



Generalized Laguerre expansions of multivariate probability densities with moments

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ABSTRACT

We generalize the well-known Laguerre series approach to approximate multivariate probability density functions (PDFs) using multidimensional Laguerre polynomials. The generalized Laguerre series, which is defined around a Gamma PDF, is suited for simulating high complex natural phenomena that deviate from Gaussianity. Combining the multivariate Laguerre approximation and Bayes theorem, an approximation to the conditional PDFs is derived. Numerical results first showed the superiority of the Gamma expansion over other numerical methods. The ability of the Gamma expansion to fit mixtures of Gaussian and super Gaussian PDFs, univariate and multivariate Lognormal PDFs, and complex geologic media is shown through different examples.

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1. Introduction

Numerical techniques to approximate multivariate PDFs are of interest for a definitive aspect of most spatially distributed and varying natural phenomena encountered in geo-science and engineering problems which are non-Gaussian and exhibit non-linear and complex patterns. Determining a probability distribution given its moments is a well-known problem, the so-called moments-problem (MP), [1–5]. Efficient techniques for solving MP are useful, since it is relatively easy in many statistical situations to determine moments, but it is extremely hard or impossible to determine the distributions themselves [1,6,7,5]. The objective of this work is to illustrate a numerical technique which is (1) suitable for treating MP for multivariate cases, (2) efficient, and (3) applicable for further research work on real-life problems.

Consider a continuous PDF $P(\mathbf{z})$ which is defined in $D^N \in [0, \infty[^N$, where N denotes the dimension of the problem. The Edgeworth expansion [8,9] is widely used, in the literature, to approximate $P(\mathbf{z})$ around a Gaussian PDF using a combination of Hermite polynomials, with coefficients defined in terms of cumulants population. Kendall and Stuart [4] and others [10–14] showed that this expansion is ill-defined, and fails to reproduce the expected behavior in the tails of the distribution. Daniels [15] explored the use of the saddlepoint approximation in mathematical statistics to overcome the drawbacks of the Edgeworth approximation. Superiority of the saddlepoint to the Edgeworth for approximating Moran's I 's reference distributions and their numerical evaluations is shown in [16]. However, in some cases, the approximation fails in the tails of the distributions. In addition, it is shown that the saddlepoint performs well for a large sample size; however, it is still not available in tails areas when the autoregressive coefficient is large [17]. Using the first three cumulants (c_1 , c_2 and c_3), Easton and Ronchetti [18] and Renshaw [19] show that the saddlepoint approximation can collapse in the lower tails of a distribution due to the necessity of having $x \geq c_1 - 0.5c_2^2/c_3$. Then, for large $|c_3|$ the approximation fails for $x \leq c_1$. Different correction methods have been implemented [20–26]. However, the values of c_3 used have generally been small in comparison with the mean and variance.

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The class of Laguerre polynomials is encountered in the applications, especially in mathematical physics problems involving the integration of Helmholtz’s equation in parabolic coordinates, in the theory of hydrogen atom, in the theory of propagation of electromagnetic waves along transmission lines, etc., [3]. The Laguerre polynomials are formally analogous to the Hermite polynomials that appear in the Edgeworth series around a Gaussian distribution. The Gamma expansion is a well-defined expansion around a non-Gaussian PDF, and it can be useful for studying highly complex natural phenomena that are non-Gaussian. Hille [27–29] and Uspensky [30] have extensively studied the convergence theories of Laguerre’s series. Tiku [31] expressed the density function of the usual χ^2 and F distributions as a series of Laguerre polynomials, and subsequently used this expression to obtain a series representation for the corresponding probability integral. Bailey [32] uses the Gamma expansion to approximate the simple stochastic epidemic in a large population. In 1973, Wilson and Wragg [7] showed the superiority of the Laguerre Gamma expansion to the approximation obtained by maximizing entropy. Later on, this expansion was employed by different authors as shown in [33,34,5,35]. More recently, Gastanaga et al. [11] use this expansion to estimate the gravitational evolution of the cosmic distribution function. In addition, the authors show the superiority of the Laguerre Gamma expansion to the Charlier expansion.

This paper focuses on the approximation of multivariate densities using high-dimensional Laguerre polynomials. Various methods using multivariate Laguerre and Legendre series are available in the literature ([36–44] and others). In addition, Qjidaa [45] shows a superiority of Laguerre moments to Legendre moments for pattern recognition and image analysis problems. However, usability of all these approximations may not be feasible from a computational point of view. In this paper, we generalize the approximation used in [38,45] to the multivariate case using generalized Laguerre polynomials. Also, several details, not discussed in [45], are outlined here. The generalized numerical approach discussed ensures that both the true distribution and the approximated solution share the same moments up to the order of approximation n used. Based on the multivariate densities’ approximation analytical expressions are derived to approximate conditional densities.

The paper is organized as follows: Section 2 revises the univariate Laguerre’s series and discusses the multivariate approximation. Conditional approximation of the conditional PDFs is derived in Section 3 based on the multivariate approximation and a sample application of Bayes theorem [46]. Numerical results for both univariate and multivariate cases are presented in Section 4. The general algorithm is presented in Appendix A. Conclusions follow.

2. Approximation of multivariate PDFs

2.1. Univariate case

For the reason of completeness, approximation of univariate PDFs with additional details is first presented. The PDF P can be written formally as an infinite series of generalized Laguerre polynomials

$$P(z) \approx P_\infty^\alpha(z) = \sum_{n=0}^\infty r_n L_n^{(\alpha)}(z) \phi_{\text{GAM}}(z), \tag{1}$$

where, $\phi_{\text{GAM}}(z)$ is the Gamma PDF,

$$\begin{aligned} \phi_{\text{GAM}}(z) &= \frac{\beta}{\Gamma(\alpha + 1)} z^\alpha \exp(-z), \\ z = \beta x \geq 0, \quad x \in \Omega \quad \text{and} \quad \alpha \geq -1 \end{aligned} \tag{2}$$

the subscript in P_∞^α denotes the number of elements kept in the expansion, and $L_n^{(\alpha)}(z)$ are the generalized Laguerre polynomials given, using $L_n^{(\alpha)}(z)$, using Rodrigues’ formula, by

$$L_n^{(\alpha)}(z) \phi_{\text{GAM}}(z) = \frac{1}{n!} \left(-\frac{d}{dz} \right)^n [z^n \phi_{\text{GAM}}(z)]. \tag{3}$$

Using the Leibniz’s theorem for differentiation of a product, the generalized Laguerre polynomials [47] can, equivalently, be written as

$$L_n^{(\alpha)}(z) = \sum_{i=0}^n \frac{(-1)^i}{i!} \binom{n + \alpha}{n - i} z^i. \tag{4}$$

