\; t < t_0 \\ k_1 t + \frac{1}{2} := L(t), \;\; -t_0 \leq t \leq t_1 \\ B_1, \;\; t > t_1. \end{cases} \qquad (13)$$

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

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

$$\rho(C, S) = f(A, B) \qquad (14)$$

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

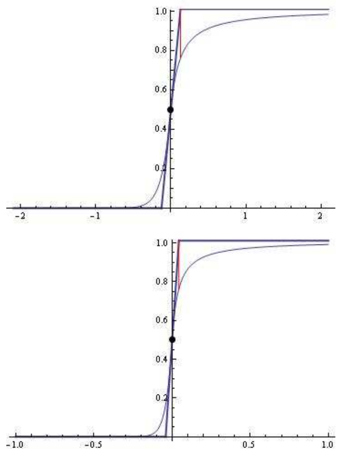

Figure 6: The function $C(t)$ for fixed $B = 2.5$, $A = 4$: a) $k = 10$; b) $k = 30$; The uniform distance: $\rho = 0.249829$.

The proof is trivial. Evidently,

$$\begin{aligned}\rho(C,S) &= \max\{\rho(C,s_2(t_1)),\rho(C,s_1(t_0))\} = \rho(C,s_2(t_1)) = B_1 - s_2(t_1)\\ &= B_1 - \frac{B}{1+Ae^{-\frac{kt_1}{1+kt_1}}}\end{aligned}$$

Further,

$$kt_1 = \frac{k}{k_1}(B_1 - \frac{1}{2}) = \frac{(1+A)^2}{AB}(B_1 - \frac{1}{2}).$$

This completes the proof of the proposition.

Some computational examples are presented in Table 2.

A	B	$f(A,B)$ $from$ (14)
4	2.5	0.249829
3.4	2.2	0.233264
3	2	0.220282

Table 2: The uniform distance $\rho(C,S)$.

By contrast, it turns out that the Hausdorff distance (H-distance) depends on the slope k and tends to zero when increasing the slope. For the H–distance d_3 between $C(t)$ and $S(t)$ we have

$$s_2(t_1 + d_3) = B_1 - d_3. \tag{15}$$

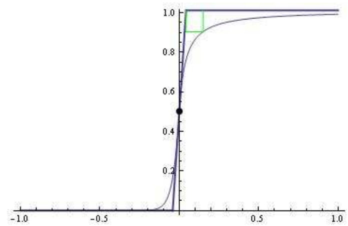

Figure 7: For fixed $k = 30$, $B = 2.5$, $A = 4$ the H–distance is $d_3 = 0.107354$.

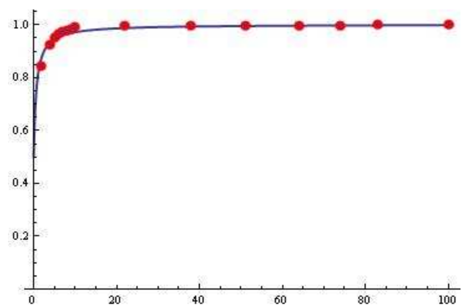

Figure 8: Epidemic data of Storm worm (normalized) fitted by $s_2(t)$ for $A = 2.41$; $B = 3.82$; $k = 1.87122$.

For example, for fixed $k = 30$, $B = 2.5$, $A = 4$ from (15) we find $d_3 = 0.107354$ (see, Figure 7). For other results, see [16]–[20].

2.3. APPLICATIONS

Often, researchers are faced with the following dilemma - how to use in practice a fixed sigmoidal function (which they believe is well models on a particular process in the field of Growth Theory) when approximating a database provided to them in a "normalized form". One possibility is to use the methodology proposed in this article for constructing piecewise smooth sigmoidal growth function.

1. Storm worm was one of the most biggest cyber threats of 2008.

$$dataStorm := \{\{1.8, 0.843\}, \{4, 0.926\}, \{5, 0.954\}, \{6, 0.967\},$$
$$\{7, 0.976\}, \{8, 0.981\}, \{9, 0.985\}, \{10, 0.991\}, \{22, 0.995\}, \{38, 0.997\},$$
$$\{51, 0.998\}, \{64, 0.9985\}, \{74, 0.999\}, \{83, 1\}, \{100, 1\}\}$$

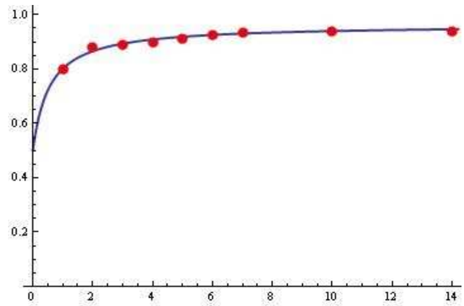

Figure 9: The $data\_CDF\_of\_ransoms\_received\_per\_adress\_in\_C_{CL}$ fitted by $s_2(t)$ for $B = 2.09,\ A = 3.18,\ k = 2.13576$.

