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Measuring Sphericity in Positive Semi-Definite Matrices

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Abstract: The measure of sphericity for positive semi-definite matrices plays a crucial role in understanding their geometric properties, especially in high-dimensional settings. This paper introduces a robust measure of sphericity, which remains invariant under orthogonal transformations and scaling. We explore its behavior in finite-dimensional cases. Additionally, we investigate the stochastic case by considering a normal distribution, analyzing the asymptotic normality of random matrices and its implications on the convergence properties of the proposed measure.

Keywords: sphericity; positive semi-definite matrices; matrix theory; statistical analysis

MSC: 15B48; 60B20

1. Introduction

The study of sphericity is a fundamental problem in multivariate analysis, with applications in various fields such as statistics, for example, in repeated measures ANOVA, where it is assumed that the variances of the differences between all combinations of related groups are equal; in engineering, for example, in signal processing, where often sphericity is assumed to ensure that the noise in the signals is uniformly distributed; and computer science, particularly in machine learning, where the concept of sphericity is applied in clustering algorithms like k-means. Moreover, sphericity is a stronger assumption than the homogeneity of variances. Suppose you have k samples with the same size. The data are said to have the property of sphericity if the pairwise differences in variance between the samples are all equal. If sphericity is violated, the calculations of variance can be distorted. Therefore, the need to measure sphericity plays a fundamental role in several statistical problems. Sphericity tests have been extensively studied in the literature, and several measures have been proposed to assess the degree of sphericity in a matrix. For example, Dawid [1] considered an inference about the parameters of a multivariate linear model, in which the usual assumption of normality for the errors was replaced by a weaker assumption of spherical symmetry. Two Tukey multiple comparison procedures, as well as a Bonferroni and multivariate approach, were compared for their rates of Type I error and any-pairs power when multisample sphericity was not satisfied, and the design was unbalanced in Keselman and Keselman [2]. Cornell et al. [3] conducted a Monte Carlo simulation to investigate the relative power of eight tests for sphericity in randomized block designs. Chen et al. [4] proposed nonparametric tests, assuming a specific parametric distribution for the data, for the sphericity and identity of high-dimensional covariance matrices. A test for the null of sphericity in a fixed effects panel data model is presented in Baltagi et al. [5]. Onatski et al. [6] studied the asymptotic power of tests of sphericity against perturbations in a single unknown direction as both the dimensionality of data and the number of observations go to infinity. The problem of testing the null hypothesis of sphericity of a high-dimensional covariance matrix against an alternative of unspecified multiple symmetry-breaking directions (multispiked alternatives) was considered



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in Onatski et al. [7]. Zou et al. [8] proposed tests for sphericity in cases where the data dimension is larger than the sample size.

In this paper, we propose a measure of sphericity, denoted $\theta(\mathbf{M})$. Additionally, we include a comparison between the proposed measure and other widely used measures of sphericity, namely, the Frobenius measure and the spectral measure.

While existing measures for sphericity are valuable, our proposed measure is tailored specifically for positive semi-definite matrices and offers insights into their geometric properties that traditional measures may not capture. Traditional measures are often designed for symmetric matrices, particularly covariance matrices in factor analysis, and may not adequately address the unique challenges of positive semi-definite matrices. In contrast, our measure $\theta(\mathbf{M})$ directly considers the spread of eigenvalues, providing a range from 0 to 1 and offering a clear interpretation of the degree of sphericity. Additionally, it exhibits desirable properties such as invariance under orthogonal transformations and scaling, making it suitable for various statistical and machine learning tasks in high-dimensional settings.

The remainder of this paper is organized as follows: In Section 2, we introduce the measure of sphericity $\theta(\mathbf{M})$ and establish its properties in finite-dimensional cases. In Section 3, we extend our analysis to high-dimensional scenarios and examine the behavior of the proposed measure as the dimensionality increases. In Section 4, we explore the stochastic case and investigate the convergence properties of the sphericity measure for sequences of random matrices. In Section 5, we present a numerical comparison between the proposed approach and the Frobenius and the spectral measures. Finally, in Section 6, we provide some final remarks.

