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Refined saddlepoint approximations for the normalizing constant of the complex Bingham quartic distribution: A change of variable approach

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Highlights

- **Statistical shape analysis is a very elegant framework for analyzing 2D and 3D labelled or unlabelled shape profile points including anatomical, mathematical, pseudo and semi-landmarks data, outline data, elastic curves, surfaces, curvature, ridges, solid shape and torsion data.**
- **Two modified saddlepoint approximation techniques have been proposed to improve the accuracy rates of approximation for the undefined normalizing constant of the CBQ distribution.**
- **The ISPA method seems more accurate than the SPIA method for approximating the normalizing constant of the CBQ planar shape distribution.**
- **The upgraded CVISPA and CVSPIA methods for the normalizing constant of the CBQ distribution numerically work better than ISPA and SPIA methods that have disregarded a change of variable with a slight reduction in computer time as well as with comparative ratios attain unity under high concentrations.**

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ABSTRACT

The complex Bingham quartic (CBQ) distribution is defined on the unit complex sphere in $\mathbb{C}^{k-1}$ and it is relevant for the statistical shape analysis of a k-point landmark data in 2D. This extended the Fisher distribution on the unit spherical shape space $S^2(1/2)$. The complex Bingham quartic (CBQ) distribution provides suitable shape parameters to comprise anisotropy. Under high concentrations, it looks like a multivariate Gaussian normal distribution but the main drawback of this planar shape distribution is that its normalizing constant does not have a simple closed explicit form representation. The present paper provides a modified approximation procedure for the indeterminate normalizing constant of the CBQ distribution based on saddlepoint approximations with a change of variable scheme. The modified saddlepoint approximations under a change of variable seem more precise as compared with the saddlepoint approximations without a change of variable approach.

1. Introduction

Modern statistical methods use models that require the computation of probabilities from complicated distributions, which can lead to intractable computations. Saddlepoint approximations can be the answer (Butler, 2007). Although the theory of saddlepoint approximations is quite complex, use of the approximations is fairly straightforward. The saddlepoint method provides an accurate approximation to the density or the distribution of a statistic, even for small tail probabilities and with very small sample sizes. This accuracy is seen not only in numerical work, but also in theoretical calculations. The basis of this method is to overcome the inadequacy of the normal approximation in the tails by tilting the random variable of interest in such a way that the normal approximation is evaluated at a point near the mean (Paolella, 2007).

1.1 Background Ideas

The moment generating function or the cumulant transform, $M_X(u)$, at a point $u \geq 0$ for a probability density function $f(x)$ is defined as

$$M_X(u) = \int_{-\infty}^{+\infty} \exp(ux) f(x) \mathrm{d}x. \tag{1}$$

Besides, the cumulant generating function, $K_X(u)$, is defined as

$$K_X(u) = \log M_X(u). \tag{2}$$

From $K_X(u)$, one can obtain $f(x)$ using the Fourier inversion formula (Feller, 1991; Billingsley, 1995)

$$f(x) = \frac{1}{2\pi i} \int_{u-i\infty}^{u+i\infty} \exp(K_X(z) - zx)\, \mathrm{d}z, \tag{3}$$

where $z = u + iy$ and $i = \sqrt{-1}$ is the imaginary unit with assuming that $K_X(u)$ is an integrable function (e.g., Huzurbazer, 1999; Stalker, 2009 and Wintner, 2013).

1.2 Simple Saddlepoint Approximations

The key to the saddlepoint method is to choose the path of integration, i.e., u in Eq. 3. Consider the following choice: set $u = u(x) \in \mathbb{R}$ that satisfies the following saddlepoint equation

$$K_X'(u) - x = 0. \tag{4}$$

According to Daniels (1954) and Field and Ronchetti (1990) the saddlepoint equation Eq. 4 has a unique real root $u > 0$ in the legitimate support $u_1 < u < u_2$ where $u_1 \geq 0$ and $u_2 \geq 0$ for every $a < x < b$. Such a point u is neither a maximum nor minimum but a saddlepoint (Fig.1) of $K_X(u) - ux$ so that $M_X(u) = \exp\big(K_X(u)\big) < \infty$, $K_X'(u)$ is a strictly increasing function of u and $K_X''(u) < \infty$ is convex.

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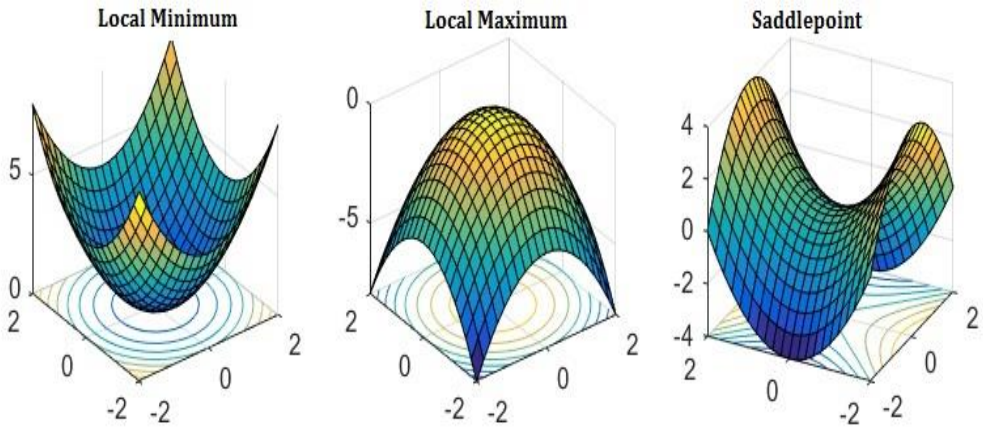

Fig. 1. Graphical representation of local minimum, local maximum and saddlepoints.

