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A Note on the Log-Alpha-Skew-Normal Model with Geochemical Applications.

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Abstract: In this paper we introduce an extension of the log-normal distribution, based on the alpha-skew-normal distribution introduced by Elal-Olivero [10]. Basic properties, moments, moment estimators, maximum likelihood estimators and a simulation study are discussed. We apply the approach developed in this paper to data sets related to neodymium and nickel concentrations in soil samples. Model fit indicates good performance of the proposed model when compared with less flexible models.

Keywords: Alpha-skew-normal distribution, Bimodality, Log-normal distribution

1 Introduction

Vistelius [27] showed that chemical element concentrations in soil samples follow an asymmetric distribution. Ahrens [1,2,3] studied chemical element concentrations using many data sets and concluded that a large part of the data sets present positive asymmetry. For most of these cases, however, a logarithm transformation reduced asymmetry leading to the formulation of the fundamental law of biochemistry: “*the concentration of a chemical element in soil samples follows a log-normal distribution*”.

Quantification of soil sources provides fundamental information for studies of weathering rates, groundwater geochemistry, and cation/nutrient cycling in ecosystems, see Miller et al. [20]. The variable solubility and mobility of cations in the soil environment, however, has made constraining the components from which soils and paleosoils are derived problematic. Apart from their occurrence in primary minerals, we know rather little about the specification, concentrations in soil solution, and solubility relations to acid-base conditions of soils for most of them. Knowledge of soil solution concentrations and the solubility of elements, in relation to soil acidity or acidity-neutralizing measures, is of great importance in studying their biochemical cycles and availability to plants. Neodymium (Nd) is present in rock, weathered rock (arene) and saprolite, sediment and soil, shallow and deep groundwater, and surface waters. Neodymium isotopes fluctuate least between bedrock and weathering products. Weathering is the breakdown and alteration of rocks and minerals at or near the Earth’s surface into products that tend towards equilibrium with the conditions found in this environment [21]. In rivers draining igneous and metamorphic terrains, preferential dissolution of silicate minerals (plagioclase, pyroxene, amphibole and garnet) may be more important and may induce a weak shift in the Nd isotopic composition. However, the Nd isotopic composition generally appears to be a good indicator of the weathered parent rock, [16, 22]. Nickel (Ni) is present in all soils, derived from parent material (lithosphere), anthropogenic deposition, or both [15]. The concentration of Ni in most cultivated soils seldom exceeds 50 mg/kg [19], but in areas in which mafic and ultramafic bedrock is present, it can rise to more than 10,000 mg/kg, [7]. Ultramafic rocks such as peridotite, dunite, and pyroxenite have the highest Ni content, followed by mafic (gabbro and basalt) and intermediate rocks, [18]. On the other hand, environmental geochemical baselines are needed in order to assess the present state of the surface environment and provide guidelines and quality standards for

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environmental legislation and political decision-making, especially in the assessment of contaminated soils, [12].

Given that support for the skew-normal distribution is the real line, it is important to modify it to deal with geochemical data as in Mateu-Figueras et al. [17] where the log-skew-normal distribution is used. This distribution is also used by Azzalini et al. [6], for family income data.

Azzalini [5] introduces the $\{SN(\lambda), \lambda \in \mathbb{R}\}$ skew-normal distribution, with asymmetry parameter λ, where $SN(0)$ is the standard normal distribution. We denote $X \sim SN(\mu,\sigma,\lambda)$ with probability density function (pdf) given by

$$f(x|\theta) = \frac{2}{\sigma}\phi(y)\,\Phi(\lambda y), \qquad x,\lambda \in \mathbb{R} \tag{1}$$

where $\theta = (\mu,\sigma,\lambda)$, $y = \frac{x-\mu}{\sigma}$, μ is a location parameter, σ a scale parameter, ϕ and Φ is the pdf $N(0,1)$ and its cumulative distribution function (cdf). Some properties of this distribution are:

$$E(X) = \mu + \sqrt{\frac{2}{\pi}}\frac{\sigma\lambda}{\sqrt{1+\lambda^2}},$$
$$Var(X) = \sigma^2\left[1 - \frac{2\lambda^2}{\pi(1+\lambda^2)}\right]. \tag{2}$$