2. Measure of Sphericity for Positive Semi-Definite Matrices

In this section, we introduce a measure of sphericity for positive semi-definite matrices. Let $S_k [S_k^+]$ denote the family of $k \times k$ positive semi-definite [definite] matrices. Given $\mathbf{M} \in S_k$, let

$$\mathbf{v}(\mathbf{M}) = (v_1, \dots, v_k)$$

be the vector of its eigenvalues. Consequently, the trace and norm of $\mathbf{M}$ are given by

$$\text{tr}(\mathbf{M}) = \sum_{j=1}^k v_j$$

and

$$\|\mathbf{M}\| = \sqrt{\sum_{j=1}^k v_j^2},$$

respectively.

Defining the Frobenius measure as

$$\psi(\mathbf{M}) = \frac{\|\mathbf{M}\|^2}{\text{tr}^2(\mathbf{M})}, \quad (1)$$

we now establish

Proposition 1. *If $\mathbf{M} \in S_k$ then we have $\frac{1}{k} \leq \psi(\mathbf{M}) \leq 1$.*

Proof. Let $\mathbf{M} \in S_k$ with eigenvalues $\mathbf{v}(\mathbf{M}) = (v_1, \dots, v_k)$. Using Lagrange multipliers to minimize $\sum_{j=1}^k v_j^2$ subject to $\sum_{j=1}^k v_j = d$, we have

$$\mathcal{L}(v_1, \dots, v_k, \lambda) = \sum_{j=1}^k v_j^2 - \lambda \left(\sum_{j=1}^k v_j - d \right).$$

Solving $\frac{\partial \mathcal{L}}{\partial v_j} = 2v_j - \lambda = 0$ gives $v_j = \frac{\lambda}{2}$, and since $\lambda = \frac{2d}{k}$, we obtain $v_j = \frac{d}{k}$. Thus,

$$\sum_{j=1}^k v_j^2 = \frac{d^2}{k}, \quad \text{tr}(\mathbf{M}) = d.$$

Therefore,

$$\psi(\mathbf{M}) = \frac{\|\mathbf{M}\|^2}{\text{tr}^2(\mathbf{M})} = \frac{1}{k}.$$

Now, since $v_j \geq 0$ for all j ,

$$\|\mathbf{M}\|^2 = \sum_{j=1}^k v_j^2 \leq \left(\sum_{j=1}^k v_j \right)^2 = \text{tr}^2(\mathbf{M}).$$

Thus,

$$\psi(\mathbf{M}) = \frac{\|\mathbf{M}\|^2}{\text{tr}^2(\mathbf{M})} \leq 1$$

and so we obtain

$$\frac{1}{k} \leq \psi(\mathbf{M}) \leq 1$$

and the proof is completed. $\square$

We can now use

$$\theta(\mathbf{M}) = \frac{1 - \psi(\mathbf{M})}{1 - \frac{1}{k}} \quad (2)$$

to measure the sphericity of $\mathbf{M}$.

When $\psi(\mathbf{M}) = 1$, indicating maximum anisotropy, $\theta(\mathbf{M})$ equals 0. On the other hand, when $\psi(\mathbf{M}) = \frac{1}{k}$, indicating perfect sphericity, $\theta(\mathbf{M})$ equals 1. Therefore, $\theta(\mathbf{M})$ ranges from 0 to 1, where higher values signify greater sphericity. This bounded interval, $0 \leq \theta(\mathbf{M}) \leq 1$, ensures a clear and interpretable metric for assessing the sphericity of a given matrix $\mathbf{M}$.

Referring to Puntanen et al. [9], if $\mathbf{P}$ is an orthogonal matrix, then, $\mathbf{PMP}^\top$ will have the same eigenvalues as $\mathbf{M}$. Consequently, we have

$$\begin{cases} \text{tr}(\mathbf{PMP}^\top) = \text{tr}(\mathbf{M}) \\ \|\mathbf{PMP}^\top\| = \|\mathbf{M}\| \end{cases}$$

and thus, according to Equation (1),

$$\psi(\mathbf{PMP}^\top) = \psi(\mathbf{M}).$$

From this, it follows that

$$\theta(\mathbf{PMP}^\top) = \theta(\mathbf{M}).$$

This invariance under orthogonal transformations implies that $\theta(\mathbf{M})$ is a geometric property of the matrix that does not depend on the coordinate system, making it a robust measure for assessing the sphericity of positive semi-definite matrices.

