A note on MLE of covariance matrix

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Summary: For a multivariate normal set up, it is well known that the maximum likelihood estimator of covariance matrix is neither admissible nor minimax under the Stein loss function. For the past six decades, a bunch of researches have followed along this line for Stein’s phenomenon in the literature. In this note, the results are two folds: Firstly, with respect to Stein type loss function we use the full Iwasawa decomposition to enhance the unpleasant phenomenon that the minimum risks of maximum likelihood estimators for the different coordinate systems (Cholesky decomposition and full Iwasawa decomposition) are different. Secondly, we introduce a new class of loss functions to show that the minimum risks of maximum likelihood estimators for the different coordinate systems, the Cholesky decomposition and the full Iwasawa decomposition, are of the same, and hence the Stein’s paradox disappears.

Keywords: Geodesic distance; Iwasawa decomposition; minimax estimator

1. Introduction

Let $X_1, \cdots, X_n$ be independent $p$-dimensional random vectors with a common multivariate normal distribution $N_p(0, \Sigma)$. A basic problem considered in the literature is the estimation of the $p \times p$ covariance matrix $\Sigma$ which is unknown and assumed to be nonsingular. It is also assumed that $n \geq p$, as such the sufficient statistic

$$A = \sum_{i=1}^n X_iX_i'$$

is positive definite with probability one. In the literature, the estimators $\phi(A)$ of $\Sigma$ are the functions of $A$. The sample space $\mathcal{S}$, the parameter space $\Theta$ and the action space $\mathcal{A}$ are taken to be the set of $p \times p$ positive definite matrices. Note that $A$ has a Wishart distribution $W(\Sigma, n)$ and the maximum likelihood estimator of $\Sigma$

$$\hat{\Sigma} = n^{-1}A,$$

which is unbiased. The general linear group $Gl(p)$ acts on the spaces $\mathcal{S}$, $\Theta$ and $\mathcal{A}$. Generally, we consider the invariance loss function $L$, namely, $L$ satisfies the condition that $L(g\phi(A)g', g\Sigma g') = L(\phi(A), \Sigma)$ for all $g \in Gl(p)$. One of the most interesting examples was introduced by Stein (see Jame and Stein, 1961),

$$L(\phi(A), \Sigma) = \text{tr}\Sigma^{-1}\phi(A) - \log\det\Sigma^{-1}\phi(A) - p,$$
where \( \text{tr} \) and \( \det \) denote the trace and the determinant of a matrix, respectively. Because \( Gl(p) \) acts transitively on the space \( \Theta \), so the best equivalent estimator exists. The minimum risk for the estimator \( \hat{\Sigma} \) is

\[
R(\hat{\Sigma}, \Sigma) = \sum_{i=1}^{p} \{ \log n - \mathcal{E}[\log \chi_{n-i+1}^2] \},
\]

where \( \mathcal{E}[X] \) denotes the expectation of random variable of \( X \). It can be easily seen that the maximum likelihood estimator is the best equivalent estimator.

Since the general linear group is not a solvable group, hence relax the condition a little bit by considering the group of \( p \times p \) lower triangular matrices with positive diagonal elements \( G_T^+ \), the loss function is also invariant under \( G_T^+ \). Using the Cholesky decomposition, we may write \( A = TT' \), where \( T \in G_T^+ \). Since \( G_T^+ \) acts transitively on the space \( \Theta \), the best equivalent estimator was established by Stein (see James and Stein, 1961) in the following

\[
\hat{\Sigma}_S = TD_S^{-1}T',
\]

where \( D_S \) is a positive diagonal matrix with elements \( d_{sii} = n + p - 2i + 1, \ i = 1, \cdots, p \). The minimum risk for the estimator \( \hat{\Sigma}_S \) is

\[
R(\hat{\Sigma}_S, \Sigma) = \sum_{i=1}^{p} \{ \log(n + p - 2i + 1) - \mathcal{E}[\log \chi_{n-i+1}^2] \}.
\]

Since the group \( G_T^+ \) is solvable, it follows from results in Kiefer (1957) that the estimator \( \hat{\Sigma}_{JS} \) is minimax.

