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A family of recurrence generated sigmoidal functions based on the Verhulst logistic function. Some approximation and modelling aspects

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Abstract In this note we construct a family of recurrence generated sigmoidal logistic functions based on the Verhulst logistic function.

We prove estimates for the Hausdorff approximation of the Heaviside step function by means of this family. Numerical examples, illustrating our results are given.

Keywords Sigmoidal functions \cdot Logistic functions \cdot Heaviside step function \cdot Hausdorff distance \cdot Upper and lower bounds.

1 Introduction

The logistic function belongs to the important class of smooth sigmoidal functions arising from population and cell growth models.

The logistic function was introduced by Pierre François Verhulst [45]–[47], who applied it to human population dynamics. Verhulst

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proposed his logistic equation to describe the mechanism of the selflimiting growth of a biological population. His equation was rediscovered by A. G. McKendrick [18] for the bacterial growth in broth and was tested using nonlinear parameter identification.

Since then the logistic function finds applications in many scientific fields, including biology, ecology, population dynamics, chemistry, demography, economics, geoscience, mathematical psychology, probability, sociology, political science, financial mathematics, statistics, fuzzy set theory, insurance mathematics to name a few [1], [2], [52], [51], [4], [15], [22], [23], [24], [21], [44], [48], [49].

Logistic functions are also used in artificial neural networks [3], [6]–[8], [9], [10], [12], [13], [11], [14]. Constructive approximation by superposition of sigmoidal functions and the relation with neural networks and radial basis functions approximations is discussed in [10]. Any neural net element computes a linear combination of its input signals, and uses a logistic function to produce the result; often called "activation" function [19], [20].

Another application area is medicine, where the logistic function is used to model the growth of tumors or to study pharmacokinetic reactions.

Definition 1. Define the logistic (Verhulst) function v on \mathbb{R} as

$$v_0(k;t) = \frac{1}{1+e^{-kt}}.$$
(1)

Note that the logistic function (1) has an inflection at its "center" (0, 1/2) and its slope κ at 0 is equal to k/4.

Definition 2. The (basic) step function is:

$$h_0(t) = \begin{cases} 0, & \text{if } t < 0, \\ 1/2, & \text{if } t = 0, \\ 1, & \text{if } t > 0, \end{cases}$$

usually known as Heaviside step function.

Definition 3. [16], [17] The Hausdorff distance (the H-distance) [16] $\rho(f,g)$ 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,

$$\rho(f,g) = \max\{\sup_{A \in F(f)} \inf_{B \in F(g)} ||A - B||, \sup_{B \in F(g)} \inf_{A \in F(f)} ||A - B||\}, \quad (2)$$

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 $||A - B|| = \max(|t_A - t_B|, |x_A - x_B|)$.

The Hausdorff approximation of the Heaviside step function by logistic functions of the form (1) is considered in [2] and the following is proved:

Theorem A. [2] The H-distance $d = \rho(h_0, s_0)$ between the Heaviside step function h_0 and the Verhulst function v_0 can be expressed in terms of the rate parameter k for any real $k \ge 2$ as follows:

$$\dot{d}_l(k) = \frac{1}{k+1} < d(k) < \frac{\ln(k+1)}{k+1},\tag{3}$$

$$d_l(k) = \frac{\ln(k+1)}{k+1} - \frac{\ln\ln(k+1)}{k+1} < d(k) < \frac{\ln(k+1)}{k+1} = d_r(k), \quad (4)$$

or

$$d(k) = \frac{\ln(k+1)}{k+1} \left(1 + O(\varepsilon(k))\right), \ \varepsilon(k) = \frac{\ln\ln(k+1)}{\ln(k+1)}.$$
 (5)

More precise estimates for the Hausdorff approximation of the Heaviside step function by Verhulst logistic function is obtained in [30].

Theorem B. [30] For the Hausdorff distance $d = \rho(h_0, s_0)$ between the Heaviside step function h_0 and the sigmoidal function v_0 the following inequalities hold for $k \geq 2$:

$$\tilde{d}_{l} = \frac{\ln(k+1)}{k+1} - \frac{\ln\ln(k+1)}{(k+1)\left(1 + \frac{1}{\ln(k+1)}\right)} < d$$

$$< \frac{\ln(k+1)}{k+1} + \frac{\ln\ln(k+1)}{(k+1)\left(\frac{\ln\ln(k+1)}{1 - \ln(k+1)} - 1\right)} = \tilde{d}_{r}.$$
(6)

2 Main Results

Let us consider the following family of recurrence generated sigmoidal logistic functions

$$v_{i+1}(t) = \frac{1}{1 + k_{i+1}e^{-k(t+v_i(t))}}, \quad i = 0, 1, 2, \dots,$$
(7)

with

$$v_{i+1}(0) = \frac{1}{2}, \quad i = 0, 1, 2, \dots,$$
 (8)

based on the Verhulst logistic function $v_0(t)$.

