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Kies Cumulative Distribution Function: Reaction Network Analysis and Related Problems

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Abstract

The Kies probability model [1] was proposed as an alternative to the extended Weibull models as it provides a more efficient fit to some real-life data sets in comparison to the aforementioned models. In the present article, it has first been shown that the dynamic Kies model is generated by a specific framework of chemical reaction networks. We will also discuss some properties of the family by Kies. Precise bounds for the Hausdorff distance between the Heaviside step function and the considered sigmoid are also given. We also define a hypothetical family of generalized Kies CDF. Some computational examples using *CAS Mathematica* are presented.

Keywords: Kies CDF, Reaction Network, Hausdorff Distance, Upper and Lower Bounds

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1 Introduction

One of the modified versions of the Weibull distribution is known as Kies Distribution and was firstly proposed by Kies (1958) [1].

The Kies probability model was proposed as an alternative to the extended Weibull models as it provides a more efficient fit to some real–life data sets in comparison to the aforementioned models.

For some modifications see [2–6].

Definition 1. *The cumulative distribution function (CDF) of the two-parameter Kies distribution is given by:*

$$F(t) = 1 - e^{-k\left(\frac{t}{1-t}\right)^a}, \tag{1}$$

where $0 < t < 1$, $k > 0$ *and* $a > 0$.

In the present work, it has first been shown that the dynamic Kies model is generated by a specific framework of chemical reaction networks.

"Confidence bands" are given for the CDF of Kies distribution (see for example [2]).

In recent years, it has become necessary to study the "saturation" of CDF to the horizontal asymptote about Hausdorff distance.

The two characteristics of "confidence bands – saturation" allow the user to choose an appropriate model when approximating specific data from different branches of scientific knowledge.

Definition 2 ([7])**.** *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,*

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

where $||.||$ *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 shifted Heaviside step–function is defined by:*

$$h_0(t) = \begin{cases} 0, & \text{if } t < t_0, \\ [0,1], & \text{if } t = t_0, \\ 1, & \text{if } t > t_0. \end{cases}$$

In this article we will also discuss some properties of the family (1).

2 Main results

2.1 The CDF of Kies distribution generated by reaction networks and based on "correcting amendments of fractional linear function – type"

In the present section we discuss the usage of the framework of chemical reaction network for the construction of dynamical model by Kies and its mathematical analysis.

Without loss of generality, let's fix the parameter $a = 1$ in the model (1).

Consider the reaction (network):

$$S \xrightarrow{k} P \tag{2}$$

($k > 0$) known in chemistry as a "first-order (FO)" reaction and in nuclear physics as "one-step exponential radioactive decay (1-SERD)".

This elementary reaction is known under several additional names due to its application to various processes such as radioactive nuclear decay, fluid dynamics, enzyme kinetics, marine ecology, physico-chemistry, etc. For some details, see Markov [8].

Reaction (2) induces the following dynamical system for the change rates of the concentrations $s = s(t)$, $p = p(t)$ of species S, P:

$$\begin{cases} \dfrac{ds(t)}{dt} = -ks(t), \\ \dfrac{dp(t)}{dt} = ks(t), \end{cases} \tag{3}$$

with $s(0) = s_0$, $p(0) = p_0$.

System (3) implies the relation

$$s + p = c = const. \tag{4}$$

When equipped with initial conditions $s(0) = s_0 = 1$, $p(0) = p_0 = 0$ from relation (4) becomes $s + p = 1$, hence $s = 1 - p$.

Substituting $s = 1-p$ in equation $p' = ks$ we obtain an autonomous ordinary differential equation for the growth function of the form

$$p' = k(1 - p) \tag{5}$$

and

$$p(t) = 1 - e^{-kt}. \tag{6}$$

Following the ideas given in [9] we consider the following hypothetical reaction (network):

$$Y \xrightarrow{\rho(t)} X \tag{7}$$

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

Reaction network (7) induces the following differential system:

$$\begin{cases} \dfrac{dy(t)}{dt} = -\rho(t)y(t), \\ \dfrac{dx(t)}{dt} = \rho(t)y(t). \end{cases} \tag{8}$$

Let $y(0) = y_0 = 1$, $x(0) = x_0 = 0$ and

$$\rho(t) = \frac{k}{(1-t)^2}.$$

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

$$x'(t) = \frac{k}{(1-t)^2}(1 - x(t)), \quad x(0) = 0. \tag{9}$$

Some computational examples using *CAS Mathematica* are given in Figs. 1–2.

Obviously, the function $x(t)$ coincides with the original Kies model (1) for fixed $a = 1$ (see Fig. 2). The model $p(t)$ (6) – dashed for the same fixed value of the "rate constant" $k = 20$ is visualized on the same graph.