In the literature, there are many developments along this approach and its ramifications, we may refer to the book of Anderson (2003) or the book of Muirhead (1982), and the references cited there, hence we omit the details. With respect to Stein loss function, we use the full Iwasawa decomposition (Terras, 1988) to enhance the Stein’s phenomenon.

2. The full Iwasawa decomposition

The Cholesky decomposition can be viewed as a partial Iwasawa decomposition. We would like to relax the conditions more by considering the full Iwasawa decomposition in this section. Some more notations are needed. Partition \( \Sigma(k) \) and \( A(k) \) as

\[
\Sigma(k) = \begin{bmatrix}
\sigma(k)_{11} & \Sigma(k)_{12} \\
\Sigma(k)_{21} & \Sigma(k)_{22}
\end{bmatrix} \quad \text{and} \quad A(k) = \begin{bmatrix}
a(k)_{11} & A(k)_{12} \\
A(k)_{21} & A(k)_{22}
\end{bmatrix},
\]

for all \( k = 1, \cdots, p \) with \( \Sigma(1) = \Sigma \) and \( A(1) = A \), also define

\[
\Sigma(k+1) = \Sigma(k)_{22} - \Sigma(k)_{21} \Sigma(k)_{12} / \sigma(k)_{11}
\]

and

\[
A(k+1) = A(k)_{22} - A(k)_{21} A(k)_{12} / a(k)_{11}.
\]

Let

\[
g(k) = \begin{bmatrix}
1 & 0 \\
-\Sigma(k)_{21} \sigma(k)_{11}^{-1} & I
\end{bmatrix} \quad \text{and} \quad h(k) = \begin{bmatrix}
1 & 0 \\
-A(k)_{21} a(k)_{11}^{-1} & I
\end{bmatrix}, \ k = 1, \cdots, p.
\]

Then we have
\[
\tilde{\Sigma}(k) = g(k) \Sigma(k) g'(k) = \begin{bmatrix} \sigma(k)_{11} & 0 \\ 0 & \Sigma(k)_{22:1} \end{bmatrix},
\]
and
\[
\tilde{A}(k) = h(k) A(k) h'(k) = \begin{bmatrix} a(k)_{11} & 0 \\ 0 & A(k)_{22:1} \end{bmatrix}, \quad k = 1, \cdots, p.
\]
Let
\[
\Sigma^* = \text{Diag}(\sigma(1)_{11}, \cdots, \sigma(p)_{11}) \quad \text{and} \quad A^* = \text{Diag}(a(1)_{11}, \cdots, a(p)_{11}).
\]
By using the full Iwasawa decomposition, we can eventually transform \(\Sigma\) and \(A\) into the diagonal matrices \(\Sigma^*\) and \(A^*\), respectively. Thus we establish the one-to-one correspondences: \(\Sigma \leftrightarrow \Sigma^*\) and \(A \leftrightarrow A^*\). By the properties of Wishart distribution (see Theorem 4.3.4, Theorem 7.3.4 and Theorem 7.3.6 of Anderson, 2003), it is easy to note that \(a(i)_{11}/\sigma(i)_{11}, i = 1, \cdots, p\) are independent \(\chi^2\) random variables with \(n - i + 1\) degrees of freedom respectively. Consider the loss function similar to the equation (3)
\[
L(\phi(A^*), \Sigma^*) = \text{tr} \Sigma^*^{-1}DA^* - \log \det \Sigma^*^{-1}DA^* - p,
\]
where \(D = \text{Diag}(d_{11}, \cdots, d_{pp})\) is a positive diagonal matrix, not depending on \(A^*\).

