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On estimation of parameters for bivariate von Mises and toroidal wrapped Gaussian torus distributions: A simulation study

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Highlights

- Circular, spherical and torus data have many special and innovative characteristics, both in terms of modeling and statistical manipulations.
- Bivariate von Mises (BvMST) and toroidal wrapped Gaussian or normal (TWNT) distributions on torus are suitable in modeling directional and orientation data.
- Acceptance-rejection simulation method based on Bingham-angular central Gaussian (BACG) distribution as an envelope can effectively be used for generating random samples from bivariate von Mises sine (BvMST) distribution.
- The maximum likelihood (ML), maximum pseudolikelihood (MPL) and moments' (M) methods are applied to estimate the parameters of the BvMST distribution and the efficiency rates are numerically calculated under a range of own R routines.
- Jammalamadaka-SenGupta simulation technique is implemented in order to produce random samples from the TWNT distribution. Furthermore, a suggested trigonometric moments' (TM) method is used for parameter estimation on the basis of variances – covariances and evaluating the corresponding efficiency rates with the machine time significantly decreased. The proposed method gives adequate and efficient estimates with distinct values of parameters.

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ABSTRACT

The bivariate von Mises sine (BvMST) and toroidal wrapped Gaussian or normal (TWNT) distributions are defined on torus and they are applicable to statistical directional analysis of orientational data in 2D. The multivariate wrapped normal distribution in p -dimension has both multivariate marginal wrapped normal models and bivariate marginal wrapped normal distributions, and thus has a theoretical merit. One drawback of the wrapped normal torus (WNT) distribution is that, unlike the sine and cosine models, it does not form an exponential family and thus additional statistical and mathematical care is required to tackle the problem. The maximum likelihood (ML), maximum pseudolikelihood (MPL) and moments' (M) methods are numerically compared with respect to their efficiency rates for estimating the corresponding parameters of the BvMST distribution. Both MPL and M methods provide good estimates relative to the estimates of the ML method under an acceptance – rejection simulation scheme with Bingham-Angular Central Gaussian (BACG) distribution as an envelope. A proposed trigonometric moments' (TM) method is derived and utilized for the purpose of parameters estimation of the TWNT distribution as compared to the traditional maximum likelihood technique. It provides efficient estimates either in small or large simulated random samples.

1. Introduction

Directional angular data are widely used in a broad variety of modern statistical studies. A variety of well-known examples include the direction of waves in oceanography, the direction of winds in meteorology and the direction of animal movements in biology. Other examples can be found in fields such as bioinformatics, evolutionary biology, molecular sciences and astronomy. In addition, circular data often derive from periodic data, for instance, event times could be bundled up to a weekly duration to give a circular periodicity (e.g., Breckling, 1989; Zhan *et al.*, 2019).

In applied sciences, there are several problems where the amount of interest is calculated as a direction. Mardia (1972) is one of the most common sources in directional statistics and describes how this kind of data can be handled in a variety of areas. One vec-

tor of unit length can be considered as a simple example of the directional data. Virtually, the directional component can be border on an angle on a unit circle, given that the orientation of the circle has been chosen, and this type of data is often known as directional data. There are many features of the directional data in statistics. One aspect of this type of orientation data is that it cannot be analyzed using standard models in Euclidean space (Nodehi *et al.*, 2018). In other words, in comparison with popular Euclidean space, the researcher comes cross various topological properties. Mardia and Jupp (2000) and Jammalamadaka and SenGupta (2001) include theoretical developments in this area of statistics. Batschelet (1981) is a further significant guide.

1.1 Representation of Torus

In geometrical science, a torus is characterized as a surface of revolution formed by rotating a circle in three-dimensional space

around an axis that is in the same plane with the circle (Gallier and Xu, 2013). This means that it is a 2D surface and hence can be parametrized by two independent variables which are obviously the two angles $0 \leq \theta_1 < 2\pi$ in the x/y -plane, around the z -axis and $0 \leq \theta_2 < 2\pi$ around the x/y -plane. The torus can be mathematically described in parametric polar coordinates form by

$$\begin{aligned} x(\theta_1, \theta_2) &= (R + r \cos \theta_1) \cos \theta_2 \\ y(\theta_1, \theta_2) &= (R + r \cos \theta_1) \sin \theta_2 \\ z(\theta_1, \theta_2) &= r \sin \theta_1 \end{aligned} \quad (1)$$

in which θ_1 and θ_2 create angles making a full circle, so that their values start and terminate on the same point, R is the distance from the tube's center to the torus's center (major radius) and r is the tube's radius (minor radius).

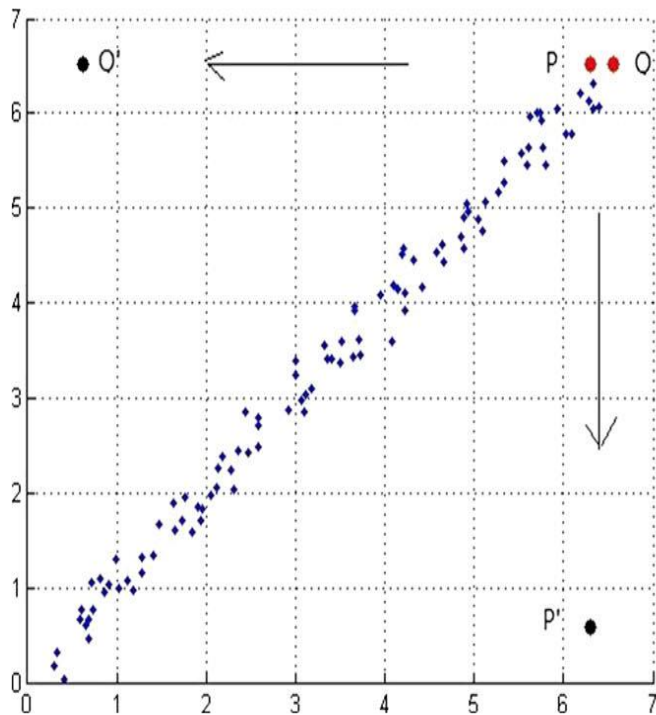
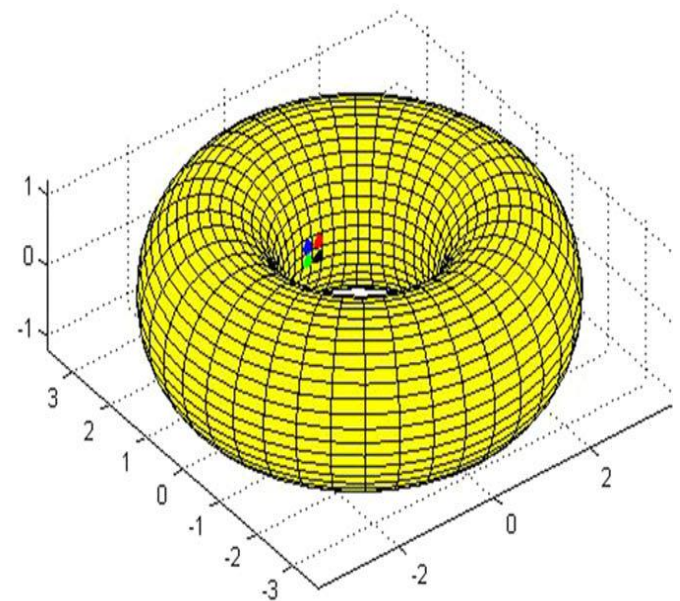


Fig.1. The different circumstances on the rectangle $[0, 2\pi] \times [0, 2\pi]$ and the torus (from Zhan et al., 2019).