The unnormalized first-order saddlepoint approximation to $f(x)$ is

$$\hat{f}_1(x) = \left(\frac{1}{2\pi K_X''(u)}\right)^{1/2} \exp(K_X(\hat{u}) - \hat{u}x). \quad (5)$$

Its error of approximation is much better than the Taylor series approximation to a function (Goutis and Casella, 1999).

1.3 Refined Saddlepoint Approximations

The saddlepoint approximation is optimal in the sense that it is based on the highly efficient numerical method of steepest descents and this efficiency can be improved using higher order expansions. Higher-order saddlepoint expansions can be obtained by expanding the function $g(u) = K_X(u) - ux$ around u to a higher order using Taylor series expansion. The unnormalized second-order saddlepoint approximation to $f(x)$ is

$$\hat{f}_2(x) = \hat{f}_1(x)\left(1 + \frac{1}{8}\kappa_4(\hat{u}) - \frac{5}{24}\kappa_3^2(\hat{u})\right), \quad (6)$$

where $\kappa_3(\hat{u}) = K_X^{(3)}(\hat{u})/\left(K_X''(\hat{u})\right)^{3/2}$ and $\kappa_4(\hat{u}) = K_X^{(4)}(\hat{u})/K_X''(\hat{u})$ (Kolassa, 1997; Goutis and Casella, 1999). The unnormalized first-order saddlepoint approximation function $\hat{f}_1(x)$ in Eq. 5 and the unnormalized second-order saddlepoint approximation function $\hat{f}_2(x)$ in Eq. 6 will not, in general, integrate to one, although it will usually not be far off and can be improved by renormalization.

1.4 Complex Bingham Quartic Distribution

The complex Bingham (CB) distribution described by Kent (1994) is a suitable distribution for modelling shapes. For example, to assess the effects of selection for body weight on the shape of mouse vertebrae into control, large and small groups of mice when a random sample of landmark configurations is available in 2D. Also, if it is of interest to study any shape differences in the brain between a group of schizophrenic patients and a group of normal individuals or for postcode recognition in image analysis or for protein matching in bioinformatics, planar statistical shape analysis provides a very elegant framework for the analysis of such 2D shape data (Dryden and Mardia, 2016).

Under high concentrations the complex Bingham (CB) distribution has a complex normal distribution with isotropy ($\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{I}_{2k-3}$) where k is the number of labelled landmarks. The complex Bingham quartic (CBQ) distribution can be constructed by adding a quartic term to the complex Bingham (CB) density. The motivation behind the CBQ distribution was to develop a distribution centred at the CB distribution, which includes anisotropy i.e., a full multivariate Gaussian distribution under high concentrations.

Let $\mathbb{C}\,S^{k-2} = \left\{\mathbf{z}: (z_1, z_2, \cdots, z_{k-1})^T, \mathbf{z}^*\mathbf{z} = \sum_{j=1}^{k-1}|z_j|^2 = 1\right\}$ denotes the unit complex sphere in $\mathbb{C}^{k-1}$. The complex Bingham (CB) density on $\mathbb{C}\,S^{k-2} \equiv S^{2k-3}$, denoted $\mathbb{C}\mathrm{B}_{k-2}(\boldsymbol{A})$ can be written in the form: $f(\mathbf{z}) = c_{\mathrm{CB}}(\mathbf{A})^{-1}\exp(\mathbf{z}^*\boldsymbol{A}\mathbf{z}), \quad \mathbf{z} \in \mathbb{C}\,S^{k-2}$,

where $\mathbf{z}^*$ represents the complex conjugate of the transpose of the complex pre-shape vector $\mathbf{z}$, the matrix $\boldsymbol{A}$ is $(k-1)\times(k-1)$ Hermitian (i.e., $\boldsymbol{A} = \boldsymbol{A}^*$) and $c_{\mathrm{CB}}(\boldsymbol{A})$ is the normalizing constant (Dryden and Mardia, 2016).

The complex Bingham quartic (CBQ) density function centred at the north pole $(0, 0, \cdots, 1)^T$ with respect to the uniform measure on $\mathbb{C}\,S^{k-2}$, denoted $\mathbb{C}\mathrm{BQ}_{k-2}(\boldsymbol{\Omega}, \boldsymbol{A}, \mathbf{B})$ can be written in terms of the partial Procrustes tangent coordinates $\mathbf{v}$ by

$$f(\mathbf{z}) = c_{\mathrm{CBQ}}(\boldsymbol{\Omega})^{-1}\exp\left(\mathbf{v}^*\boldsymbol{A}\mathbf{v} + (\mathbf{1} - \mathbf{v}^*\mathbf{v})\mathrm{Re}(\mathbf{v}^T\boldsymbol{B}\mathbf{v})\right), \quad (7)$$

where $\boldsymbol{\Omega}$ is a $(2k-4)\times(2k-4)$-dimensional real symmetric (reduced) concentration matrix, $\boldsymbol{A}$ and $\boldsymbol{B}$ are $(k-2)\times(k-2)$ complex Hermitian matrices and $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ is the normalizing constant (Kent *et al.*, 2006). For k landmarks in 2 dimensions there are $(2k-4)$ mean parameters and $(2k-4)\times(2k-3)/2$ covariance parameters that are identifiable.

