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A NOTE ON THE LOG–LOGISTIC AND TRANSMUTED LOG–LOGISTIC MODELS. SOME APPLICATIONS

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ABSTRACT: The Hausdorff approximation of the shifted Heaviside function by Log-logistic and quadratic transmuted Log-logistic sigmoid functions is investigated and an expression for the error of the best approximation is obtained. The results of numerical examples performed in the programming environment Mathematica confirm our theoretical conclusions. Some applications in the field of biochemical processes and debugging theory are also explored.

AMS Subject Classification: 41A46, 68N30

Key Words: log–logistic model, quadratic transmuted log–logistic model, shifted Heaviside function $h_{t_0}(t)$, Hausdorff approximation, upper and lower bounds, debugging theory

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1. INTRODUCTION

A very good kinetic interpretation of Log–logistic dose–time response curves can be found in [5]. We will follow a brief statement from the cited article. In the context of kinetics mechanisms yielding Verhulst model [1]–[3] (see, also [7]–[9]), the logistic equation is defined as:

$$\frac{dM^*(t)}{dt} = kM^*(t)(1 - M^*(t)) \tag{1}$$

where k is the rate constant. The general solution is

$$1 - M^*(t) = \frac{1}{1 + e^{k(t-t_0^*)}}.$$

At time $t = 0$ we have

$$1 - M_0^* = \frac{1}{1 + e^{-kt_0^*}}; \ \ M_0^* = M^*(0),$$

i.e.

$$t_0^* = \frac{1}{k}\left(\ln\left(\frac{1}{M_0^*} - 1\right)\right).$$

We consider the following generalization of logistic model. Let the function $M(t)$ is defined my the following nonlinear equation:

$$\left(\frac{M}{1-M}\right)^{\frac{1}{\beta}} = 1 + \frac{k(t-t_0)}{\beta}. \tag{2}$$

After differentiation of both sides of Eq. (2), and after simple calculation we get the following differential equation for the new Log–logistic function $M(t)$:

$$\frac{dM(t)}{dt} = kM^{1-\frac{1}{\beta}}(1-M)^{1+\frac{1}{\beta}}, \tag{3}$$

where β is a shape parameter. For $\beta \to \infty$ the equation (3) reduces to equation (1). The Eq. (3) provides a parametric interpolation formula between the predictions of the logistic equation ($\beta \to \infty$) and second order kinetics ($\beta = 1$). The equation (2) can be rewritten as:

$$1 - M = \frac{1}{1 + \left(1 + \frac{k(t-t_0)}{\beta}\right)^{\beta}}.$$

For $0 < \frac{1}{\beta}$ it is possible to force $M = 0$ at $t = 0$ by setting $t_0 = 0$. With this condition the equation reduces to the simple form

$$1 - M = \frac{1}{1 + \left(\frac{t}{\alpha}\right)^{\beta}},$$

where the time constant, defined by $\alpha = \frac{\beta}{k}$ is a scale parameter.

The Log–logistic equation can be written as:

$$M(t) = \frac{t^{\beta}}{\alpha^{\beta} + t^{\beta}}. \tag{4}$$

In this article we study the Hausdorff approximation of the shifted Heaviside function $h_{t_0}(t)$ by Log–logistic and quadratic transmuted Log–logistic cumulative distribution functions (see, for instance [20]).

We give a software modules within the programming environment CAS Mathematica for illustrating the results. Some applications in the field of biochemical processes and debugging theory have also explored.

2. PRELIMINARIES

Definition 1. [20] Let T be a random variable with cumulative distribution function (c.d.f.) $C(t)$.

Then a general transmuted family (called k– transmuted family) is defined as:

$$M(t) = C(t) + (1 - C(t)) \sum_{i=1}^{k} \lambda_i \left(C(t)\right)^i \tag{5}$$

with $\lambda_i \in [-1, 1]$ for $i = 1, 2, \ldots, k$ and $-k \leq \sum_{i=1}^{k} \lambda_i < 1$.

For the quadratic transmuted family, see Shaw et Buckley [10]. Shaw et al. [10], Gupta et al. [12] study a new model which generalizes the Log–logistic function [13]. The Log–logistic distribution (also known as the Fisk distribution [11]) is a widely used lifetime distribution. For other results, see [21].