From (8) we have $k_{i+1} = e^{\frac{k}{2}}$ for $i = 0, 1, 2, \dots,$

Denoting the number of recurrences by p, we can consider various cases.

Special case 1. Let p = 1. In this case we find from (7)–(8):

$$v_1(t) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kt} e^{\frac{-k}{1 + e^{-kt}}}}$$
(9)

The H-distance $d_1 = \rho(h_0, v_1)$ between the Heaviside step function h_0 and the sigmoidal function v_1 satisfies the relation:

$$v_1(d_1) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kd_1} e^{\frac{-k}{1 + e^{-kd_1}}}} = 1 - d_1.$$
(10)

The following theorem gives upper and lower bounds for $d_1 = d_1(k)$

Theorem 2.1 The H-distance $d_1(k)$ between the function h_0 and the function v_1 can be expressed in terms of the rate parameter k for any real $k \ge e$ as follows:

$$d_{l_1} = \frac{1}{\frac{1}{\frac{1}{4}(k^2 + 4k + 16)}} < d_1 < \frac{\ln\frac{1}{4}(k^2 + 4k + 16)}{\frac{1}{4}(k^2 + 4k + 16)} = d_{r_1}.$$
 (11)

Proof. We define the functions

$$F_1(d_1) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kd_1} e^{\frac{-k}{1 + e^{-kd_1}}}} - 1 + d_1$$
(12)

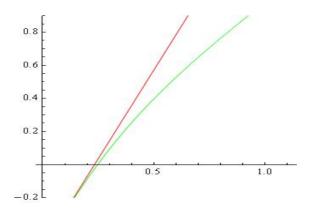


Figure 1: The functions $F_1(d_1)$ and $G_1(d_1)$ for k = e.

$$G_1(d_1) = -\frac{1}{2} + \frac{1}{16}(k^2 + 4k + 16)d_1.$$
 (13)

From Taylor expansion

$$\frac{1}{1+e^{\frac{k}{2}}e^{-kd_1}e^{\frac{-k}{1+e^{-kd_1}}}} - 1 + d_1 - \left(-\frac{1}{2} + \frac{1}{16}(k^2 + 4k + 16)d_1\right) = O(d_1^2)$$

we see that the function $G_1(d_1)$ approximates $F_1(d_1)$ with $d_1 \to 0$ as $O(d_1^2)$ (cf. Fig.1).

In addition $G'_1(d_1) > 0$ and for $k \ge e$

$$G_1(d_{l_1}) < 0; \quad G_1(d_{r_1}) > 0.$$

This completes the proof of the inequalities (11).

Some computational examples using relations (10) and (11) are presented in Table 1.

Special case 2. Let p = 2. In this case we find from (7)–(8):

$$v_2(t) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kt} e^{\frac{-k}{1 + e^{-\frac{k}{2}} e^{-kt} e^{\frac{-k}{1 + e^{-kt}}}}}$$

k	d_{l_1}	$d_1 \mod by (10)$	d_{r_1}
e	0.116747	0.247348	0.250743
3	0.108108	0.23192	0.2405
10	0.025641	0.0743631	0.0939375
20	0.00806452	0.0297465	0.0388732
50	0.00147275	0.00731424	0.00960327

Table 1: Bounds for $d_1(k)$ computed by (10) and (11) for various rates k

The H-distance $d_2 = \rho(h_0, v_2)$ between the Heaviside step function h_0 and the sigmoid function v_2 satisfies the relation:

$$v_2(d_2) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kd_2} e^{\frac{-k}{1 + e^{-\frac{k}{2}} e^{-kd_2} e^{\frac{-k}{1 + e^{-kd_2}}}}}} = 1 - d_2.$$

The following theorem gives upper and lower bounds for $d_2 = d_2(k)$

Theorem 2.2 The H-distance $d_2(k)$ between the function h_0 and the function v_2 can be expressed in terms of the rate parameter k for any real $k \ge e$ as follows:

$$d_{l_2} = \frac{1}{\frac{1}{16}(k^3 + 4k^2 + 16k + 64)} < d_2 < \frac{\ln\frac{1}{16}(k^3 + 4k^2 + 16k + 64)}{\frac{1}{16}(k^3 + 4k^2 + 16k + 64)} = d_{r_2}.$$
(14)