The CBQ density on $\mathbb{C}\,S^{k-2}$ can also be rewritten in $(2k-4)$-dimensional real coordinates (Kent *et al.*, 2006)

$$\mathbf{x} = (\mathrm{Re}(\mathbf{v})^T, \mathrm{Im}(\mathbf{v})^T)^T \quad (8)$$

by

$$f(\mathbf{z}) = c_{\mathrm{CBQ}}(\boldsymbol{\Omega})^{-1}\exp\left(-\tfrac{1}{2}(\mathbf{x}^T\boldsymbol{\Omega}\,\mathbf{x} - (\mathbf{x}^T\mathbf{x})\mathbf{x}^T\boldsymbol{\Omega}^{(\mathrm{as})}\,\mathbf{x})\right) \quad (9)$$

where

$$\boldsymbol{\Omega}^{(\mathrm{as})} = \frac{1}{2}\begin{pmatrix} \boldsymbol{\Omega}_{11} - \boldsymbol{\Omega}_{22} & \boldsymbol{\Omega}_{12} + \boldsymbol{\Omega}_{21} \\ \boldsymbol{\Omega}_{21} + \boldsymbol{\Omega}_{12} & \boldsymbol{\Omega}_{11} - \boldsymbol{\Omega}_{22} \end{pmatrix}$$

is a $(k-2)\times(k-2)$ real symmetric matrix that summarizes the whole anti-complex-symmetric information in the reduced concentration matrix $\boldsymbol{\Omega}$ of the CBQ planar shape distribution.

According to Kent *et al.* (2006) the normalizing constant of the complex Bingham quartic (CBQ) can be derived as

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) = \pi\int_0^1 c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s)\big)s^{k-3}\,\mathrm{d}s, \quad (11)$$

where

$$\boldsymbol{\Psi}(s) = -\frac{\mathbf{1}}{2}\big(s\boldsymbol{\Omega} + s^2\boldsymbol{\Omega}^{(\mathrm{as})}\big), \quad 0 \le s \le 1, \quad (12)$$

is also a real symmetric $(2k-4)\times(2k-4)$ matrix and $c_{\mathrm{Bing}}(\cdot)$ is the normalizing constant of the real Bingham distribution on S^{2k-5}. Thus, the normalizing constant for the complex Bingham quartic (CBQ) distribution has been reduced to a one-dimensional integral of normalizing constants for the Bingham distribution.

So far, no closed form of representation for the normalizing constant of the complex Bingham quartic distribution $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ is

known. The search for numerical techniques of optimal approximation for $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ is an indispensable aim of full identification.

1.5 Objectives

The main purpose of this article is to modify two proposed saddlepoint approximation methods for the normalizing constant of the complex Bingham quartic distribution $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ that appeared in Ganeiber and Kent (2010) viz., the second order integrated saddlepoint approximations (ISPA) and the second order saddlepoint approximations of integration (SPAI). The technique of changing of variables has been used in the present process of modification. The target aims of the current scheme of changing of variable are

- To simplify the numerical integration method using Gauss-Legendre quadrature rule with equal or unequal weights and uniformly abscissas or nodes.
- To improve (or develop) the accuracy of performance of the ISPA and SPAI techniques with an extra closeness of their numerical results under either low or high concentrations.

2. Materials and Methods

Consider the real Bingham distribution on the unit sphere S^{k-2} i.e., $\|\mathbf{x}\| = \mathbf{x}^T\mathbf{x} = 1$ with parameter matrix $\boldsymbol{A}$ where $\boldsymbol{A} = \boldsymbol{\Gamma\Lambda\Gamma^T}$ is a $(k-1)\times(k-1)$ symmetric matrix with a diagonal non-zero eigenvalues matrix $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_{k-1})$ and an orthogonal matrix $\boldsymbol{\Gamma}$ whose columns are standardized eigenvectors. According to Ganeiber and Kent (2010) the normalizing constant for the real Bingham distribution $c_{\mathrm{Bing}}(\mathbf{A})$ can be rewritten as a function of a probability density function of a convolution central scaled chi squared χ_1^2 variates, $f(1, \mathbf{A})$. More specifically,

$$c_{\mathrm{Bing}}(\mathbf{A}) = \frac{(2\pi)^{(k-1)/2}}{|2\mathbf{A}|^{1/2}} f(1, \mathbf{A}). \tag{13}$$

Kent *et al.* (2006) have shown that the second order saddlepoint approximation for the normalizing constant of the real Bingham distribution is given by

$$\hat{c}_{\mathrm{Bing}}(\mathbf{A}) = \left[2\pi^{2k-5}/K''(\hat{u}) \prod_{i=1}^{2k-4}(\lambda_i - \hat{u})\right]^{1/2} \times \exp\left(-\hat{u} + \frac{1}{8}\kappa_4(\hat{u}) - \frac{5}{24}\kappa_3^2(\hat{u})\right), \tag{14}$$

where λ_i are the eigenvalues of $-\mathbf{A}$.

The normalizing constant for the complex Bingham quartic (CBQ) can be mathematically written as asymptotic representation defined by

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) \approx \pi \sum_{i=1}^{n} w_i c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s_i)\big) s_i^{k-3}. \tag{15}$$

Under low concentrations, the uniform nodes are suitable to evaluate numerically the integrand in Eq. 11. On the other hand, further care is needed under high concentrations to suit the behaviour of $c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s_i)\big)$.