Elal-Olivero [10] introduced the $\{ASN(\alpha), \alpha \in \mathbb{R}\}$ the alpha-skew-normal distribution, with shape parameter α, so that $ASN(0)$ corresponds to the standard normal distribution. That is, $X \sim ASN(\mu,\sigma,\alpha)$ and its pdf is given by

$$f(x|\theta) = \left(\frac{(1-\alpha y)^2+1}{\sigma(2+\alpha^2)}\right)\phi(y), \qquad x,\alpha \in \mathbb{R} \tag{3}$$

where $y = \frac{x-\mu}{\sigma}$, $\theta = (\mu,\sigma,\alpha)$, μ is a location parameter, σ a scale parameter and $\phi(\cdot)$ denotes the pdf of the $N(0,1)$. Some properties for this distribution are

$$E(X) = \mu - \frac{2\alpha\sigma}{2+\alpha^2},$$
$$M_X(t) = \left[1 - \alpha\sigma t\left(\frac{2-\alpha\sigma t}{2+\alpha^2}\right)\right]\exp\left(\mu t + \frac{\sigma^2 t^2}{2}\right). \tag{4}$$

More recently, Bolfarine et al. [8] proposed a bimodal version for the log-skew-normal distribution version of the bimodal distribution introduced in Elal-Olivero et al. [11]. Therefore, we can say that the random variable X follows the log-bimodal-skew-normal distribution (LBSN) if its density function is given by

$$f(x|\theta) = \frac{2}{\sigma x}\left(\frac{1+\alpha y^2}{1+\alpha}\right)\phi(y)\Phi(\lambda y), \tag{5}$$

where $x > 0, \mu \in \mathbb{R}, \sigma > 0, \lambda \in \mathbb{R}, \alpha > 0,$ with parameter vector $\theta = (\mu,\sigma,\lambda,\alpha)$ and $y = \frac{\log(x)-\mu}{\sigma}$. We denote $X \sim LBSN(\mu,\sigma,\lambda,\alpha)$.

This paper focuses on introducing the log-alpha-skew-normal distribution so that the log-normal model is a special case and hence the model can be used for modeling chemical data. This model is flexible in the sense that for some values of α it is suitable for fitting bimodal data, similar to the model studied by Bolfarine et al. [8].

The paper is organized as follows. In Section 2 we introduce the log-alpha-skew-normal distribution, its basic properties, moments, log-likelihood function and Fisher information matrix. In Section 3 we conduct a simulation study. Section 4 illustrates application to real data sets related to concentrations of nickel and neodymium in soil samples from the Mining Department of Universidad de Atacama in Chile.

2 The log-alpha-skew-normal distribution

In this section we define the new distribution by presenting its pdf and study some of its properties and moments.

2.1 Density and properties

Definition 2.1. If the density of the random variable X has pdf given by

$$f(x|\theta) = \left(\frac{(1-\alpha y)^2+1}{(2+\alpha^2)\sigma x}\right)\phi(y), \qquad x > 0,\ \alpha \in \mathbb{R} \tag{6}$$

where $y = \frac{\log(x)-\mu}{\sigma}$, then we say that X is distributed according to the log-alpha-skew-normal distribution (LASN) with parameter $\theta = (\mu,\sigma,\alpha)$. We denote $X \sim LASN(\mu,\sigma,\alpha)$.