The associated Laguerre polynomials are orthogonal over D with respect to the measure $d\zeta = \phi_{\text{GAM}}(z) dz$

$$\int_\Omega L_i^{(\alpha)}(z) L_j^{(\alpha)}(z) d\zeta = \frac{\Gamma(i + \alpha + 1)}{i! \Gamma(\alpha + 1)} \delta_{ij}. \tag{5}$$

On the most important aspect of the Laguerre polynomials is the fact that the PDF P can be written formally in a series of the form

$$P(z) \approx P_\infty^\alpha(z) = \sum_{n=0}^\infty r_n L_n^{(\alpha)}(z) \phi_{\text{GAM}}(z), \tag{6}$$

where, the subscript in P_n^α denotes the order of approximation. For example, the approximation of order n is given by

$$P(z) \approx P_n^\alpha(z) = \sum_{k=0}^n r_k L_k^{(\alpha)}(z) \phi_{\text{GAM}}(z). \tag{7}$$

The question of how to select parameters α , and β is not addressed in [45]. A way of calculating these parameters is by considering the following conditions

$$\int_{\Omega} P(z) L_i^{(\alpha)}(z) dz = 0, \quad \text{for } i = 1, 2. \tag{8}$$

Then, the coefficients r_1 and r_2 are identically zero, and $\alpha = (2m_1^2 - m_2)/(m_2 - m_1^2)$, and $\beta = m_1/(m_2 - m_1^2)$. For more details, see Appendix B. The coefficients r_n can be calculated by multiplying the right- and the left-hand side of Eq. (1) by $L_m^{(\alpha)}(z)$ and integrating over Ω , that is

$$r_n = \frac{n! \Gamma(\alpha + 1)}{\Gamma(n + \alpha + 1)} \int_{\Omega} P(z) L_n^{(\alpha)}(z) dz. \tag{9}$$

If the parameters $\alpha = 0$ and $\beta = 1$, one gets the original Laguerre polynomials $L_n(z)$ and the analysis is unchanged. Note that, using Eqs. (3) and (7), another equivalent expression to the coefficients r_n can be obtained by

$$\begin{aligned} r_n &= \frac{n! \Gamma(\alpha + 1)}{\Gamma(n + \alpha + 1)} \int_{\Omega} P(x) \left[\sum_{i=0}^n \frac{(-1)^i}{i!} \binom{n + \alpha}{n - i} \beta^i x^i \right] dx \\ &= \frac{n! \Gamma(\alpha + 1)}{\Gamma(n + \alpha + 1)} \sum_{i=0}^n \frac{(-1)^i}{i!} \binom{n + \alpha}{n - i} \beta_i \int_{\Omega} P(x) x^i dx \\ &= \frac{n! \Gamma(\alpha + 1)}{\Gamma(n + \alpha + 1)} \sum_{i=0}^n \frac{(-1)^i}{i!} \binom{n + \alpha}{n - i} \beta^i m_i, \end{aligned} \tag{10}$$

where m_i is the i th-moment of P . Obviously the first n moments of P_n^α are m_1, m_2, \dots, m_n and the integral condition $\int_D P_n^\alpha(z) dz = 1$ is also satisfied. For the convergence theories analysis, we refer to [27–30,3].

2.2. Multivariate case

Let X_1, \dots, X_N be N scalar real random values, with joint probability distribution function $P(\mathbf{z})$. Then, a generalization of Eq. (1) to the multivariate case can be written as

$$\begin{aligned} P(\mathbf{z}) \approx P_n^\alpha(\mathbf{z}) &= \sum_{n=0}^{\infty} \sum_{i_1=1}^N \dots \sum_{i_n=1}^N r_{i_1 \dots i_n} \frac{(-1)^n}{n b^m(i_1)! \dots n b^m(i_n)!} \left(\frac{d}{dz_{i_1}} \dots \frac{d}{dz_{i_n}} \right) [z_1^{i_1} \dots z_N^{i_n} \phi_{\text{GAM}}(\mathbf{z})] \\ &= \sum_{n=0}^{\infty} \sum_{i_1=1}^N \dots \sum_{i_n=1}^N r_{i_1 \dots i_n} L_{i_1 \dots i_n}^{(\alpha)}(\mathbf{z}) \phi_{\text{GAM}}(\mathbf{z}), \end{aligned} \tag{11}$$

where, $\alpha = (\alpha_1, \dots, \alpha_N)$, $n b^m(i_k)$ is the number of indices in $\{i_1, \dots, i_m\}$ equal to i_k , $\phi_{\text{GAM}}(\mathbf{z}) = \prod \phi_{\text{GAM}}(z_i)$ (where $\mathbf{z} = (z_1, \dots, z_N)^T$) is a generalization of the univariate Gamma distribution [36,38,44,45], and the high-dimensional Laguerre polynomial satisfies

$$\begin{aligned} L_{i_1 \dots i_n}^{(\alpha)}(\mathbf{z}) \phi_{\text{GAM}}(\mathbf{z}) &= \frac{(-1)^n}{n_{i_1}! \dots n_{i_n}!} \frac{d}{dz_{i_1}} \dots \frac{d}{dz_{i_n}} [z_1^{i_1} \dots z_N^{i_n} \phi_{\text{GAM}}(\mathbf{z})] \\ &= \prod_{k=1}^n L_{n b^m(i_k)}^{(\alpha_{i_k})}(z_{i_k}) \phi_{\text{GAM}}(\mathbf{z}), \quad \alpha_{i_k} \in \{\alpha_1, \dots, \alpha_N\}, \end{aligned} \tag{12}$$

and they are orthogonal with respect to the measure $d\zeta = \phi_{\text{GAM}}(\mathbf{z}) d\mathbf{z}$, that is

$$\int_{\Omega^n} L_{i_1 \dots i_n}^{(\alpha)}(\mathbf{z}) L_{j_1 \dots j_n}^{(\beta)}(\mathbf{z}) d\zeta = \frac{\Gamma(i_1 + \alpha_{i_1} + 1) \dots \Gamma(i_n + \alpha_{i_n} + 1)}{i_1! \dots i_n! \Gamma(\alpha_{i_1} + 1) \dots \Gamma(\alpha_{i_n} + 1)} \delta_{i_1 j_1} \dots \delta_{i_n j_n}. \tag{13}$$