The distribution is used to model in fields such as biostatistics, population dynamic, medical research [6] and economics.

The (c.d.f.) of Log–logistic distribution is given by:

$$C(t) = \frac{t^\beta}{\alpha^\beta + t^\beta}, \quad t \in [0, \infty).$$

Definition 2. The (c.d.f.) of quadratic transmuted Log–logistic family is defined by:

$$M_1(t) = \frac{t^\beta}{\alpha^\beta + t^\beta} \left(1 + \lambda - \lambda \frac{t^\beta}{\alpha^\beta + t^\beta}\right). \tag{6}$$

Remark. From (5) we have

$$M_1(t) = C(t) + (1 - C(t)) \left(\lambda_1 C(t) + \lambda_2 C^2(t)\right)$$

If $\lambda_2 = 0$ and $\lambda_1 = \lambda$ we have

$$\begin{aligned} M_1(t) &= C(t) + (1 - C(t))\, \lambda C(t) \\ &= \tfrac{t^\beta}{\alpha^\beta + t^\beta} + \left(1 - \tfrac{t^\beta}{\alpha^\beta + t^\beta}\right) \lambda \tfrac{t^\beta}{\alpha^\beta + t^\beta} \\ &= \tfrac{t^\beta}{\alpha^\beta + t^\beta} \left(1 + \lambda - \lambda \tfrac{t^\beta}{\alpha^\beta + t^\beta}\right). \end{aligned} \tag{7}$$

Definition 3. The shifted interval Heaviside function is defined as [17]:

$$h_{t_0}(t) = \begin{cases} 0, & \text{if} \quad t < t_0, \\ [0,1], & \text{if} \quad t = t_0, \\ 1, & \text{if} \quad t > t_0\ . \end{cases} \tag{8}$$

We will note that the determination of compulsory in area of the Software Reliability Theory components, such as confidence intervals and confidence bounds, should also be accompanied by a serious analysis of the value of the best Hausdorff approximation of the function $h_{t_0}(t)$ by cumulative functions of type (4) and (6) - the subject of study in the present paper.

Definition 4. [16] 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 $||A - B|| = \max(|t_A - t_B|, |x_A - x_B|)$.

3. MAIN RESULTS

3.1. A NOTE ON THE LOG–LOGISTIC FAMILY (4)

We see that $M(\alpha) = \frac{1}{2}$. The one–sided Hausdorff distance d between the function $h_\alpha(t)$ and the function (4) satisfies the relation

$$M(\alpha + d) = 1 - d. \tag{9}$$

The following theorem gives upper and lower bounds for d

Theorem 1. *For the one–sided Hausdorff distance $d = d(\alpha, \beta)$ between $h_\alpha(t)$ and the sigmoid (4) the following inequalities hold for $\frac{\beta}{\alpha} \geq 2$:*

$$d_l = \frac{1}{1 + \frac{\beta}{\alpha}} < d < \frac{\ln\left(1 + \frac{\beta}{\alpha}\right)}{1 + \frac{\beta}{\alpha}} = d_r. \tag{10}$$

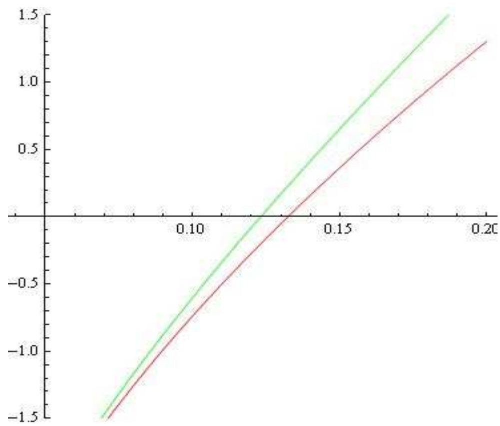

Figure 1: The functions $F(d)$ and $G(d)$.

Proof. Let us examine the function:

$$F^*(d) = M(\alpha + d) - 1 + d. \tag{11}$$

From (9) we find

$$\ln \frac{1-d}{d} = \beta \ln \frac{\alpha + d}{\alpha} = \beta \ln \left(1 + \frac{d}{\alpha}\right)$$

Consider the function

$$F(d) = \beta \ln \left(1 + \frac{d}{\alpha}\right) - \ln(1-d) - \ln \frac{1}{d}.$$

From

$$F'(d) = \frac{\beta}{\alpha} \frac{1}{1 + \frac{d}{\alpha}} + \frac{1}{1-d} + \frac{1}{d} > 0$$

we conclude that function F is increasing.