That (6) is a density can be verified by direct integration. Using the notation previously established, we have the following properties:

1. $f(x|\mu,\sigma,\alpha=0) = \frac{1}{\sigma x}\phi\left(\frac{\log(x)-\mu}{\sigma}\right), \quad x > 0.$
2. $\lim_{\alpha\to\infty} f(x|\mu,\sigma,\alpha) = \frac{y^2}{\sigma x}\phi(y), \quad x > 0.$

Remark 2.1. Property 1 establishes that the new distribution contain to the log-normal distribution as $\alpha = 0$. The second result indicates that as $\alpha \to \infty$ the new distribution converges to a log-gamma-type distribution.

Figure 1 depicts graphs of the new density for some parameter combinations. Notice its bimodal nature for some values of α.

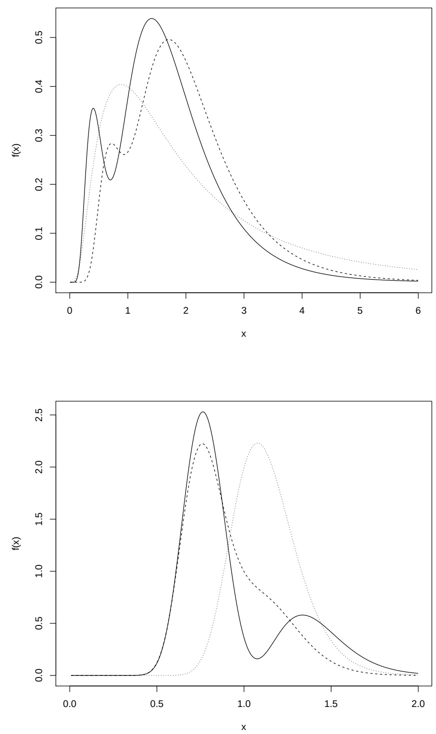

Fig. 1: Top panel: LASN(0,0.5,-1.5) (solid line), LBSN(0,0.5,1,2) (dashed line) and LSN(0,1,1) (dotted line). Panel below: LASN(0,0.2,3) (solid line), LBSN(0,0.2,-0.5,1) (dashed line) and LSN(0,0.2,1) (dotted line)

2.2 Moments

In this section we present moments and moment estimators for the LASN distribution. We make use of the moment generating function presented in (4). That is, if $X \sim LASN(\mu,\sigma,\alpha)$ and $Y \sim ASN(\mu,\sigma,\alpha)$ then it can be verified that

$$\begin{aligned} E(X^r) &= E(\exp(rY)) = M_Y(r) \\ &= \left[1-\alpha\sigma r\left(\frac{2-\alpha\sigma r}{2+\alpha^2}\right)\right]\exp\left(\mu r+\frac{\sigma^2 r^2}{2}\right), \end{aligned}$$

where $r = 1,2,3,\ldots$.

Using this result, it can be verified that

1. $E(X) = \left[1-\alpha\sigma\left(\frac{2-\alpha\sigma}{2+\alpha^2}\right)\right]\exp\left(\mu+\frac{\sigma^2}{2}\right)$;
2. $E(X^2) = \left[1-4\alpha\sigma\left(\frac{1-\alpha\sigma}{2+\alpha^2}\right)\right]\exp\left(2(\mu+\sigma^2)\right)$,

from where $Var(X)$ can be computed. Note that the expressions for the moment estimators are relatively simple, because the method needs to solve the following equations for μ, σ and α

$$\left[1-\alpha\sigma r\left(\frac{2-\alpha\sigma r}{2+\alpha^2}\right)\right]\exp\left(\mu r+\frac{\sigma^2 r^2}{2}\right) = m_r,$$

where $m_r = n^{-1}\sum_{i=1}^n x_i^r$, $r = 1,2,3$. Those equations can be solved using numerical procedures, for instance, using the *nleqslv* package [13] available in the R software [23]. This us allow to obtain the moment estimators $(\widehat{\mu}_M, \widehat{\sigma}_M, \widehat{\alpha}_M)$ of the vector (μ,σ,α).

