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A MODIFIED THREE–PARAMETER KIES CUMULATIVE DISTRIBUTION FUNCTION IN THE LIGHT OF REACTION NETWORK ANALYSIS

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ABSTRACT: In the present article we consider a new modified three–parameter Kies c.d.f. $F^*(t) = 1 - e^{-k\left(\frac{t}{1-k_1 t}\right)^a}$ where $0 < t < \frac{1}{k_1}$, $k > 0$, $k_1 > 0$ and a is a positive integer. We consider the following hypothetical reaction network: $Y \overset{\rho_a(t)}{\longrightarrow} X_a$ where $\rho_a(t) = \frac{kat^{a-1}}{(1-k_1 t)^{a+1}}$ is the "rate function". The new model can be written for the growth function in the form: $x'_a(t) = \frac{kat^{a-1}}{(1-k_1 t)^{a+1}}(1 - x_a(t));\quad x_a(0) = 0$. For each value of a, the reader can make quantitative and qualitative relationships between the modified model and that generated by the more general reaction scheme of the form: $S + X \underset{k_1}{\overset{k}{\rightleftarrows}} X + \cdots + X = aX$. It can be concluded that in many cases these reaction networks lead to similar results. In Appendix we discuss some distributional properties of the new three parameter Kies distribution. Some computational examples using *CAS Mathematica* are presented.

AMS Subject Classification: 41A46
Key Words: c.d.f. of modified Kies distribution, reaction network analysis

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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].

The cumulative distribution function (CDF) of the two-parameter Kies distribution is given by

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

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

Definition 1. We define the following modified three–parameter Kies cumulative distribution function as

$$F^*(t) = 1 - e^{-k\left(\frac{t}{1-k_1 t}\right)^a}. \tag{1}$$

where $0 < t < \frac{1}{k_1}$, $k > 0$, $k_1 > 0$ and a is a positive integer.

In the present work, it has first been shown that the dynamical modified model (1) is generated by a specific framework of chemical reaction networks. We will also discuss some properties of the family (1).

2. MAIN RESULTS

2.1. THE C.D.F. OF MODIFIED MODEL (1) GENERATED BY REACTION NETWORKS AND BASED ON "CORRECTING AMENDMENTS OF FRACTIONAL FUNCTION –TYPE"

In the present Section we discuss the usage of the framework of chemical reaction network for the construction of dynamical model (1) and its mathematical analysis.

The case $a = 1$.

Consider the reaction (network):

$$S \overset{\rho=k-k_1}{\longrightarrow} P \tag{2}$$

where ρ is the difference of two reaction constants k and k_1, which are used by the researcher in generating and studying dynamic models of the same type. 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 in [7]–[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:

$$\begin{cases} \dfrac{ds(t)}{dt} = -(k-k_1)s(t) \\ \dfrac{dp(t)}{dt} = (k-k_1)s(t) \end{cases} \tag{3}$$

with $s(0) = s_0 = 1$; $p(0) = p_0 = 0$. We obtain an autonomous ordinary differential equation for the growth function with the solution

$$p(t) = 1 - e^{-(k-k_1)t}. \tag{4}$$

We consider the following hypothetical reaction (network):

$$Y \overset{\rho_1(t)}{\longrightarrow} X_1 \tag{5}$$

wherein $\rho_1(t)$ is the "rate function". Reaction network (5) induces the following differential system

$$\begin{cases} \dfrac{dy(t)}{dt} = -\rho_1(t)y(t) \\ \dfrac{dx_1(t)}{dt} = \rho_1(t)y(t). \end{cases} \tag{6}$$

Let $y(0) = y_0 = 1$; $x_1(0) = x_{1,0} = 0$ and

$$\rho_1(t) = \frac{k}{(1-k_1t)^2}.$$

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

$$x_1'(t) = \frac{k}{(1-k_1t)^2}(1 - x_1(t)); \quad x_1(0) = 0. \tag{7}$$

Obviously, the function $x_1(t)$ coincides with the proposed new model (1) for $a = 1$. Some computational examples using *CAS Mathematica* are given in Fig. 1–2. Comparisons between models $p(t)$ (dashed) and $x_1(t)$ (blue) are given in Fig. 2. From the comparison of the two models it can be concluded that with the model (1) (with $a = 1$) 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.