**Theorem 1.** With respect to the likelihood loss function (Stein type loss function), the best estimator invariant with respect to one-to-one transformations \(\Sigma \to \Sigma^*, A \to A^*\), is \(\hat{\Sigma}_I = D_0^{-1}A^*\). The minimum risk is 
\[
E_L(\phi(A^*), I) = \sum_{i=1}^{p} \left\{ \log(n - i + 1) - E[\log \chi_{n-i+1}^2] \right\} - p.
\]

**Proof.** Take \(\Sigma = I\), and then note that
\[
E_L(\phi(A^*), I) = E[\text{tr}DA^* - \log \det DA^* - p]
\]
\[
= \sum_{i=1}^{p} (n - i + 1)d_{ii} - \sum_{i=1}^{p} \log d_{ii} - \sum_{i=1}^{p} E[\log \chi_{n-i+1}^2] - p.
\]
The minimum of (15) occurs at \(d_{ii} = 1/(n - i + 1), i = 1, \cdots, p\). Since \(A^*\) also acts transitively on the space \(\Theta\), so the best equivalent estimator exists, which is of the form
\[
\hat{\Sigma}_I^* = D_0^{-1}A^*,
\]
where \(D_0\) is a diagonal matrix with elements \(d_{0ii} = n - i + 1, i = 1, \cdots, p\). Thus the minimum risk for the estimator \(\hat{\Sigma}_I^*\) is
\[
R(\hat{\Sigma}_I^*, \Sigma^*) = \sum_{i=1}^{p} \left\{ \log(n - i + 1) - E[\log \chi_{n-i+1}^2] \right\}.
\]
Since the group of positive diagonal matrices is a subset of \(G_+\), which is solvable, thus the group of positive diagonal matrices is also solvable. And hence, by the results of Kiefer (1957) the estimator \(\hat{\Sigma}_I^*\) is minimax.
for \( p \geq 2 \). The equality in (18) holds when \( \hat{\Sigma}_I^* = \hat{\Sigma}_S = \hat{\Sigma} \): namely, (i) the components are independent or (ii) as the sample size \( n \to \infty \). With respect to the Stein loss function, the minimum risk functions are different based on the full Iwasawa decomposition and based on the Cholesky decomposition.

We may note that each \( a_{(i)11}/(n - i + 1) \) is the maximum likelihood estimator of \( \sigma_{(i)11} \), and is unbiased, for all \( i = 1, \cdots, p \). For each component, \( a_{(i)11}/(n - i + 1) \) is admissible for \( \sigma_{(i)11}, i = 1, \cdots, p \). Note that saying \( n^{-1}A \) is the maximum likelihood estimator of \( \Sigma \) is the same as to say that \( D_0^{-1}A^* \) is the maximum likelihood estimator of \( \Sigma^* \). Thus, the results of the equation (18) lead to a paradox that the property of maximum likelihood estimators for the different coordinate systems is not consistent with respect to the Stein type loss function. This motives us to further study whether a suitable loss function exists so that the maximum likelihood estimators can be invariant under reparameterizations.

3. The geodesic distance

Since the space of positive definite symmetric matrices is a non-Euclidean space, it is more natural to use a metric on a Riemannian metric space. The Riemannian metric can be defined with the help of the fundamental form \( ds^2 = \text{tr}(W^{-1}dW)^2 \), where \( dW \) denotes the matrix of differentials. This is invariant under the transformation \( W \to VW \), where \( V \) is any fixed elements of \( \text{Gl}(p) \). Let \( \mathcal{P}_p \) be the set of square symmetric positive definite matrices, this set is a representation space of the group \( \text{Gl}(p) \). An element \( V \in \text{Gl}(p) \) operates on \( \mathcal{P}_p \) according to \( M \to VMV^T \). On \( \text{Gl}(p) \), any maximal compact subgroup \( \Delta \) of \( \text{Gl}(p) \) can be represented in the form \( \Delta = \{ \rho \Delta \mid \rho \in \text{Gl}(p) \} \) can be considered as a representation space of \( \text{Gl}(p) \). Since \( \Delta = V^{-1}\mathcal{O}(p)V, V \in \text{Gl}(p) \), thus the all maximal compact subgroup are conjugate. Conjugate subgroups yield equivalent representation spaces, hence it is sufficiently enough to only consider the orthogonal group \( \mathcal{O}(p) \) as the maximal compact group of \( \text{Gl}(p) \). The map \( V\mathcal{O}(p) \to M = WW' \) establishes an equivalence between the representation spaces \( \text{Gl}(p)/\mathcal{O}(p) \) and \( \mathcal{P}_p \) of \( \text{Gl}(p) \). And hence the \( ds^2 \) defines an invariant metric on \( \mathcal{P}_p \). The tangent space to \( \mathcal{O}(p) \) is \( so(p) \), the vector space of skew-symmetric \( p \times p \) matrices. Thus \( \dim \mathcal{O}(p) = \dim so(p) = p(p - 1)/2 \). And hence \( \dim \text{Gl}(p)/\mathcal{O}(p) = \dim \text{Gl}(p) - \dim \mathcal{O}(p) = p(p + 1)/2 - p(p - 1)/2 = p \).