The coefficients $r_{i_1 \dots i_n}$ are given by

$$\begin{aligned}
 r_{i_1 \dots i_n} &= a_{i_1 \dots i_n} \int_{D^n} P(\mathbf{z}) L_{i_1 \dots i_n}^{(\alpha)}(\mathbf{z}) d\mathbf{z} \\
 &= a_{i_1 \dots i_n} \int_{D^n} P(\mathbf{X}) \prod_{k=1}^n L_{nb^n(i_k)}^{(\alpha_{i_k})}(\beta X_{i_k}) d\mathbf{x} \\
 &= a_{i_1 \dots i_n} \int_{D^n} P(\mathbf{X}) \prod_{k=1}^n \left[\sum_{j_k=0}^{nb^n(i_k)} \frac{(-1)^{j_k}}{j_k!} \binom{n+\alpha}{n-j_k} \beta_{i_k}^{j_k} X_{i_k}^{j_k} \right] d\mathbf{x} \\
 &= a_{i_1 \dots i_n} \int_{D^n} P(\mathbf{X}) \left[\prod_{k=1}^n \left(\sum_{j_k=0}^{nb^n(i_k)} \frac{(-1)^{j_k}}{j_k!} \binom{n+\alpha}{n-j_k} \beta_{i_k}^{j_k} \right) \prod_{k=1}^n X_{i_k}^{j_k} \right] d\mathbf{x} \\
 &= a_{i_1 \dots i_n} \left[\prod_{k=1}^n \left(\sum_{j_k=0}^{nb^n(i_k)} \frac{(-1)^{j_k}}{j_k!} \binom{n+\alpha}{n-j_k} \beta_{i_k}^{j_k} \right) \int_{D^n} P(\mathbf{X}) \left[\prod_{k=1}^n X_{i_k}^{j_k} \right] d\mathbf{x} \right] \\
 &= a_{i_1 \dots i_n} \left[\prod_{k=1}^n \left(\sum_{j_k=0}^{nb^n(i_k)} \frac{(-1)^{j_k}}{j_k!} \binom{n+\alpha}{n-j_k} \beta_{i_k}^{j_k} \right) m_{j_1 \dots j_n} \right], \tag{14}
 \end{aligned}$$

where, $a_{i_1 \dots i_n} = \frac{i_1! \dots i_n! \Gamma(\alpha_{i_1} + 1) \dots \Gamma(\alpha_{i_n} + 1)}{\Gamma(i_1 + \alpha_{i_1} + 1) \dots \Gamma(i_n + \alpha_{i_n} + 1)}$, $m_{j_1 \dots j_n} = E(X_1^{j_1} X_2^{j_2} \dots X_n^{j_n})$ is the $(j_1 + j_2 + \dots + j_n)$ -th-moment of the multivariate PDF P and α_i and β_i are the parameters of the univariate Gamma PDF $\phi_{\text{GAM}}(z_i)$.

The general algorithm for implementing the multivariate approximation is presented in [Appendix A](#).

Corollary 1. *The multivariate Gamma distribution, $\phi_{\text{GAM}}(\mathbf{z})$, is built on an independence kernel; however, the coefficients $r_{i_1 \dots i_n}$ (Eq. (14)) of the Gamma expansion are calculated such that all the moments up to order n of the true distribution P coincide with the moments of the approximated solution P_n^α . Then, the expansion can capture dependence in the true distribution as shown in the numerical examples. We particularly have $\int_{\Omega} P_n^\alpha(\mathbf{z}) d\mathbf{z} = 1$.*

3. Approximation of conditional PDFs

This sections derives an analytical approximation to the conditional PDF of a random variable X_i . The variable X_i has a density P_{X_i} which can be computed, as the marginal of P_X , by $P(x_i) = \int_{\Omega_{n-1}} P(\mathbf{x}) d\mathbf{x}_i$, where, $d\mathbf{x}_i = dx_1 \dots dx_{i-1} dx_{i+1} \dots dx_n$. The conditional density of X_i given $\text{DEV} = \{X_1 = x_1, \dots, X_{i-1} = x_{i-1}, X_{i+1} = x_{i+1}, \dots, X_n = x_n\}$ is defined by $P(x_i/\text{DEV}) = P(\mathbf{x})/P(\mathbf{x}^i)$, where, $\mathbf{x}^i = (x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$ and the marginal density of the vector $\mathbf{X}^i = (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_n)$ is calculated by $P(\mathbf{x}^i) = \int_{\Omega} P(\mathbf{x}^i) dx_i$. Using Eq. (12), Eq. (11) can be written as

$$P(\mathbf{z}) = P_n^\alpha(\mathbf{z}) = \sum_{n=0}^{\infty} \sum_{i_1=1}^N \dots \sum_{i_n=1}^N \bar{r}_{i_1 \dots i_n} L_{nb^n(i)}^{(\alpha)}(z_i) \phi_{\text{GAM}}(z_i), \tag{15}$$

where, $\bar{r}_{i_1 \dots i_n} = r_{i_1 \dots i_n} L_{j_1 \dots j_m}^{(\alpha)}(\mathbf{z}^i) \phi_{\text{GAM}}(\mathbf{z}^i)$ and $\{j_1, \dots, j_m\}$ is a subset of $\{i_1 \dots i_n\} \setminus \{i\}$. Thus, the conditional PDF of X_i given DEV can be expressed by

$$P(z_i/\text{DEV}) \approx P_n^\alpha(z_i/\text{DEV}) = \sum_{n=0}^{\infty} \sum_{i_1=1}^N \dots \sum_{i_n=1}^N \bar{r}_{i_1 \dots i_n} L_{nb^n(i)}^{(\alpha)}(z_i) \left[\int_D P_{\mathbf{X}}(\mathbf{z}) d\mathbf{z}_i \right]^{-1} \phi_{\text{GAM}}(z_i). \tag{16}$$

The Gamma expansion provides better results than the Edgeworth series concerning the non-negativity densities as we will show later. However in some cases, the Gamma expansion (P_n^α) provides a negative PDF around the origin. To analyze this problem a simple method to fit a quadratic $P_{\text{Corr},n}^\alpha(x) = ax^2 + bx + c$ over the interval $[0, x^*]$ can be used. This method is presented by the following steps shown in [Fig. 1](#):

- Find the minimal value, x^* , of x in $]0, R]$ (i.e., $\Omega = [0, R]$ is the range of the variable X) such that: $\int_0^x P_n^\alpha(s) ds > \frac{1}{3} x P_n^\alpha(x)$. Then, $x^* = \min\{x \in]0, R] \text{ and } x^* > x_0 / \int_0^x P_n^\alpha(s) ds > \frac{1}{3} x P_n^\alpha(x) \text{ and } P_n^\alpha(x_0) = 0\}$; For example, [Fig. 1](#) shows the value x^* such that $x^* > x_0$ and the $(A - B) > \frac{1}{3} x^* q$, where A and B are respectively the areas of $ox_0^* p x_0$ and $ox_0 o$, $x^* q$ is the area of the rectangle $ox^* p q$.
- Find the coefficients a , b and c of $P_{\text{Corr},n}^\alpha(x)$ such that:
 - (a) $P_{\text{Corr},n}^\alpha$ passes through $(0, P_n^\alpha(0))$ and $(x^*, P_n^\alpha(x^*))$; In [Fig. 1](#), $(0, P_n^\alpha(0))$ and $(x^*, P_n^\alpha(x^*))$ are $(0, 0)$ and (x^*, q) , respectively.
 - (b) $\int_0^{x^*} P_{\text{Corr},n}^\alpha(s) ds = \int_0^{x^*} P_n^\alpha(s) ds$. This equation corresponds to the areas of $ox^* p$ and $(A - B)$ shown in [Fig. 1](#).