2.3 Likelihood function

Let $X_1,\ldots,X_n$ be a random sample from the distribution of the random variable $X \sim LASN(\mu,\sigma,\alpha)$, so that the log-likelihood function for θ and $y_i = \frac{\log(x_i)-\mu}{\sigma}$ is given by

$$\begin{aligned} l(\theta) &= -\frac{n}{2}\log(2\pi) - n\log(\sigma) - n\log(2+\alpha^2) - \frac{1}{2}\sum_{i=1}^n y_i^2 \\ &\quad - \sum_{i=1}^n \log(x_i) + \sum_{i=1}^n \log((1-\alpha y_i)^2+1). \end{aligned} \tag{7}$$

Differentiating (7) above with respect to the model parameters, we arrive at the following likelihood equations:

$$\frac{\partial l}{\partial \mu} = 2\alpha\sum_{i=1}^n \frac{1-\alpha y_i}{(1-\alpha y_i)^2+1} + \sum_{i=1}^n y_i = 0 \tag{8}$$

$$\frac{\partial l}{\partial \sigma} = \sum_{i=1}^n y_i^2 + 2\alpha\sum_{i=1}^n \frac{(1-\alpha y_i)y_i}{(1-\alpha y_i)^2+1} - n = 0 \tag{9}$$

$$\frac{\partial l}{\partial \alpha} = \frac{n\alpha}{2+\alpha^2} + \sum_{i=1}^n \frac{(1-\alpha y_i)y_i}{(1-\alpha y_i)^2+1} = 0. \tag{10}$$

The maximum likelihood estimator for $\theta = (\mu,\sigma,\alpha)$ is obtained by solving the system of equations $(8)-(10)$, which has to be done numerically. The derivation of the observed information matrix is also obtained using numerical procedures. Initial values for those procedures can be obtained although the moment estimators.

2.4 Fisher information matrix

The log-likelihood function for θ=(μ,σ,α) and $y = \frac{\log(x)-\mu}{\sigma}$ based on a single observation X, is given by

$$\begin{aligned} l(\theta) &= -\frac{1}{2}\log(2\pi) - \log(\sigma) - \log(2+\alpha^2) - \frac{1}{2}y^2 \\ &\quad - \log(x) + \log((1-\alpha y)^2+1). \end{aligned} \tag{11}$$

2.4.1 Score function:

$$\begin{aligned} \frac{\partial l(\theta;x)}{\partial \mu} &= \frac{2\alpha(1-\alpha y)}{\sigma[(1-\alpha y)^2+1]} + \frac{y}{\sigma}, \\ \frac{\partial l(\theta;x)}{\partial \sigma} &= \frac{2\alpha y(1-\alpha y)}{\sigma[(1-\alpha y)^2+1]} - \frac{1}{\sigma} + \frac{y^2}{\sigma}, \\ \frac{\partial l(\theta;x)}{\partial \alpha} &= \frac{-2y(1-\alpha y)}{(1-\alpha y)^2+1} - \frac{2\alpha}{2+\alpha}. \end{aligned}$$

The second derivatives of $l(\theta;x)=l(\theta)$ are:

$$\frac{\partial^2 l(\theta)}{\partial\mu^2}=\frac{2\alpha^2}{\sigma^2[(1-\alpha y)^2+1]}-\frac{4\alpha^2(1-\alpha y)^2}{\sigma^2[(1-\alpha y)^2+1]^2}-\frac{1}{\sigma^2},$$

$$\frac{\partial^2 l(\theta)}{\partial\mu\partial\sigma}=\frac{(4\alpha^2 y-2\alpha)[(1-\alpha y)^2+1]-4\alpha^2 y(1-\alpha y)^2}{\sigma^2[(1-\alpha y)^2+1]^2}-\frac{2y}{\sigma^2},$$

$$\frac{\partial^2 l(\theta)}{\partial\mu\partial\alpha}=\frac{2-4\alpha y}{\sigma[(1-\alpha y)^2+1]}+\frac{4\alpha y(1-\alpha y)^2}{\sigma[(1-\alpha y)^2+1]^2},$$

