SOME GEOMETRY OF THE CONE OF NONNEGATIVE DEFINITE MATRICES AND WEIGHTS OF ASSOCIATED $\bar{\chi}^2$ DISTRIBUTION

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Abstract. Consider the test problem about matrix normal mean M with the null hypothesis M=O against the alternative that M is nonnegative definite. In our previous paper (Kuriki (1993, Ann. Statist., 21, 1379–1384)), the null distribution of the likelihood ratio statistic has been given in the form of a finite mixture of χ^2 distributions referred to as $\bar{\chi}^2$ distribution. In this paper, we investigate differential-geometric structure such as second fundamental form and volume element of the boundary of the cone formed by real nonnegative definite matrices, and give a geometric derivation of this null distribution by virtue of the general theory on the $\bar{\chi}^2$ distribution for piecewise smooth convex cone alternatives developed by Takemura and Kuriki (1997, Ann. Statist., 25, 2368–2387).

Key words and phrases: One-sided test for covariance matrices, symmetric cone, mixed volume, second fundamental form, volume element.

1. Introduction

Let $A = (a_{ij})$ be a $p \times p$ symmetric random matrix whose components are independently distributed according to the normal distributions $a_{ii} \sim N(\mu_{ii}, 1)$ and $\sqrt{2}a_{ij} \sim N(\sqrt{2}\mu_{ij}, 1)$ (i < j). The joint distribution of A is written as

$$\frac{1}{(2\pi)^{p(p+1)/4}} \exp\left\{-\frac{1}{2} \operatorname{tr} (A-M)^2\right\} \cdot 2^{p(p-1)/4} \prod_{i < j} da_{ij},$$

where $M = (\mu_{ij})$ is the mean matrix.

Let S_p be the set of $p \times p$ real symmetric matrices. Let S_p^+ be the closed convex cone formed by $p \times p$ real nonnegative definite matrices, that is,

$$\mathcal{S}_p^+ = \{W \in \mathcal{S}_p \mid W \ge O\},\$$

where > denotes the Löwner order.

The statistical problems we consider here are one-sided tests about the matrix mean M for testing

(1.1)
$$H_0: M = O \text{ against } H_1: M \in \mathcal{S}_p^+,$$

and for testing

(1.2)
$$H_1: M \in \mathcal{S}_p^+ \text{ against } H_2: M \in \mathcal{S}_p.$$

The likelihood ratio test statistics for (1.1) and (1.2) are shown to be

(1.3)
$$\bar{\chi}_{01}^2 = \operatorname{tr} A^2 - \max_{M \in \mathcal{S}_p^+} \operatorname{tr} (A - M)^2 = \sum_{l_i > 0} l_i^2$$

and

(1.4)
$$\bar{\chi}_{12}^2 = \max_{M \in \mathcal{S}_p^+} \operatorname{tr}(A - M)^2 = \sum_{l_i < 0} l_i^2,$$

respectively, where $l_1 \geq \cdots \geq l_p$ are the eigenvalues of the random matrix A. The critical regions are given by $\bar{\chi}_{01}^2 > c$ and $\bar{\chi}_{12}^2 > c'$ for some critical values c and c'. Note that the marginal distributions of $\bar{\chi}_{01}^2$ and $\bar{\chi}_{12}^2$ under H_0 are identical because the null distribution of -A is equivalent to that of A.

The testing problem (1.1) and the corresponding distribution of $\bar{\chi}_{01}^2$ (1.3) arise as the limit of one-sided likelihood ratio tests for testing the equality of two covariance matrices against that one covariance matrix is greater than the other covariance matrix in the sense of Löwner order, when the degrees of freedom go to infinity. In this setting, Sakata (1997) derived the distribution of $\bar{\chi}_{01}^2$ under H_0 when p=2. Moreover, Kuriki (1993) proved that when H_0 holds the distribution of $\bar{\chi}_{01}^2$ has a form of a finite mixture of χ^2 distributions referred to as $\bar{\chi}^2$ distribution (e.g. Shapiro (1988), Robertson *et al.* (1988)):

(1.5)
$$P(\bar{\chi}_{01}^2 \le a) = \sum_{i=0}^{p(p+1)/2} w_{p(p+1)/2-i} G_{p(p+1)/2-i}(a),$$

where $G_d(\cdot)$ denotes the cumulative distribution function of χ^2 distribution with d degrees of freedom. The weights $\{w_d\}$ in (1.5) are mixing probabilities satisfying $w_d \geq 0$ and $\sum w_d = 1$. Actually the joint distribution of $\bar{\chi}_{01}^2$ and $\bar{\chi}_{12}^2$ under H_0 is a mixture of independent χ^2 distributions with the same weights:

(1.6)
$$P(\bar{\chi}_{01}^2 \le a, \bar{\chi}_{12}^2 \le b) = \sum_{i=0}^{p(p+1)/2} w_{p(p+1)/2-i} G_{p(p+1)/2-i}(a) G_i(b).$$

Kuriki (1993) gave an integral expression of the weights for a general p as well as a method to evaluate them numerically.