Note that the choice of x^* ensures that $P_{\text{Corr},n}^\alpha$ exists, is unique, and has a value of $b \geq 0$, that is, the fitted quadratic is non-negative as shown in the next section.

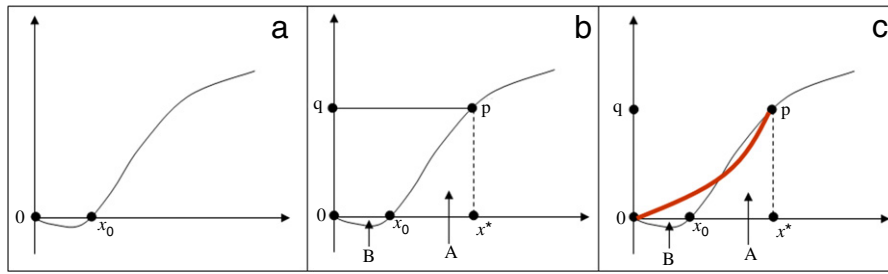


Fig. 1. Non-negativity analysis procedure.

Table 1

Relative difference between the target cumulants of Cases 1 and 2, and the cumulants obtained using the developed approach, Wang’s approach, and the Gillespie and Renshaw’s approximation based on a Poisson and Negative binomial moment structure.

	Case 1			Case 2		
	p^{W_3}	p^{GRP_3}	P_3^α	p^{W_3}	p^{GRNB_3}	P_3^α
\tilde{c}_1	1.42	0.43	0.00001	−0.106	1.17	0.00002
\tilde{c}_2	−3.63	−1.7	−0.00004	−21.08	2.66	−0.00005
\tilde{c}_3	−13.28	−2.38	−0.00007	−34.22	−9.05	−0.00008

4. Numerical results

Different numerical examples are presented in this section. Superiority of the discussed approach to other methods is first illustrated. The capability of fitting a univariate mixture of Gaussian and Laplace (super Gaussian) distributions is shown in Examples 2 and 3. Approximations to bivariate lognormal distributions and conditional distribution are presented in Example 4. Example 5 illustrates the approximation of a real complex two-dimensional image. All runs were performed on a 3.2 GHz Intel(R) Xeon (TM) PC with 2 GB of RAM.

Example 1 (Validation). In this example, we compare the technique discussed above to the corrected saddlepoint approximation [48, Appendix C] using just two and three cumulants, and the saddlepoint approximations [25] based on a Poisson and Negative binomial moment structure.

First define the relative difference $\tilde{c}_n = 100(\hat{c}_n - c_n)/c_n$, where c_n denotes the n th cumulant of the target distribution and \hat{c}_n the n th cumulant of the approximation.

The approximations by Wang [48], and Gillespie and Renshaw [25] present problems when the third order cumulant is large in comparison with the mean and the variance. The subscripts W_3 , GRP_3 , and $GRNB_3$ denote third-order truncation under Wang’s improvements, Gillespie and Renshaw’s improvements based on a Poisson, and Gillespie and Renshaw’s improvements based on a Negative Binomial, respectively.

We consider the cases studied by Gillespie and Renshaw [25] where the target cumulants are given by

Case 1: $c_1 = 13.84, c_2 = 26.57,$ and $c_3 = 82.87$

Case 2: $c_1 = 12, c_2 = 18,$ and $c_3 = 100.$

The results obtained for Cases 1 and 2 are shown in Table 1. For both cases, the table shows that the developed approach estimates the target means and variances within $10^{-5}\%$, while the best result for the other methods is above 2.66%. The error rate using the other methods is over 9% for c_3 . Whilst the method developed involves a very small loss of accuracy in c_3 .

Example 2 (Mixture of Gaussian Distributions). Consider first a mixture of two normal PDFs to obtain interesting shapes. Let

$$f(x) = a_1 \left(\frac{0.8}{\sqrt{2\pi}} \exp \left\{ -\frac{1}{2}x^2 \right\} + \frac{0.2}{\sqrt{2\pi}} \exp \left\{ -\frac{1}{2}(x - 4)^2 \right\} \right), \tag{17}$$

a mixture of the $N(0, 1)$ and $N(4, 1)$ densities with weights 0.8 and 0.2, respectively. a_1 is 1 over the integral $\int_0^8 f(x)dx$. Fig. 2 (left) shows that f is fitted well by using the generalized Gamma expansion P_{12}^α . The relative error is of order 10^{-4} as shown in Fig. 2 (right). The moments of f and P_{12}^α are compared as shown in Table 2. This table shows that the difference between the moments is smaller than 10^{-6} , and then Corollary 1 is numerically validated for the univariate case.

The degree of approximation achieved using Laguerre polynomials is shown by fitting another density function defined by

$$\bar{P}_1(x) = (2/\pi x^5)^{\frac{1}{2}} \exp\{-(1 - x/2)^2/(x/2)\}. \tag{18}$$

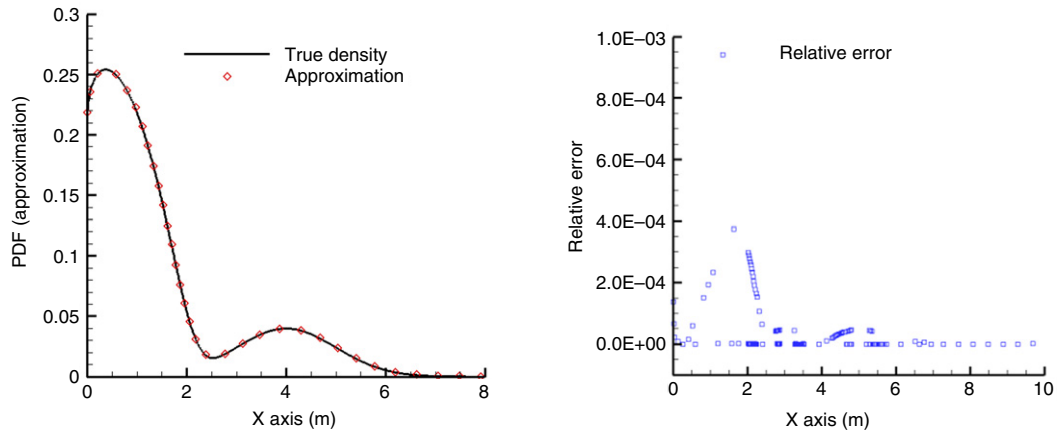


Fig. 2. Values of $f(x)$ (solid line) with corresponding values of fitted Gamma expansion $P_{12}^\alpha(x)$ (diamond) (left), and relative error plot (right).