**Proposition 1.** A geodesic segment \( T(t) \) through \( I \) and \( Y \) in \( \mathcal{P}_p \) has the form: \( T(t) = \exp(tU^TBU), 0 \leq t \leq 1 \), where \( Y \) has the spectral decomposition: \( Y = U \exp(B)U = \exp(U^TBU) \), for \( U \in \mathcal{O}(p) \) and \( B = \text{Diag}(b_1, \cdots, b_p), b_i \in R, i = 1, \cdots, p \). The length of the geodesic segment is \( (\sum_{i=1}^p b_i^2)^{1/2} \).

The proof of Proposition 1 can be found in the book of Terras (1988). For any given two points \( \Sigma_1 \) and \( \Sigma \) of \( \mathcal{P}_p \), the geodesic distance is defined to be \( \sum_{i=1}^p \log^2 \lambda_i \), where \( \lambda_i, i = 1, \cdots, p \), are the zeros of charactistic polynomial \( \det(\lambda \Sigma - \Sigma_1) \). A loss function \( L \) is invariant iff \( L \) can be written as a function of the eigenvalues of \( \phi(A) \). Hence from geometric point of view, with the help of Proposition 1 we may naturally consider the compatible, coordinate-invariant loss function \( L_G(\phi(A), \Sigma) = \sum_{i=1}^p \log^2 \lambda_i \), where \( \lambda_i, i = 1, \cdots, p \) denote the eigenvalues of \( \Sigma^{-1}\phi(A) \). And the risk function is denoted by \( R_G(\hat{\Sigma}_G, \Sigma)(= \mathcal{E}[L_G(\phi(A), \Sigma)]) \), where \( \hat{\Sigma}_G \) be the corresponding estimator based on the
geodesic distance loss function on $P$. Without loss the generality we may take $\Sigma = I$ as Stein did. Write $d = (d_1, \ldots, d_p)^T$. The following studies are comparable to the results in Section 7.8. of Anderson (2003). Let $\text{Var}[X]$ denote the variance of random variable $X$.

**Theorem 2.** With respect to the geodesic distance loss function on $P$, $L_G(\phi(A), I) = \sum_{i=1}^p \log^2(d_i, \lambda_i)$, where $\lambda_i$ denotes the $i$-th largest eigenvalue of $\phi(A)$ and $d_i$ is a positive constant, $\forall i = 1, \ldots, p$, let $C = \{d|E[d, \lambda_i] \leq e, \forall i = 1, \ldots, p\}$. Then on the set $C$ the minimum of risk function $R_G(\hat{\Sigma}_G, I)$ occurs at $d_i = \exp\{-E[\log\lambda_i]\}, \forall i = 1, \ldots, p$, and its minimum risk is $\sum_{i=1}^p \text{Var}[\log\lambda_i]$.

**Proof.** Note that $\partial E[\sum_{i=1}^p \log^2(d_i, \lambda_i)]/\partial d_i = 0$ implies that $E[\log(d_i, \lambda_i)/d_i] = 0, \forall i = 1, \ldots, p$, which is the same as the conditions that $\log d_i + E[\log\lambda_i] = 0, \forall i = 1, \ldots, p$. By Jensen inequality, we have that $0 = \log d_i + E[\log\lambda_i], \forall i = 1, \ldots, p$. Let $d_0$ be the point so that $\log d_i = -E[\log\lambda_i], \forall i = 1, \ldots, p$. Then $d_0$ is the critical point for the risk function $R_G(\hat{\Sigma}_G, I)$.