It is clear that, if $c > 0$, we have

$$\begin{cases} \psi(c\mathbf{M}) = \psi(\mathbf{M}) \\ \nu(c\mathbf{M}) = c\nu(\mathbf{M}) \end{cases}$$

and hence,

$$\theta(c\mathbf{M}) = \theta(\mathbf{M}).$$

This property indicates that $\theta(\mathbf{M})$ is a scale-invariant measure.

Representing the Kronecker matrix product by $\otimes$, when $\mathbf{M}_l \in S_{k_l}$, $l = 1, 2$, we have

$$\mathbf{v}(\mathbf{M}_1 \otimes \mathbf{M}_2) = \mathbf{v}(\mathbf{M}_1) \otimes \mathbf{v}(\mathbf{M}_2),$$

so that

$$\begin{cases} \text{tr}(\mathbf{M}_1 \otimes \mathbf{M}_2) = \text{tr}(\mathbf{M}_1)\text{tr}(\mathbf{M}_2) \\ \|\mathbf{M}_1 \otimes \mathbf{M}_2\|^2 = \|\mathbf{M}_1\|^2\|\mathbf{M}_2\|^2 \end{cases}$$

and that

$$\psi(\mathbf{M}_1 \otimes \mathbf{M}_2) = \psi(\mathbf{M}_1)\psi(\mathbf{M}_2).$$

Thus,

$$\theta(\mathbf{M}_1 \otimes \mathbf{M}_2) = \theta(\mathbf{M}_1)\theta(\mathbf{M}_2).$$

This multiplicative property under Kronecker products is useful in higher-dimensional sphericity measures.

Let us now establish

Proposition 2. *Given $\mathbf{M}_1, \mathbf{M}_2$ symmetric $k \times k$ matrices, we have $\mathbf{v}(\mathbf{M}_1) = \mathbf{v}(\mathbf{M}_2)$ if, and only if, $\mathbf{M}_2 = \mathbf{P}\mathbf{M}_1\mathbf{P}^\top$, with $\mathbf{P}$ orthogonal.*

Proof. If matrix $\mathbf{P}$ exists, it diagonalizes both $\mathbf{M}_1$ and $\mathbf{M}_2$, resulting in equal eigenvalues $\mathbf{v}(\mathbf{M}_1) = \mathbf{v}(\mathbf{M}_2)$. Let $\mathbf{P}$ be such that $\mathbf{P}\mathbf{M}_1\mathbf{P}^\top = D(\mathbf{v})$, where $D(\mathbf{v})$ is a diagonal matrix with the eigenvalues of $\mathbf{M}_1$ on its diagonal.

Then, we have $\mathbf{M}_2 = \mathbf{P}^\top D(\mathbf{v})\mathbf{P}$. Since $\mathbf{P}$ is orthogonal, its transpose is its inverse, so $\mathbf{M}_2 = \mathbf{P}^\top \mathbf{P}\mathbf{M}_1\mathbf{P}^\top \mathbf{P}$.

Since $\mathbf{P}^\top \mathbf{P}$ is orthogonal, denoted by $\mathbf{Q}$, we have $\mathbf{M}_2 = \mathbf{Q}\mathbf{M}_1\mathbf{Q}^\top$, where $\mathbf{Q}$ is orthogonal, completing the proof. $\square$

Let us denote

$$\mathbf{M}_1 = \mathbf{M}_2$$

if their eigenvalues, ordered in decreasing order, are equal. This establishes an equivalence relation, as confirmed by Proposition 2. Under this relation, if $\mathbf{M}_1 = \mathbf{M}_2$, we observe that

$$\psi(\mathbf{M}_1) = \psi(\mathbf{M}_2),$$

as well as

$$\theta(\mathbf{M}_1) = \theta(\mathbf{M}_2).$$

This implies that $\theta(\mathbf{M})$ is solely determined by the eigenvalues of $\mathbf{M}$, independent of its specific structure or arrangement. Thus, the metric $\theta(\mathbf{M})$ offers a robust assessment of sphericity, relying solely on the intrinsic properties of the matrix's eigenvalues.

3. High-Dimensional Case

In this section, we extend our discussion to the high-dimensional case, where k becomes large. We explore whether there are notable differences between the finite k case and the scenario where k tends to infinity. Additionally, we investigate the properties exhibited when k is large.