Table 2

Comparison between the moments of f and P_{12}^α .

Moments	f	P_{12}^α
m_0	1.00000000000000	1.00000000000000
m_1	1.34424607894811	1.34424607894842
m_2	3.80825580894909	3.80825580894931
m_3	14.7317701683029	14.7317701683037
m_4	65.2494548410070	65.2494548410076
m_5	310.247430105884	310.247430105891

Table 3

Values of $\overline{P_1}(x)$ with corresponding values of the fitted third-order Edgeworth (P_3 in Eq. (C.1)), Saddlepoint approximation (Eq. (C.2)) and Gamma (P_3^α in Eq. (7)) expansions.

x	$f(x)$	$P_3^\alpha(x)$ Laguerre	P_3 Edgeworth	P_3 Saddlepoint
0.1616	0.0002	0.0865	1.7456	no-value
0.5656	0.7179	0.5767	0.6863	no-value
1.0505	0.6129	0.6385	-0.5837	no-value
1.5353	0.3397	0.3947	-0.5269	2.6472
2.0202	0.1835	0.1883	0.0706	2.6531
2.5050	0.1018	0.0837	0.2501	2.1259
3.0707	0.0534	0.0402	0.0861	1.3715
3.5555	0.0317	0.0281	-0.0055	0.8351
4.0404	0.0193	0.0215	-0.0160	0.4628
4.5252	0.0120	0.0158	-0.0068	0.2359
5.0101	0.0076	0.0106	-0.0016	0.1114
6.0606	0.0030	0.0033	0.0000	0.0173
6.5454	0.0020	0.0016	0.0000	0.0066
7.0303	0.0013	0.0007	0.0000	0.0024
7.5151	0.0009	0.0002	0.0000	0.0008
8.0000	0.0006	0.0000	0.0000	0.0002

First, a comparison between the third-order Edgeworth (P_3 in Eq. (C.1)), saddlepoint approximation (P_3 in Eq. (C.2)) and Gamma expansion (P_3^α in Eq. (7)) for fitting $\overline{P_1}$ is shown in Table 3. This table shows that P_3^α fits well $\overline{P_1}$ while the Edgeworth expansion (P_3) predicts negative probabilities and allows for negative densities. Thus, the Edgeworth expansion is not strictly well defined. The first three cumulants of $\overline{P_1}$ are given by $c_1 = 1.33$, $c_2 = 0.83$ and $c_3 = 1.60$. Then, the saddlepoint approximation (Eq. (C.2)) is only defined for $x \geq c_1 - 0.5c_2^2/c_3 = 1.11$; thus the saddlepoint approximation fails in the region $x < c_1$ as shown in Table 3.

Comparable values of P_n^0 (i.e., using original Laguerre polynomials) and P_n^α (i.e., using generalized Laguerre polynomials) shown in Fig. 3, for $n = 8$ and 12, shows a typical superiority of P_n^α to P_n^0 . Increasing the order n does not always lead to a better fit as presented in Fig. 4.

Note that, in some cases and as shown in Fig. 3 (right), the fitted distributions are negative near to the origin. This problem can be solved using the technique explained above to obtain the results presented in Fig. 5.

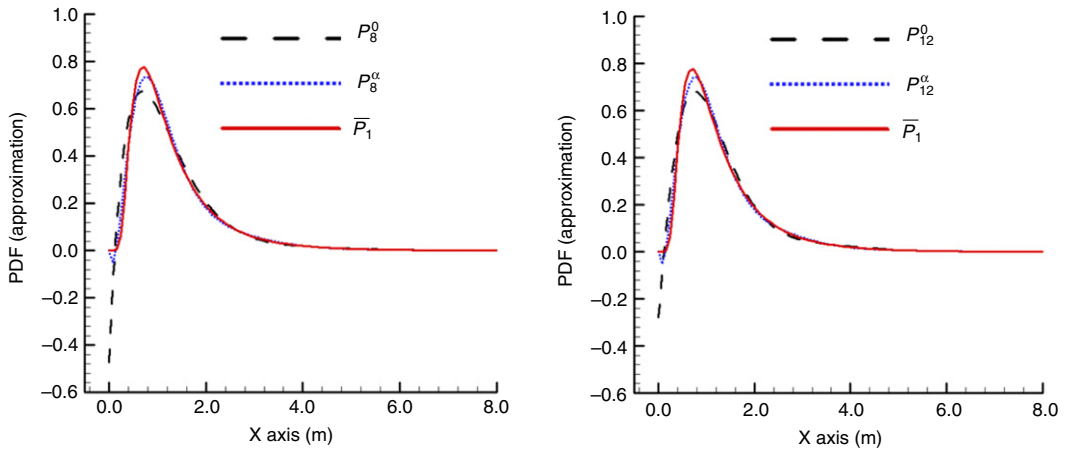


Fig. 3. Values of $\bar{P}_1(x)$ with corresponding values of the fitted Gamma expansions P_8^0 and P_8^α (left) and P_{12}^0 and P_{12}^α (right).

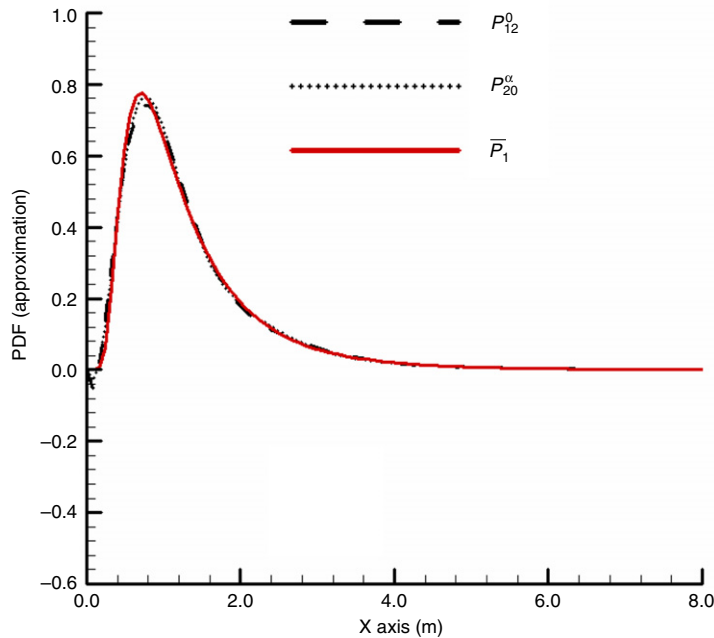


Fig. 4. Two higher-order Gamma expansions comparison.