We tried to give a mathematical justification for the model proposed by Kies.

In all likelihood, he was guided by such considerations in defining the probability distribution.

From the comparison of the two models it can be concluded that with the Kies model for a short time interval can be achieved a good approximation of specific data, such as those arising from the field of Population Dynamics, Debugging Theory and Computer Viruses Propagation.

2.2 Some Properties

For the "saturation" d to the horizontal asymptote using model (1) in the Hausdorff sense [7] we have

$$F(d) = 1 - d. \tag{10}$$

For example, for fixed $k = 20$ we find $d = 0.10232$. For $k = 40$ we have $d = 0.0642257$ and for $k = 80$ we find $d = 0.0389784$ (see Fig. 3).

The following is valid.

Theorem. *For $k \geq 2$, for the "saturation" d we have*

$$0 < d < \frac{\ln(k+1)}{k+1} := d_r. \tag{11}$$

```
k = Input["k"];(* 20 *)
Print["k = ", k];
x0 = Input["Input initial condition - x[0]"]; (* 0 *)
Print["Initial condition x0 = ", x0];
t0 = Input["Input t0"];
Print["t0 = ", t0];
t1 = Input["Input t1"];
Print["t1 = ", t1];
Print["The solution of the differential equation"];
NDSolve[{x'[t] == k / (1 - t)^2 * (1 - x[t]), x[0] == x0}, {x}, {t, t0, t1}];
Plot[Evaluate[{x[t]} /. First[%]], {t, t0, t1}, AxesOrigin → {0, 0}]
```

```
k = 20
Initial condition x0 = 0
t0 = 0
t1 = 0.99
The solution of the differential equation
```

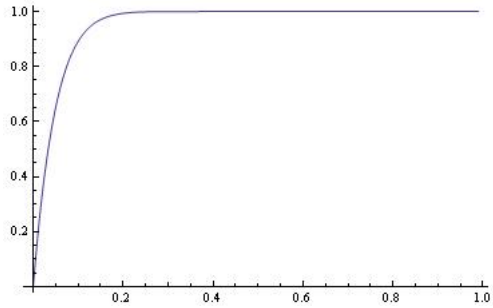

Figure 1: Module in the software environment *CAS Mathematica* for solving and visualizing the solution of the differential equation (9).

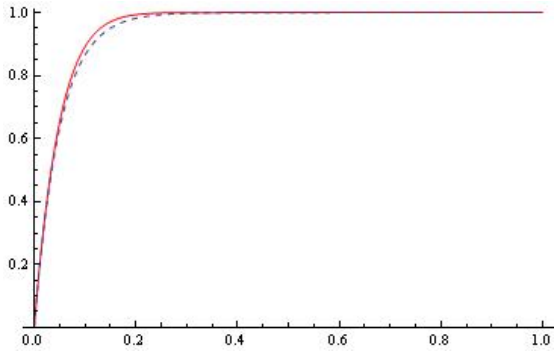

Figure 2: For fixed $k = 20$ the original Kies model (1)-red and model $p(t)$ (6)-dashed.

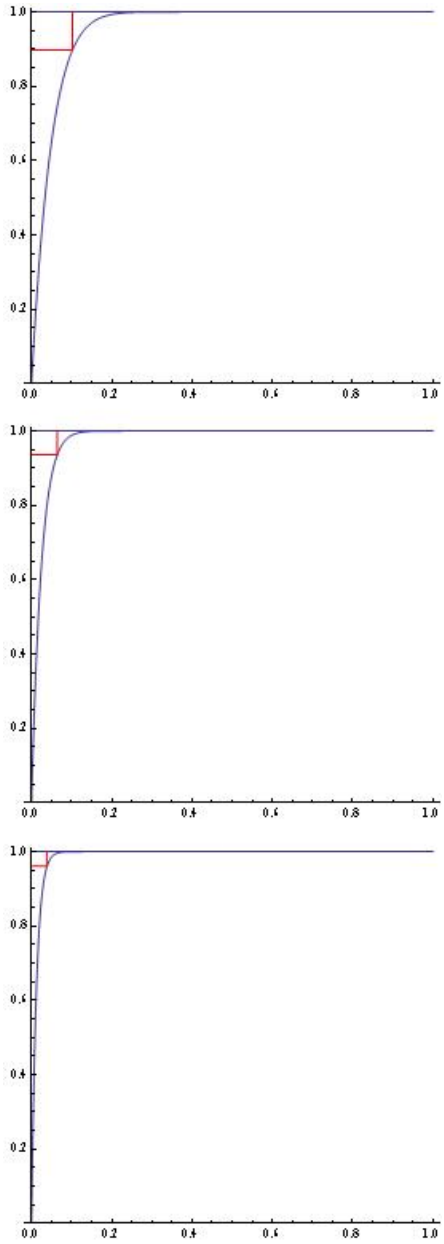

Figure 3: The function $F(t)$ (1) for fixed $a = 1$: a) $k = 20$, $d = 0.10232$, b) $k = 40$, $d = 0.0642257$, c) $k = 80$, $d = 0.0389784$.