There are three types of torus depending on the relative sizes of the minor radius, r and the major radius, R viz., the ring torus if $R > r$, horn torus if $R = r$ which is tangent to itself at the point $(0,0,0)$ and spindle torus if $R < r$ (e.g., Pinkall, 1986).

Bivariate circular data are represented on a torus as the 2-fold Cartesian product of unit circles i.e., $T^2 = S^1 \times S^1$ where it is defined with the interval $T^2 \equiv [0, 2\pi] \times [0, 2\pi] \equiv (-\pi, \pi) \times (-\pi, \pi)$ and therefore the four points $(0,0)$, $(0, 2\pi)$, $(2\pi, 0)$, $(2\pi, 2\pi)$ are overlapping. The torus clearly has a different topological structure to the rectangle $[0, 2\pi] \times [0, 2\pi]$. The correlation changes significantly after moving from P to P' and Q to Q' . For torus plotting, as shown in Fig. 1, the modified points, P' and Q' are very similar to the original ones, P and Q , respectively.



Two important directional distribution, the wrapped normal and the von Mises, match the Gaussian distribution on Euclidean circle space. The von Mises distribution, for instance, belongs to the exponential family and it is a natural circular analogue of the univariate normal distribution if the variability inside the circular variable is minimal. The conditional distributions are also von Mises in the multivariate framework, while its marginal distributions are not. Other circular distribution close to univariate normal is the wrapped Gaussian or normal (WN) distribution. By wrapping a normal distribution around the circle, this distribution is converted to a symmetrical wrapped normal distribution, but unfortunately it does not a member of exponential family. Fortunately, the convolution of p wrapped normal variables is also wrapped normal (e.g., Jammalamadaka and SenGupta, 2001; Nodehi et al., 2018).

Johnson and Wehrly (1978) suggest the toroidal (bivariate) wrapped normal distribution while Baba (1981) offers the multivariate wrapped normal distribution. Estimation of the wrapped Gaussian parameters including the univariate situations leads to face numerical tough solutions for finding a convergence of an infinite sum series. This is one of the major motives in which some authors, e.g., Fisher (1987) and Breckling (1989) proposed to approximate this distribution via the von Mises distribution. An alternative estimation approach based on moments is proposed in this paper.

1.2 Objectives

The core aims of this article are

- [1] To highlight some common estimation frameworks for the parameters of bivariate von Mises sine torus (BvMST) distribution viz., the maximum likelihood (ML), maximum pseudolikelihood (MPL) and moments' (M) methods,
- [2] To numerically compare the statistical relative efficiency rates of the MPL and M techniques in [1] with that for the traditional ML method after generating random samples using an efficient modern acceptance-rejection simulation method based on Bingham-angular central Gaussian (BACG) distribution as an envelope under either low or high concentrations,
- [3] To propose and derive the trigonometric moments for estimating the parameters of the toroidal wrapped normal torus (TWNT) distribution based on variances-covariances instead of ML and MPL methods due to their computational burden,
- [4] To numerically evaluate the efficiency rates for the suggested trigonometric moments' (TM) method in [3] as compared to the standard maximum likelihood (ML) after producing random samples using Jammalamadaka-SenGupta simulation plan with high precision and reliance.

2. Theoretical Background

In this section theoretic foundations from the modern literature on both the bivariate von Mises and toroidal wrapped Gaussian (normal) distributions on the torus are briefly discussed. They are the basis for statistical addressing the main targets of the current paper.

2.1 Bivariate von Mises Torus Distribution

A bivariate circular distribution for modeling torsional angles in molecules is proposed by Singh *et al.* (2002). Mardia (1975) and Mardia and Patrangenaru (2005) suggest an extended form of circular modeling but this particular case has some desirable properties among the negligible redundancy class. In the situation of two random angles $-\pi \leq \theta_1 < \pi$ and $-\pi \leq \theta_2 < \pi$ lie on the torus, the proposed bivariate von Mises probability density function is of the form

$$f(\theta_1, \theta_2) = [C(\kappa_1, \kappa_2, \mathbf{A})]^{-1} \exp\{\kappa_1 \cos(\theta_1 - \mu_1) + \kappa_2 \cos(\theta_2 - \mu_2) + [\cos(\theta_1 - \mu_1) \sin(\theta_2 - \mu_2)] \times \mathbf{A}[\cos(\theta_1 - \mu_1) \sin(\theta_2 - \mu_2)]^T\}, \quad (2)$$

where $\kappa_1 \geq 0$ and $\kappa_2 \geq 0$ describe the concentration parameters for the circular random variables θ_1 and θ_2 , $-\pi \leq \mu_1, \mu_2 < \pi$, the 2×2 matrix $\mathbf{A} = (a_{ij})$ contains parameters for the dependence between θ_1 and θ_2 and $C(\cdot)$ is a normalizing constant. This model has eight parameters. A variety of sub-models with only five parameters have been appeared (Singh *et al.*, 2002) to imitate the behavior of bivariate normal distribution with five parameters. Three sub-models are considered viz., the bivariate von Mises sine torus (BvMST), the bivariate von Mises cosine torus with positive intersection (BvMCTPI) and the bivariate von Mises cosine with negative intersection (BvMCTNI) distributions (Mardia *et al.*, 2007).