Example 3 (Laplace Distributions). The Laplace distribution, sometime termed *super Gaussian*, is given by

$$h(x) = \frac{1}{2b} \exp(|x - \mu|/b) / a_3 = \frac{1}{2b} \begin{cases} \exp((\mu - x)/b) / a_3 & \text{if } x < \mu \\ \exp((x - \mu)/b) / a_3 & \text{if } x \geq \mu, \end{cases}$$

where μ is a location parameter and $b > 0$ is a scale parameter. The constant a_3 is used to ensure that $\int_5^{15} h(x)dx = 1$. The developed method fits very well to the corresponding Laplace distribution for $(\mu = 10, b = 1, \alpha \approx -0.990, \beta \approx 0.099, a_3 \approx 0.065)$ as shown in Fig. 6 (left). A relative error of order of 10^{-3} is obtained with good approximation of the tails as shown in Fig. 6 (right).

Example 4 (Bivariate Distributions). In this example, we consider the joint distribution $L(x, y)$ of two *correlated* continuous zero-mean random variables, X and Y , that are lognormally distributed. $L(x, y)$ is given by

$$L(x, y) = \frac{1}{2\pi xy\sigma_1\sigma_2\sqrt{1 - \rho^2}} \exp[-q/2]/a_4, \quad -1 < \rho < 1$$

and $q = \frac{1}{1 - \rho^2} (\ln(x/\sigma_1)^2 + \ln(y/\sigma_2)^2 - 2\rho \ln(x/\sigma_1) \ln(y/\sigma_2)),$

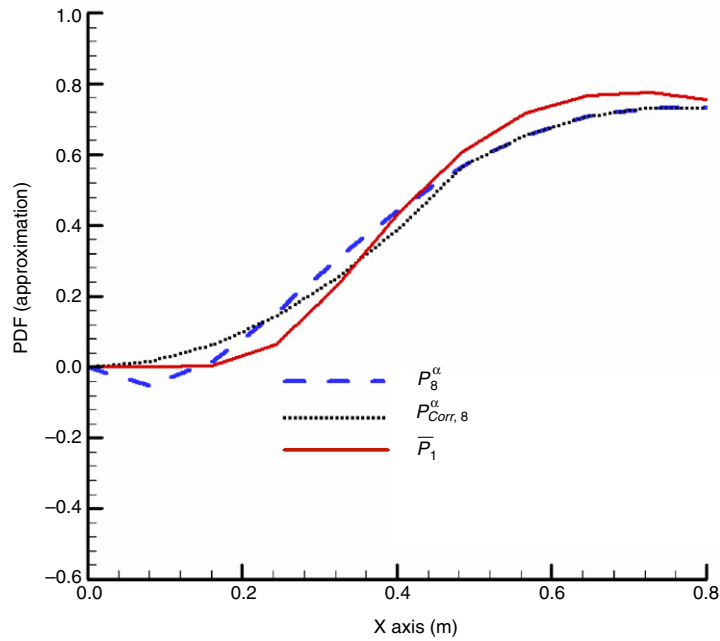


Fig. 5. Values of $\bar{P}_1(x)$ with corresponding values of the fitted Gamma expansion P_8^α and the non-negative correction $P_{Corr,8}^\alpha$.

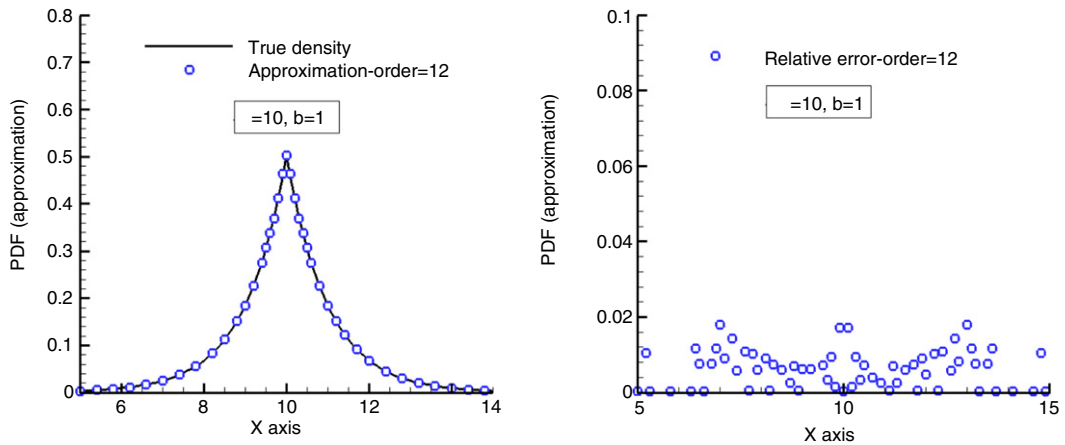


Fig. 6. Values of Laplace distribution $h(x)$ with corresponding values of fitted Gamma expansion $P_{12}^\alpha(x)$ (squares) (left), and relative error plot (right). $\mu = 10, b = 1$.

where ρ is the correlation coefficient of X and Y [49]. The constant a_3 is used to ensure that $\int_{0.01}^1 \int_{0.01}^1 L(x, y) dx dy = 1$. Fig. 7 shows that the Gamma expansion fits well to L for ($\sigma_1 = 0.2, \sigma_2 = 0.2, \rho = 0.8, \alpha = 0, \beta = 1, a_3 \approx 0.919$). A relative error of order 10^{-4} is obtained as shown in Fig. 8.

The relative error map for the moments of L and P_{12}^α is reported in Fig. 9. The relative error obtained is of order 10^{-3} . For $y = 0.58$, the conditional PDF $P_8^\alpha(x/y)$ in Eq. (16) is compared to $\bar{P}_2(x/y)$ as shown in Fig. 10, and very well results are obtained. Now, if the equation $P_n^\alpha(x, y) = P_n^\alpha(y)P_n^\alpha(x/y)$ is used, then $P_n^\alpha(x, y)$ can be reconstructed to fit $\bar{P}_2(x, y)$.

Example 5 (Complex Geological Image). The approach is validated by reconstructing 2D horizontal sections of a 3D fluvial reservoir. The data sets used are available in the Stanford V Reservoir Data Set [50]. The channel configurations in the horizontal sections are complex as shown in Fig. 11 (left). The integral of the distribution over $[0, 100]^2$ is one. Fig. 11 (middle) shows the reconstructed image by Laguerre series of order 31. A relative error of order 10^{-3} is obtained as shown in Fig. 11 (right). This example shows the ability of fitting very complex images.