The case $a = 2$.

```
Print["The new model"];

Print["x'[t] ==k/(1-k1*t)^2*(1-x[t])"];

k = Input["reaction constant k"]; (* 20 *)
Print["k = ", k];
k1 = Input["reaction constant k1"]; (* 0.9 *)
Print["k1 = ", k1];
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 - k1 * t)^2 * (1 - x[t]), x[0] == x0}, {x}, {t, t0, t1}];
Plot[Evaluate[{x[t]} /. First[%]], {t, t0, t1}, AxesOrigin → {0, 0}]
```

```
The new model
x'[t] ==k/(1-k1*t)^2*(1-x[t])
k = 20
k1 = 0.9
Initial condition x0 = 0
t0 = 0
t1 = 1
The solution of the differential equation
```

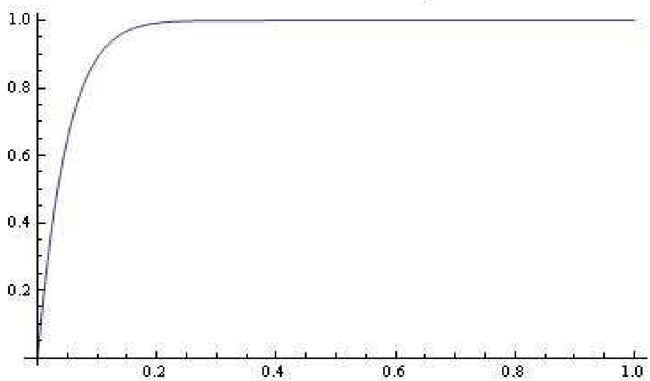

Figure 1: Simple Module in *CAS Mathematica* for solving and visualizing the solution of the differential equation (7).

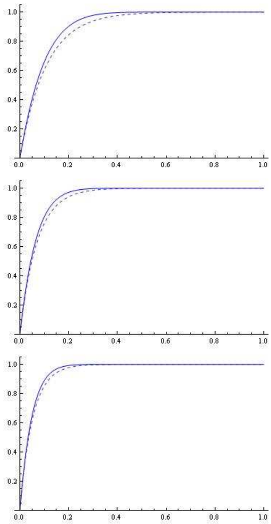

Figure 2: Comparisons between models $p(t)$ (dashed) and $x_1(t)$ (blue): a) $k = 10$, $k_1 = 0.7$; b) $k = 15$, $k_1 = 0.8$; c) $k = 20$, $k_1 = 0.9$.

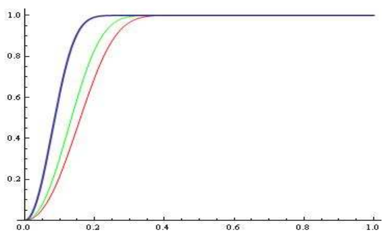

Figure 3: The solution $x_2(t)$ of equation (8) for fixed $k_1 = 0.9$ and $k = 20,\ 30,\ 80$.

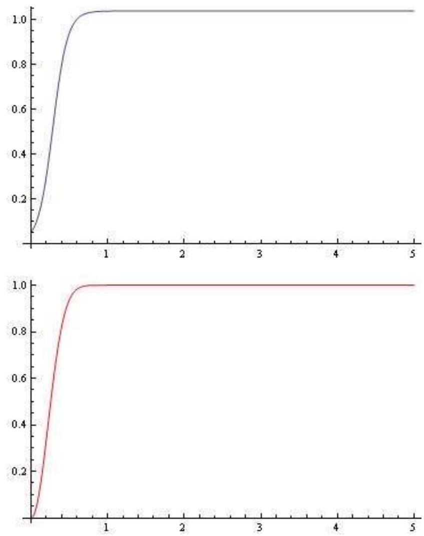

Figure 4: For fixed $k = 10$, $k_1 = 0.1$: a) the solution of the system (10) for the growth function $x(t)$; b) the solution of our model $x_2(t)$ (in the case $a = 2$).