Proof. We define the functions

$$F_2(d_2) = \frac{1}{1 + e^{\frac{k}{2}} e^{-kd_2} e^{\frac{-k}{1+e^{-\frac{k}{2}}e^{-kd_2}e^{\frac{-k}{1+e^{-kd_2}}}}}} = 1 - d_2$$
(15)

$$G_2(d_2) = -\frac{1}{2} + \frac{1}{64}(k^3 + 4k^2 + 16k + 64)d_2.$$
 (16)

From Taylor expansion

$$F_2(d_2) - G_2(d_2) = O(d_2^2)$$

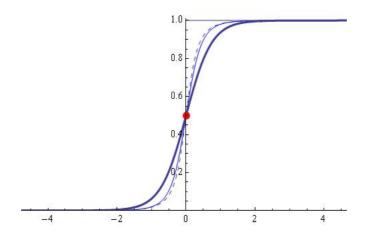


Figure 2: Reaction rate k = e. The graphics: Verhulst function - v_0 (thick), recurrence generated function - v_1 (blue) and recurrence generated function - v_2 (dashed); $d_1 = 0.247348$, $d_2 = 0.224001$.

we see that the function $G_2(d_2)$ approximates $F_2(d_2)$ with $d_2 \to 0$ as $O(d_2^2)$.

In addition $G'_2(d_2) > 0$ and for k > e

$$G_2(d_{l_2}) < 0; \quad G_2(d_{r_2}) > 0.$$

This completes the proof of the inequalities (14).

The recurrence generated sigmoidal logistic functions $v_0(t), v_1(t)$ and $v_2(t)$ are visualized on Fig. 2 Print "Calculation of the value of the Hausdorff distance d between the Heaviside step function h(t) and the recurrence generated family of logistic functions $V_{\{i+1\}}(t) = \frac{1}{1 + k_{\{i+1\}} e^{-k(t+V_{i}(t))}}; i=0, 1, 2, \dots$ on the base of the sigmoidal Verhulst function $V_0(t) = \frac{1}{1 + e^{-kt}}$ in terms of the reaction rate"]; k = Input[" k"]; (*2.7 *) Print["The reaction rate - k = ", k]; i = Input[" i"]; (*1 *) Print["i=", i]; Print["Number of recursions i+1=", i+1]; k1 = Exp[k/2];Print["The rate - k1 = ", k1]; k2 = Exp[k/2];Print["The rate - k2 = ", k2]; Print["The recurrence generated logistic function V1(t): "]; V1 (t) = $\frac{1}{1 + k1 * Exp[-k (t+1/(1 + Exp[-k * t]))]};$ $Print \left["V1(t) = ", \frac{1}{1 + k1 + Exp[-k(t+1/(1 + Exp[-k + t]))]} \right];$ Print["The recurrence generated logistic function V2(t): "]; $V2 (t) = \frac{1}{1 + k2 * Exp\left[-k \left(t + \frac{1}{1 + k1 * Exp\left[-k (t + 1/(1 + Exp\left[-k * t\right]))\right]}\right)\right]}$ $\Pr["V2(t) = ", \frac{1}{1 + k2 * Exp\left[-k\left(t + \frac{1}{1 + k1 * Exp\left[-k(t+1)(1 + Exp\left[-k * t1))\right]}\right)\right]};$

Figure 3: Module in CAS Mathematica.

Print["The basic sigmoidal Verhulst function V0(t): "];

$$V0 (t) = \frac{1}{1 + Exp[-k + t]};$$

$$Print \left["V0 (t) = ", \frac{1}{1 + Exp[-k + t]} \right];$$

1

Print["The following nonlinear equation is used to determination
of the Hausdorff distance d between the Heaviside step function h(t)
and the recurrence generated logistic function V1(t): "];

```
m = 1 / (1 + Exp[k / 2] * Exp[-k * d] * Exp[-k / (1 + Exp[-k * d])]) - 1 + d;
```