For simplicity and without loss of generality, assume that $a_{11} = a_{12} = a_{21} = a_{22} = \eta$ and $\mu_1 = \mu_2 = 0$. The corresponding probability density function for bivariate von Mises sine torus (BvMST) distribution can be written as

$$f_S(\theta_1, \theta_2) = [C(\kappa_1, \kappa_2, \eta)]^{-1} f_S^*(\theta_1, \theta_2)$$

where

$$C(\kappa_1, \kappa_2, \eta) = 4\pi^2 \sum_{m=0}^{\infty} \binom{2m}{m} \left(\frac{\eta}{2}\right)^{2m} \kappa_1^{-m} I_m(\kappa_1) \kappa_2^{-m} I_m(\kappa_2) \quad (3)$$

is the normalizing constant (Singh *et al.*, 2002), $I_m(\cdot)$ is a modified Bessel function of the first kind of order m and

$$f_S^*(\theta_1, \theta_2) = \exp\{\kappa_1 \cos \theta_1 + \kappa_2 \cos \theta_2 + \eta \sin \theta_1 \sin \theta_2\}. \quad (4)$$

The parameter $-\infty < \eta < \infty$ is a familiar measure of dependence between the circular random variables θ_1 and θ_2 . If $\eta = 0$, then θ_1 and θ_2 are independent with each having univariate von Mises distribution. Moreover, under considerable concentration with excluding the normalization constant, the probability density function for the bivariate von Mises sine torus (BvMST) distribution in Eq. 4 becomes

$$\begin{aligned} f_S^*(\theta_1, \theta_2) &\approx \exp\left[\kappa_1 \left(1 - \frac{\theta_1^2}{2}\right) + \kappa_2 \left(1 - \frac{\theta_2^2}{2}\right) + \eta \theta_1 \theta_2\right] \\ &= \exp(\kappa_1 + \kappa_2) \exp\left(-\frac{1}{2}(\kappa_1 \theta_1^2 + \kappa_2 \theta_2^2 + 2\eta \theta_1 \theta_2)\right) \\ &= C_1 \exp\left(-\frac{1}{2}[\theta_1 \ \theta_2] \begin{bmatrix} \kappa_1 & -\eta \\ -\eta & \kappa_2 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}\right) \\ &= C_1 \exp\left(-\frac{1}{2} \boldsymbol{\theta}^T \Sigma_1^{-1} \boldsymbol{\theta}\right), \end{aligned} \quad (5)$$

where $C_1 = \exp(\kappa_1 + \kappa_2)$, since

$$\cos \theta_i = 1 - \frac{\theta_i^2}{2!} + \frac{\theta_i^4}{4!} + O(\theta_i^6) \approx 1 - \frac{\theta_i^2}{2!}$$

and

$$\sin \theta_i = \theta_i - \frac{\theta_i^3}{3!} + \frac{\theta_i^5}{5!} + O(\theta_i^7) \approx \theta_i$$

for $i = 1, 2$ up two terms approximation. For Σ_1 to be existent positive definite matrix and for unimodality purpose, $\kappa_1 > 0$, $\kappa_2 > 0$, $-\infty < \eta < \infty$ and $\kappa_1 \kappa_2 > \eta^2$ should be held. The BvMST distribution is bimodal in the case of $\kappa_1 \kappa_2 < \eta^2$ (Singh *et al.*, 2002).

Assume that $a_{11} = a_{12} = a_{21} = a_{22} = \gamma_1$ and $\mu_1 = \mu_2 = 0$, the correspond probability density function for bivariate von Mises cosine torus distribution with positive interaction (BvMCTPI) is given by

$$f_{\text{CPI}}(\theta_1, \theta_2) = [C(\kappa_1, \kappa_2, \gamma_1)]^{-1} f_{\text{CPI}}^*(\theta_1, \theta_2)$$

where the normalizing constant $C(\kappa_1, \kappa_2, \gamma_1)$ has an explicit formula similar to that of Eq. 3 except η is replaced by γ_1 and

$$f_{\text{CPI}}^*(\theta_1, \theta_2) = \exp\{\kappa_1 \cos \theta_1 + \kappa_2 \cos \theta_2 + \gamma_1 \cos(\theta_1 - \theta_2)\} \quad (6)$$

In a similar manner to Eq. 5 and under considerable concentration with overlooking the normalizing constant, the probability density function for the bivariate von Mises cosine torus distribution with positive interaction (BvMCTPI) in Eq. 6 becomes

$$\begin{aligned} f_{\text{CPI}}^*(\theta_1, \theta_2) &= C_2 \exp\left(-\frac{1}{2}[\theta_1 \ \theta_2] \begin{bmatrix} \kappa_1 + \gamma_1 & -\gamma_1 \\ -\gamma_1 & \kappa_2 + \gamma_1 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}\right) \\ &= C_2 \exp\left(-\frac{1}{2} \boldsymbol{\theta}^T \Sigma_2^{-1} \boldsymbol{\theta}\right). \end{aligned} \quad (7)$$

where $C_2 = \exp(\kappa_1 + \kappa_2)$. For Σ_2 to be existent positive definite matrix, $\kappa_1 + \gamma_1 > 0$, $\kappa_2 + \gamma_1 > 0$ and $(\kappa_1 + \gamma_1)(\kappa_2 + \gamma_1) > \gamma_1^2$ should be held

Furthermore, suppose that $a_{11} = a_{12} = a_{21} = a_{22} = \gamma_2$ and $\mu_1 = \mu_2 = 0$, the correspond probability density function for the bivariate von Mises cosine torus distribution with negative interaction (BvMCTNI) is given by

$$f_{\text{CNI}}(\theta_1, \theta_2) = [C(\kappa_1, \kappa_2, \gamma_2)]^{-1} f_{\text{CNI}}^*(\theta_1, \theta_2)$$

where the normalizing constant $C(\kappa_1, \kappa_2, \gamma_2)$ has an explicit formula similar to that of Eq. 3 except η is replaced by γ_2 and

$$f_{\text{CNI}}^*(\theta_1, \theta_2) = \exp\{\kappa_1 \cos \theta_1 + \kappa_2 \cos \theta_2 - \gamma_2 \cos(\theta_1 - \theta_2)\} \quad (8)$$

(see, Kent *et al.*, 2008). In a similar manner to Eq. 5 and under considerable concentration with excluding the normalization constant, the probability density function for the bivariate von Mises cosine torus distribution with negative interaction (BvMCTNI) in Eq. 8 becomes

$$\begin{aligned} f_{\text{CNI}}^*(\theta_1, \theta_2) &= C_3 \exp\left(-\frac{1}{2}[\theta_1 \ \theta_2] \begin{bmatrix} \kappa_1 - \gamma_2 & \gamma_2 \\ \gamma_2 & \kappa_2 - \gamma_2 \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}\right) \\ &= C_3 \exp\left(-\frac{1}{2} \boldsymbol{\theta}^T \Sigma_3^{-1} \boldsymbol{\theta}\right). \end{aligned} \quad (9)$$

where $C_3 = \exp(\kappa_1 + \kappa_2)$. For Σ_3 to be existent positive definite matrix, $\kappa_1 - \gamma_2 > 0$, $\kappa_2 - \gamma_2 > 0$ and $(\kappa_1 - \gamma_2)(\kappa_2 - \gamma_2) > \gamma_2^2$ should be held. So, under large concentration about $\boldsymbol{\theta}^T = (\theta_1, \theta_2) = (0, 0)$, each of the three models behaves as a bivariate Gaussian distribution with inverse matrices, have the constraints of symmetric positive definiteness, of the form

$$\begin{aligned} \Sigma_1^{-1} &= \begin{bmatrix} \kappa_1 & -\eta \\ -\eta & \kappa_2 \end{bmatrix}, \quad \Sigma_2^{-1} = \begin{bmatrix} \kappa_1 + \gamma_1 & -\gamma_1 \\ -\gamma_1 & \kappa_2 + \gamma_1 \end{bmatrix}, \\ \Sigma_3^{-1} &= \begin{bmatrix} \kappa_1 - \gamma_2 & \gamma_2 \\ \gamma_2 & \kappa_2 - \gamma_2 \end{bmatrix}. \end{aligned}$$