2.1 ISPA and SPIA Methods

Two methods are explored in Ganeiber and Kent (2010) to evaluate the normalizing constant of the CBQ distribution based on the saddlepoint approximations. The first approach is an integrated saddlepoint approximation (ISPA) in which $c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s_i)\big)$ is approximated by the corresponding second-order saddlepoint approximation and then evaluate the integral numerically using Gauss-Legendre quadrature rule with unequal weights and non-uniform abscissas or nodes. The second suggestion is the saddlepoint of integration approximation (SPIA) i.e., evaluating the integration numerically and next applying the second-order saddlepoint approximation.

One notable drawback of the numerical quadrature is the need to pre-compute (or look up) the requisite weights and nodes. Uniform nodes are not a suitable choice to compute numerically the integrand function in Eq. 11 for the normalizing constant of the complex Bingham quartic (CBQ) distribution, especially for $k > 3$ and under high concentrations. Under maximum concentrations, $c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s_i)\big)s_i^{k-3}$ gets steeper/has a sharp peak, which is imperative to carefully choose a smaller subinterval width h over the interval $[0,1]$ for achieving acceptable accuracy.

2.2 ISPA and SPIA Methods with a Change of Variable

A change of variable scheme is an alternative statistical technique to overcome the drawbacks of implementing the Gauss-Legendre quadrature rule under either low or high concentrations. Uniform nodes and equal or unequally weights can be used under the scheme of a change of variable. This approach will simplify the numerical integration technique under consideration as well as a high acceptable accuracy can be attained.

It is known in multivariate analysis that the quadratic form $\mathbf{x}^T\boldsymbol{\Omega}\,\mathbf{x}$ has the same distribution as $\mathbf{y}^T\boldsymbol{\Lambda}\,\mathbf{y} = \sum_{i=1}^{k-1}\lambda_i y_i^2$ where y_i are independent standardized normal variables and $\boldsymbol{\Lambda}$ is a $(k-1)\times(k-1)$ diagonal matrix of the eigenvalues, $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_{k-1}$, of the concentration matrix – $\boldsymbol{\Omega}$ (see, Mardia, *et al.*, 1979). So, without loss of generality, it can be assumed that $\boldsymbol{\Omega} = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_{k-1})$ and then $v = \sum_{i=1}^{k-1}\lambda_i\chi_1^2$ holds as well as it can also be approximated by $\bar{\lambda}\chi_{k-1}^2$ with probability density function

$$f(v) = \frac{1}{2^{(k-1)/2}\Gamma\big((k-1)/2\big)} v^{\frac{(k-1)}{2}-1}\exp\left(-\frac{1}{2}v\right), \quad 0 < v < \infty,$$

and cumulative density function

$$F(v) = \frac{\gamma\left(\frac{k-1}{2}, \frac{v}{2}\right)}{\Gamma\big((k-1)/2\big)},$$

where $\Gamma(\cdot)$ is the gamma function and

$$\gamma\left(\frac{k-1}{2}, \frac{v}{2}\right) = \left(\frac{v/2}{(k-1)/2}\right)\Gamma\left(\frac{k-1}{2}\right)\exp\left(-\frac{1}{2}v\right) \times \sum_{j=1}^{\infty}\frac{(v/2)^j}{\Gamma\left(\frac{(k-1)}{2}+j+1\right)}$$

is the lower incomplete gamma function (Abramowitz and Stegun, 1972).

The normalizing constant for the complex Bingham quartic (CBQ) in Eq. 11 can be rewritten as

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) = \pi\int_0^1 h(s)f(s)\,\mathrm{d}s, \tag{16}$$

where

$$h(s) = \frac{c_{\mathrm{Bing}}\big(\boldsymbol{\Psi}(s)\big)s^{k-3}}{f(s)} \tag{17}$$

Let $\tau = F(s)$ and $\mathrm{d}\tau = f(s)\mathrm{d}s$. For the purpose of changing of variable it is necessary to choose the probability density function $f(s)$ so that the function $h(s)$ will be nearly constant. A good test case is $\boldsymbol{\Omega}^{(\mathrm{as})} = \mathbf{0}$ and $\boldsymbol{\Omega} = \mathrm{c}\mathbf{I}$, a multiple of the identity matrix with $\mathrm{c} > 0$. The expression of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ in Eq. 16 can be rewritten as

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) = \pi\int_0^1 h\big(s(\tau)\big)\,\mathrm{d}\tau. \tag{18}$$

In practice, one can use the quadrature rules to approximate the definite integral in Eq. 18 by a summation of the form

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) \approx \pi\sum_{i=1}^{n} w_i h\big(\boldsymbol{\Psi}(s_i)\big). \tag{19}$$

The normalizing constant of the real Bingham distribution in Eq. 13 can be simplified as

$$c_{\text{Bing}}\big(\boldsymbol{\Psi}(s_i)\big) = \frac{(2\pi)^{(k-1)/2}}{|2\boldsymbol{\Psi}(s_i)|^{1/2}}\left(\frac{1}{2^{(k-1)/2}\Gamma\big((k-1)/2\big)}\right) \times \bar{\lambda}\big(\boldsymbol{\Psi}(s_i)\big)^{\frac{k-1}{2}-1}\exp\left(-\frac{1}{2}\bar{\lambda}\big(\boldsymbol{\Psi}(s_i)\big)\right). \quad (20)$$