$$\frac{\partial^2 l(\theta)}{\partial\sigma^2}=\frac{(6\alpha^2 y^2-4\alpha y)[(1-\alpha y)^2+1]-4\alpha^2 y^2(1-\alpha y)^2}{\sigma^2[(1-\alpha y)^2+1]^2}+\frac{1}{\sigma^2}-\frac{3y^2}{\sigma^2},$$

$$\frac{\partial^2 l(\theta)}{\partial\sigma\partial\alpha}=\frac{(2y-4\alpha y^2)[(1-\alpha y)^2+1]+4\alpha y^2(1-\alpha y)^2}{\sigma[(1-\alpha y)^2+1]^2},$$

$$\frac{\partial^2 l(\theta)}{\partial\alpha^2}=\frac{2y^2[(1-\alpha y)^2+1]-4y^2(1-\alpha y)^2}{[(1-\alpha y)^2+1]^2}-\frac{4-2\alpha^2}{(2+\alpha^2)^2}.$$

After extensive algebraic manipulations, it follows that the Fisher information matrix is given by

$$I(\theta)=\begin{pmatrix}\frac{4\alpha^2 b_0-\alpha^2+2}{\sigma^2(2+\alpha^2)} & \frac{4\alpha^2 b_1-2\alpha}{\sigma^2(2+\alpha^2)} & -\frac{4\alpha b_1+2}{\sigma(2+\alpha^2)}\\ \frac{4\alpha^2 b_1-2\alpha}{\sigma^2(2+\alpha^2)} & \frac{4\alpha^2 b_2+2\alpha^2+4}{\sigma^2(2+\alpha^2)} & \frac{4\alpha(1-b_2)}{\sigma(2+\alpha^2)}\\ -\frac{4\alpha b_1+2}{\sigma(2+\alpha^2)} & \frac{4\alpha(1-b_2)}{\sigma(2+\alpha^2)} & \frac{4b_2(\alpha^2+2)-4\alpha^2}{(2+\alpha^2)^2}\end{pmatrix},$$

where $Z\sim N(0,1)$ and $b_k=E\left[Z^k\frac{(1-\alpha Z)^2}{(1-\alpha Z)^2+1}\right]$, $k=0,1,2,$ which has to be evaluated numerically.

On the other hand, where $\alpha=0$, the Fisher information matrix is

$$I(\theta)=\begin{pmatrix}\frac{1}{\sigma^2} & 0 & -\frac{1}{\sigma}\\ 0 & \frac{2}{\sigma^2} & 0\\ -\frac{1}{\sigma} & 0 & 1\end{pmatrix},$$

which is singular. Using the methodology introduced by Rotnitzky et al. [24], with a suitable reparametrization, as used by Chiogna [9], Salinas et al. [25], Elal-Olivero [10], among others, a non-singular matrix is obtained.

3 Simulation study

In order to verify the performance of the procedure estimation, we present a brief simulation study. We fix the location and scale parameters at the standard values, i.e., $\mu=0$ and $\sigma=1$. The values for α were chosen in the set $\{-1.5,-0.5,0.1,1\}$, i.e., two values that provide two modes in the distribution and two values that produce an unimodal distribution. The sample sizes vary in the set $\{50,100,200\}$. For values drawn from the model, we can use the algorithm presented by Elal-Olivero [10] in his Proposition 3.5 and apply the exponential transformation.

We then apply the maximum likelihood estimators and estimate the standard errors using the Hessian matrix. We present the average bias (AB) and the mean of the standard errors (SE). Results are presented in Table 1. Note that the bias is acceptable for all cases, considering that the sample sizes are relatively small. However, the bias for all parameters appears greater for the cases where $|\alpha|$ is not close to zero. On the other hand, the mean of the standard errors also decreases when n increases, suggesting good performance of the estimators in finite samples.