Recently, Takemura and Kuriki (1997) have developed a general theory on $\bar{\chi}^2$ distribution for any convex cone alternatives when the cone has a piecewise smooth boundary. The weights of $\bar{\chi}^2$ distribution have been shown to be expressed in terms of integrals with respect to volume element measure involving the elementary symmetric function of the eigenvalues of second fundamental form at the boundary of the cone. As we shall show in the next section, S_p^+ is a typical example of the cone whose boundary is piecewise smooth. In this paper, we investigate the differential-geometric structure such as second fundamental form and volume element at the boundary of the cone S_p^+ , and give a geometric derivation of the weights of $\bar{\chi}^2$ distribution for $\bar{\chi}^2_{01}$ and $\bar{\chi}^2_{12}$ by virtue of the general theory by Takemura and Kuriki (1997).

The main results are given in Sections 2 and 3. Differential-geometric structure of the cone \mathcal{S}_p^+ of nonnegative definite matrices are discussed in Section 2. The general procedure of Takemura and Kuriki (1997) consists of evaluation of three quantities at each point of the boundary of the cone: i) the normal cone, ii) the second fundamental form with respect to an arbitrary direction of the normal cone, and iii) the volume

element. Corresponding quantities to i)-iii) for the cone S_p^+ are given in Subsections 2.1, 2.2, and 2.3, respectively. Using these, we obtain the weights of $\bar{\chi}^2$ distribution for $\bar{\chi}_{01}^2$ and $\bar{\chi}_{12}^2$ in Section 3. Relevant definitions and results of Takemura and Kuriki (1997) are summarized in the Appendix. Although we give geometric results on S_p^+ as far as required in applying the theory by Takemura and Kuriki (1997), we remark that these results may be of independent interest and may be useful in other problems of multivariate statistics and related fields.

2. Geometric structure of the boundary of \mathcal{S}_p^+

In this section we inspect and reveal the differential-geometric structure of the boundary of \mathcal{S}_p^+ . The normal cone at the boundary of \mathcal{S}_p^+ is determined in Subsection 2.1. The second fundamental form of the boundary of \mathcal{S}_p^+ is given in Subsection 2.2. The volume element of the boundary of \mathcal{S}_p^+ is given in Subsection 2.3. These three quantities shall be used in the succeeding Section 3 in order to derive the weights $\{w_d\}$ of the $\bar{\chi}^2$ distribution in (1.6) with the help of Theorem A.1 of the Appendix.

As related works with this section, Ohara et al. (1996) discussed geometric structure of the cone of positive definite matrices (set of interior points of \mathcal{S}_p^+) in view of dualistic geometry. Full treatment of the cone of positive definite matrices as a symmetric cone is found in Faraut and Korányi (1994).

2.1 Normal cone at the boundary

We identify the space of real symmetric matrices S_p with the Euclidean space $R^{p(p+1)/2}$ by the map

$$W = (w_{ij}) \in \mathcal{S}_p \leftrightarrow (w_{11}, \dots, w_{pp}, \sqrt{2}w_{12}, \dots, \sqrt{2}w_{p-1,p}) \in \mathbb{R}^{p(p+1)/2}$$

and the corresponding inner product

(2.1)
$$\langle W_1, W_2 \rangle = \operatorname{tr} W_1 W_2$$

$$= \sum_i w_{1ii} w_{2ii} + \sum_{i < j} (\sqrt{2} w_{1ij}) (\sqrt{2} w_{2ij})$$

for $W_1 = (w_{1ij})$, $W_2 = (w_{2ij}) \in \mathcal{S}_p$. The norm is $||W|| = \sqrt{\operatorname{tr}(W^2)}$. Note that the likelihood ratio statistics $\bar{\chi}_{01}^2$ (1.3) and $\bar{\chi}_{12}^2$ (1.4) are squared norms of the orthogonal projection of A onto \mathcal{S}_p^+ and its dual cone $(\mathcal{S}_p^+)^*$, respectively.