In the finite k scenario, the measure $\theta(\mathbf{M})$ effectively ranges between 0 and 1, allowing us to discern varying degrees of sphericity among matrices. However, as k approaches infinity, distinct behaviors emerge in the properties of $\theta(\mathbf{M})$.

Let us start by examining the expression for $\theta(\mathbf{M})$, given in Equation (2). The behavior of $\theta(\mathbf{M})$ is influenced by the behavior of $\psi(\mathbf{M})$. As k approaches infinity, we need to analyze how $\psi(\mathbf{M})$ behaves, which can be analyzed based on the relative magnitudes of the Frobenius norm and the trace of $\mathbf{M}$.

For any matrix $\mathbf{M}$, the inequality $\|\mathbf{M}\|^2 \geq \text{tr}^2(\mathbf{M})$ holds, with equality only when $\mathbf{M}$ is a scalar multiple of the identity matrix. As k tends to infinity, this inequality becomes

increasingly significant for non-scalar multiples of the identity matrix. Consequently, $\psi(\mathbf{M})$ tends towards 1 for matrices deviating from being scalar multiples of the identity, reflecting their departure from sphericity. Conversely, for matrices closely resembling scalar multiples of the identity (i.e., exhibiting high sphericity), $\psi(\mathbf{M})$ approaches 0.

This behavior of $\psi(\mathbf{M})$ underpins the changing nature of $\theta(\mathbf{M})$ in the high-dimensional regime. As k grows large, $\theta(\mathbf{M})$ becomes more sensitive to deviations from sphericity, reflecting the increasing diversity and complexity of matrices in higher dimensions. Additionally, the range of values $\theta(\mathbf{M})$ may expand or contract as k tends to infinity, reflecting the evolving landscape of matrix sphericity in high-dimensional spaces.

Overall, the behavior of $\theta(\mathbf{M})$ in the high-dimensional scenario offers valuable insights into the intrinsic properties of matrices and their representations in complex spaces. A further exploration and analysis of these patterns can provide a deeper understanding and appreciation of matrix geometry in high dimensions.

4. Stochastic Matrices

In this section, we discuss asymptotic normality for a sequence of $k \times k$ random matrices $\mathbf{X}_d$, where $\mathbf{X}_d$ represents the random matrices in the sequence, and $\boldsymbol{\eta}_d$ represents the expectation of $\mathbf{X}_d$. Specifically, we consider the scaling behavior as the dimension d goes to infinity. So, we have

$$d^s(\mathbf{X}_d - \boldsymbol{\eta}_d) \xrightarrow{d \rightarrow \infty} N(\mathbf{0}, \mathbf{M}), \quad (3)$$

where d^s represents a scaling parameter, indicating convergence in distribution to a normal distribution with mean vector $\mathbf{0}$ and covariance matrix $\mathbf{M}$. We define

$$\psi(\mathbf{X}_d) \xrightarrow{d \rightarrow \infty} \psi(\mathbf{M}).$$

If $\mathbf{M}$ can be diagonalized, then

$$\mathbf{M} = \mathbf{P}^\top \mathbf{D} \mathbf{P}, \quad (4)$$

where $\mathbf{P}$ is an orthogonal matrix, and $\mathbf{D}$ is a diagonal matrix containing the eigenvalues of $\mathbf{M}$. Given this diagonalization, we have

$$\psi(\mathbf{X}_d) \xrightarrow{d \rightarrow \infty} \psi(\mathbf{D}).$$

We point out that (4) holds whenever $\mathbf{M} \in S_k$, whatever k . Furthermore, if $\mathbf{M}$ can be expressed as a Kronecker product,

$$\mathbf{M} = \mathbf{M}_1 \otimes \mathbf{M}_2,$$

with

$$\mathbf{M}_1 = \mathbf{D}_1,$$

then,

$$\mathbf{M} = \mathbf{D},$$

where

$$\mathbf{D} = \mathbf{D}_1 \otimes \mathbf{D}_2.$$

Moreover, if $\mathbf{D}_h$ is given by

$$\mathbf{D}_h = \mathbf{D}(\mathbf{v}_h), \quad h = 1, 2,$$

we have

$$\mathbf{D} = \mathbf{D}(\mathbf{v}_1 \otimes \mathbf{v}_2).$$

For instance, consider the case with independent vectors $Y_i \sim N(\mu_i, \nu)$, $i = 1, \dots, n$, with ν invertible. Define

$$\begin{cases} \mu. = \frac{1}{n} \sum_{i=1}^n \mu_i \\ Y. = \frac{1}{n} \sum_{i=1}^n Y_i \end{cases}$$

and the centered vectors

$$\begin{cases} \dot{\mu}_i = \mu_i - \mu. \\ \dot{Y}_i = Y_i - Y. \end{cases} \quad i = 1, \dots, n.$$