The reaction network (5) with the "rate function" ρ_2

$$\rho_2(t) = \frac{2kt}{(1-k_1t)^3}$$

induces the growth function $x_2(t)$ as the solution of differential equation:

$$x_2'(t) = \frac{2kt}{(1-k_1t)^3}(1-x_2(t)); \quad x_2(0) = 0. \tag{8}$$

Obviously, the function $x_2(t)$ coincides with the proposed new model (1) for the case $a = 2$. The solution $x_2(t)$ of equation (8) for fixed $k_1 = 0.9$ and $k = 20, 30, 80$ is depicted on Fig. 3.

Remark.

Formally, we consider the following reaction equation

$$S + X \underset{k_1}{\overset{k}{\rightleftarrows}} X + X \tag{9}$$

The reaction network (9) induces the following differential system:

$$\begin{cases} \dfrac{ds}{dt} &= -ks(t)x(t) + k_1x^2(t) \\ \dfrac{dx}{dt} &= ks(t)x(t) - k_1x^2(t) \end{cases} \tag{10}$$

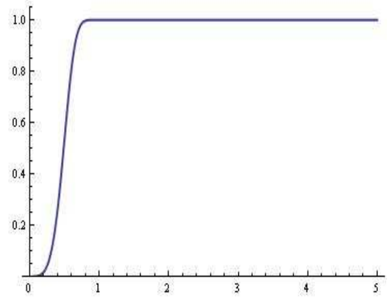

Figure 5: The solution $x_a(t)$ for $a = 4$, $k = 10$ and $k_1 = 0.1$.

The solution of the system (10) for the growth function $x(t)$ for $k = 10$, $k_1 = 0.1$, $s(0) = 1$, $x(0) = 0.05$ is visualized on Fig. 4a (blue). For fixed $k = 10$, $k_1 = 0.1$ the solution of our model $x_2(t)$ (in the case $a = 2$) is depicted on Fig. 4b (red). From the comparison of the two models $x(t)$ and $x_2(t)$ it can be concluded that in many cases reaction networks $S + X \underset{k_1}{\overset{k}{\rightleftarrows}} X + X$ and $Y \overset{\rho_2(t)}{\longrightarrow} X_2$ lead to similar results.

The general case.

We consider the following hypothetical reaction network:

$$Y \overset{\rho_a(t)}{\longrightarrow} X_a \tag{11}$$

where

$$\rho_a(t) = \frac{kat^{a-1}}{(1 - k_1 t)^{a+1}}.$$

is the "rate function". Evidently

$$\begin{cases} \dfrac{dy(t)}{dt} &= -\rho_a(t) y(t) \\ \dfrac{dx_a(t)}{dt} &= \rho_a(t) y(t). \end{cases} \tag{12}$$

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

$$x'_a(t) = \frac{kat^{a-1}}{(1 - k_1 t)^{a+1}} (1 - x_a(t)); \quad x_a(0) = 0. \tag{13}$$

For example, the solution $x_a(t)$ for $a = 4$, $k = 10$ and $k_1 = 0.1$ is visualized on Fig. 5. For each value of a, the reader can make quantitative and qualitative relationships between the modified Kies model (1) and that generated by the more general reaction scheme of the form:

$$S + X \underset{k_1}{\overset{k}{\rightleftarrows}} X + X + \cdots + X = aX.$$

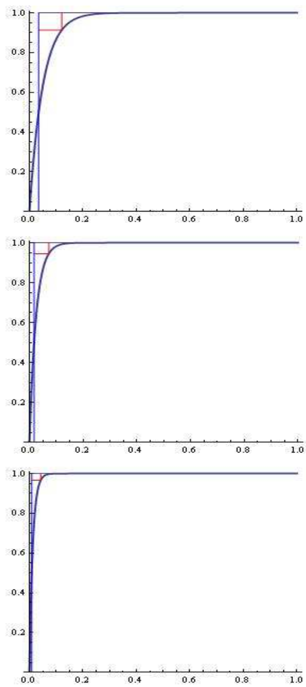

Figure 6: a) $k = 20$, $k_1 = 0.1$, $t_0 = 0.0345377$, $d = 0.0864126$; b) $k = 40$, $k_1 = 0.1$, $t_0 = 0.0172987$, $d = 0.0547859$; c) $k = 80$, $k_1 = 0.1$, $t_0 = 0.00865684$, $d = 0.0395849$.