Consider the function

$$G(d) = \left(1 + \frac{\beta}{\alpha}\right) d - \ln \frac{1}{d}. \tag{12}$$

From Taylor expansion we obtain $G(d) - F(d) = O(d^2)$.

Hence $G(d)$ approximates $F(d)$ with $d \to 0$ as $O(d^2)$ (see Fig. 1).

In addition $G'(d) > 0$.

Further, for $\frac{\beta}{\alpha} \geq 2$ we have

$$G\left(\frac{1}{1 + \frac{\beta}{\alpha}}\right) = 1 - \ln \left(1 + \frac{\beta}{\alpha}\right) < 0,$$

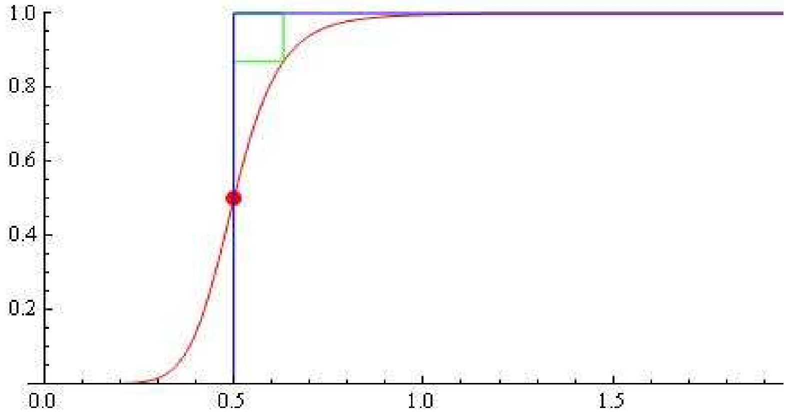

Figure 2: The model (4) for $\beta = 8.2$, $\alpha = 0.5$; H–distance $d = 0.130267$, $d_l = 0.0574713$, $d_r = 0.164165$.

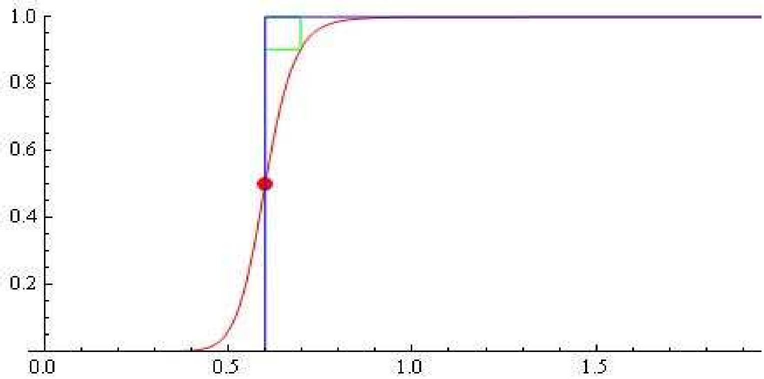

Figure 3: The model (4) for $\beta = 15$, $\alpha = 0.6$; H–distance $d = 0.0964897$, $d_l = 0.0384615$, $d_r = 0.125311$.

$$G\left(\frac{\ln\left(1+\frac{\beta}{\alpha}\right)}{1+\frac{\beta}{\alpha}}\right) = \ln\ln\left(1+\frac{\beta}{\alpha}\right) > 0.$$

This completes the proof of the theorem.

The model (4) for $\beta = 8.2$, $\alpha = 0.5$ is visualized on Fig. 2.

From the nonlinear equation (9) and inequalities (10) we have: $d = 0.130267$, $d_l = 0.0574713$, $d_r = 0.164165$.

The model (4) for $\beta = 15$, $\alpha = 0.6$ is visualized on Fig. 3.