When the fluctuations of variance in θ_1 and θ_2 are sufficiently small, then it follows that (θ_1, θ_2) in the BvMST distribution follows roughly a bivariate normal distribution with parameters

$$\sigma_1^2 = \frac{\kappa_2}{\kappa_1 \kappa_2 - \eta^2}, \quad \sigma_2^2 = \frac{\kappa_1}{\kappa_1 \kappa_2 - \eta^2}, \quad \rho = \frac{\eta}{(\kappa_1 \kappa_2)^{1/2}}$$

and (θ_1, θ_2) in the BvMCTPI distribution has approximately a bivariate normal distribution with parameters

$$\sigma_1^2 = \frac{\kappa_2 + \gamma_1}{(\kappa_1 + \gamma_1)(\kappa_2 + \gamma_1) - \gamma_1^2}, \quad \sigma_2^2 = \frac{\kappa_2 + \gamma_1}{(\kappa_1 + \gamma_1)(\kappa_2 + \gamma_1) - \gamma_1^2},$$

$$\rho = \frac{\gamma_1}{\{(\kappa_1 + \gamma_1)(\kappa_2 + \gamma_1)\}^{1/2}}$$

and so on.

2.1.1 Marginal and Conditional Probability Densities

The marginal and conditional probability functions are so important to discuss in this paper for the reason that the new simulation scheme suggested by Kent *et al.* (2018) for the bivariate von Mises sine and cosine distributions on torus depends upon deriving such functions and it is used into the generation process of random samples in this investigation.

Let the directional random variables θ_1 and θ_2 be distributed according to the probability density function of the BvMST distribution in Eq. 4. Define new parameters ψ and ω by $\kappa_2 = \psi \cos \omega$ and $\eta \sin \theta_1 = \psi \sin \omega$, so that

$$\psi = (\kappa_2^2 + \eta^2 \sin^2 \theta_1)^{1/2}, \quad \tan \omega = (\eta / \kappa_2) \sin \theta_1.$$

Write $\psi = \psi(\theta_1)$ and $\omega = \omega(\theta_1)$ to underline the dependent restriction on θ_1 . Then without loss of generalization, the marginal probability density function of θ_1 with overlooking the normalization constant for the BvMST distribution in Eq. 4 is given by

$$f_S^*(\theta_1) = \int_{-\pi}^{\pi} f_S^*(\theta_1, \theta_2) d\theta_2$$

$$= 2\pi I_0(\psi(\theta_1)) \exp(\kappa_1 \cos \theta_1) \quad (10)$$

where $I_0(\cdot)$ is a modified Bessel function of the first kind of order $m = 0$. The marginal density function of θ_2 can be derived in a similar way. Furthermore, the conditional probability density function of θ_2 given θ_1 is

$$f_S^*(\theta_2|\theta_1) = \frac{f_S^*(\theta_1, \theta_2)}{f_S^*(\theta_1)}$$

$$= \frac{1}{2\pi I_0(\psi(\theta_1))} \exp\{\psi(\theta_1) \cos(\theta_2 - \omega(\theta_1))\}. \quad (11)$$

Thus, the conditional probability density function of θ_2 given θ_1 in Eq. 11 is a von Mises distribution with concentration parameter $\psi(\theta_1)$ and mean angle $\omega(\theta_1)$.

The corresponding marginal and conditional probability density functions for the circular random variables θ_1 and θ_2 in both bivariate von Mises cosine torus with positive intersection (BvMCTPI) or negative intersection distributions (BvMCTNI) as shown in Eq. 6 and Eq. 8, respectively, can be derived using the same mathematical steps.

2.1.2 Log-Densities for Comparing Models

The bivariate probability density functions for the BvMST, BvMCTPI and BvMCTNI distributions can be depicted graphically by plotting contours i.e., a 3D surface $(\theta_1, \theta_2, f(\theta_1, \theta_2))$ in the plane by projecting the level curves $f(\theta_1, \theta_2) = c$ for selected constant c . The multivariate contour diagrams can be used to demonstrate certain comparative claims. The main features are more conveniently contrasted by plotting the logarithm probability densities with omitting the normalizing constants, as many statisticians

do not presume that missing the normalization constants would influence the results for comparison purposes (e.g., Mardia *et al.*, 2008). In addition, after multiplying it by a constant, the logarithm of any member of the exponential family of directional distributions does not mutate and the plots of the log densities will be visible even in the tails. The contour representation of the joint probability density function offers an insight into how the parameters index the concentrated amount of probability along the curve.

The values of parameters for each of the three probability distributions can be chosen to match any predetermined positive definite inverse covariance matrices viz., Σ_1^{-1} , Σ_2^{-1} and Σ_3^{-1} , respectively. Comparing the probability density functions of the three directional distributions yields,

- [1] altering the sign of η , γ_1 and γ_2 in the BvMST, BvMCTPI and BvMCTNI distributions, respectively, causes a reflection in the axes,
- [2] the bimodality of the BvMST distribution happens only if $\kappa_1 \kappa_2 < \eta^2$,
- [3] the bimodality of the BvMCTPI and BvMCTNI distributions occurs in the case of positive $\kappa_1 = \kappa_2$ with negative $\gamma_1 = \gamma_2$,
- [4] for small $\eta \approx -\gamma_1$ the BvMST and BvMCTPI distributions are approximately the same,
- [5] for large $\gamma_1 \approx -\gamma_2$ the BvMCTPI and BvMCTNI distributions are similar to each other,

the case of mutating (θ_1, θ_2) to $(\theta_2, -\theta_1)$ is similar to changing the sign of η in the BvMST model, but also enables the contour plots of the BvMST and BvMCTPI distributions to be rotated (which cannot be done by changing the values of the parameter of dependence, γ_1 (Mardia *et al.*, 2009).