The method developed herein can be coupled with a maximum entropy procedure [51] to determine the optimal order. The process consists in estimating the density for different orders and finding the optimal one as the one for which the entropy reaches maximum.

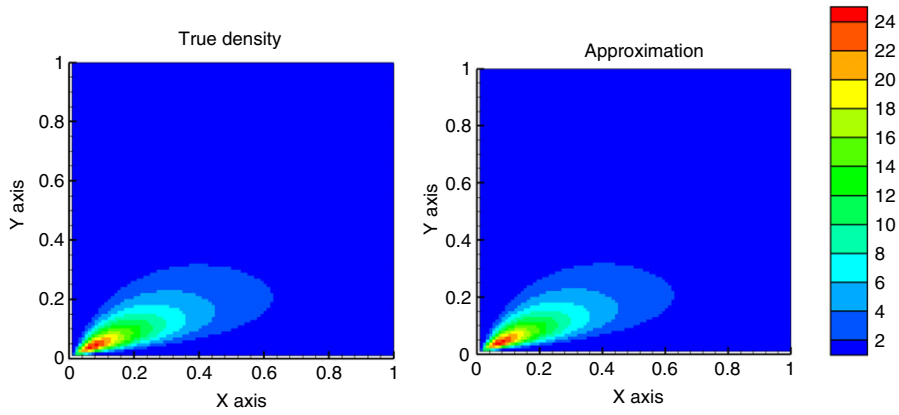


Fig. 7. Values of $L(x, y)$ (left) with corresponding values of the fitted bivariate Gamma expansion $P_{12}^{\alpha}(x, y)$ (right). $\sigma_1 = 0.2, \sigma_2 = 0.2$.

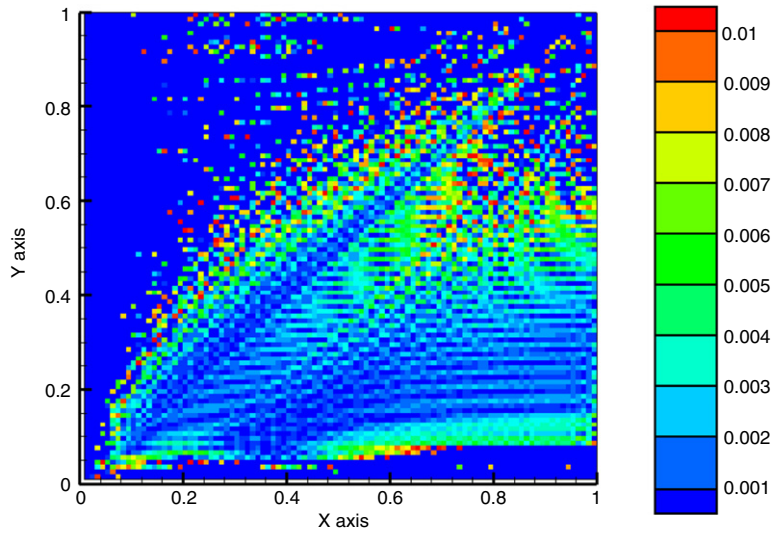


Fig. 8. Relative error map. $\sigma_1 = 0.2, \sigma_2 = 0.2$.

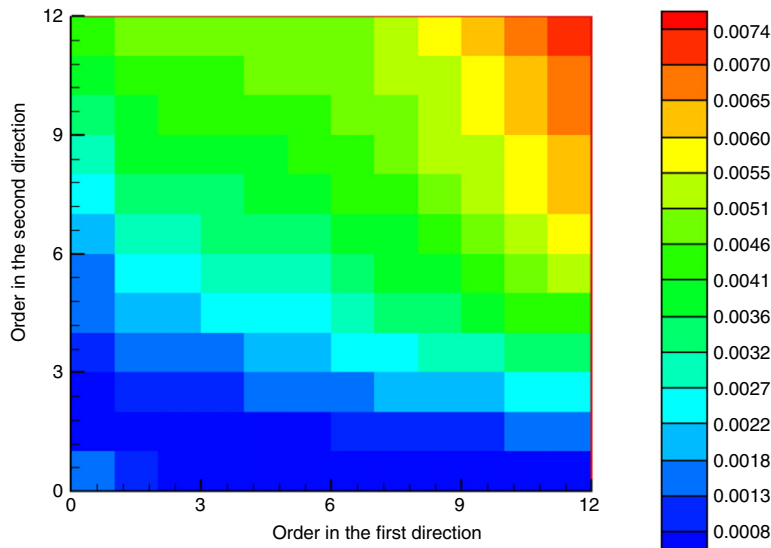


Fig. 9. Relative error map from the comparison between the moments of L and P_{12}^{α} . $\sigma_1 = 0.2, \sigma_2 = 0.2$.

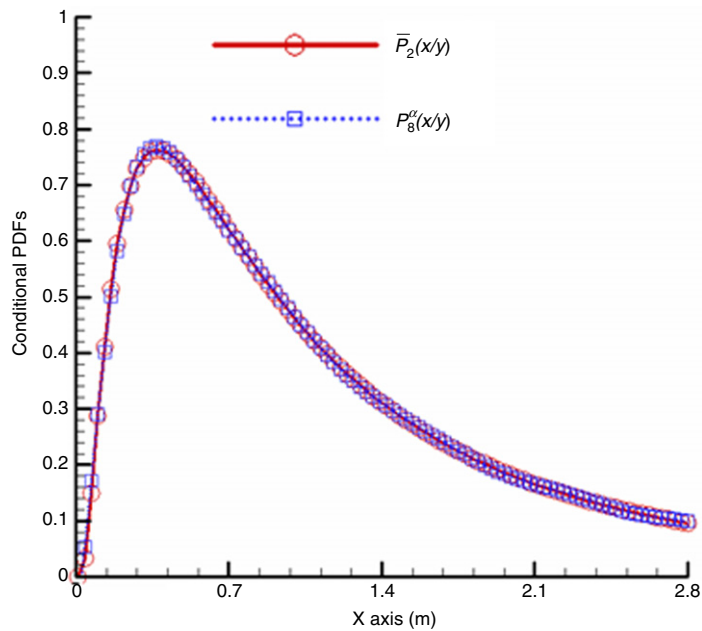


Fig. 10. Values of $\bar{P}_2(x/y)$ with corresponding values of the fitted conditional Gamma expansion $P_8^\alpha(x, /y) \cdot y = 0.58$.