We prove more precise bounds for d. Using the same notations as in Theorem 1, we state the following

Theorem 2. *For* α, $\beta \in R$

$$\begin{aligned}\tilde{d}_l &= \frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}} - \frac{\ln\ln(1+\frac{\beta}{\alpha})}{(1+\frac{\beta}{\alpha})\left(1+\frac{1}{\ln(1+\frac{\beta}{\alpha})}\right)} < d < \frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}} \\ &+ \frac{\ln\ln(1+\frac{\beta}{\alpha})}{(1+\frac{\beta}{\alpha})\left(\frac{\ln\ln(1+\frac{\beta}{\alpha})}{1-\ln(1+\frac{\beta}{\alpha})}-1\right)} = \tilde{d}_r.\end{aligned} \tag{13}$$

Proof. Evidently, the second derivative of (12)

$$G''(d) = -\frac{1}{d^2} < 0$$

has a constant sign on $[\frac{1}{1+\frac{\beta}{\alpha}}, \frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}}]$.

The straight line, defined by the points $\left(\frac{1}{1+\frac{\beta}{\alpha}}, G\left(\frac{1}{1+\frac{\beta}{\alpha}}\right)\right)$, $\left(\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}}, G\left(\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}}\right)\right)$, and the tangent to $G(d)$ at the point $\left(\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}}, G\left(\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}}\right)\right)$, cross the abscissa at the points

$$\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}} + \frac{\ln\ln(1+\frac{\beta}{\alpha})}{(1+\frac{\beta}{\alpha})\left(\frac{\ln\ln(1+\frac{\beta}{\alpha})}{1-\ln(1+\frac{\beta}{\alpha})}-1\right)},$$

$$\frac{\ln(1+\frac{\beta}{\alpha})}{1+\frac{\beta}{\alpha}} - \frac{\ln\ln(1+\frac{\beta}{\alpha})}{(1+\frac{\beta}{\alpha})\left(1+\frac{1}{\ln(1+\frac{\beta}{\alpha})}\right)},$$

respectively.

This completes the proof of the Theorem 2.

We note that the improved bounds (13) are more precise than (10).

3.2. A NOTE ON THE QUADRATIC TRANSMUTED LOG–LOGISTIC CUMULATIVE SIGMOID (5)

We consider the following family:

$$M_1^*(t) = \frac{t^\beta}{\alpha^\beta + t^\beta}\left(1+\lambda-\lambda\frac{t^\beta}{\alpha^\beta+t^\beta}\right). \tag{14}$$

Let t_0 is the positive root of the nonlinear equation

$$M_1^*(t_0) - \frac{1}{2} = 0. \tag{15}$$

The one–sided Hausdorff distance d_1 between the function $h_{t_0}(t)$ and the function (14) satisfies the relation

$$M_1^*(t_0+d_1) = 1-d_1. \tag{16}$$

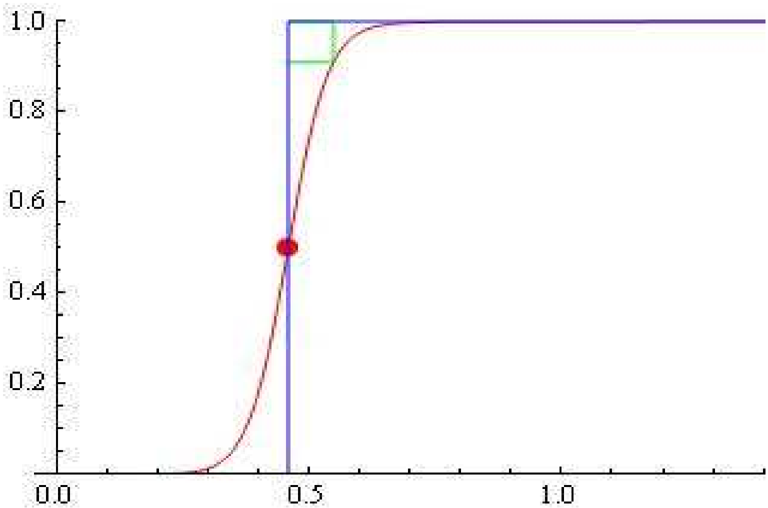

Figure 4: The model (14) for $\lambda = 0.96$, $\alpha = 0.5$, $\beta = 10$, $t_0 = 0.459127$; H–distance $d_1 = 0.0891484$, $d_{l_1} = 0.0649963$, $d_{r_1} = 0.177663$.