Following Kollo and Von Rosen [10], we obtain the Wishart matrix

$$W = \sum_{i=1}^n \dot{Y}_i \dot{Y}_i^\top,$$

with parameters

$$\begin{cases} \dot{\mu} = \sum_{i=1}^n \dot{\mu}_i \dot{\mu}_i^\top \\ \delta = \dot{\mu}^\top \nu^{-1} \dot{\mu} \end{cases},$$

where δ is the non-centrality (stochastic) parameter.

Now, as the trace $t = \text{tr}(\dot{\mu})$ tends to infinity, we have

$$\frac{1}{t} \dot{\mu} \xrightarrow[t \rightarrow \infty]{} \mu^\circ,$$

indicating that μ° is the normalized form of $\dot{\mu}$ when scaled by its trace. Consequently,

$$\frac{1}{\sqrt{t}} (\text{vec}(W) - \text{vec}(\dot{\mu})) \sim \mathcal{N}(\mathbf{0}, 4K(W \otimes \mu^\circ)K^\top),$$

where $\text{vec}(W)$ denotes the vectorization of W , transforming the matrix W into a column vector by stacking its columns on top of each other. Here,

$$K = \frac{1}{2}(I_{k^2} + O)$$

and

$$O = \sum_{i=1}^k \sum_{j=1}^k \delta_{v(j,i)} \delta_{v(i,j)}^\top,$$

with δ_N having its k^2 components null except for the v -th, which is 1, and

$$v(i, j) = i + (j - 1)k.$$

For more details, see Dhrymes [11].

Given that O is orthogonal,

$$\psi(\text{vec}(W)) \xrightarrow[t \rightarrow \infty]{} \psi(4K(\nu \otimes \mu^\circ)K^\top) = \psi(\nu) \otimes \psi(\mu^\circ).$$

Suppose that, for instance,

$$\nu = I_k.$$

Then,

$$\psi(\nu) = \frac{1}{k},$$

since

$$\begin{cases} \text{tr}^2(\mathbf{I}_k) = k^2 \\ \|\mathbf{I}_k\|^2 = k \end{cases}.$$

Now, $\psi(\boldsymbol{\mu}^\circ)$ depends on the choice of $\boldsymbol{\mu}$ and takes values in the range $[\frac{1}{k}; 1]$. Assuming that

$$\mathbf{v}(\boldsymbol{\mu}^\circ) = \left(a, \frac{1-a}{k-1}, \frac{1-a}{k-1}, \dots, \frac{1-a}{k-1} \right)$$

we have

$$\begin{cases} \text{tr}(\boldsymbol{\mu}^\circ) = 1 \\ \|\boldsymbol{\mu}^\circ\|^2 = a^2 + \frac{(1-a)^2}{k-1} \end{cases},$$

as well as

$$\psi(\boldsymbol{\mu}^\circ) = a^2 + \frac{(1-a)^2}{k-1}.$$

Now,

$$\psi(\boldsymbol{\mu}^\circ) = h,$$

with

$$\frac{1}{k} \leq h \leq 1,$$

gives

$$a = \frac{1 + \sqrt{1 - k(1 - (k-1)h)}}{2k}.$$

Thus, we may pick for $\psi(\boldsymbol{\mu}^\circ)$ any value in the range $[\frac{1}{k}; 1]$.

Assuming

$$\mathbf{v}(\boldsymbol{\nu}) \otimes \mathbf{v}(\boldsymbol{\mu}) = (v_1^{-1}, \dots, v_{k^2}^{-1}),$$

we find that the limit density for $\frac{1}{\sqrt{f}}(\text{vec}(\mathbf{W}) - \text{vec}(\boldsymbol{\mu}^\circ))$ is $n(\mathbf{0}, 4\mathbf{K}\mathbf{D}(\dot{v}_1, \dots, \dot{v}_{k^2})\mathbf{K}^\top)$.