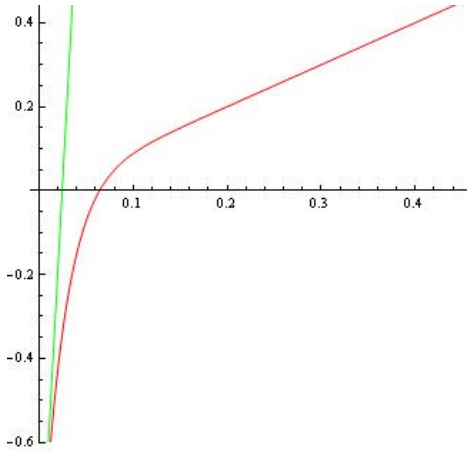

Figure 4: The functions $G(d)$ (red) and $H(d)$ (green) for fixed $k = 40$, $d = 0.0642257$.

Table 1: Bounds for d computed by (10) and (11) for various values of k.

k	d computed by (10)	d_r computed by (11)
100	0.03299	0.0456943
300	0.0140239	0.0189605
1000	0.00522654	0.00690185
3000	0.0020578	0.00266801

Sketch of the proof. Insofar as the proof is based on a technique proposed in [10], we will only note that from (10) it is easy to see that $d = d(k)$ is the only positive root of the nonlinear equation

$$G(d) := F(d) - 1 + d = 0. \tag{12}$$

Evidently, the function

$$H(d) := -1 + (1 + k)d \tag{13}$$

approximates $G(d)$ with $d \to 0$ as $\mathcal{O}(d^2)$ (see, for example Fig. 4). The functions G and H are increasing and $H(d_r) > 0$ for $k \geq 2$. □

Remark. We will explicitly note that the estimate (11) 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 (10), and, moreover, it is necessary double precision operation.

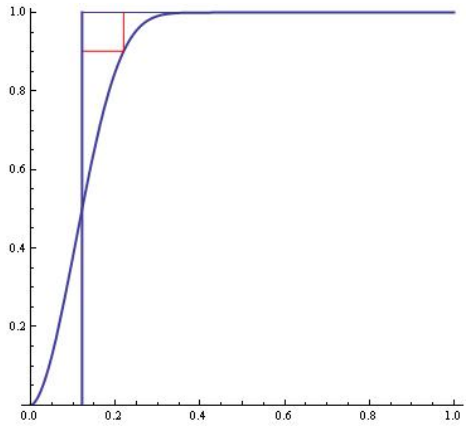

Figure 5: The function $F(t)$ for $k = 20$, $a = 1.7$, $t_0 = 0.121554$, H-distance $d = 0.098216$.

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

Consider the function $F(t)$ for $k > 0$, $a > 0$. Let t_0 is the "median level", i.e. $F(t_0) = \frac{1}{2}$. For the H–distance between Heaviside function h_0 and the sigmoidal function $F(t)$ we have:

$$F(t_0 + d) = 1 - d. \tag{14}$$

For example, for fixed $k = 20$, $a = 1.7$, $t_0 = 0.121554$ we find from nonlinear equation (14) $d = 0.098216$ (see Fig. 5). For other results, see [11–20].

2.3 Concluding remarks

Tadmor and Tanner [21, 22] construct a new class of accurate filters for processing piecewise smooth spectral data:

$$\sigma_{adapt}(t) := \begin{cases} e^{-\frac{c_q t^q}{1-t^2}}, & |t| < 1, \\ 0, & |t| \geq 1, \end{cases} \tag{15}$$

where

$$c_q = 2^q . \frac{3}{8} . \frac{18q^2 + 3q + 14}{9q^2 + 6q + 2}.$$

Some properties of the $\sigma_{adapt}(t)$ are considered in [23].