Moreover, we may note that $\partial^2 E[\sum_{i=1}^p \log^2(d_i, \lambda_i)]/\partial^2 d_i = 2E[(1 - \log d_i)\lambda_i/d_i^2], \forall i = 1, \ldots, p$. By the Jensen inequality, we may note that $E[(1 - \log d_i)\lambda_i] \geq (1 - \log E[\lambda_i]) \geq 0, \forall i = 1, \ldots, p$. Then, on the set $C$, we have $\partial^2 E[\sum_{i=1}^p \log^2(d_i, \lambda_i)]/\partial^2 d_i \geq 0, \forall i = 1, \ldots, p$, and $\partial^2 E[\sum_{i=1}^p \log^2(d_i, \lambda_i)]/\partial d_i \partial d_j = 0, \forall i \neq j$. Thus the risk function $R_G(\hat{\Sigma}_G, I)$ is convex and has an unique minimum on the set $C$. Since the set $C$ is a connected set, and $d_0 \in C$, and hence, the theorem follows.

Theorem 2 provides us a new class of loss functions for statistical inference. Although Theorem 2 looks simple mathematically, it provides us an intrinsically new approach to make statistical inference. With respect to the geodesic distance loss function, we may see that MLE is invariant under different parameterizations, and more importantly, the Stein’s paradox disappears. Those results are tremendously different from what have existed in the literature with respect to Stein type loss functions.

To obtain the best equivalent estimator with respect to geodesic distance loss function, the quantities $\exp\{-E[\log\lambda_i]\}, \forall i = 1, \ldots, p$, which can be viewed as the geometric means of the distributions, are needed to be evaluated. Some often seen cases are illustrated in the followings:

I. The full Iwasawa decomposition form. Based on the one-to-one transformation: $\Sigma \leftrightarrow \Sigma^*$ and $A \leftrightarrow A^*$, as such using the geodesic distance on $P$, namely, to use the loss function $L_G(DA^*, I) = \sum_{i=1}^p \log^2(d_i, \lambda_i^*)$, where $\lambda_i^*, i = 1, \ldots, p$ are the eigenvalues of $A^*$. Thus, $\mathcal{E}[L_G(DA^*, I)] = \mathcal{E}[\sum_{i=1}^p \log^2(d_i, \lambda_i^*)]$. Thus, by Theorem 2 the minimum of it occurs at $d_{ii} = \exp\{-E[\log(\lambda_{ii})]\}] = \exp\{-E[\log(\lambda_{ii}^*)]\}, \forall i = 1, \ldots, p$. Thus the geometric estimator $\hat{\Sigma}_{GI}$ of $\Sigma^*$ is that $\hat{\Sigma}_{GI} = D^* A^*$, where $D^*$ is a diagonal matrix with elements $d_{ii}^* = \exp\{-E[\log(\lambda_{ii}^*)]\}, i = 1, \ldots, p$ and $A^*$ in (13). Since $A^*$ is a diagonal matrix, the group of positive diagonal matrices is solvable, and hence by the results of Kiefer (1957) this geometric estimator $\hat{\Sigma}_{GI}$ is minimax. And its minimum risk is $R_G(\hat{\Sigma}_{GI}, I) = \sum_{i=1}^p \text{Var}[\lambda_{ii}^*] + \sum_{i=1}^p \{\log(n - i + 1) - E[\log(\lambda_{n-i+1}^*)]\}^2, i.e., R_G(\hat{\Sigma}_{GI}, I) < R_G(\hat{\Sigma}_I, I)$, where $\hat{\Sigma}_I$ is defined in (16). Thus we may conclude that the Stein estimator $\hat{\Sigma}_I^*$ is inadmissible with respect to geodesic distance loss function.