Let $\alpha = \text{tr}(\boldsymbol{\Omega})$ and

$$\bar{\lambda}_i = \frac{1}{k-1}\text{tr}\big(\boldsymbol{\Psi}(s_i)\big) = \frac{1}{k-1}\text{tr}\left(-\frac{\mathbf{1}}{2}\big(s_i\boldsymbol{\Omega} + s_i^2\boldsymbol{\Omega}^{(\text{as})}\big)\right) = -\frac{\alpha}{2(k-1)}s_i,$$

where $\text{tr}\big(\boldsymbol{\Omega}^{(\text{as})}\big) = 0$. Moreover,

$$|2\boldsymbol{\Psi}(s_i)|^{1/2} = \sqrt{2}\left|-\frac{\mathbf{1}}{2}\big(s_i\boldsymbol{\Omega} + s_i^2\boldsymbol{\Omega}^{(\text{as})}\big)\right|^{1/2} \approx \sqrt{2}\left|-\frac{\mathbf{1}}{2}(s_i\boldsymbol{\Omega})\right|^{1/2} = \frac{1}{\sqrt{2}}\left(-\frac{s_i}{2}\right)^{(k-1)/2},$$

and the normalizing constant in Eq. 20 becomes

$$c_{\text{Bing}}\big(\boldsymbol{\Psi}(s_i)\big) = c_g s_i^{k-2}\exp\left(-\frac{1}{\delta}s_i\right), \quad (21)$$

where

$$c_g = \frac{\sqrt{2}\pi^{(k-1)/2}\left(\frac{\alpha}{2(k-1)}\right)^{\frac{(k-1)}{2}-1}}{\alpha\Gamma\big((k-1)/2\big)}$$

and

$$\delta = \frac{4(k-1)}{\alpha}.$$

Notice that the final representation for the normalizing constant of the real Bingham distribution in Eq. 21 is proportional to the probability density function of gamma distribution with scale and shape parameters $(k-1)/2$ and δ, respectively. Thus, the normalizing constant for the complex Bingham quartic (CBQ) distribution in Eq. 19 reduces to

$$c_{\text{CBQ}}(\boldsymbol{\Omega}) = \pi\sum_{i=1}^{n} w_i\left(\frac{\sqrt{2}\pi^{\frac{(k-1)}{2}}\left(\frac{\alpha}{2(k-1)}\right)^{\frac{(k-1)}{2}-1}}{\alpha\Gamma\left(\frac{(k-1)}{2}\right)}\right) \times s_i^{2k-5}\exp\left(-\frac{1}{4(k-1)}\alpha s_i\right). \quad (22)$$

Notice also that the last expression of $h\big(\boldsymbol{\Psi}(s_i)\big)$ in Eq. 22 is proportional to the probability density function of gamma distribution with scale and shape parameters $2k-4$ and δ, respectively. So, the integral of a gamma density function over the interval $[0,1]$ is less than 1. Thus, the function $h\big(\boldsymbol{\Psi}(s_i)\big)$ must be truncated over the interval $[0,1]$,

$$h^*\big(\boldsymbol{\Psi}(s_i)\big) = \frac{h\big(\boldsymbol{\Psi}(s_i)\big)}{H(1)}, \quad (23)$$

where

$$H(1) = \int_0^1 \frac{\sqrt{2}\pi^{\frac{(k-1)}{2}}\left(\frac{\alpha}{2(k-1)}\right)^{\frac{(k-1)}{2}-1}}{\alpha\Gamma\left(\frac{(k-1)}{2}\right)} s^{(2k-4)-1} \times \exp\left(-\frac{1}{4(k-1)/\alpha}s\right)\text{d}s,$$

with distribution function $H^*\big(\boldsymbol{\Psi}(s_i)\big) = H\big(\boldsymbol{\Psi}(s_i)\big)/H(1)$.

For the purpose of suitable numerical integration, it is straightforward to use equal weights $w_i = \frac{1}{n}$, $i = 1,2,\cdots,n$ with the following suggested nodes

$$s_i = H^{*-1}(\tau_i) = H^{*-1}\left(\frac{i-0.5}{n}\right). \quad (24)$$

The cumulative distribution function $H^*(\text{s})$ is strictly increasing. Therefore, the equation

$$H^*(\text{s}) = \tau, \qquad 0 \le \tau \le 1 \quad (25)$$

has a unique solution, $\text{s} = \xi_\tau$, say, and $H^{*-1}(\tau)$ is the unique quantile of order τ for the scaled/truncated gamma distribution and it is also an increasing function over the interval $[0,1]$ (David and Nagaraja, 2003).

The integrated saddlepoint approximation (ISPA) for the complex Bingham quartic (CBQ) distribution $\hat{c}_{\text{CBQ,CVISPA}}(\boldsymbol{\Omega})$, say, can be evaluated by finding firstly the second-order saddlepoint approximation for the truncated gamma distribution in Eq. 23 and next evaluating the numerical integration for the obtained saddlepoint approximation with equal weights and uniform nodes or abscissas. Let

$$c_{\text{CBQ}}(\boldsymbol{\Omega}) = \pi\sum_{i=1}^{n} w_i h^*\big(\boldsymbol{\Psi}(s_i)\big). \quad (26)$$

Then

$$\hat{c}_{\text{CBQ,CVISPA}}(\boldsymbol{\Omega}) = \pi\sum_{i=1}^{n} w_i \hat{h}^*\big(\boldsymbol{\Psi}(s_i)\big). \quad (27)$$