For the "data_Storm"– normalized (see, [11] for some details) the fitted model

$$s_2(t) = \frac{B}{1 + Ae^{-\frac{kt}{1+kt}}}$$

for $A = 2.41$; $B = 3.82$; $k = 1.87122$ is depicted on Fig. 8.

2. For the

$$data\_CDF\_of\_ransoms\_received\_per\_adress\_in\_C_{CL} :=$$
$$\{\{1, 0.80\}, \{2, 0.88\}, \{3, 0.89\}, \{4, 0.9\}, \{5, 0.91\}, \{6, 0.92\}, \{7, 0.93\},$$
$$\{10, 0.935\}, \{14, 0.94\}\}$$

the fitted model $s_2(t)$ for $B = 2.09,\ A = 3.18,\ k = 2.13576$ is depicted on Fig. 9.

3. We will consider the following interesting example. The applicability of the model (11) is proved in simulation study to "neck cumulative cancer data" in [15] (appropriate scaling has been selected for this dataset). "Neck cancer data" is divided into two datasets containing specific grouped data:

$$dataNeckcancer1 := \{\{0.01, 0\}, \{0.025, 0.067\}, \{0.05, 0.1\},$$
$$\{0.075, 0.2\}, \{0.1, 0.234\}, \{0.125, 0.281\}, \{0.15, 0.42\}, \{0.2, 0.502\}\}$$

and

$$dataNeckcancer2 := \{\{0.2, 0.522\}, \{0.225, 0.668\}, \{0.25, 0.708\},$$
$$\{0.275, 0.733\}, \{0.3, 0.749\}, \{0.325, 0.8\}, \{0.35, 0.82\}, \{0.375, 0.84\},$$
$$\{0.4, 0.853\}, \{0.425, 0.867\}, \{0.45, 0.887\}, \{0.475, 0.893\}, \{0.5, 0.9\},$$
$$\{0.525, 0.906\}, \{0.55, 0.91\}, \{0.575, 0.913\}, \{0.6, 0.92\}, \{0.625, 0.927\},$$
$$\{0.65, 0.933\}, \{0.675, 0.957\}, \{0.7, 0.96\}, \{0.725, 0.967\}, \{0.75, 0.977\},$$
$$\{0.775, 0.983\}, \{0.8, 0.99\}, \{0.825, 0.997\}, \{0.85, 1\}\}$$

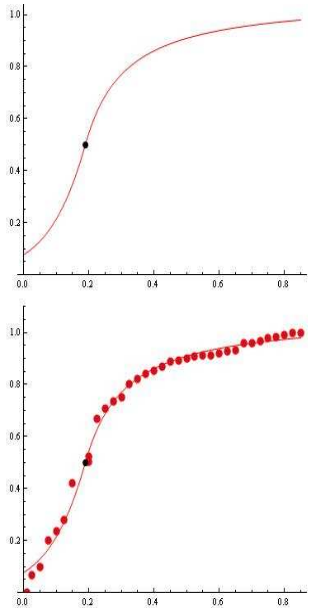

Figure 10: The "dataNeckcancer1" and "dataNeckcancer2" fitted by $s_1^*(t)$ and $s_2^*(t)$ for $A = 5.2,\ B = 5.2,\ k = 10.6996,\ r = 0.189648$.

We will use model $S^*(s_1^*, s_2^*)$:

$$s_1^*(t) = \frac{B}{1 + Ae^{-k(t-r)}}, \quad 0 < t < r \approx 0.2$$

to approximate "dataNeckcancer1" and

$$s_2^*(t)\frac{B}{1 + Ae^{-\frac{k(t-r)}{1+k(t-r)}}}, \quad t > r$$

to approximate "dataNeckcancer2".

For the actual data in the specified period the our new model for

$$A = 5.2,\ B = 5.2,\ k = 10.6996,\ r = 0.189648$$

is depicted on Fig. 10. Of course, when using similar models - of the type (11), the Kolmogorov-Smirnov test must be applied in the case when the parameters of the model are estimated from grouped data (see, for example [14]) .