II. The Cholesky decomposition form, can be viewed as a partial Iwasawa decomposition. Riemannian geometry yields an invariant volume element $dv$ on $P$, it
is of the form \( dv = (\det A)^{-(p+1)/2} (dA) \), where \((dA) = \prod_{1 \leq j \leq i \leq p} da_{ij} \) with \( da_{ij} \) being the Lebesgue measure on \( R^{p(p+1)/2} \). This \( dv \) is the invariant \( d \)-form \((d = p(p + 1)/2) \) on \( \mathcal{P}_p \). Normalization is not necessary because this invariant \( d \)-form is not a probability measure. Note that this \( d \)-form is still invariant under \( G_T^+ \). With the Cholesky decomposition \( A = TT' \) and differentiate at \( T = I : dA = dT + dT' \). Thus \( da_{ii} = 2 dt_{ii} \), and for \( i > j \), \( da_{ij} = dt_{ij} \). Then the \( d \)-form becomes to \( dv = 2^p \prod_{i=1}^{p} t_{ii}^{-1} (dt_i) \), where \((dt_i) \) denotes the wedge product. Let \( \etr(A) \) denote \( \exp(\text{tr}A) \) and write \( T = ((t_{ij})) \). Similarly, we do the Cholesky decomposition for the scale parameter as \( \Sigma = \Theta \Theta' \), where \( \Theta = ((\theta_{ij})) \) is a lower triangular matrix. Take \( \Sigma = I \), the Wishart density of \( A \) then becomes to the following density function

\[
\frac{2^{p-pn/2}}{\Gamma_p(n/2)} \etr\left(-\frac{1}{2} TT'\right) \prod_{i=1}^{p} t_{ii}^{p-i},
\]

where \( \Gamma_p(a) = \pi^{p(p-1)/4} \prod_{i=1}^{p} \Gamma(a - (i - 1)/2) \). This is essentially called the Bartlett decomposition in the literature. Note that \( T \) is a lower triangular matrix which has the eigenvalues \( t_{ii}, i = 1, \cdots, p \). With respect to the geodesic distance loss function, the density function (19) can be further reduced to the product of the densities with \( n - i + 1 \) degrees of freedom, \( i = 1, \cdots, p \). Thus, the risk function of geodesic distance loss function is \( I_{LG}(\phi(A), I) = \mathcal{E}(\sum_{i=1}^{p} \log^2 (d_{ii} t_{ii})) \). By Theorem 2, the minimum of it occurs at \( d_{ii} = \exp\{-\mathcal{E}[\log^2 t_{ii}]\} = \exp\{-\mathcal{E}[\log^2 \chi_{n-i}^2]\}, \forall_{i} = 1, \cdots, p \). Let \( d_{0i} = \exp\{-\mathcal{E}[\log^2 t_{ii}]\}, \forall_{i} = 1, \cdots, p \), and write \( T_0 = ((t_{0ij})) \), where \( t_{0ij} = t_{ij} \) if \( i \neq j \) and \( t_{0ij} = (d_{0i} t_{ii})^{1/2} \), \( i = 1, \cdots, p, j = 1, \cdots, i \). We may note that \( t_{0}^2 \) is the unbiased MLE of \( \theta_{ii}' \), \( \forall_{i} = 1, \cdots, p \). Thus, the best equivalent estimator is of the form \( \Sigma_{GC} = T_0 T_0' \) and its minimum risk is \( R_G(\Sigma_{GC}, I) = \sum_{i=1}^{p} \text{Var} [\log \chi_{n-i}^2] \). Since the group \( G_T^+ \) is solvable, it follows from results in Kiefer (1957) that the estimator \( \Sigma_{GC} \) in minimax with respect to geodesic distance loss function.

This minimum risk is equivalent to that in Example 1, which indicates that with respect to the geodesic distance loss function on the space of positive definite symmetric matrices the minimum risks of maximum likelihood estimators with the different coordinate systems, the Cholesky decomposition and the full Iwasawa decomposition, are of the same. These results are quite different from what have existed in the literature based on the Stein type loss function, see Section 2 for the details. Moreover, note that \( R_G(\Sigma_S, I) = \sum_{i=1}^{p} \mathcal{E}[\log^2 (\chi_{n-i}^2/n + p - 2i + 1)] \), where \( \Sigma_S \) is defined in (5). It is easy to see that \( R_G(\Sigma_S, I) = R_G(\Sigma_{GC}, I) + \sum_{i=1}^{p} \{ \log (n + p - 2i + 1) - \mathcal{E}[\log \chi_{n-i}^2] \}^2 \), i.e., \( R_G(\Sigma_{GC}, I) < R_G(\Sigma_S, I) \). Thus we may conclude that the Stein estimator \( \Sigma_S \) is inadmissible with respect to geodesic distance loss function.