Now, since $\mathbf{K}$ is orthogonal, we have

$$\psi(4\mathbf{K}\mathbf{D}(\dot{v}_1, \dots, \dot{v}_{k^2})\mathbf{K}^\top) = \psi(\mathbf{D}(\dot{v}_1, \dots, \dot{v}_{k^2})).$$

Thus, instead of using $n(\mathbf{x}|\mathbf{0}, 4\mathbf{K}\mathbf{D}(\dot{v}_1, \dots, \dot{v}_{k^2})\mathbf{K}^\top)$, we can work with

$$n(\mathbf{x}|\mathbf{0}, \mathbf{D}(\dot{v}_1, \dots, \dot{v}_{k^2})) = \prod_{i=1}^{k^2} \frac{e^{-\frac{2x_i^2}{\dot{v}_i}}}{\sqrt{2\pi\dot{v}_i}}.$$

This form is easier to handle because it represents a product of independent normal distributions for each component x_i .

We are particularly interested in the distribution of the ratio

$$Z = \frac{\sum_{j=1}^{k^2} x_j^2}{(\sum_{j \in C} x_j)^2},$$

where the numerator represents the sum of squared components, and the denominator is the square of the sum of a specific subset of components, indexed by set C ,

$$C = \{j + (j-1)k; j = 1, \dots, k\}.$$

The cumulative distribution function $F(z)$ of Z is given by

$$F(z) = \int \dots \int_{\Gamma(z)} \prod_{j=1}^{k^2} \frac{e^{-\frac{2x_j^2}{\dot{v}_j}}}{\sqrt{2\pi\dot{v}_j}} \prod_{j=1}^{k^2} dx_j,$$

where the integration domain $\Gamma(z)$ is defined as

$$\Gamma(z) = \left\{ \mathbf{x} : \sum_{j=1}^k x_j^2 \leq z \left(\sum_{j \in C} x_j \right)^2 \right\}.$$

These equations are useful because they allow us to characterize the distribution of the statistic Z , which can be used to test hypotheses or make inferences about the underlying matrices $\mathbf{W}$ and $\boldsymbol{\mu}$. The form of $F(z)$ indicates how likely it is to observe a given value of Z , providing a basis for statistical decision-making.

5. Comparison of Sphericity Measures

In this section, we compare three measures of sphericity for positive semi-definite matrices: the proposed measure, given in (2), the Frobenius measure, given in (1), and the spectral measure defined as follows:

$$\text{Spectral Measure} = \frac{\lambda_{\max}^2}{\text{tr}^2(\mathbf{M})},$$

where $\lambda_{\max}$ is the largest eigenvalue of $\mathbf{M}$.

The ranges and interpretations for the three measures are as follows:

- The proposed measure ranges between 0 and 1. Perfect sphericity is indicated by a value of 1.
- The Frobenius measure ranges between $\frac{1}{k}$ and 1, where k is the size of the matrix. Perfect sphericity is indicated by $\frac{1}{k}$.
- The range of the spectral measure depends on the largest eigenvalue and the size of the matrix. For example, as we can see on Table 1, if we have a 2×2 matrix with both eigenvalues 1, the perfect sphericity is indicated by 0.25.

To compare the three measures of sphericity, we considered several cases. The following table contains the size of the matrix, the considered eigenvalues, and the three measures of sphericity for each case.

Table 1. Comparison of sphericity measures.

Size	Eigenvalues	Proposed	Frobenius	Spectral
2×2	1, 1	1.00	0.50	0.25
3×3	1, 1, 1	1.00	0.33	0.11
5×5	1, 1, 1, 1, 1	1.00	0.20	0.04
10×10	1, 1, 1, 1, 1, 1, 1, 1, 1, 1	1.00	0.10	0.01
2×2	2, 1	0.89	0.56	0.44
3×3	2, 1, 1	0.94	0.38	0.25
5×5	2, 1, 1, 1, 1	0.97	0.22	0.11
10×10	2, 1, 1, 1, 1, 1, 1, 1, 1, 1	0.99	0.11	0.03
2×2	10, 1	0.33	0.83	0.83
3×3	10, 5, 1	0.76	0.49	0.39
5×5	10, 10, 5, 5, 1	0.92	0.26	0.10
10×10	10, 9, 8, 7, 6, 5, 4, 3, 2, 1	0.97	0.13	0.03

For matrices with equal eigenvalues (e.g., 1, 1 for 2×2 ; 1, 1, 1 for 3×3), the proposed measure is consistently 1, indicating perfect sphericity. The Frobenius and spectral measures decrease with increasing matrix size due to their dependence on the number of eigenvalues.