The saddlepoint of integration approximation (SPIA) for the complex Bingham quartic (CBQ) distribution $\hat{c}_{\text{CBQ,CVSPIA}}(\boldsymbol{\Omega})$, say, can be evaluated by finding firstly the integration numerically with equal weights and uniform nodes or abscissas and therewith applying the second-order saddlepoint approximation. Let

$$g(1) = \pi\sum_{i=1}^{n} w_i h^*\big(\boldsymbol{\Psi}(s_i)\big). \quad (28)$$

The cumulant generating function, $K_g\big(\hat{u};\boldsymbol{\Psi}(s_i)\big)$ for $g(1)$ is given by

$$K_g(\hat{u};\boldsymbol{\Psi}) = \log\left[\pi\sum_{i=1}^{n} w_i\exp\Big(K_i\big(\hat{u};\boldsymbol{\Psi}(s_i)\big)\Big)\right]$$

and

$$\hat{c}_{\text{CBQ,CVSPIA}}(\boldsymbol{\Omega}) = \hat{g}(1) = \left(\frac{1}{2\pi K_g''}\right)^{1/2}\exp\big(K_g - \hat{u}\big) \times (1+T), \quad (29)$$

where

$$T = \frac{1}{8}\kappa_4(\hat{u}) - \frac{5}{24}\kappa_3^2(\hat{u}).$$

In triangle case of $k = 3$ unlabelled or labelled landmarks data, the $(2k-4)\times(2k-4)$ concentration matrix $\boldsymbol{\Omega}$ reduces to a 2×2 diagonal matrix of the form

$$\boldsymbol{\Omega} = \begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}$$

and $\boldsymbol{\Psi}(s)$ becomes

$$\boldsymbol{\Psi}(s) = -\frac{1}{2}\begin{pmatrix}\lambda_1 s(1-s)+\lambda_2 s^2 & 0\\ 0 & \lambda_2 s(1-s)+\lambda_1 s^2\end{pmatrix}.$$

According to Kent (1982) and Kent *et al.*, (2006), the relationship between the normalizing constant of the complex Bingham quartic distribution $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ and the normalizing constant of the 5-parameter Fisher-Bingham (FB5) or Kent distribution $c_{\mathrm{FB5}}(\kappa,\beta)$ is given by

$$c_{\mathrm{CBQ}}(\boldsymbol{\Omega}) = \frac{\pi}{2}\exp(-\kappa)\, c_{\mathrm{FB5}}(\kappa,\beta), \tag{30}$$

where $\kappa \geq 0$ represents the concentration parameter and $0 \leq \beta \leq \kappa/2$ (unimodality case) determines the ovalness or the ellipticity of the contours of the distribution. Moreover, the concentration κ and ovalness β parameters for the FB5 distribution and the concentration parameters, λ_1 and $\lambda_2 \geq \lambda_1$ for the CBQ distribution are related by

$$\kappa = \frac{1}{8}(\lambda_1+\lambda_2),$$

and

$$\beta = \frac{1}{16}(\lambda_2-\lambda_1).$$

The normalizing constant for the 5-parameter Fisher-Bingham (FB5) is defined as

$$c_{\mathrm{FB5}}(\kappa,\beta) = 2\pi\sum_{j=1}^{\infty}\frac{\Gamma\left(j+\frac{1}{2}\right)}{\Gamma(j+1)}\beta^{2j}\left(\frac{1}{2}\kappa\right)^{-2j-\frac{1}{2}} I_{2j+\frac{1}{2}(\kappa)}, \tag{31}$$

where $I_{\eta(\kappa)}$ is the modified Bessel function and $\Gamma(\cdot)$ is the gamma function (Kent, 1982).

For $k > 3$, a simple closed form representation for the true $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ is not available. For example, in the case of $k = 4$ landmarks data, the $(2k-4)\times(2k-4)$ concentration matrix $\boldsymbol{\Omega}$ reduces to a 4×4 diagonal matrix of the form

$$\boldsymbol{\Omega} = \begin{pmatrix}\lambda_1 & 0 & 0 & 0\\ 0 & \lambda_2 & 0 & 0\\ 0 & 0 & \lambda_3 & 0\\ 0 & 0 & 0 & \lambda_4\end{pmatrix}$$

and saddlepoint approximations for $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ are needed with or without a change of variable approach.

3. Results and Discussions

Practical performance assessments for the second-order saddlepoint approximations with and without a change of variable scheme are required.