Define

$$S_{r,p} = \{ W \in S_p \mid \operatorname{rank} W = r \},\$$

and

$$\begin{split} \mathcal{S}_{r,p}^+ &= \mathcal{S}_{r,p} \cap \mathcal{S}_p^+ \\ &= \{ W \in \mathcal{S}_p \mid W \geq O, \operatorname{rank} W = r \}. \end{split}$$

Then we have a partition of the boundary ∂S_p^+ of S_p^+ :

$$\partial \mathcal{S}_p^+ = \mathcal{S}_{p-1,p}^+ \cup \cdots \cup \mathcal{S}_{1,p}^+ \cup \mathcal{S}_{0,p}^+.$$

Fix $W_0 \in \mathcal{S}_{r,p}^+$. The spectral decomposition of W_0 is denoted by $W_0 = H_{10}\Lambda_0 H_{10}'$, where $\Lambda_0 = \operatorname{diag}(l_{10}, \ldots, l_{r0})$ with $l_{10} \geq \cdots \geq l_{r0} > 0$ and H_{10} is a $p \times r$ matrix such

that $H_{10}'H_{10}=I_r$. Let H_{20} be a $p\times (p-r)$ matrix such that $H_0=(H_{10},H_{20})$ is $p\times p$ orthogonal. The normal cone of \mathcal{S}_p^+ at W_0 , defined by

$$(2.2) N(\mathcal{S}_{p}^{+}, W_{0}) = \{ Y \in \mathcal{S}_{p} \mid \text{tr} Y(Z - W_{0}) \leq 0, \forall Z \in \mathcal{S}_{p}^{+} \},$$

is given in the following.

LEMMA 2.1. The normal cone (2.2) of S_p^+ at $W_0 \in S_{r,p}^+$ is

$$N(\mathcal{S}_{p}^{+}, W_{0}) = \{-H_{20}Y_{22}H_{20}' \mid Y_{22} \in \mathcal{S}_{p-r}^{+}\}$$

$$= \left\{-H_{0}YH_{0}' \mid Y = \begin{pmatrix} O & O \\ O & Y_{22} \end{pmatrix}, Y_{22} \in \mathcal{S}_{p-r}^{+}\right\}$$

with the dimension

$$\dim N(\mathcal{S}_p^+, W_0) = (p-r)(p-r+1)/2.$$

PROOF. Put

$$M(W_0) = \left\{ -H_0 Y H_0' \mid Y = \begin{pmatrix} O & O \\ O & Y_{22} \end{pmatrix}, Y_{22} \in \mathcal{S}_{p-r}^+ \right\}.$$

From the definition of

$$N(\mathcal{S}_{p}^{+}, W_{0}) = \left\{ -H_{0}YH_{0}' \middle| \operatorname{tr} \begin{pmatrix} Y_{11} & Y_{12} \\ {Y_{12}'} & Y_{22} \end{pmatrix} \begin{pmatrix} Z_{11} - \Lambda_{0} & Z_{12} \\ {Z_{12}'} & Z_{22} \end{pmatrix} \geq 0, \forall Z \in \mathcal{S}_{p}^{+} \right\},\,$$

it holds obviously that

$$N(\mathcal{S}_p^+, W_0) \supset M(W_0).$$

The proof of the converse is as follows. Fix a point in S_p as

$$-H_{0}V{H_{0}}' = -\left(\begin{array}{cc} H_{10} & H_{20} \end{array} \right) \left(\begin{array}{cc} V_{11} & V_{12} \\ {V_{12}}' & V_{22} \end{array} \right) \left(\begin{array}{cc} {H_{10}}' \\ {H_{20}}' \end{array} \right) \in \mathcal{S}_{p}$$

such that

$$(2.3) -H_0VH_0' \notin M(W_0).$$

Case 1) If V_{22} is not nonnegative definite, there exist $-\lambda < 0$, a negative eigenvalue of V_{22} , and the corresponding eigenvector v. Putting

$$Z = \begin{pmatrix} \Lambda_0 & O \\ O & vv' \end{pmatrix} \in \mathcal{S}_p^+,$$

we see that

$$\mathrm{tr} \bigg\{ V \bigg(Z - \left(\begin{matrix} \Lambda_0 & O \\ O & O \end{matrix} \right) \bigg) \bigg\} = - \lambda v' v < 0.$$

Case 2) If $V_{11} \neq O$, we can choose $\varepsilon > 0$ such that

$$Z = \begin{pmatrix} \Lambda_0 - \varepsilon V_{11} & O \\ O & O \end{pmatrix} \in \mathcal{S}_p^+$$

and

$$\operatorname{tr}\left\{V\bigg(Z-\begin{pmatrix}\Lambda_0 & O\\ O & O\end{pmatrix}\bigg)\right\}=-\varepsilon\operatorname{tr}{V_{11}}^2<0.$$

Case 3) If $V_{11} = O$ and $V_{12} \neq O$, we can choose a sufficiently small number $\varepsilon > 0$ such that

$$Z = \begin{pmatrix} \Lambda_0 + I_r & -\varepsilon V_{12} \\ -\varepsilon V_{12}' & \varepsilon^2 V_{12}' V_{12} \end{pmatrix} \in \mathcal{S}_p^+$$

and

$$\operatorname{tr}\left\{V\bigg(Z-\left(\begin{smallmatrix} \Lambda_{0} & O \\ O & O \end{smallmatrix} \right) \bigg)\right\} = -2\varepsilon\operatorname{tr}V_{12}V_{12}{'} + \varepsilon^{2}\operatorname{tr}V_{12}V_{22}V_{12}{'} < 0.$$