2.2 Toroidal Wrapped Normal Torus Distribution

Assume that Θ is a unit vector of angles following a multivariate p -variate wrapped normal torus distribution; that is,

$$\theta_j = \mathbf{x}_j \bmod 2\pi \quad (12)$$

for $j = 1, 2, \dots, p$ where the modulo operation is performed componentwise and $\mathbf{x}$ has the multivariate probability density function with zero mean vector, $\boldsymbol{\mu} = (\mu_1, \mu_2, \dots, \mu_p)^T = (0, 0, \dots, 0)^T$ and $p \times p$ symmetric positive definite variance - covariance matrix $\boldsymbol{\Sigma} > \mathbf{0}$ (Kent *et al.*, 2009)

$$f_{MN}(\mathbf{x}; \boldsymbol{\Sigma}) = (2\pi)^{-\frac{p}{2}} |\boldsymbol{\Sigma}|^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \mathbf{x}^T \boldsymbol{\Sigma}^{-1} \mathbf{x}\right) \quad (13)$$

with $-\infty < x_j < \infty$. The probability density function for the multivariate wrapped normal torus (MWNT) distribution is given by

$$f_{MWNT}(\boldsymbol{\Theta}; \boldsymbol{\Sigma}) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \dots \sum_{k_p=-\infty}^{\infty} f_{MN}(\boldsymbol{\Theta} + 2\pi \mathbf{k}; \boldsymbol{\Sigma}) \quad (14)$$

where $\boldsymbol{\Theta} = (\theta_1, \theta_2, \dots, \theta_p)^T \in [0, 2\pi)^p$ and $\mathbf{k} = (k_1, k_2, \dots, k_p)^T$ is a set of integers (Johnson and Wehrly, 1977; Coles, 1998).

In the case $p = 2$, $\sigma_{11} = \sigma_{22} = \sigma^2 > 0$ and the $\sigma_{12} = \sigma_{21} = \sigma^2 \rho$, the probability density function in Eq. 14 is converted to a toroidal (bivariate) wrapped normal torus (TWNT) distribution for $\boldsymbol{\Theta} = (\theta_1, \theta_2)^T \in [0, 2\pi)^2$ with zero mean vector $\boldsymbol{\mu} = (\mu_1, \mu_2)^T = (0, 0)^T$, $\mathbf{k} = (k_1, k_2)^T$ and symmetric positive definite variance - covariance matrix

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma^2 & \sigma^2 \rho \\ \sigma^2 \rho & \sigma^2 \end{bmatrix}. \quad (15)$$

The corresponding probability density function for the toroidal (bivariate) wrapped normal torus (TWNT) distribution is

$$f_{\text{TWNT}}(\boldsymbol{\theta}; \boldsymbol{\Sigma}) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} f_{\text{MN}}((\theta_1, \theta_2)^T + 2\pi(k_1, k_2)^T; \boldsymbol{\Sigma}) \quad (16)$$

and the parameters to be estimated are σ^2 and the correlation coefficient between θ_1 and θ_2 , $-1 \leq \rho \leq 1$.

3. Materials and Methods

The first approach of inference for the bivariate von Mises sine torus (BvMST), the bivariate von Mises cosine torus with positive interaction (BvMCTPI) and the bivariate von Mises cosine torus with negative interaction (BvMCTNI) distributions as well as for the toroidal (bivariate) wrapped normal torus (TWNT) distribution is the statistical estimation. In this section, only three estimation methodologies for the parameters of only the BvMST and the TWNT distributions are briefly discussed.

3.1 Maximum Likelihood Technique

The ordinal protocol of statistical estimation is the maximum likelihood (ML) estimators dependent on a random sample of size n . For the bivariate von Mises sine torus (BvMST) distribution of zero means (omitted normalizing constant) as in Eq. 4, the ML estimators are obtained by maximizing or optimizing the likelihood function

$$L(\kappa_1, \kappa_2, \eta; \boldsymbol{\theta}) = \exp \left(\kappa_1 \sum_{i=1}^n \cos(\theta_{1i}) + \kappa_2 \sum_{i=1}^n \cos(\theta_{2i}) + \eta \sum_{i=1}^n \sin(\theta_{1i}) \sin(\theta_{2i}) \right). \quad (17)$$

The maximum likelihood estimators (MLE's) for κ_1 , κ_2 and η as well as the corresponding standard errors are numerically calculated under the `nlm` estimation routine in R from the Hessian matrix (Mardia et al., 2009)

$$\mathbf{H} = \begin{bmatrix} G_{\theta_1, \theta_1} & G_{\theta_1, \theta_2} \\ G_{\theta_2, \theta_1} & G_{\theta_2, \theta_2} \end{bmatrix} = \begin{bmatrix} -\kappa_1 \cos \theta_1 - \eta \sin \theta_1 \sin \theta_2 & \eta \cos \theta_1 \cos \theta_2 \\ \eta \cos \theta_1 \cos \theta_2 & -\kappa_2 \cos \theta_2 - \eta \sin \theta_1 \sin \theta_2 \end{bmatrix}.$$

The usual maximum likelihood (ML) estimators of σ^2 and ρ for the toroidal (bivariate) wrapped normal torus (TWNT) distribution in Eq. 16 are also acquired by optimizing the likelihood function

$$L = \prod_{i=1}^n \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} f_{\text{MN}}((\theta_{1i}, \theta_{2i})^T + 2\pi(k_1, k_2)^T; \boldsymbol{\Sigma}). \quad (18)$$

The optimization problem can be solved using numerical methods such as the Nelder - Mead simplex algorithm under R environment. This is quite computationally intensive, however. Also, as this mathematical issue is not convex, the results may depend upon the chosen initial value and no guarantee whatsoever that the global optimum will be found. Another proposed technique of numerical approximation is based on Jensen's inequality. This method has been applied to both the circular and the toroidal cases (Roy et al., 2014).

3.2 Maximum Pseudolikelihood Technique

Define the pseudolikelihood function (Besag, 1975) selected according to a random sample of size n for the bivariate von Mises sine torus (BvMST) distribution of zero means and omitted normalizing constant in Eq. 4 by

$$PL = (2\pi)^{-4} \prod_{j=1}^2 \prod_{i=1}^n \left(I_0(\kappa_{j,\text{rest}}^i) \right)^{-1} \exp(\kappa_{j,r}^i \cos(\theta_{ji})) \quad (19)$$

where $I_0(\cdot)$ is a modified Bessel function of the first kind of order $m = 0$ and

$$\kappa_{j,r}^i = \left(\kappa_j^2 + [\eta \sin(\theta_j)]^2 \right)^{1/2}.$$

The estimation of parameters based on the pseudolikelihood approach accomplishes by maximizing the PL function in Eq. 19 with respect to the only 3 unidentified parameters (Mardia et al., 2008).

The parameter estimation based on the maximum pseudolikelihood (MPL) approach for the toroidal (bivariate) wrapped normal torus (TWNT) distribution in Eq. 16 is deliberately excluded in this research because of presence several numerical problems of convergence for the infinite sums.

3.3 Moments' Technique

The approach of moments by Mardia et al. (2008) could be used to obtain good estimates for the parameters κ_1 , κ_2 and η of the bivariate von Mises sine torus (BvMST) distribution with zero means and omitted normalizing constant in Eq. 4. The reader can return back to that paper for extra detail.