2.2. SOME PROPERTIES. RELATED PROBLEMS

1. For the one–sided Hausdorff approximation [9] of the shifted Heaviside function (at the median level t_0) by $x_1(t)$ we have

$$x_1(t_0 + d) = 1 - d. \tag{14}$$

For example, for fixed

a) $k = 20$, $k_1 = 0.1$ we find $t_0 = 0.0345377$; $d = 0.0864126$;

b) $k = 40$, $k_1 = 0.1$ we have $t_0 = 0.0172987$; $d = 0.0547859$;

c) $k = 80$, $k_1 = 0.1$ we find $t_0 = 0.00865684$; $d = 0.0395849$

(see, Fig. 6).

For other results, see [10]–[19], [23].

2. We construct a new class of accurate filters

$$Q_i(t; k; k_1)(t) := e^{-k\left(\frac{t}{1-k_1 t}\right)^i}; \quad i = 2, 4, 6, \ldots, \tag{15}$$

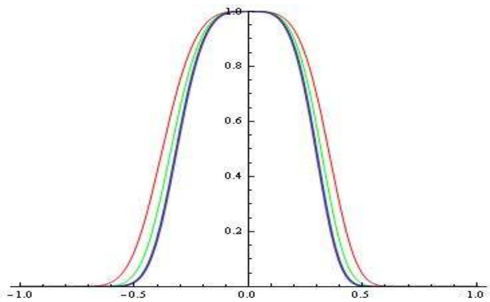

Figure 7: The factor $Q_i(t;k;k_1)$ from (15) as "exponentially filter" for fixed $i = 4$, $k_1 = 0.1$: a) $k = 40$ (red); b) $k = 60$ (green); c) $k = 80$ (thick).

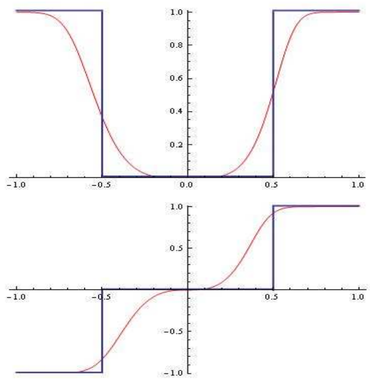

Figure 8: a) Approximation by $F_4^*(t)$ for $k = 15$, $k_1 = 0.1$; b) Approximation by $F_3^*(t)$ for $k = 22$, $k_1 = 0.1$.

The factor $Q_i(t;k;k_1)$ from (15) for some values of k, k_1, i is visualized on Fig. 7.

3. We define the following activation function based on $Q_i(t;k;k_1)$:

$$F_i^*(t;k;k_1) = \frac{1 - Q_i(t;k;k_1)}{1 + Q_i(t;k;k_1)}. \tag{16}$$

In antenna-feeder technique most often occurred signals are of types shown on Fig. 8. For i even, the corresponding approximation using model (16) is shown in Fig. 8 a. For i odd, the corresponding approximation using new activation function $F_i^*(t;k;k_1)$ is shown in Fig. 8 b.

4. Let $t = b\cos\theta + c$, where θ is the azimuthal angle and c is the phase difference.

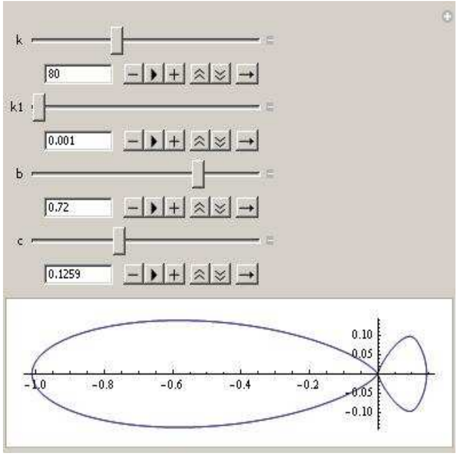

Figure 9: A typical antenna diagram using $F(\theta)$ for $a = 7$, $k = 80$, $k_1 = 0.001$, $b = 0.72$, $c = 0.1259$. (Software tool in *CAS Mathematica*)