The three cases 1)-3) above cover (2.3) and we obtain

$$N(\mathcal{S}_p^+, W_0) \subset M(W_0).$$

This completes the proof. \Box

Remark 2.1. $\mathcal{S}_{p-1,p}^+$ is a smooth surface of the boundary $\partial \mathcal{S}_p^+$ of \mathcal{S}_p^+ in the sense that the normal cone at any point on $\mathcal{S}_{p-1,p}^+$ is one dimensional. $\mathcal{S}_{r,p}^+$, $r=0,\ldots,p-2$, form singularities of $\partial \mathcal{S}_p^+$ in the sense that the dimensions of the corresponding normal cones are greater than one. \mathcal{S}_p^+ is a typical example of piecewise smooth cone defined in the Appendix.

2.2 Second fundamental form

We proceed to derive the second fundamental form at $W_0 \in \mathcal{S}_{r,p}^+$ with respect to the direction of the normal cone (2.2). In order to do this we introduce a local coordinate system $X = (x_{ij}) = \begin{pmatrix} X_{11} & X_{12} \\ X_{12}' & X_{22} \end{pmatrix}$ of \mathcal{S}_p in the neighborhood of W_0 as

$$\begin{split} \mathcal{S}_p \ni W &= W_0 + H_0 X H_0{}' \\ &= \left(\begin{array}{ccc} H_{10} & H_{20} \end{array} \right) \left(\begin{array}{ccc} \Lambda_0 + X_{11} & X_{12} \\ X_{12}{}' & X_{22} \end{array} \right) \left(\begin{array}{ccc} H_{10}{}' \\ H_{20}{}' \end{array} \right). \end{split}$$

In this coordinate system W_0 is represented as X = O. We note here that for a $p \times p$ orthogonal matrix H, the transform $W \mapsto HWH'$ is orthogonal and preserves the inner product (2.1), because

(2.4)
$$\operatorname{tr}(HW_1H')(HW_2H') = \operatorname{tr}W_1W_2.$$

Hence, the new coordinate system X, that is, $(x_{11}, \ldots, x_{pp}, \sqrt{2}x_{12}, \ldots, \sqrt{2}x_{p-1,p})$, is also orthonormal.

Here we can take $\partial/\partial x_{ii}$ $(r+1 \leq i \leq p)$, $\partial/\partial(\sqrt{2}x_{ij})$ $(r+1 \leq i < j \leq p)$ as an orthonormal basis of $N(\mathcal{S}_p^+, W_0)$, and therefore, $\partial/\partial x_{ii}$ $(1 \leq i \leq r)$, $\partial/\partial(\sqrt{2}x_{ij})$ $(1 \leq i \leq r, i < j \leq p)$ as an orthonormal basis of $N(\mathcal{S}_p^+, W_0)^{\perp} = T_{W_0}(\mathcal{S}_{r,p}^+)$, which is the tangent space of $\mathcal{S}_{r,p}^+$ at W_0 .

In the neighborhood of W_0 , $W \in \mathcal{S}_{r,p}^+$ is equivalent to

$$X_{22} = X_{12}'(\Lambda_0 + X_{11})^{-1}X_{12},$$

because $\Lambda_0 + X_{11}$ is positive definite in the neighborhood of W_0 . Fix a particular direction of the normal cone $\tilde{W} = -H_{20}YH_{20}' \in N(\mathcal{S}_p^+, W_0)$, where $Y = (y_{ij}) \in \mathcal{S}_{p-r}^+$. Then, the second fundamental form with respect to the normal direction \tilde{W} becomes

(2.5)
$$H(W_0, \tilde{W}) = \frac{\partial^2 \operatorname{tr}(Y X_{22})}{\partial ((x_{ii})_{1 \le i \le r}, (\sqrt{2} x_{ij})_{1 \le i \le r, i < j \le p})^2} \Big|_{W_0}.$$

The (k, l)-th element of X_{22} is

$$(2.6) x_{k+r,l+r} = (X'_{12}(\Lambda_0 + X_{11})^{-1}X_{12})_{kl}$$

$$= (x_{1,k+r}, \dots, x_{r,k+r})(\Lambda_0 + X_{11})^{-1} \begin{pmatrix} x_{1,l+r} \\ \vdots \\ x_{r,l+r} \end{pmatrix}, 1 \le k, l \le p-r.$$