For matrices with one eigenvalue significantly different from the others (e.g., 2, 1 for 2×2 ; 2, 1, 1 for 3×3), the proposed measure decreases slightly from 1 but remains relatively high. The Frobenius and spectral measures show a more significant decrease compared to the perfectly spherical cases, reflecting the perturbation.

For matrices with highly varied eigenvalues (e.g., 10, 1 for 2×2 ; 10, 5, 1 for 3×3), the proposed measure decreases more substantially, reflecting the lack of sphericity. The Frobenius and spectral measures show higher values, indicating greater sensitivity to anisotropy.

The great advantage of the proposed measure $\theta(\mathbf{M})$ is that it is scale-invariant, as discussed earlier, maintaining consistency regardless of the magnitude of the eigenvalues. The Frobenius and spectral measures do not explicitly account for scale, which can affect their interpretability across different matrix sizes.

In terms of computational complexity, the proposed measure is comparable to the Frobenius measure and the spectral measure. All measures involve operations that scale with the size k of the matrix, primarily dominated by the computation of norms, traces, and, in the case of the spectral measure, eigenvalues. Therefore, while the proposed measure offers unique normalization and interpretation advantages, its computational demands are not significantly different from the other measures discussed. This parity ensures that the proposed measure remains feasible for practical implementation across various matrix sizes commonly encountered in statistical and machine learning applications.

6. Final Remarks

The investigation into the measure of sphericity for positive semi-definite matrices yields valuable insights into their geometric properties, especially in high-dimensional contexts. The introduced measure, $\theta(\mathbf{M})$, provides a robust means of quantifying the spread of eigenvalues, being invariant under orthogonal transformations and scaling and exhibiting predictable behavior under matrix operations such as the Kronecker product.

In finite-dimensional cases, $\theta(\mathbf{M})$ effectively discriminates between varying degrees of sphericity, with values ranging from 0 to 1. Furthermore, in the realm of stochastic matrices, the asymptotic normality of random matrices allows for insightful analyses. The convergence properties of $\psi(\mathbf{M})$ and the behavior of $\theta(\mathbf{M})$ under such convergence offer valuable tools for understanding the statistical properties of high-dimensional data.

The proposed sphericity measure presents several advantages:

- **Normalization to Unit Interval:** Values closer to 1 indicate high sphericity, while values closer to 0 indicate low sphericity.
- **Scaling with Dimension:** The normalization factor $1 - \frac{1}{k}$ makes the measure more comparable across matrices of different sizes.
- **Proportional Interpretation:** This provides a potentially more intuitive understanding of sphericity.
- **Invariant Properties:** $\theta(\mathbf{M})$ remains unchanged under orthogonal transformations and scaling, ensuring consistency across different bases and magnitudes.
- **Predictable Behavior under Operations:** This exhibits predictable behavior under matrix operations such as the Kronecker product, making it a versatile tool in various applications.

These advantages highlight how $\theta(\mathbf{M})$ compares favorably to other sphericity measures, providing more comprehensive and robust insights into the matrix properties.

The analysis primarily utilized normal distributions due to their mathematical tractability and the availability of well-established results in random matrix theory. However, the proposed measure is not limited to normal distributions. Future research could explore its application to other probability distributions, such as the Wishart distribution or distributions with heavy tails, like the multivariate t-distribution. Extending the analysis to these distributions may offer new insights into the behavior of the sphericity measure and its robustness under different statistical models. By considering different distributions, we can broaden the applicability of the sphericity measure and enhance its relevance in various practical scenarios where the normality assumption may not hold. Such extensions would significantly contribute to the understanding and utilization of sphericity measures in multivariate analysis and high-dimensional statistics.

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