Print[m, " = 0"];

```
Print["The unique positive root of the equation is the searched value of d:"]
FindRoot[1 / (1 + Exp[k / 2] + Exp[-k + d] + Exp[-k / (1 + Exp[-k + d])]) - 1 + d, \{d, 0.5\}]
Print["The following nonlinear equation is used to determination
of the Hausdorff distance d between the Heaviside step function h(t)
and the recurrence generated logistic function V2(t): "];
m1 = 1 / (1 + Exp[k/2] + Exp[-k + d] + Exp[-k / (1 + Exp[k/2] + Exp[-k + d] + Exp[-k / (1 + Exp[-k + d])])) - 1 + d;
Print[m1, " = 0"];
Print["The unique positive root of the equation is the searched value of d:"]
FindRoot [1 / (1 + Exp[k / 2] * Exp[-k * d] * Exp[-k / (1 + Exp[k / 2] * Exp[-k * d] * Exp[-k / (1 + Exp[-k * d])])) -
  1 + d, \{d, 0.5\}]
f[d] := 1 / (1 + k1 * Exp[-k * d] * Exp[-k / (1 + Exp[-k * d])])
g[d] := 1 / (1 + Exp[-k * d])
h[d] := 1 / (1 + Exp[k/2] + Exp[-k + d] + Exp[-k / (1 + Exp[k/2] + Exp[-k + d] + Exp[-k / (1 + Exp[-k + d])]))
g3 = Plot[f[d], \{d, -5, 5\}, PlotRange \rightarrow \{0, 1.01\}, PlotStyle \rightarrow \{Blue\}, AspectRatio \rightarrow 0.5];
g4 = Plot[g[d], \{d, -5, 5\}, PlotRange \rightarrow \{0, 1.01\}, PlotStyle \rightarrow \{Thick\}, AspectRatio \rightarrow 0.5];
g5 = Plot[h[d], \{d, -5, 5\}, PlotRange \rightarrow \{0, 1.01\}, PlotStyle \rightarrow \{Dashed\}, AspectRatio \rightarrow 0.5];
Print["The graphics: Verhulst funktion - V0 (thick),
```

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recurrence generated function - V1 (blue) and recurrence generated function - V2 (dashed):"] Show[g3, g4, g5, Plot[1, {t, 0, 5}, PlotRange \rightarrow Full]]
```

Figure 4: Module in CAS Mathematica.

Theorem 2.3 For given p, the H-distance $d_p(k)$ between the function h_0 and the function v_p can be expressed in terms of the rate parameter k for any real $k \ge e$ as follows:

$$d_{l_p} = \frac{1}{\frac{1}{2^{2p}} \left(k^{p+1} + \sum_{i=0}^{p} 2^{2(i+1)} k^{p-i} \right)} < d_p < \frac{\ln \left(\frac{1}{2^{2p}} \left(k^{p+1} + \sum_{i=0}^{p} 2^{2(i+1)} k^{p-i} \right) \right)}{\frac{1}{2^{2p}} \left(k^{p+1} + \sum_{i=0}^{p} 2^{2(i+1)} k^{p-i} \right)} = d_{r_p}.$$
 (17)

Proof. We note that the function

$$G_p(d_p) = -\frac{1}{2} + \frac{1}{2^{2(p+1)}} \left(k^{p+1} + \sum_{i=0}^p 2^{2(i+1)} k^{p-i} \right) d_p.$$

approximates $F_p(d_p)$ with $d_p \to 0$ as $O(d_p^2)$. In addition $G'_p(d_p) > 0$ and for $k \ge e$

$$G_p(d_{l_p}) < 0; \quad G_p(d_{r_p}) > 0.$$

This completes the proof of the inequalities (17).

Remarks. A function which is close to the step function is the cut (or ramp) function.

About approximation of the cut function by logistic and squashing functions see, [6], [5], [15], [25], [28].

The Hausdorff approximation of the Heaviside interval step function by the logistic and other sigmoid functions is discussed from various computational and modelling aspects in [30] (see also [26]–[43]).

The most frequently used non-linear activation function is a sigmoid function, which is modified from a binary step function and is in a form of [50]:

$$f(t) = \frac{1}{1 + e^{-\frac{t}{\tau}}}$$

where τ is a tunable number and referred as the temperature of the neuron.

Based on the methodology proposed in the present note, the reader may formulate the corresponding approximation problems on his/her own.

3. Conclusions

To achieve our goal, we obtain new sharper estimates for the Hdistance between a step function and its best approximating family of recurrence generated sigmoidal logistic functions based on the Verhulst logistic function.

Numerical examples, illustrating our results are given.

We propose a software module within the programming environment CAS Mathematica for the analysis of the considered family of logistic functions.

The module offers the following possibilities:

- generation of the logistic functions under user defined values of the reaction rate k and number of recursions p;

- calculation of the H-distance $d_p = \rho(h_0, v_p), \ p = 0, 1, 2, \dots, p$ between the Heaviside function h_0 and the sigmoidal functions $v_0, v_1, v_2, \dots, v_p$;

- software tools for animation and visualization.

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