Table 1: Simulation study for the LASN model. AB and SE denote the average bias and the average of the estimated standard errors respectively.

true α	parameter	$n=50$ AB (SE)	$n=100$ AB (SE)	$n=200$ AB (SE)
-1.5	μ	0.050 (0.167)	0.034 (0.117)	0.016 (0.083)
	σ	-0.087 (0.082)	-0.057 (0.062)	-0.033 (0.046)
	α	-0.268 (0.501)	-0.132 (0.310)	-0.080 (0.210)
-0.5	μ	0.076 (1.475)	0.040 (0.845)	0.040 (0.694)
	σ	-0.110 (0.097)	-0.074 (0.073)	-0.048 (0.053)
	α	-0.155 (1.741)	-0.099 (0.941)	-0.064 (0.721)
0.1	μ	-0.096 (5.305)	-0.067 (3.416)	-0.038 (2.716)
	σ	-0.057 (0.096)	-0.042 (0.069)	-0.023 (0.050)
	α	-0.052 (5.458)	-0.034 (3.596)	-0.018 (2.811)
1.0	μ	-0.417 (3.082)	-0.301 (1.604)	-0.224 (0.802)
	σ	-0.077 (0.094)	-0.057 (0.072)	-0.035 (0.054)
	α	-0.259 (3.514)	-0.217 (1.856)	-0.210 (0.925)

4 Illustrations with real data sets

To illustrate the applicability of the proposed model, we provide two real data sets. They related to neodymium and nickel concentrations in soil samples obtained from the Mining Department of Universidad de Atacama, Chile. To compare the fit of the various models, Akaike information criterion (AIC) [4], the consistent version of the AIC criterion (CAIC) [14] and the Bayesian information criterion (BIC) [26] are used.

In Illustration 1 the LASN, LBSN and LSN models are fitted to the neodymium concentration data set. In Illustration 2, we fit the same models to the nickel concentration data set studied in Bolfarine et al. [8]. Figures 2 and 3 depict the model fits for the three models with the neodymium data set (Illustration 1) and nickel data set (Illustration 2) respectively.

4.1 Illustration 1. Neodymium concentration

Table 2 presents basic descriptive statistics for the data set. We use the notation $\sqrt{b_1}$ and b_2 to represent sample asymmetry and kurtosis coefficients. Additionally, the moment estimators for this data set are $\widehat{\mu}_M=3.69$, $\widehat{\sigma}_M=0.577$ and $\widehat{\alpha}_M=1.216$. These values can be used as

Table 2: Descriptive statistics for the Neodymium

Data set	n	$\overline{X}$	S^2	$\sqrt{b_1}$	b_2
Nd	86	35.020	1171.741	3.648	18.216

initial values to initialize the maximization procedure of the log-likelihood function for the LASN model.

Table 3: Parameter estimates of the LSN, LBSN and LASN models.

Parameter estimates	LSN	LBSN	LASN
μ	2.826(0.222)	2.258(0.144)	3.749(0.107)
σ	0.835(0.140)	0.777(0.076)	0.645(0.051)
λ	0.989(0.598)	1.543(0.381)	-
α	-	3.607(2.241)	0.986(0.273)
AIC	752.663	750.254	748.757
CAIC	752.956	750.747	749.050
BIC	760.026	760.071	756.120

Table 3 depicts maximum likelihood estimates for parameters in the LSN, LBSN and LASN models; to compare the models, AIC, CAIC and BIC criteria are used. These criteria suggest that the LASN model fits the data better than the other models. Moreover, estimated standard deviations for the LASN model are smaller than for the other models, leading to shorter confidence intervals.