For $k = 3$ labelled landmarks data, Table 1 shows numerical results of the exact value of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$, second- order integrated saddlepoint approximation $\hat{c}_{\mathrm{CBQ,ISPA}}(\boldsymbol{\Omega})$, second-order saddlepoint of integration approximation, $\hat{c}_{\mathrm{CBQ,SPIA}}(\boldsymbol{\Omega})$, second- order integrated saddlepoint approximation (ISPA) with a change of variable, $\hat{c}_{\mathrm{CBQ,CVISPA}}(\boldsymbol{\Omega})$ and second-order saddlepoint integration approximation (SPIA) with a change of variable, $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\boldsymbol{\Omega})$ with various values of κ, $\beta = 0.4\kappa$, λ_1, λ_2 and $n = 1000$. Evaluating the exact values for the normalizing constant of the Kent distribution $c_{\mathrm{FB5}}(\kappa,\beta)$ in Eq. 31 is carried out using the R function **`fb5.series`**, `which` accompanies Kent (1982). Both $\hat{c}_{\mathrm{CBQ,ISPA}}(\boldsymbol{\Omega})$ and $\hat{c}_{\mathrm{CBQ,SPIA}}(\boldsymbol{\Omega})$ give less precise estimates when the concentration parameters λ_1 and λ_2 tend to zero. Furthermore, both $\hat{c}_{\mathrm{CBQ,CVISPA}}(\boldsymbol{\Omega})$ and $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\boldsymbol{\Omega})$ have improved the numerical estimations of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ under either low or high concentrations as compared to $\hat{c}_{\mathrm{CBQ,ISPA}}(\boldsymbol{\Omega})$ and $\hat{c}_{\mathrm{CBQ,SPIA}}(\boldsymbol{\Omega})$ without a change of variable scheme. Fig. 1 plots the exact values of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ along with the numerical results of the 4 saddlepoint approximation approaches, 2 without a change of variable and 2 with a change of variable scheme. As the concentration parameters into $\boldsymbol{\Omega}$ tend to infinity, the ratios between $\hat{c}_{\mathrm{CBQ,ISPA}}(\boldsymbol{\Omega})$, $\hat{c}_{\mathrm{CBQ,SPIA}}(\boldsymbol{\Omega})$, $\hat{c}_{\mathrm{CBQ,CVISPA}}(\boldsymbol{\Omega})$ and $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\boldsymbol{\Omega})$ and the true values of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ tend to unity and these results agree with that of Kume and Wood (2005), i.e.,

$$\lim_{\kappa\to\infty}\frac{\hat{c}_{\mathrm{CBQ,ISPA}}(\boldsymbol{\Omega})}{c_{\mathrm{CBQ}}(\boldsymbol{\Omega})} = \lim_{\kappa\to\infty}\frac{\hat{c}_{\mathrm{CBQ,SPIA}}(\boldsymbol{\Omega})}{c_{\mathrm{CBQ}}(\boldsymbol{\Omega})} = 1$$

and

$$\lim_{\kappa\to\infty}\frac{\hat{c}_{\mathrm{CBQ,CVISPA}}(\boldsymbol{\Omega})}{c_{\mathrm{CBQ}}(\boldsymbol{\Omega})} = \lim_{\kappa\to\infty}\frac{\hat{c}_{\mathrm{CBQ,CVSPIA}}(\boldsymbol{\Omega})}{c_{\mathrm{CBQ}}(\boldsymbol{\Omega})} = 1.$$

These practical remarks are shown in Fig. 2.

Table 1

Numerical results of the true values of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ and four proposed saddlepoint approximation techniques (Triangle case, $k = 3$).

λ_1	λ_2	κ	β	c_{CBQ} True	$\hat{c}_{\mathrm{CBQ}}$ ISPA	$\hat{c}_{\mathrm{CBQ}}$ SPIA	$\hat{c}_{\mathrm{CBQ}}$ CVISPA	$\hat{c}_{\mathrm{CBQ}}$ CVSPIA
0.4	3.6	0.5	0.2	19.89	12.56	11.92	14.41	12.22
1.6	14.4	2	0.8	8.22	5.41	5.07	6.11	5.12
4	36	5	2	3.29	2.34	2.22	2.68	2.35
8	72	10	4	1.65	1.29	1.21	1.33	1.26
12	108	15	6	1.09	0.90	0.85	0.94	0.86
20	180	25	10	0.66	0.57	0.55	0.59	0.57
60	540	75	30	0.22	0.20	0.19	0.21	0.20
80	720	100	40	0.17	0.15	0.14	0.16	0.15
100	900	125	50	0.14	0.12	0.11	0.13	0.12
140	1260	175	70	0.10	0.08	0.08	0.09	0.08
160	1440	200	80	0.09	0.07	0.07	0.08	0.07
200	1800	250	100	0.08	0.06	0.06	0.07	0.07
220	1980	275	110	0.07	0.05	0.05	0.07	0.06
400	3600	500	200	0.03	0.04	0.04	0.03	0.03

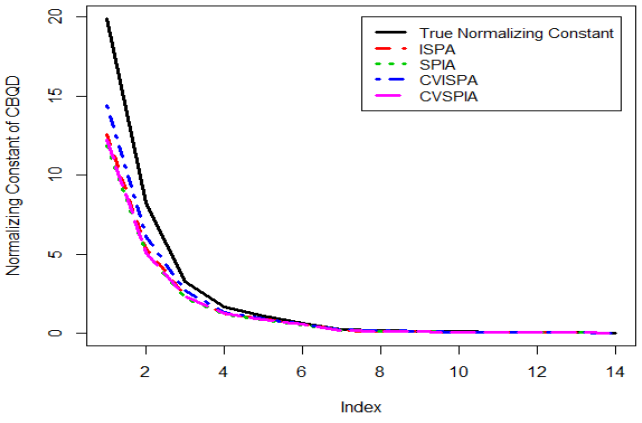

Fig. 1. Graphical representation for the numerical results of the true values of $c_{\mathrm{CBQ}}(\boldsymbol{\Omega})$ along with the numerical results of the four proposed saddlepoint approximation methods.