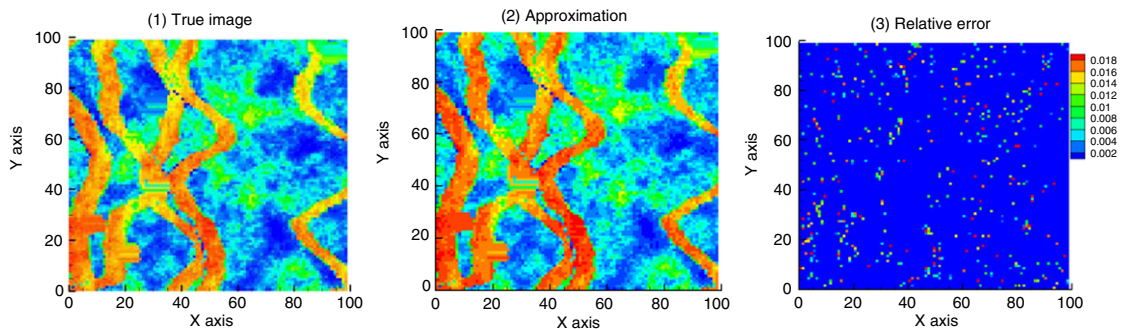


Fig. 11. A horizontal 2D section of a fluvial reservoir.

5. Conclusions

This paper presented the multivariate Gamma expansion as an alternative to the well-known multivariate Edgeworth series and saddlepoint approximation for modeling multivariate non-Gaussian PDFs as a function of its lower order moments. The search for an alternative expansion is motivated by the fact that the Gaussian PDF, which is used as the parent distribution for the Edgeworth series, is not strictly well-defined for describing positive variates, such as the density field. The basis of the multivariate Gamma expansion is given by the high-dimensional generalized Laguerre polynomials. Based on that, an analytical expression to the conditional PDFs is developed by decomposing the high-dimensional Laguerre and Hermite polynomials into products of one-dimensional polynomials and using Bayes theorem. In addition, an efficient solution is proposed to avoid, if there exist, negative values around the origin.

The results first showed that the Gamma expansion is more accurate than the Edgeworth and the saddlepoint approximations, and it fits well mixtures of Gaussian, super Gaussian, and Lognormal PDFs. In addition, the conditional PDFs are fitted well using the conditional densities approximations derived above. Furthermore, it is shown that Gamma expansion reconstructs very complex geologic images. The method developed showed that the approximated solutions reproduce the high-order statistics of the true distributions. The numerical examples show that true distributions share with the approximated solutions the same high-order moments.

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Appendix A. General numerical algorithm

The program developed reads two input files “*name_file.par*” and “*name_file.data*”, and generates one output file “*name_file.out*” that contain the values of the approximated solution at the grid nodes given in “*name_file.par*”.

The input parameter and data files are stored in “*name_file.par*” and “*name_file.data*”, respectively. These files contain the key parameters of the program and the high-order moments of the multivariate distribution to be approximated. The main function, of calculating the approximated values at the grid nodes, uses the input data and then evaluates the coefficients r using its expression given in Eq. (15). Finally, it builds the gamma expansion by evaluating the Laguerre polynomials and Gamma PDF on the points of the grid. The general algorithm can be summarized as the following:

Algorithm. Multivariate approximation using generalized gamma expansion.

Class_read_input

1. **Read** input parameter file
2. **Read** input data file

Class_macum

3. **Loop 1** over the grid nodes: $i = 1, \dots, NN$ (NN : number of grid nodes)
- 3.1. **Loop 2** over the order: $k = 1, \dots, n$ (n : order of approximation)

3.1.1. **k-Loops** over the dimension: $i_1, \dots, i_k = 1, \dots, N$ (N : dimension)

integer test = 1

calculate r_{i_1, \dots, i_k} from Eq. (14)

Evaluate $L_{i_1, \dots, i_k}^{(\alpha)}(\mathbf{z})$ using Eq. (11)

Evaluate $\phi_{\text{GAM}}(\mathbf{z})$

Multiply $r_{i_1, \dots, i_k} \times L_{i_1, \dots, i_k}^{(\alpha)}(\mathbf{z}) \times \phi_{\text{GAM}}(\mathbf{z})$

Update the sum

end k-Loops

end Loop 2

end Loop 1

Appendix B. Laguerre’s parameters calculation

In this appendix, we derive analytical expressions to α , and β ensuring that the fitted distribution has its first and second moments equal to m_1 and m_2 , respectively. For that, two integral conditions are needed

$$\int_D P(x)L_n^{(\alpha)}(\beta x)dx = 0, \quad \text{for } n = 1, 2. \quad (\text{B.1})$$

Using the expressions of $L_n^{(\alpha)}$ in Eq. (3), Eq. (B.1) can be written as

$$\begin{cases} \alpha + 1 - \beta m_1 = 0 \\ \frac{(\alpha + 1)(\alpha + 2)}{2} - (\alpha + 2)\beta m_1 + \beta^2 \frac{m_2}{2} = 0. \end{cases} \quad (\text{B.2})$$

The solution to the system of Eqs. (B.2) is

$$\alpha = \frac{2m_1^2 - m_2}{m_2 - m_1^2}, \quad \text{and} \quad \beta = \frac{m_1}{m_2 - m_1^2}, \quad (\text{B.3})$$

or in terms of cumulants

$$\alpha = \frac{c_1^2}{c_2} - 1, \quad \text{and} \quad \beta = \frac{c_1}{c_2}. \quad (\text{B.4})$$

Note that, if $m_1 = 1$ and $m_2 = 2$, then, using Eqs. (B.1) and (B.3), $\alpha = 0$ and $\beta = 1$.

Appendix C. Edgeworth and saddlepoint approximations

Edgeworth approximation. The third order Edgeworth expansion [4] is given by

$$P(x) \approx P_3(x) = \left[1 + \frac{1}{6}s_3H_3\left(\frac{x}{\sigma}\right)\sigma + \frac{1}{24}s_4H_4\left(\frac{x}{\sigma}\right)\sigma^2 + \frac{1}{72}s_3^2H_6\left(\frac{x}{\sigma}\right)\sigma^2 \right] \phi_{\text{GAU}}(x), \quad (\text{C.1})$$

where H_k is the k th-order Hermite polynomial and ϕ_{GAU} is the Gaussian PDF.

Saddlepoint approximation. The third-order saddlepoint approximation [19] can be written as

$$P(x) = P_3(x) = (4\pi\theta(x))^{-1/4} \exp\{-(1/6c_3^2)[c_2^3 - 3c_2\theta(x) + 2\theta(x)^{3/2}]\}, \quad (\text{C.2})$$

where $\theta(x) = c_2^2 + 2c_3(x - c_1)$. This approximation is defined under the condition $\theta(x) > 0$ or equivalently for $x \geq c_1 - 0.5c_2^2/c_3$. Then for large $|c_3|$ the approximation fails for $x \leq c_1$. Wang [48] proposes multiplying c_3 with a corrective term $l(t) = \exp(-c_2b^2t^2/2)$, where $b > 0$ is an appropriately chosen constant.

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