Differentiating (2.6) twice with respect to $(x_{ii})_{1 \le i \le r}$, $(\sqrt{2}x_{ij})_{1 \le i \le r, i < j \le p}$, and putting $X_{11} = O$ and $X_{12} = O$, we see that the nonvanishing terms of (2.5) are only

$$\left. \frac{\partial^2 x_{m+r,n+r}}{\partial (\sqrt{2}x_{i,k+r})\partial (\sqrt{2}x_{j,l+r})} \right|_{W_0} = \frac{\delta_{ij}}{l_{i0}} \cdot \frac{\delta_{km}\delta_{ln} + \delta_{kn}\delta_{lm}}{2},$$

 $1 \leq i, j \leq r, 1 \leq k, l, m, n \leq p - r$, where δ_{ij} denotes the Kronecker delta. Hence,

$$\left.\frac{\partial^2 \operatorname{tr}(YX_{22})}{\partial (\sqrt{2}x_{i,k+r})\partial (\sqrt{2}x_{j,l+r})}\right|_{W_0} = \frac{\delta_{ij}}{l_{i0}} \cdot y_{kl},$$

and other contributions are zero. Now we have established the following.

LEMMA 2.2. The nonvanishing part of the second fundamental form at $W_0 = H_{10}\Lambda_0 H_{10}' \in \mathcal{S}_{r,p}^+$ with respect to the direction $\tilde{W} = -H_{20}YH_{20}' \in N(\mathcal{S}_p^+, W_0)$ is

$$H(W_0, \tilde{W}) = \left(rac{\delta_{ij}}{l_{i0}} \cdot y_{kl}
ight) = {\Lambda_0}^{-1} \otimes Y.$$

Here $H_0 = (H_{10}, H_{20})$ is $p \times p$ orthogonal, and \otimes denotes the Kronecker product.

We now proceed to evaluate the elementary symmetric functions of the eigenvalues of second fundamental form $H(W_0, \tilde{W})$. Let $\tilde{\Lambda} = \text{diag}(\tilde{l}_1, \dots, \tilde{l}_{p-r})$ be the eigenvalues of Y and let

$$\operatorname{tr}_m H(W_0, \tilde{W}) = \operatorname{tr}_m(\Lambda_0^{-1} \otimes Y) = \operatorname{tr}_m(\Lambda_0^{-1} \otimes \tilde{\Lambda})$$

denote the m-th trace of $H(W_0, \tilde{W})$. (For the definition of m-th trace, see the Appendix, or Appendix A.7 of Muirhead (1982).)

LEMMA 2.3. For $\Lambda = \operatorname{diag}(l_i)_{1 \leq i \leq r}$ and $\tilde{\Lambda} = \operatorname{diag}(\tilde{l_i})_{1 \leq i \leq p-r}$, it holds

$$\det(\Lambda)^{p-r} \operatorname{tr}_{m}(\Lambda^{-1} \otimes \tilde{\Lambda}) = \sum_{(q,\bar{q})} \frac{\det(l_{i}^{q_{j}})_{1 \leq i,j \leq r}}{\prod_{1 \leq i < j \leq r} (l_{i} - l_{j})} \cdot \frac{\det(\tilde{l}_{i}^{q_{j}})_{1 \leq i,j \leq p-r}}{\prod_{1 \leq i < j \leq p-r} (\tilde{l}_{i} - \tilde{l}_{j})},$$

where the summation $\sum_{(q,\bar{q})}$ is over the set of integers

$$(q_1,\ldots,q_r,\bar{q}_1,\ldots,\bar{q}_{p-r})\in Q_{r,p}(-m+r(p-r)+r(r-1)/2)$$

with

$$Q_{r,p}(n) = \left\{ (q_1, \dots, q_r, \bar{q}_1, \dots, \bar{q}_{p-r}) \in \pi_p \;\middle|\; q_1 > \dots > q_r, \bar{q}_1 > \dots > \bar{q}_{p-r}, \sum_{j=1}^r q_j = n \right\}$$

and π_p denotes the set of all permutations of $\{p-1, p-2, \ldots, 0\}$.

PROOF. Define the generating function by

$$\Phi(x) = \sum_{m=0}^{r(p-r)} (-1)^m x^{r(p-r)-m} \det(\Lambda)^{p-r} \operatorname{tr}_m(\Lambda^{-1} \otimes \tilde{\Lambda}).$$