Let

$$\begin{aligned} p_1 =& \frac{\alpha^\beta(-t_0^\beta - \alpha^\beta + \lambda t_0^\beta)}{(\alpha^\beta + t_0^\beta)^2}, \\ q_1 =& 1 + \frac{2\beta\lambda t_0^{3\beta-1}}{(\alpha^\beta + t_0^\beta)^3} - \frac{\beta(1+3\lambda)t_0^{2\beta-1}}{(\alpha^\beta + t_0^\beta)^2} + \frac{\beta(1+\lambda)t_0^{\beta-1}}{\alpha^\beta + t_0^\beta}. \end{aligned}$$

The following theorem gives upper and lower bounds for d_1

Theorem 3. *For the one–sided Hausdorff distance d_1 between $h_{t_0}(t)$ and the sigmoid (14) the following inequalities hold for:*

$$2.1q_1 > e^{1.05}$$

$$d_{l_1} = \frac{1}{2.1q_1} < d_1 < \frac{\ln(2.1q_1)}{2.1q_1} = d_{r_1}. \tag{17}$$

The proof follows the ideas given in this note and will be omitted.

The model (14) for $\lambda = 0.96$, $\alpha = 0.5$, $\beta = 10$, $t_0 = 0.459127$ is visualized on Fig. 4.

4. SOME APPLICATIONS

1. The Hill's function is used frequently to study biochemical processes in the living cell (see, e.g. [14], [15]). Hill's model is concerned with the reaction network:

$$C + \beta T \longleftrightarrow C_\beta,$$

where C denotes a protein that binds up to β molecules of ligand T and C_β is a ligand–protein complex. The coefficient β describes the number of binding sites on the protein.

All ligands bind simultaneously. Assuming that both the forward and backward reactions are allowed applying the mass action law we obtain for the rate of the ligand concentration a simple expression.

We may assume that this expression equals zero, because the ligand concentration is much bigger than the protein concentration and thus dot change in time. From the latter equation one easily derive the expression for the dose response curve (the Hill's function) which relates the amount of free ligands, t, to the fraction of ligand–bound proteins (e.g. receptors) in the system, φ.

In biochemistry, the proportion of the bound macromolecules is often described by Hill's equation [4]:

$$\varphi = \frac{\frac{t^\beta}{K}}{1 + \frac{t^\beta}{K}},$$

where K denotes the dissociation constant.

When β is an integer, this formula can be explained by chemical kinetics. In many cases, the value of β is not an integer. For example, for the binding of oxygen to haemoglobin, we have $\beta \approx 2.8$ [14].

In the case $K = \alpha^\beta$ we have the Log–logistic function

$$M(t) = \frac{t^\beta}{\alpha^\beta + t^\beta}.$$

The function $M(t)$ is the general Hill time–response equation

$$1 - M(t) = \frac{1}{1 + \left(\frac{t}{\alpha}\right)^\beta}$$

that describes the temporal transformation of the population mechanism [15].

Now it is clear how important is the study of the phenomenon "super saturation", to which we devoted the Theorems 1–2.

2. The research of each new model in the field of debugging and test theory compulsory passes through the experimental phase with imposed in practice databases.

Month Index	System Days (Days)	System Days (Cumulative)	Failures	Cumulative Failures
1	961	961	7	7
2	4170	5131	3	10
3	8789	13,920	14	24
4	11,858	25,778	8	32
5	13,110	38,888	11	43
6	14,198	53,086	8	51
7	14,265	67,351	7	58
8	15,175	82,526	19	77
9	15,376	97,902	17	94
10	15,704	113,606	6	100
11	18,182	131,788	11	111
12	17,760	149,548	4	115
13	18,352	167,900	0	115

Table 1: Field failure data [18].

One of them is the data provided in [18]. The operating time of the software is 167,900 days. 115 failures are detected for these days which contain 71 unique failures.

Table 1 shows the failures data which are united for each of the 13 months.

Dataset included [19] Year 2000 compatibility modifications, operating system upgrade, and signaling message processing.

Below, we will illustrate the fitting of this data, for example, with the $M(t)$ model, and will show the connection to discussed in this article - approximate task.

The fitted model

$$M(t) = N\frac{t^\beta}{\alpha^\beta + t^\beta}$$

based on the data of Table 1 for the estimated parameters: $N = 115$; $\alpha = 5.93046$; $\beta = 3.15179$ is plotted on Fig. 5.