A few approaches to parameter estimation for the toroidal (bivariate) wrapped normal torus (TWNT) distribution in Eq. 16 have been discussed in literature of directional statistics. Jammalamadaka and Sarma (1988) set forth a moment-based approach that unfortunately fails in many practically relevant cases by returning a matrix $\boldsymbol{\Sigma}$ that is not positive definite. The work in this paper produces an improvement to the method of estimation based on moments with a guarantee of positive definiteness for the variance - covariance matrix $\boldsymbol{\Sigma}$.

If $\boldsymbol{\delta}$ is 2×1 vector of integer coefficients and $\boldsymbol{\theta} = (\theta_1, \theta_2)^T$, then

$$\mathbb{E}[\cos(\boldsymbol{\delta}^T \boldsymbol{\theta})] = \exp \left(-\frac{1}{2} \boldsymbol{\delta}^T \boldsymbol{\Sigma} \boldsymbol{\delta} \right)$$

$$\mathbb{E}[\sin(\boldsymbol{\delta}^T \boldsymbol{\theta})] = 0.$$

In particular, for $j, k = 1, 2$, the first order trigonometric moments are

$$\mathbb{E}[\cos(\theta_1)] = \exp \left(-\frac{1}{2} \sigma_{11} \right) = c_1, \quad \text{say}$$

$$\mathbb{E}[\sin(\theta_1)] = 0$$

$$\mathbb{E}[\cos(\theta_2)] = \exp \left(-\frac{1}{2} \sigma_{22} \right) = c_2,$$

$$\mathbb{E}[\sin(\theta_2)] = 0$$

$$\mathbb{E}[\cos(\theta_1 \pm \theta_2)] = \exp \left(-\frac{1}{2} (\sigma_{11} \pm 2\sigma_{12} + \sigma_{22}) \right)$$

$$\mathbb{E}[\sin(\theta_1 \pm \theta_2)] = 0 \quad (20)$$

Let $\mathbf{c} = (c_1, c_2)^T$ be a vector and write $\mathbf{D} = \text{diag}(\mathbf{c})$. Merging the two forms of the last two equations yields the second order trigonometric moments

$$\mathbb{E}[\cos(\theta_1) + \cos(\theta_2)] = c_1 c_2 \cosh(\sigma_{12}) = a_{12}, \quad \text{say}$$

$$\mathbb{E}[\sin(\theta_1) + \sin(\theta_2)] = c_1 c_2 \sinh(\sigma_{12}) = b_{12}$$

$$\mathbb{E}[\sin(\theta_1) + \cos(\theta_2)] = 0 \quad (21)$$

where

$$\cosh(\sigma_{12}) = \left(\frac{e^{2\sigma_{12}} + 1}{2e^{\sigma_{12}}} \right) \quad \text{and} \quad \sinh(\sigma_{12}) = \left(\frac{e^{2\sigma_{12}} - 1}{2e^{\sigma_{12}}} \right).$$

Store the coefficients $\{a_{jk}\}$ and $\{b_{jk}\}$ in the symmetric squared matrices

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}.$$

The variance – covariance matrices, un form of a matrix, for the co-sines and sines can be written as

$$\text{var}(\cos \Theta) = \mathbf{DAD} - \mathbf{cc}^T$$

$$\text{var}(\sin \Theta) = \mathbf{DBD},$$

$$\text{cov}(\cos \Theta, \sin \Theta) = \mathbf{0}.$$

Thus, the variance – covariance matrix Σ in Eq. 15 can be retrieved from the trigonometric moments using the equation

$$\Sigma_{\Theta} = \sinh^{-1}(\mathbf{D}^{-1} \text{var}(\sin \Theta) \mathbf{D}^{-1}) \quad (22)$$

(Mardia et al., 2009). These results suggest the trigonometric moments' (TM) method for estimating Σ of the toroidal (bivariate) wrapped normal torus (TWNT) distribution from an $n \times 2$ matrix of torus data i.e.,

- [1] For the angles θ_1 and θ_2 , compute the sample first order trigonometric moments in Eq. 20 and rotate each angle, such that the points of the resultant vector are towards the positive horizontal x-axis.
- [2] For the angles θ_1 and θ_2 , calculate the sample second trigonometric moments in Eq. 21 and use Eq. 22 to produce an estimate of Σ_{Θ} i.e., $\hat{\Sigma}_{\Theta} = \hat{\Sigma}_{\Theta}$.

This modified estimation technique has an innovation to represent the first order and the second order trigonometric moments for the angles θ_1 and θ_2 in form of matrices which makes it easier to implement in R environment for assessing the corresponding efficiency rates relative to statistical estimators based on the maximum likelihood (ML) method.

3.4 Relative Efficiency Rate

The relative efficiency rate, $0 \leq \text{ER} \leq 1$, of the maximum pseudolikelihood and moments' estimates for the parameters of the bivariate von Mises sine torus (BvMST) distribution compared to the standard maximum likelihood method and for the parameters of the toroidal wrapped normal torus (TWNT) distribution as compared to the standard maximum likelihood method can be evaluated using the same approach of Wood (1993) for the Bingham distribution and Davison (2003). For the bivariate von Mises sine torus (BvMST) distribution, the first step of numerical calculation of the relative efficiency rate under R environment is finding the Fisher information matrices based on ML, MPL and moment (M) methods and denoted by $I_{\text{ML}}(\kappa_1, \kappa_2, \eta)$, $I_{\text{MPL}}(\kappa_1, \kappa_2, \eta)$ and $I_{\text{M}}(\kappa_1, \kappa_2, \eta)$, respectively. Thus, the efficiency rate of estimation based on MPL method relative to estimation based on ML method can be obtained as

$$\text{RER}_{\text{MPL}|\text{ML}} = \frac{I_{\text{MPL}}(\kappa_1, \kappa_2, \eta)}{I_{\text{ML}}(\kappa_1, \kappa_2, \eta)}. \quad (23)$$

Moreover, the efficiency rate of estimation based on M method relative to estimation based on ML method can also be obtained as

$$\text{RER}_{\text{M}|\text{ML}} = \frac{I_{\text{M}}(\kappa_1, \kappa_2, \eta)}{I_{\text{ML}}(\kappa_1, \kappa_2, \eta)}. \quad (24)$$

For the toroidal wrapped normal torus (TWNT) distribution, the efficiency rate estimation based on trigonometric moments

(TM) method relative to estimation based on maximum likelihood (ML) method can also be obtained as

$$\text{RER}_{\text{TM}|\text{ML}} = \frac{I_{\text{TM}}(\sigma^2, \rho)}{I_{\text{ML}}(\sigma^2, \rho)}. \quad (25)$$

4. Results and Discussion

The investigation in the current article depends upon generating random samples from both the bivariate von Mises sine torus (BvMST) distribution in Eq. 4 and the toroidal wrapped normal torus (TWNT) distribution in Eq. 16.