Then, for example, typical antenna diagram using

$$F(\theta) = \frac{1}{a}\left|1 - e^{\frac{-k(b\cos\theta+c)^a}{(1-k_1(b\cos\theta+c))^a}}\right|$$

for $a = 7$, $k = 80$, $k_1 = 0.001$, $b = 0.72$, $c = 0.1259$ is plotted on Fig. 9. The question of the optimality of $Q_i(t;k;k_1)$ in the light of Tadmor and Tanner approach [20]–[22] can be considered open.

5. A new class of "adaptive functions" with "polynomial variable transfer". Consider the following modified Kies model for $a = 1$:

$$F_1(t) := 1 - e^{-\frac{k(t)t}{1-k_1(t)t}} \tag{17}$$

where

$$k(t) = \sum_{i=0}^{n} a_i t^i; \quad k_1(t) = \sum_{i=0}^{n} b_i t^i.$$

The simulation for fixed $a_0 = 0, a_1 = 0.3, a_2 = -0.6, a_3 = 0.6$ and $b_0 = 0, b_1 = 0.1, b_2 = 0.01, b_3 = -0.001$ is visualized on Fig. 10.

For the corresponding emitting chart $|F_1(\theta)|$, $t = b\cos\theta + c$ and fixed $n = 3$, $a_0 = 0.05, a_1 = 0.1, a_2 = -0.9, a_3 = 0.7$, $b_0 = 0.01, b_1 = 0.055, b_2 = 0.1, b_3 = -0.001$, $b = 0.68$, $c = 0.97$ see Fig. 11. We will explicitly note that in this new formulation the model (17) has many degrees of freedom (the coefficients of the polynomials $k(t)$

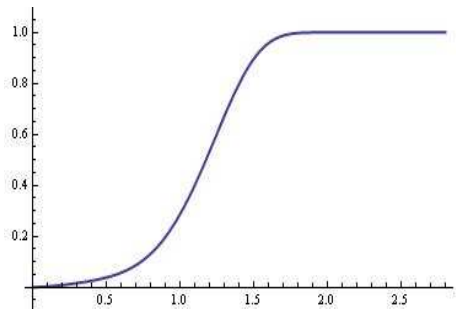

Figure 10: Simulation with the model (17).

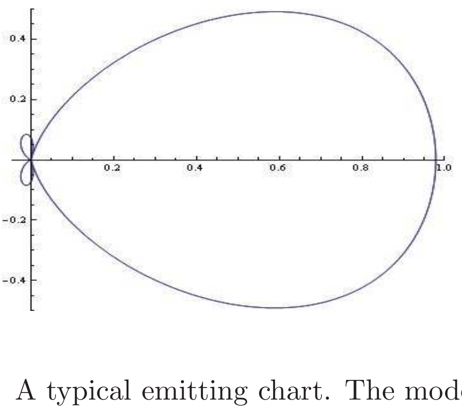

Figure 11: A typical emitting chart. The model $|F_1(\theta)|$.

and $k_1(t)$), and this makes it attractive in the study and simulation of some dynamical models.

3. APPENDIX: DISTRIBUTIONAL PROPERTIES OF THE THREE-PARAMETER KIES DISTRIBUTION

We present below some distributional properties of the three-parameter Kies distribution following [4] and taking in attention the corrections made in [26].

Proposition 1. *The probability density function, the rate (hazard) function, and the quantile function of the three-parameter Kies distribution are given by*

$$\begin{aligned} f(t) &= ak \exp\left\{-k\left(\frac{t}{1-k_1 t}\right)^a\right\} \frac{t^{a-1}}{(1-k_1 t)^{a+1}} I_{t\in\left[0,\frac{1}{k_1}\right)} \\ h(t) &= ak \frac{t^{a-1}}{(1-k_1 t)^{a+1}} I_{t\in\left[0,\frac{1}{k_1}\right)} \\ q(p) &= \frac{d(p)}{k_1(1+d(p))}. \end{aligned} \tag{18}$$

We denote above by $I_{(\cdot)}$ the indicator function and by $d(\cdot)$

$$d(p) = k_1\left[\frac{1}{k}\ln\left(\frac{1}{1-p}\right)\right]^{\frac{1}{a}} \tag{19}$$

for $p \in (0,1)$.