The example results show a good fit by the presented model $M(t)$.

The fitted model

$$M_1(t) = N\frac{t^\beta}{\alpha^\beta + t^\beta}\left(1 + \lambda - \lambda\frac{t^\beta}{\alpha^\beta + t^\beta}\right)$$

based on the Dataset for the estimated parameters: $N = 115$; $\alpha = 17.8094$; $\beta = 1.71172$; $\lambda = 2.92657$ is plotted on Fig. 6.

The approximation of these data by quadratic transmuted function provides very good results.

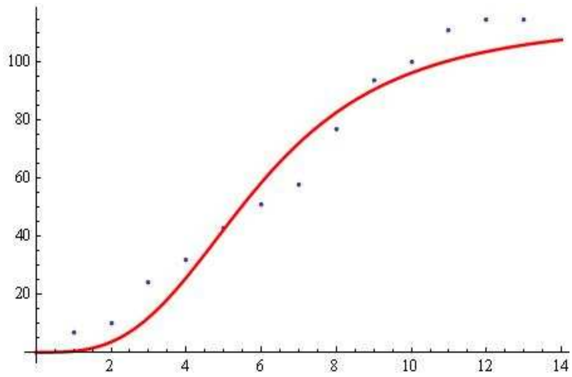

Figure 5: Approximation solution by $M(t)$.

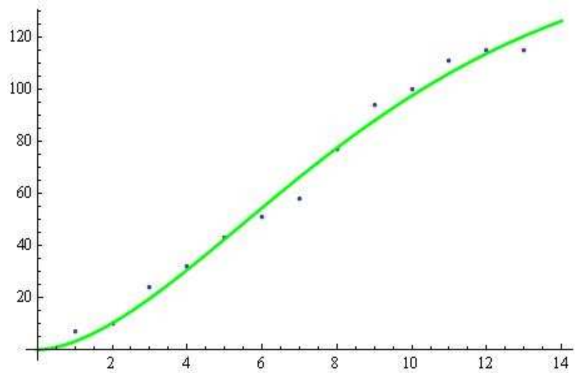

Figure 6: Approximation solution by model $M_1^*(t)$.

The given comparison shows that in some cases the quadratic transmuted Log–logistic software reliability model is better than that of Log–logistic software reliability model (see, Fig. 7).

Obviously, studying of phenomenon "super saturation" is mandatory element along with other important components - "confidence bounds" and "confidence intervals" when dealing with questions from Software Reliability Models domain.

For some software reliability models, see [22]–[39].

We hope that the results will be useful for specialists in this scientific area.

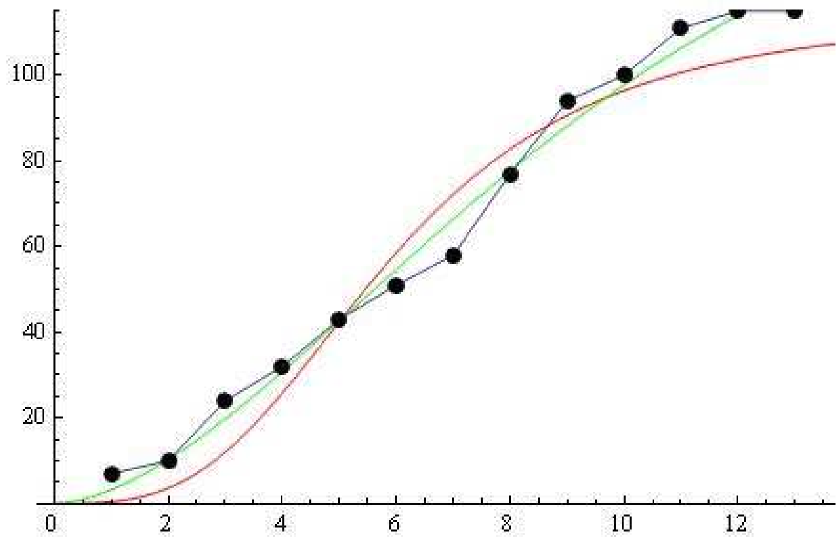

Figure 7: Comparison between Log-logistic (red) and quadratic transmuted Log–logistic (green) models.

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