2.4. APPENDIX. NEW CLASS OF GROWTH FUNCTION GENERATED BY REACTION NETWORKS AND BASED ON ”CORRECTING AMENDMENTS OF FRACTIONAL LINEAR FUNCTION –TYPE”

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

$$Y + X \xrightarrow{\rho(t)} 2X \tag{16}$$

wherein $\rho(t)$ is the ”rate function”.

The symbol $2X$ in (16) is an abbreviation for $X + X$.

Reaction network (16) induces the following differential system

$$\begin{cases} \dfrac{dy(t)}{dt} & = & -\rho(t)y(t)x(t) \\ \dfrac{dx(t)}{dt} & = & \rho(t)y(t)x(t) \end{cases} \tag{17}$$

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

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

Let

$$\rho(t) = \frac{k}{B(1+kt)^2}.$$

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

$$x'(t) = \frac{k}{B(1+kt)^2} x(t)(B - x(t)); \quad x(0) = \frac{1}{2}. \tag{18}$$

Some computational examples using *CAS Mathematica* are given in Fig. 11–12. Obviously, the function $x(t)$ coincides with the second component $s_2(t)$ of the defined and studied in detail in this article hypothetical piecewise smooth sigmoidal growth function $S(s_1(t), s_2(t))$ (see, Fig. 12). The new model has been applied to simulate biological growth data sets coming from various fields of science. For other results, see [21]–[36].

2.5. CONCLUDING REMARKS

The example (”dataNeckcancer”) we have chosen is very instructive.

```
k = Input["k"];(* 100 *)
Print["k = ", k];
B = Input["B"];(* 2.5 *)
Print["B = ", B];
x0 = Input["Input initial condition - x[0]"]; (* 0.5 *)
Print["Initial condition x0 = ", x0];
t0 = Input["Input t0"];
Print["t0 = ", t0];
t1 = Input["Input t1"];
Print["t1 = ", t1];
A = 2 * B - 1
Print["The solution of the differential equation"];
NDSolve[{x'[t] == (k / B) / (1 + k * t)^2 * x[t] * (B - x[t]), x[0] == x0}, {x}, {t, t0, t1}];
Plot[Evaluate[{x[t]} /. First[%]], {t, t0, t1}, AxesOrigin → {0, 0}]
```

```
k = 100
B = 2.5
Initial condition x0 = 0.5
t0 = 0
t1 = 1
4.
The solution of the differential equation
```

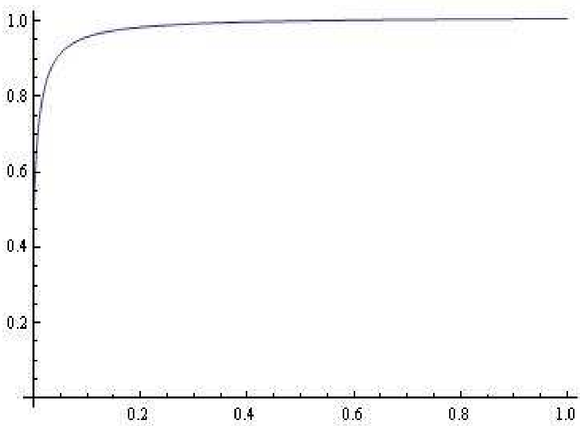

Figure 11: Module in the software environment *CAS Mathematica* for solving and visualizing the solution of the differential equation (18).

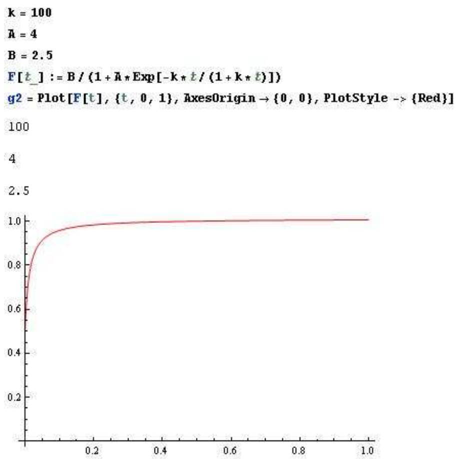

Figure 12: The component $s_2(t)$ of the function $S(s_1(t), s_2(t))$ for $k = 100$, $B = 2.5,\ A = 4$.

It justifies the new conceptual trends discussed in this article and the proposed software tools for analysis and visualization of data arising in general in the field of "growth theory".

It is envisaged that the model described in this paper will be implemented in software environments Distributed e–Testing software environments Cluster (DeTC) and distributed e–learning platform (DisPeL) for learning purposes [37].

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