The simulation from the BvMST distribution is implemented in R environment according to the acceptance – rejection (AR) simulation approach of Kent et al. (2018) using Bingham–Angular Central Gaussian (BACG) distribution as an envelope.

The simulation from the TWNT distribution is straightforward. $x_j, j = 1, 2$ is simulated from the bivariate normal distribution $f_{\text{MN}}(\mathbf{x}; \Sigma)$ in Eq. 13 with $p = 2$ using Choleski factorization or spectral decomposition or singular value decomposition methods and then the simulated angles θ_1 and θ_2 formed componentwise by Eq. 12 and simulation steps are repeated until getting the required random sample of size n . The simulation scheme is suggested by Jammalamadaka and SenGupta (2001).

For the bivariate von Mises sine torus (BvMST) distribution, the above suggested simulation scheme is implemented in R routine for each configuration (κ, η) and a random sample of size $n = 100$ is generated. Furthermore, for assessing the relative efficiencies of the maximum pseudolikelihood and moments' techniques in comparison with the traditional maximum likelihood for the parameters of the bivariate von Mises sine torus (BvMST) distribution in Eq. 4, assume that the concentration parameters $\kappa_1 = \kappa_2 = \kappa$, say, are unknown, $\mu_1 = \mu_2 = 0$ is known and η is unknown. Table 1 gives numerical relative efficiency rates of estimation based on MPL method compared to estimation based on ML method for the bivariate von Mises sine torus distribution with $\kappa_1 = \kappa_2 = \kappa = 1, 2, \dots, 15$ and $\eta = 0.5, 1, 2, 4, 6, 8, 10$. Fig. 2 graphically presents the corresponding relative efficiency rates in Table 1. It is clear from both Table 1 and Fig. 2 that for small η the efficiency rates of MPL method in comparison with the ML method are close to unity i.e., both MPL and ML have the same efficiency rates. If $\eta = 0$, the efficiency rate of the MPL relative to the ML method is unity i.e. it has full efficient relative level, since in this case $f_S^*(\theta_1, \theta_2) = f_S^*(\theta_1|\theta_2) f_S^*(\theta_2|\theta_1)$.

The aforementioned improvement in efficiency rate as κ increases should therefore only be expected to occur, for fixed η , for those regions in Fig. 2 in which $\kappa > \eta$. This is indeed the case, and the efficiency rate is greater than 0.90 for all pairs of configurations (κ, η) in Fig. 2. For $\kappa < \eta$, the joint probability distribution of the angles θ_1 and θ_2 is bimodal, and in this situation the efficiency appears to be a quadratic function of κ , with greater efficiency rates for small κ and κ close to η . Table 2 also shows numerical relative efficiency rates of estimation based on M method as compared to estimation based on ML method for the bivariate von Mises sine torus (BvMST) distribution with $\kappa_1 = \kappa_2 = \kappa = 1, 2, \dots, 15$ and $\eta = 0.5, 1, 2, 4, 6, 8, 10$. Similar comments can be written for the numerical estimates in Table 2 close to the remarks on the findings in Table 1 although the MPL method seems more efficient than the M method when using the statistical criteria of comparison between the efficiency rates in subsection 3.4.

Table 1

The numerical relative efficiency rates of estimation based on MPL method compared to estimation based on ML method for the bivariate von Mises sine torus (BvMST) distribution with $\kappa_1 = \kappa_2 = \kappa = 1, 2, \dots, 15$ and $\eta = 0.5, 1, 2, 4, 6, 8, 10$.

	$\eta = 0.5$	$\eta = 1$	$\eta = 2$	$\eta = 4$	$\eta = 6$	$\eta = 8$	$\eta = 10$
κ	$RER_{MPL/ML}$	$RER_{MPL/ML}$	$RER_{MPL/ML}$	$RER_{MPL/ML}$	$RER_{MPL/ML}$	$RER_{MPL/ML}$	$RER_{MPL/ML}$
1	0.96	0.94	0.92	0.90	0.94	0.96	0.98
2	0.97	0.94	0.95	0.89	0.91	0.95	0.96
3	0.97	0.95	0.95	0.91	0.88	0.91	0.95
4	0.97	0.97	0.96	0.94	0.90	0.87	0.91
5	0.98	0.97	0.97	0.95	0.93	0.86	0.87
6	0.98	0.97	0.97	0.95	0.95	0.88	0.85
7	0.98	0.98	0.97	0.95	0.95	0.92	0.86
8	0.98	0.98	0.98	0.96	0.95	0.95	0.87
9	0.98	0.98	0.98	0.96	0.95	0.96	0.91
10	0.98	0.98	0.98	0.97	0.96	0.97	0.92
11	0.99	0.98	0.98	0.97	0.96	0.97	0.92
12	0.99	0.98	0.98	0.97	0.97	0.98	0.95
13	0.99	0.98	0.98	0.97	0.97	0.98	0.96
14	0.99	0.99	0.98	0.97	0.97	0.99	0.97
15	0.99	0.99	0.98	0.98	0.97	0.99	0.98

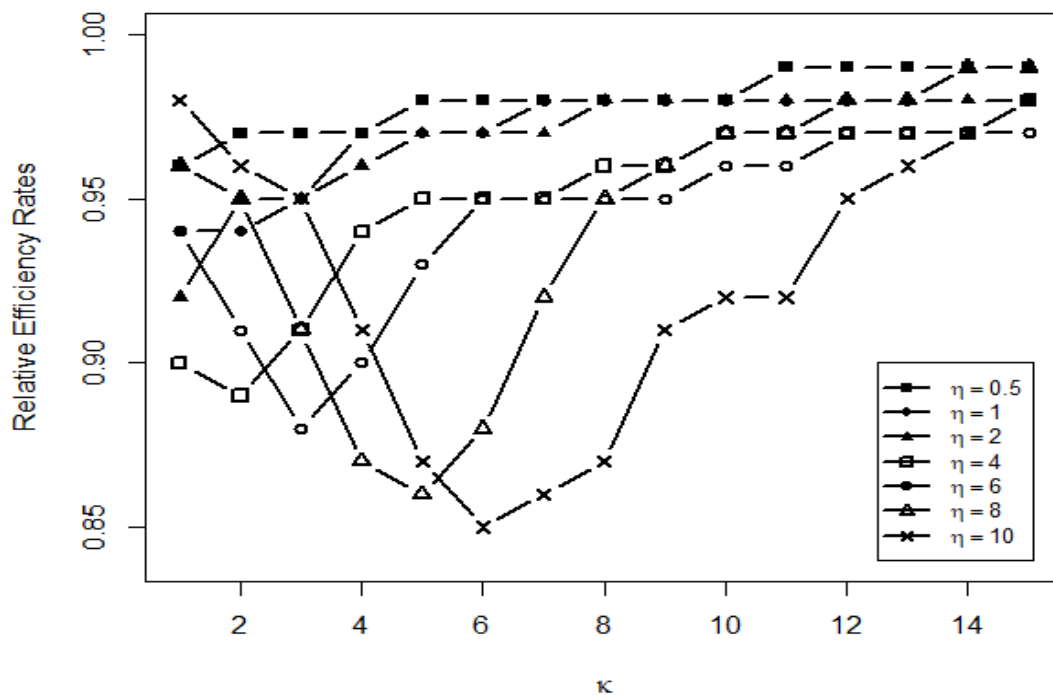


Fig 2. The efficiency rates of estimation based on MPL method compared to estimation based on ML method for the bivariate von Mises sine torus distribution with $\kappa_1 = \kappa_2 = \kappa = 1, 2, \dots, 15$ and $\eta = 0.5, 1, 2, 4, 6, 8, 10$.