The moments and the mean residual life function are presented in the following proposition.

Proposition 2. *The n-th moment of a Kies distributed random variable ξ is*

$$\mu_n \equiv E[\xi^n] = \frac{1}{k_1^n}\sum_{i=0}^{n}\left\{\binom{n}{i}\sum_{j=0}^{\infty}\frac{(-1)^{i+j}(i)_j}{j!}\left[\begin{array}{c}\frac{\gamma\left(\frac{j}{a}+1,\frac{k}{k_1^a}\right)k_1^j}{k^{\frac{j}{a}}} \\ +\frac{k^{\frac{i+j}{2a}}}{k_1^{\frac{i+j}{2}}}\exp\left(-\frac{k}{2k_1^a}\right)W_{-\frac{i+j}{2a},\frac{a-i-j}{2a}}\left(\frac{k}{k_1^a}\right)\end{array}\right]\right\}. \tag{20}$$

If $t < \frac{1}{2k_1}$, then the mean residual life function is

$$m(t) = \frac{e^{\frac{k}{k_1^a}\eta(t)}}{k_1 a}\left[\begin{array}{c} \sum\limits_{j=0}^{\infty} \frac{(-1)^j (2)_j k_1^{j+1}\left[\Gamma\left(\frac{j+1}{a}\right)-\gamma\left(\frac{j+1}{a},\frac{k}{k_1^a}\eta(t)\right)-\Gamma\left(\frac{j+1}{a},\frac{k}{k_1^a}\right)\right]}{j! k^{\frac{j+1}{a}}} \\ +e^{-\frac{k}{2k_1^a}} \sum\limits_{j=0}^{\infty} k^{\frac{j+1-a}{2a}} k_1^{-\frac{j+1-a}{2}} \Delta_j\left(\frac{k}{k_1^a}\right) \end{array}\right]. \quad (21)$$

Otherwise, if $t > \frac{1}{2k_1}$, *then*

$$m(t) = \frac{1}{k_1 a} e^{\frac{k\eta(t)}{2k_1^a}} \sum_{j=0}^{\infty} k^{\frac{j+1-a}{2a}} k_1^{-\frac{j+1-a}{2}} (\eta(t))^{-\frac{j+1+a}{2a}} \Delta_j\left(\frac{k}{k_1^a}\eta(t)\right). \quad (22)$$

The functions $\eta(t)$ *and* $\Delta_j(x)$ *above are defined as*

$$\begin{aligned} \eta(t) &= k_1^a\left(\frac{t}{1-k_1 t}\right)^a \\ \Delta_j(t) &= \frac{(-1)^j (2)_j W_{-\frac{j+1+a}{2a},-\frac{j+1}{2a}}(t)}{j!}. \end{aligned} \quad (23)$$

We can recover the moment generating function from formula (20):

Proposition 3. *The moment generating function of a Kies distributed random variable is*

$$\psi(t) = \sum_{0}^{\infty} \frac{\mu_n}{n!} t^n, \quad (24)$$

where μ_n *is given in* (20).

We present below the tail behavior of the Kies distribution in the terms of risk management – VaR (value at risk), AVaR (averaged value at risk, also known as CVaR or expected shortfall), and expectiles. In fact the VaR is the opposite of the quantile function for the left tail and it is just the quantile for the right tail. The AVaR, as its name shows, is the averaged of the VaR. For convenience we shall consider integration over the quantile function. In such a way left and right related to the $AVaR$ terms are defined as

$$\begin{aligned} Q^-(\epsilon) &= \frac{1}{\epsilon}\int_0^{\epsilon} q(t)\,dt \\ Q^+(\epsilon) &= \frac{1}{1-\epsilon}\int_{\epsilon}^{1} q(t)\,dt. \end{aligned} \quad (25)$$