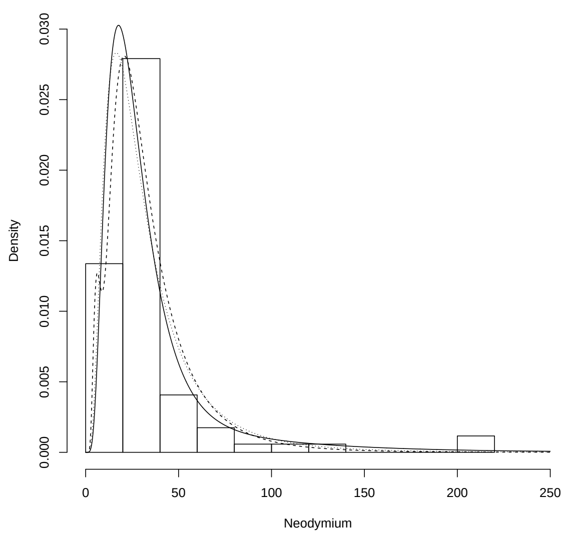

Fig. 2: Fitting of the LASN (solid line), LBSN (dashed line) and LSN (dotted line)

4.2 Illustration 2. Nickel concentration

We consider now the nickel data set using the same models as in the previous illustration. Table 4 presents basic descriptive statistics for the data set. For this data set, the moment estimators are $\widehat{\mu}_M = 2.279$, $\widehat{\sigma}_M = 0.704$ and $\widehat{\alpha}_M = -1.221$.

Table 4: Descriptive statistics for the Nickel

Data set	n	$\overline{X}$	S^2	$\sqrt{b_1}$	b_2
Ni	86	21.337	276.861	2.440	12.043

Table 5: Parameter estimates of the LSN, LBSN and LASN models.

Parameter estimates	LSN	LBSN	LASN
μ	3.486(0.155)	1.785(0.164)	2.372(0.092)
σ	0.980(0.128)	0.779(0.077)	0.633(0.050)
λ	-1.596(0.588)	1.254(0.297)	-
α	-	4.957(3.467)	-1.201(0.268)
AIC	671.010	665.684	665.638
CAIC	671.306	666.184	665.935
BIC	678.338	675.455	672.966

Table 5 presents the maximum likelihood estimates for the data set under study for the LSN, LBSN and LASN models. The AIC, CAIC and BIC indicate that the LBSN and LASN models fit the data set quite similarly. However, under the principle of parsimony the LASN is preferred over the LBSN model.

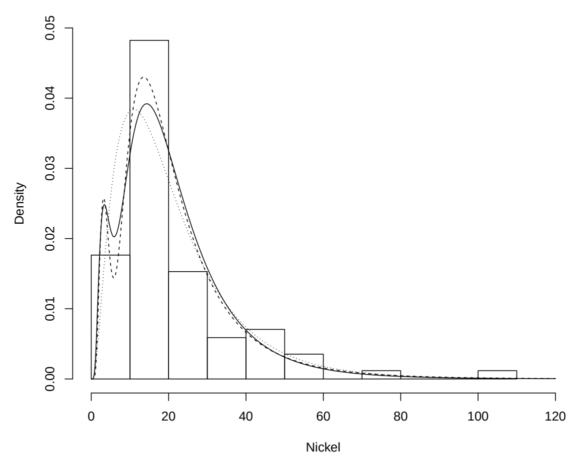

Fig. 3: Fitting of the LASN (solid line), LBSN (dashed line) and LSN (dotted line)

4.3 Final conclusions

This paper presents a new model that has a smaller number of parameters, the log-alpha-skew-normal model which, as shown, presents good fit in dealing with chemical data. Properties such as moments and maximum likelihood estimation are discussed. Special cases of the model are the log-normal and a gamma type model. It also makes Ahrens' law more flexible.

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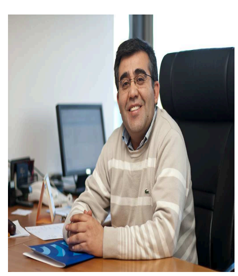

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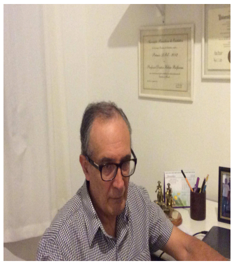

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