Then

$$(2.7) \qquad \Phi(x) = \det(\Lambda)^{p-r} \det(xI_r \otimes I_{p-r} - \Lambda^{-1} \otimes \tilde{\Lambda})$$

$$= \left(\prod_{i=1}^r l_i^{p-r}\right) \cdot \prod_{i=1}^r \prod_{j=1}^{p-r} \left(x - \frac{\tilde{l}_j}{l_i}\right)$$

$$= \prod_{i=1}^r \prod_{j=1}^{p-r} (l_i x - \tilde{l}_j)$$

$$= \det \begin{pmatrix} (xl_1)^{p-1} & \cdots & xl_1 & 1 \\ \vdots & & \vdots & \vdots \\ (xl_r)^{p-1} & \cdots & xl_r & 1 \\ \tilde{l}_1^{p-1} & \cdots & \tilde{l}_1 & 1 \\ \vdots & & \vdots & \vdots \\ \tilde{l}_{p-r}^{p-1} & \cdots & \tilde{l}_{p-r} & 1 \end{pmatrix}$$

$$/ \left[\prod_{1 \leq i \leq i \leq r} (xl_i - xl_j) \prod_{1 \leq i \leq i \leq r} (\tilde{l}_i - \tilde{l}_j)\right].$$

By the Laplace expansion of the determinant in (2.7), we have

$$\begin{split} \Phi(x) &= \sum_{(q,\bar{q})} (-1)^{r(r+1)/2 + \sum_{j=1}^{r} (p-q_j)} \frac{\det((xl_i)^{q_j})_{1 \leq i,j \leq r}}{\prod_{1 \leq i < j \leq r} (xl_i - xl_j)} \cdot \frac{\det(\tilde{l}_i^{\bar{q}_j})_{1 \leq i,j \leq p-r}}{\prod_{1 \leq i < j \leq p-r} (\tilde{l}_i - \tilde{l}_j)} \\ &= \sum_{(q,\bar{q})} (-1)^{r(r+1)/2 + \sum_{j=1}^{r} (p-q_j)} x^{\sum_{j=1}^{r} q_j - r(r-1)/2} \\ &\times \frac{\det(l_i^{q_j})_{1 \leq i,j \leq r}}{\prod_{1 \leq i < j \leq r} (l_i - l_j)} \cdot \frac{\det(\tilde{l}_i^{\bar{q}_j})_{1 \leq i,j \leq p-r}}{\prod_{1 \leq i < j \leq p-r} (\tilde{l}_i - \tilde{l}_j)}. \end{split}$$

Comparing the coefficients of $(-1)^m x^{r(p-r)-m}$, we prove the lemma. \square

Remark 2.2. The polynomial $\det(l_i^{q_j})/\prod(l_i-l_j)$ is called Schur function, which is symmetric and homogeneous in l_i (Macdonald (1995)).

2.3 Volume element

In addition to the normal cone and the second fundamental form, in order to apply Theorem A.1 of the Appendix for the cone of nonnegative matrices \mathcal{S}_p^+ , we have to know the concrete form of the volume element measure of $\mathcal{S}_{r,p}^+$. As a matter of fact, this volume element has been introduced by Theorem 2 of Uhlig (1994) as a carrier measure of the singular Wishart distribution. However, the expression he obtained is insufficient for our purpose, because he did not determine the multiplicative constant of the volume element, which is essential for our derivation. Therefore we give our derivation of the volume element including the multiplicative constant.

Before proceeding we prepare several facts on Stiefel manifolds. Let $\mathcal{V}_{r,p} = \{H_1 : p \times r \mid H_1'H_1 = I_r\}$ be the Stiefel manifold. Let H_2 be $p \times (p-r)$ such that $H = (H_1, H_2) = (h_1, \dots, h_r, h_{r+1}, \dots, h_p)$ is $p \times p$ orthogonal. Then the differential form for the invariant measure on $\mathcal{V}_{r,p}$ at H_1 is

$$dH_{r,p} = dH_{r,p}(H_1) = \bigwedge_{i=1}^{r} \bigwedge_{j=i+1}^{p} h_j' dh_i.$$

The integral over $\mathcal{V}_{r,p}$ is

$$\int_{\mathcal{V}_{r,p}} dH_{r,p}(H_1) = \frac{2^r \pi^{pr/2}}{\Gamma_r(p/2)}, \quad \Gamma_r\left(\frac{p}{2}\right) = \pi^{r(r-1)/4} \prod_{i=1}^r \Gamma\left(\frac{p-i+1}{2}\right).$$

Let

$$W = (w_{ij}) = H_1 \Lambda H_1' \in \mathcal{S}_{r,p},$$

where $\Lambda = \operatorname{diag}(l_1, \ldots, l_r)$, $l_1 \geq \cdots \geq l_r$, and $H_1 \in \mathcal{V}_{r,p}$. Then, the volume element of $\mathcal{S}_{r,p}$ can be written as follows.