Proposition 4. *Let $\epsilon \in (0,1)$. Then the terms Q^- and Q^+ at level ϵ are*

$$\begin{aligned} Q^-(\epsilon) &= \frac{\mu_1}{\epsilon} - \frac{1-\epsilon}{\epsilon}\left[q(\epsilon) + m(q(\epsilon))\right] \\ Q^+(\epsilon) &= q(\epsilon) + m(q(\epsilon)), \end{aligned} \tag{26}$$

where the functions $q(\cdot)$ and $m(\cdot)$ are given in equations (1), (21), and (22). The ϵ-expectile, $\epsilon < \frac{1}{2}$, is the solution of the following equation

$$(1-2\epsilon)\, m(y)\, \overline{F}(y) + (1-\epsilon)(y-\mu_1) = 0, \tag{27}$$

where the functions $m(\cdot)$ is as above, $\overline{F}(t) = 1 - F(t)$ is the complementary cumulative distribution function (also known as survival function), and μ_1 is the first moment given in equation (20).

Proof. Let us denote $x^- := \max(-x, 0)$ and $x^+ := \max(x, 0)$. We shall use the following statement

$$E\left[(\xi - y)^+\right] = m(y)\, \overline{F}(y)$$

– for more details see [27]. Let us consider first the term $Q^-(\cdot)$. Using the change of variables $s = q(t) \Leftrightarrow t = F(s)$ and the fact $x^- = x^+ - x$, we obtain

$$\begin{aligned} Q^-(\epsilon) &= \frac{1}{\epsilon}\int_0^{\epsilon} q(t)\, dt = \frac{1}{\epsilon}\int_0^{q(\epsilon)} s f(s)\, ds = \frac{E\left[\xi I_{\xi < q(\epsilon)}\right]}{\epsilon} \\ &= \frac{q(\epsilon)\, P(\xi < q(\epsilon))}{\epsilon} - \frac{E\left[(\xi - q(\epsilon))^-\right]}{\epsilon} \\ &= q(\epsilon) - \frac{E\left[(\xi - q(\epsilon))^+\right]}{\epsilon} + \frac{E\left[\xi - q(\epsilon)\right]}{\epsilon} \end{aligned} \tag{28}$$

$$= \frac{\mu_1}{\epsilon} - \frac{1-\epsilon}{\epsilon}\left[q(\epsilon) + m(q(\epsilon))\right].$$

Using [24] we derive for $Q^+(\epsilon)$

$$\begin{aligned} Q^+(\epsilon) &= q(\epsilon) + \frac{E\left[(\xi - q(\epsilon))^+\right]}{1-\epsilon} \\ &= q(\epsilon) + \frac{m(q(\epsilon))\, \overline{F}(q(\epsilon))}{1-\epsilon} \\ &= q(\epsilon) + m(q(\epsilon)). \end{aligned} \tag{29}$$

Formula (27) follows from equation (2) from [25] and from the mentioned above relation $x^- = x^+ - x$.

This completes the proof of the proposition.

Following Section 3 of [4] we may establish the following scheme for fitting the three-parameter Kies distribution. Let we have n-observation – t_1, t_2,...,t_n. Then the log-maximum likelihood function is

$$l\left(a,k,k_1\right) = n\ln\left(ak\right) - k\sum_{i=1}^{n}\left(\frac{t_i}{1-k_1t_i}\right)^a + (a-1)\sum_{i=1}^{n}\ln t_i - (a+1)\sum_{i=1}^{n}\ln\left(1-k_1t_i\right). \tag{30}$$

The derivatives w.r.t. a, k, and k_1 lead to the following system

$$\begin{aligned} &\frac{n}{a} + \sum_{i=1}^{n}\ln\frac{t_i}{1-k_1t_i}\left(1-k\left(\frac{t_i}{1-k_1t_i}\right)^a\right) = 0 \\ &\frac{n}{k} - \sum_{i=1}^{n}\left(\frac{t_i}{1-k_1t_i}\right)^a = 0 \\ &\sum_{i=1}^{n}\frac{t_i}{1-k_1t_i}\left(a+1-ka\left(\frac{t_i}{1-k_1t_i}\right)^a\right) = 0. \end{aligned} \tag{31}$$

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