Consider the following hypothetical family:

$$F_i(t; k) = 1 - e^{-k\left(\frac{t^i}{1-t^i}\right)} = 1 - Q_i(t; k), \quad i = 1, 2, \ldots \tag{16}$$

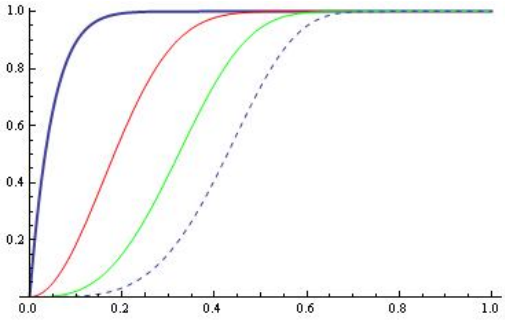

Figure 6: The model $F_i(t;k)$ for $i = 1, 2, 3, 4$ and fixed $k = 20$.

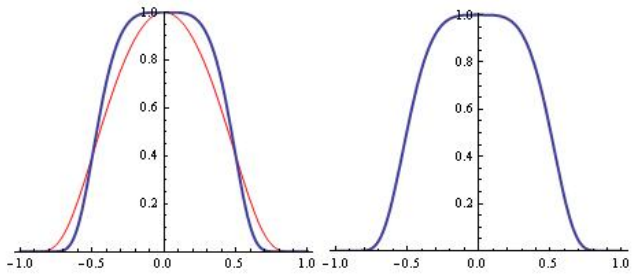

Figure 7: a) The Tadmor-Tanner exponentially optimal filter for $q = 2$ and $q = 4$, b) The factor $Q_4(k;t)$ from (16) for $k = 10$.

The model $F_i(t;k)$ for $i = 1, 2, 3, 4$ and fixed $k = 20$ is visualized on the Fig. 6. The modified adaptive functions of type $F_i(t;k)$ find application in the field of antenna-feeder analysis. Some comparisons between the Tadmor-Tanner filter $\sigma_{adapt}(t)$ and the new factor $Q_i(t;k)$ from (16) are illustrated in Fig. 7.

We define the following activation function based on $Q_i(t;k)$:

$$F_i^*(t;k) = \frac{1 - Q_i(t;k)}{1 + Q_i(t;k)}. \tag{17}$$

In antenna-feeder technique most often occurred signals are of types shown on Fig. 8. For i even, the corresponding approximation using model (17) is shown in Fig. 8a. For i odd, the corresponding approximation using new activation function $F_i^*(t;k)$ is shown in Fig. 8b.

Let $t = b\cos\theta + c$, where θ is the azimuthal angle and c is the phase difference. Then, for example, typical radiation pattern using $|F_i(b\cos\theta + c;k)|$ for $i = 5$, $k = 240$, $b = 0.33$, $c = 0.073$ is plotted on Fig. 9.

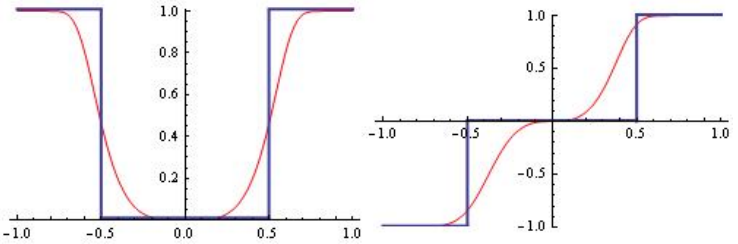

Figure 8: a) Approximation by $F_4^*(t)$ for $k = 15$, b) Approximation by $F_3^*(t)$ for $k = 22$.

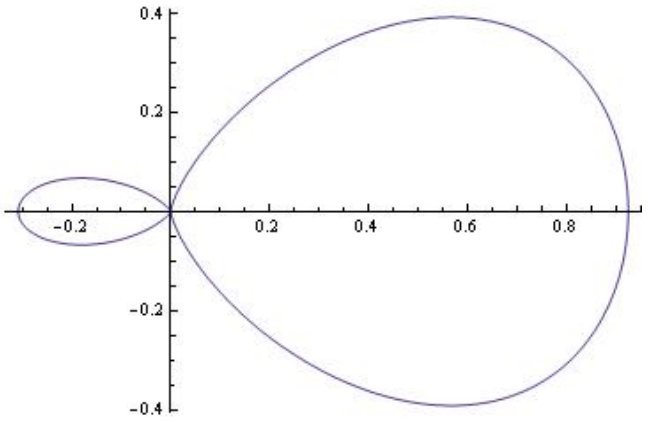

Figure 9: A typical radiation pattern using $|F_i(b\cos\theta + c; k)|$ for $i = 5$, $k = 240$, $b = 0.33$, $c = 0.073$.

In this article we consider only some aspects related to the disclosure of intrinsic properties of some proposed "adaptive functions" in a purely methodological aspect. The question of the optimality of $Q_i(t; k)$ can be considered open.

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