LEMMA 2.4. The volume element of $S_{r,p}$ at W is

$$\begin{split} dW_{r,p} &= dW_{r,p}(W) \\ &= 2^{r(r-1)/4 + r(p-r)/2} \prod_{1 \le i \le j \le r} (l_i - l_j) \prod_{i=1}^r l_i^{p-r} \prod_{i=1}^r dl_i dH_{r,p}(H_1). \end{split}$$

PROOF. Proof is similar to the derivation of the second fundamental form in Subsection 2.2. Fix an arbitrary point $W_0 \in \mathcal{S}_{r,p}$ and write $W_0 = H_{10}\Lambda_0H_{10}'$, $\Lambda_0 = \operatorname{diag}(l_1,\ldots,l_r)$, $l_1 \geq \cdots \geq l_r$. We want to obtain the volume element at W_0 . Fix some H_{20} such that $H_0 = (H_{10},H_{20}) = (h_1,\ldots,h_r,h_{r+1},\ldots,h_p)$ is $p \times p$ orthogonal. As in Subsection 2.2 we take the elements of $X = H_0'(W - W_0)H_0$, $W \in \mathcal{S}_p$, as a local coordinate system.

Now we consider the exterior derivative $dX = (dx_{ij})$ of the matrix $X = H_0'(W - W_0)H_0$ at W_0 where W (and hence $H_0'WH_0$) is restricted in $\mathcal{S}_{r,p}$. Let $W = H_1\Lambda H_1'$ be the spectral decomposition of W. As a function of H_1 we choose H_2 such that $H = (H_1, H_2)$ is $p \times p$ orthogonal. Write the exterior derivatives of H and Λ as $dH = (dH_1, dH_2) = (dh_1, \ldots, dh_r, dh_{r+1}, \ldots, dh_p)$ and $d\Lambda = \operatorname{diag}(dl_1, \ldots, dl_r)$. Then

(2.8)
$$dX = d(H_0'(W - W_0)H_0)$$

$$= H_0'dWH_0$$

$$= H_0' \Big(dH \operatorname{diag}(\Lambda_0, O)H_0' + H_0 \operatorname{diag}(d\Lambda, O)H_0' + H_0 \operatorname{diag}(\Lambda_0, O)dH'\Big)H_0$$

$$= \begin{pmatrix} H_{10}'dH_1\Lambda_0 & O \\ H_{20}'dH_1\Lambda_0 & O \end{pmatrix} + \begin{pmatrix} d\Lambda & O \\ O & O \end{pmatrix} + \begin{pmatrix} \Lambda_0 dH_1'H_{10} & \Lambda_0 dH_1'H_{20} \\ O & O \end{pmatrix}.$$

It is seen that the $(p-r) \times (p-r)$ lower-right block of $dX = (dx_{ij})$ consists of zeros, that is, $dx_{ij} = 0$ $(r+1 \le i, j)$. Therefore as already remarked at the beginning of Subsection 2.2, we can take $\partial/\partial x_{ii}$ $(1 \le i \le r)$, $\partial/\partial (\sqrt{2}x_{ij})$ $(1 \le i \le r, i < j \le p)$ as an orthonormal basis for the tangent space $T_{W_0}(\mathcal{S}_{r,p})$. Taking the exterior product, we can evaluate the volume element of $\mathcal{S}_{r,p}$ at W_0 as

$$dW_{r,p} = \bigwedge_{i=1}^{r} dx_{ii} \bigwedge_{i=1}^{r} \bigwedge_{j=i+1}^{p} d(\sqrt{2}x_{ij}).$$

Now it follows form (2.8) that

$$dx_{ii} = dl_i,$$
 $1 \le i \le r,$ $dx_{ij} = (l_i - l_j)h_j'dh_i,$ $1 \le i \le r,$ $1 \le r,$

Therefore

$$dW_{r,p} = 2^{r(r-1)/4 + r(p-r)/2} \prod_{1 \le i \le j \le r} (l_i - l_j) \prod_{i=1}^r l_i^{p-r} \prod_{i=1}^r dl_i \bigwedge_{i=1}^r \bigwedge_{j=i+1}^p h_j' dh_i$$

and this proves the lemma. \Box

Corollary 2.1. Let ∂U be the surface of the unit ball

$$U = \{ W \in \mathcal{S}_p \mid \operatorname{tr} W^2 \le 1 \}.$$

The volume element of $S_{r,p} \cap \partial U$ at $W = H_1 \Lambda H_1'$, $\operatorname{tr} \Lambda^2 = 1$, is

$$dU_{r,p} = dU_{r,p}(W) = 2^{r(r-1)/4 + r(p-r)/2} \prod_{1 \le i < j \le r} (l_i - l_j) \prod_{i=1}^r l_i^{p-r} d\mu_r(l) dH_{r,p}(H_1),$$

where $d\mu_r(l)$ is the volume element of the surface

$$\{l = (l_1, \dots, l_r) \mid {l_1}^2 + \dots + {l_r}^2 = 1\}$$

of the unit ball.