**III. The orthogonal decomposition form.** Stein (1956) considered the rotation-equivariant estimator of \( \Sigma \). The class of rotation-equivariant estimators of covariance matrix is constituted of all the estimators that have the same eigenvectors as the sample covariance matrix. Let \( \lambda_i \) denotes the \( i \)-th largest eigenvalue of \( \Sigma^{-1} A \). Also write \( A = \mathbf{ULU}' \), where \( \mathbf{L} \) is a diagonal matrix with eigenvalues \( l_i, i = 1, \cdots, p \) and \( \mathbf{U} \) being the corresponding orthogonal matrix. Similarly, write \( \Sigma = \mathbf{HH}' \), where \( \mathbf{G} \) is a diagonal matrix with eigenvalues \( \gamma_i, i = 1, \cdots, p \) and \( \mathbf{H} \) being the corresponding orthogonal matrix. Take \( \Sigma = I \), thus for the class of rotation-equivariant estimators the minimum risk function based on the geodesic distance loss function is \( \mathcal{E}[L_G(\phi(A), I)] = \mathcal{E}[\sum_{i=1}^{p} \log^2 (d_{ii} l_i)] \), and its minimum occurs at \( d_{ii} = \exp\{-\mathcal{E}[\log l_i]\}, \forall_{i} = 1, \cdots, p \). Thus, the best rotation-
equiavariant estimator is of the form $\hat{\Sigma}_{GO} = UD^*LU'$, where $D^*$ is a diagonal matrix with elements $d^*_{ii} = \exp\{-\mathcal{E}[\log l_i]\}, i = 1, \cdots, p$. On the other hand, the risk function based on the Stein loss function is $\mathcal{E}L(\phi(A), I) = \mathcal{E}[\text{tr}DL - \log\det DL - p] = \sum_{i=1}^p d_{ii}\mathcal{E}[l_i] - \sum_{i=1}^p \log d_{ii} - \sum_{i=1}^p \mathcal{E}[\log l_i] - p$. The minimum of it occurs at $d^{-1}_{ii} = \mathcal{E}[l_i], \forall i = 1, \cdots, p$.

Thus, with respect to Stein loss function the best rotation-equivariant estimator for $\Sigma$ is of the form $\Sigma_O = UD^*LU'$, where $D^*_0$ is a diagonal matrix with elements $d^*_{0ii} = 1/\mathcal{E}[l_i], i = 1, \cdots, p$. Similarly, we may also note that $R_G(\Sigma_O, I) = R_G(\Sigma_{GO}, I) + \sum_{i=1}^p \{\log \mathcal{E}[l_i] - \mathcal{E}[\log l_i]\}^2$, i.e., $R_G(\Sigma_{GO}, I) < R_G(\Sigma_O, I)$. Thus, under the orthogonal decomposition the Stein type estimator $\hat{\Sigma}_O$ is inadmissible with respect to geodesic distance loss function.

Via the result of Askey (1980), the joint density function of eigenvalues is of the form

$$2^{-np/2} \prod_{i=1}^p \frac{\Gamma(3/2)}{\Gamma((1+i)/2)\Gamma((n-p+i)/2)} l_i^{n+i-1} \exp{-l_i/2} \prod_{i<j} \{|l_i - l_j|\}. \quad (20)$$

It is easy to see that $\mathcal{E}[\prod_{i=1}^p \{l_i/(n-p+i)\}] = 1$. However, we have difficulty to find out the explicit form for the marginal density function of sample eigenvalue $l_i, i = 1, \cdots, p$, and open this type Selberg integral as a conjecture.