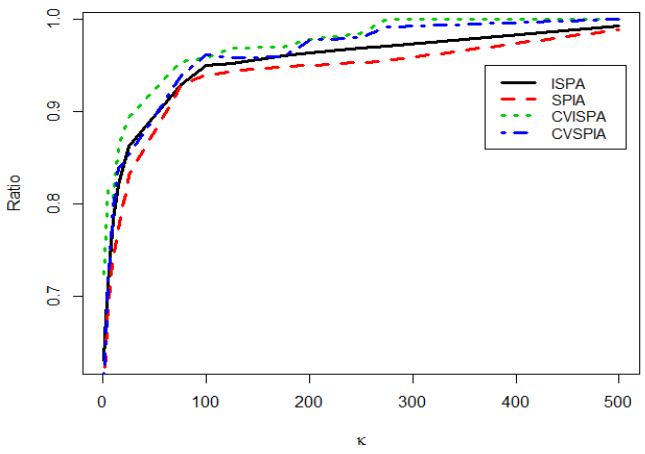

Fig. 2. Graphical representation for the ratios of the four saddlepoint approximation approaches with the true values of $c_{\mathrm{CBQ}}(\mathbf{\Omega})$.

For $k = 4$ labelled landmarks data of two dimensions, Table 2 shows numerical outputs of $\hat{c}_{\mathrm{CBQ,ISPA}}(\mathbf{\Omega})$, $\hat{c}_{\mathrm{CBQ,SPIA}}(\mathbf{\Omega})$, $\hat{c}_{\mathrm{CBQ,CVISPA}}(\mathbf{\Omega})$ and $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\mathbf{\Omega})$ with different values of low and high concentration parameters and $n = 1000$. All results of saddlepoint approximation methods under consideration are close to each other under high concentrations. However, the differences between $\hat{c}_{\mathrm{CBQ,CVISPA}}(\mathbf{\Omega})$ and $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\mathbf{\Omega})$ are closer than that of $\hat{c}_{\mathrm{CBQ,ISPA}}(\mathbf{\Omega})$ and $\hat{c}_{\mathrm{CBQ,SPIA}}(\mathbf{\Omega})$. It can be used the `system.time` function in R environment as a rough benchmark to compare the 4 saddlepoint approximation schemes with respect to the fastness of getting their numerical outputs. With increasing λ_1, λ_2, λ_3 and λ_4, the second-order saddlepoint integration approximation (SPIA), $\hat{c}_{\mathrm{CBQ,SPIA}}(\mathbf{\Omega})$ and second-order saddlepoint integration approximation (SPIA) with a change of variable, $\hat{c}_{\mathrm{CBQ,CVSPIA}}(\mathbf{\Omega})$ are faster than the second- order integrated saddlepoint approximation (ISPA), $\hat{c}_{\mathrm{CBQ,ISPA}}(\mathbf{\Omega})$ and second-order integrated saddlepoint approximation (ISPA) with a change of variable, $\hat{c}_{\mathrm{CBQ,CVISPA}}(\mathbf{\Omega})$.

4. Conclusions

In summary, the proposed saddlepoint approximation methods for the normalizing constant of the complex Bingham quartic distribution $c_{\mathrm{CBQ}}(\mathbf{\Omega})$ work well with or without a change of variable. Even though all the methods are based on second order saddlepoint approximations, nevertheless in practice the integrated saddlepoint approximation (ISPA) technique is more accurate than the saddlepoint integration approximation (SPIA) technique but the latter could be used for all concentration parameters of the complex Bingham quartic distribution with a slight reduction in computer time.

A change of variable scheme under second-order saddlepoint approximations has simplified the numerical integration method using Gauss-Legendre quadrature rule with equal or unequal weights and uniformly abscissas or nodes. It also has improved the precision rates of approximation for $c_{\mathrm{CBQ}}(\mathbf{\Omega})$ with an extra closeness of their numerical outputs under either low or high concentrations. For $k \geq 3$ labelled or unlabelled landmarks data in 2D, the four proposed saddlepoint approximation methods with and without a change of variable scheme yield reasonable and extremely accurate approximations to the normalizing constant of the CBQ distribution over the whole range of choices for the reduced concentration matrix $\mathbf{\Omega}$ with comparative ratios rise to unity when the concentration parameters tend to infinity.

Table 2

Numerical outputs of the four suggested saddlepoint approximation techniques ($k = 4$) for $c_{\mathrm{CBQ}}(\mathbf{\Omega})$.

λ_1	λ_2	λ_3	λ_4	$\hat{c}_{\mathrm{CBQ}}$ ISPA	$\hat{c}_{\mathrm{CBQ}}$ SPIA	$\hat{c}_{\mathrm{CBQ}}$ CVISPA	$\hat{c}_{\mathrm{CBQ}}$ CVSPIA
1	0	0	0	15.24	13.22	16.04	14.91
1	1	0	0	14.91	12.91	14.98	13.89
1	1	1	0	14.55	12.57	14.68	13.63
10	0	0	0	3.11	2.21	3.13	2.29
10	10	0	0	2.86	2.20	2.91	2.31
10	10	10	0	2.54	2.01	2.67	2.16
25	0	0	0	1.01	0.87	1.06	0.94
25	25	0	0	0.97	0.85	1.01	0.90
25	25	25	0	0.91	0.81	0.93	0.85
50	0	0	0	0.52	0.42	0.53	0.44
50	50	0	0	0.50	0.41	0.51	0.43
50	50	50	0	0.49	0.43	0.50	0.42
100	0	0	0	0.14	0.13	0.15	0.14
100	100	0	0	0.13	0.12	0.14	0.13
100	100	100	0	0.11	0.11	0.12	0.12

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