Table 2

The numerical relative efficiency rates of estimation based on moments' (M) method compared to estimation based on ML method for the bivariate von Mises sine torus (BvMST) distribution with $\kappa_1 = \kappa_2 = \kappa = 1, 2, \dots, 15$ and $\eta = 0.5, 1, 2, 4, 6, 8, 10$.

κ	$\eta = 0.5$	$\eta = 1$	$\eta = 2$	$\eta = 4$	$\eta = 6$	$\eta = 8$	$\eta = 10$
	RER _{M ML}	RER _{M ML}	RER _{M ML}	RER _{M ML}	RER _{M ML}	RER _{M ML}	RER _{M ML}
1	0.86	0.84	0.81	0.80	0.81	0.87	0.90
2	0.86	0.84	0.82	0.77	0.80	0.86	0.91
3	0.87	0.86	0.82	0.79	0.77	0.88	0.91
4	0.87	0.87	0.83	0.81	0.80	0.85	0.91
5	0.88	0.88	0.83	0.82	0.82	0.84	0.91
6	0.89	0.88	0.83	0.82	0.83	0.83	0.89
7	0.89	0.88	0.84	0.82	0.83	0.85	0.89
8	0.89	0.89	0.84	0.83	0.83	0.81	0.89
9	0.89	0.89	0.85	0.83	0.83	0.82	0.91
10	0.90	0.89	0.85	0.84	0.84	0.80	0.92
11	0.90	0.91	0.86	0.84	0.84	0.86	0.92
12	0.91	0.91	0.86	0.84	0.84	0.86	0.93
13	0.91	0.91	0.86	0.85	0.85	0.87	0.94
14	0.92	0.92	0.87	0.85	0.85	0.90	0.95
15	0.92	0.92	0.88	0.86	0.85	0.91	0.95

For the toroidal wrapped normal torus (TWNT) distribution, the acceptance – rejection simulation scheme with BACG distribution as an envelope is implemented in  routine for each configuration (σ^2, ρ) from 10 random sample of size $n = 100$ and from other 10 random samples of size $n = 1000$. Table 3 provides the numerical relative efficiency rates of estimation based on the trigonometric moments' (TM) method compared to estimation based on ML method for the toroidal wrapped normal torus (TWNT) distribution with different values of σ^2 and ρ . It is clear that the relative efficiency rates are improved for $n = 1000$ as compared to the

random sample of size $n = 100$ i.e., the determined size of any random sample from the TWNT distribution under this simulation scheme has a direct positive impact on the efficiency rates for the trigonometric moments' method of estimation. Moreover, for fixed σ^2 , the estimates of the trigonometric moments' method are also improved with increasing ρ . The results in Table 3 show also that for fixed ρ , the trigonometric moments' method seem to have good estimates with increasing σ^2 in comparison with the ML method.

Table 3

The numerical relative efficiency rates of estimation based on trigonometric moments' (TM) method compared to estimation based on ML method for the toroidal wrapped normal torus (TWNT) distribution with different values of σ^2 and ρ .

True Values of Parameters			TMM Estimates		Relative Efficiency Rates (RER _{TM ML})
σ^2	ρ	n	$\hat{\sigma}_{TMM}^2$	$\hat{\rho}_{TMM}$	
1.00	0.05	100	0.75	0.02	0.52
1.00	0.30	100	0.79	0.20	0.57
10.0	0.05	100	7.11	0.02	0.61
10.0	0.30	100	7.82	0.21	0.64
10.0	0.50	100	7.95	0.37	0.66
10.0	0.70	100	8.02	0.58	0.69
10.0	0.90	100	8.13	0.76	0.73
50.0	0.50	100	39.1	0.41	0.75
50.0	0.70	100	41.8	0.60	0.78
50.0	0.90	100	42.8	0.79	0.81

True Values of Parameters			TMM Estimates		Relative Efficiency Rates (RER _{TM ML})
σ^2	ρ	n	$\hat{\sigma}_{TMM}^2$	$\hat{\rho}_{TMM}$	
1.00	0.05	1000	0.84	0.03	0.61
1.00	0.30	1000	0.86	0.24	0.68
10.0	0.05	1000	8.34	0.03	0.71
10.0	0.30	1000	8.77	0.25	0.78
10.0	0.50	1000	8.83	0.42	0.79
10.0	0.70	1000	8.93	0.62	0.83
10.0	0.90	1000	9.31	0.81	0.86
50.0	0.50	1000	42.1	0.44	0.89
50.0	0.70	1000	45.1	0.64	0.90
50.0	0.90	1000	46.7	0.84	0.94

5. Conclusions

In summary, the special features of the bivariate von Mises sine torus (BvMST) and the toroidal wrapped normal torus (TWNT) distributions are briefly discussed. Three possible estimation techniques for their parameters are presented viz., the maximum likelihood (ML), maximum pseudolikelihood (MPL) and moments' (M) methods. The ML, MPL and M methods are numerically compared with respect to their efficiency rates for estimating the corresponding parameters of BvMST distribution. Both PML and M methods yield reasonable and extremely accurate numerical estimates relative to the estimates of ML method with supporting an acceptance-rejection (AR) simulation scheme and using BACG distribution as an envelope.

The trigonometric moments' method seems to provide numerical estimates for the parameters of the TWNT model after implementation the Jammalamadaka-SenGupta simulation scheme with acceptable accuracy at a small computational cost as compared to the traditional ML technique. Most statistical estimation approaches can, in principle, be generalized to the p -torus, but parameter estimation on this product manifold is still an open issue due to the exponential computational complexity when dealing with high dimensions, whereas others may have an increasing difficulty of obtaining a positive definite parameter matrix such as Σ . The Expectation-Maximization (EM) and Markov Chain Monte Carlo (MCMC) numerical algorithms are alternative techniques for future investigations on the high dimensional manifolds and could be used to get parameters' estimates for all probability density functions of the BvMST, BvMCTPI, BvMCTNI and TWTN models.

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