4. General remarks

Entropy (expectation of likelihood loss function) not only plays an important role in information theory, but also is a core in statistical theory. For the past six decades, quadratic loss function and likelihood loss function are oftenly adopted to study the Stein’s phenomenon for the covariance matrix estimation, for the details see the Section 7.8. of Anderson (2003) or the Section 4.3. of Muirhead (1982). Via the full Iwasawa decomposition, Theorem 1 tells us that the likelihood (Stein type) loss function is not invariant to arbitrary reparameterizations of $\mathcal{P}_p$. To overcome the drawbacks, Riemannian metric is a natural way to be adopted as a loss function for a non-Euclidean space $\mathcal{P}_p$. Due to the diffeomorphism invariance of risk function based on the geodesic distance, we may anticipate that the minimum risks of the MLEs may not only be invariant to reparameterizations but also the Stein paradox disappear with respect to geodesic distance loss function. Examples 1 and 2 tell us that the minimum risks of the MLEs of covariance matrices under the different coordinate systems, the Cholesky decomposition and the full Iwasawa decomposition, are of the same with respect to the geodesic distance loss function. Examples 1 and 2 also indicate that the MLE of covariance matrix is minimax with respect to the geodesic distance loss function on $\mathcal{P}_p$. This note will inevitably have an impact on statistical inference because the statisticians have to reconsider the adoption of the MLE of covariance matrix, which, however, had been constantly warned not to use for a long time since Stein’s phenomenon occurred.

If the quantity $d_i = \exp\{-\mathcal{E}[\log \lambda_i]\}$ in Theorem 2 can be approximated by the quantity $d_i = 1/\mathcal{E}[\lambda_i], \forall i = 1, \cdots, p$, then we have that $\hat{\Sigma}^*_G = \hat{\Sigma}^*_I$ and $\hat{\Sigma}_{GO} = \hat{\Sigma}_O$ approximtly. Moreover, $R_G(\hat{\Sigma}^*_G, I) = R_G(\hat{\Sigma}^*_I, I) = R_G(\hat{\Sigma}_{GC}, I) < R_G(\hat{\Sigma}_S, I)$ approximtly. We omit the details.

Example 3 points out the fact that based on the orthogonal decomposition, the analytical difficulty to find out the marginal expectations will be accompanied with the orthogonal decomposition due to the Selberg type integral which involves the Vandermonde determinant. Similar difficulty will occur when to obtain the density functions of $\min_{1 \leq i \leq p}\{l_i\}$ and $\max_{1 \leq i \leq p}\{l_i\}$ (for details see Edelman, 1989). When $p, n \to \infty$ such that
\[ \lim_{n \to \infty} p/n = y \in [0,1], \] for a Wishart matrix Edelman (1989) proved that the geometric means of \( E[\log(\min_{1 \leq i \leq p} \{ l_i \}/n)] = \log(1 - \sqrt{y})^2 + o(1) \) and \( E[\log(\max_{1 \leq i \leq p} \{ l_i \}/n)] = \log(1 + \sqrt{y})^2 + o(1) \), respectively.

With respect to Stein loss function, Stein (1956) made statistical inference focused on the special case \( \Sigma = I \), it is sufficient enough due to the invariance consideration. For the main purpose of focusing on statistical inference in this note, we adopt the same structure as Stein did. However, this will sacrifice the development of distribution theory of arbitrary covariance \( \Sigma \). For this purpose, the elegant zonal polynomials have been incorporated, we may refer the book of Muirhead (1982) for the details.

The invariance nature of geodesic distance loss function suggests that it should be the way to deal with state-of-the-art covariance matrix estimators for the interesting and timely large dimensional case. For the large dimensional case, the sample size is required to be the same order of dimension. The empirical density of eigenvalues of Wishart matrix \( A \) converges to the Marchenko-Paster law in the limit when \( p, n \to \infty \) such that \( c = p/n \) is fixed \( 0 \leq c \leq 1 \). The geometric mean of this distribution is \(-1 - [(1 - y)\log(1 - y)]/y\), where \( y = \lim_{n \to \infty} p/n \).

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