PROOF. Each element of $S_{r,p}$ is uniquely written as tW with t > 0 and $W \in S_{r,p} \cap \partial U$. We consider the pair (t,W) as a coordinate system of $S_{r,p}$. Then the tangent space $T_{tW}(S_{r,p})$ is the direct sum of span $\{\partial/\partial t\}$ and $T_W(S_{r,p} \cap \partial U)$. In addition span $\{\partial/\partial t\}$ and $T_W(S_{r,p} \cap \partial U)$ are orthogonal because of tr $W^2 = 1$. Therefore, the volume element of $S_{r,p}$ at tW is written as

(2.9)
$$dW_{r,p}(tW) = dt \times t^{\dim(\mathcal{S}_{r,p} \cap \partial U)} dU_{r,p}(W),$$

where

$$\dim(\mathcal{S}_{r,p}\cap\partial U)=pr-rac{1}{2}r(r-1)-1.$$

Let $l = (l_1, \dots, l_r) \in \{l \mid {l_1}^2 + \dots + {l_r}^2 = 1\}$. The Lebesgue measure of R^r at tl is decomposed as

(2.10)
$$\prod_{i=1}^{r} d(tl_i) = dt \times t^{r-1} d\mu_r(l).$$

Putting t=1, the claim follows immediately from Lemma 2.4, (2.9) and (2.10). \Box

Remark 2.3. As mentioned in Muirhead (1982) and Uhlig (1994), we have to be careful because the sign of each h_i is not uniquely determined. If we integrate with respect to $dH_{r,p}$ over the whole $\mathcal{V}_{r,p}$, we have to divide by 2^r .

Remark 2.4. In Uhlig (1994), the inner product of S_p is not defined explicitly. If we adopt (2.1) as the inner product of S_p and regard $S_{r,p}$ as a submanifold of S_p , the constant $2^{r(r-1)/4+r(p-r)/2}$ is necessary in the expression of the volume element which does not appear in Theorem 2 of Uhlig (1994).

3. Weights of $\bar{\chi}^2$ distribution for \mathcal{S}_p^+

Now we can evaluate the weights $\{w_d\}$ of the $\bar{\chi}^2$ distribution in (1.6) by virtue of Theorem A.1 of the Appendix. What we want to do here is to evaluate the expression (A.1) in the case where the cone is \mathcal{S}_p^+ . First of all, note that p in (A.1) should be replaced by p(p+1)/2.

By Lemma 2.1, we see that $D_m(\partial S_p^+)$ which appears in (A.1) is nonempty only if m is of the form m = (p-r)(p-r+1)/2. Therefore, the double integral in (A.1) for m = (p-r)(p-r+1)/2 is written as

$$(3.1) I_{r,p}(i) = \int_{\mathcal{S}_{r,p}^+ \cap \partial U} \left[\int_{N(\mathcal{S}_{p}^+,W) \cap \partial U} \operatorname{tr}_{i-(p-r)(p-r+1)/2} H(W,\tilde{W}) dV(\tilde{W};W) \right] dU_{r,p}(W),$$

where $dV(\tilde{W};W)$ is the volume element of $N(\mathcal{S}_p^+,W)\cap \partial U$ at \tilde{W} , and the summation $\sum_{m=1}^i$ in (A.1) can be replaced by the summation over r such that $1\leq (p-r)(p-r+1)/2\leq i$.

Let $W = H_1 \Lambda H_1' \in \mathcal{S}_{r,p}^+$ be the spectral decomposition, where $\Lambda = \operatorname{diag}(l_1, \ldots, l_r)$, $l_1 \geq \cdots \geq l_r > 0$, and $H_1 \in \mathcal{V}_{r,p}$. Lemma 2.1 states that $\tilde{W} \in N(\mathcal{S}_p^+, W) \cap \partial U$ holds if and only if $\tilde{W} = -H_2 Y H_2'$ for $Y \in \mathcal{S}_{p-r}^+ \cap \partial U$, where H_2 is a $p \times (p-r)$ matrix such that (H_1, H_2) is orthogonal. Here, by the same argument of orthogonal transformation as in Subsection 2.3, the volume element of $N(\mathcal{S}_p^+, W) \cap \partial U$ at $\tilde{W} = -H_2 Y H_2'$ is easily shown to be $dU_{p-r,p-r}(Y)$. Then, by Lemma 2.2, (3.1) reduces to

$$(3.2) I_{r,p}(i) = \int_{\mathcal{S}_{r,p}^+ \cap \partial U} \left[\int_{\mathcal{S}_{p-r}^+ \cap \partial U} \operatorname{tr}_{i-(p-r)(p-r+1)/2} (\Lambda^{-1} \otimes Y) dU_{p-r,p-r}(Y) \right] dU_{r,p}(W).$$

Let $Y = \tilde{H}\tilde{\Lambda}\tilde{H}'$ be the spectral decomposition, where $\tilde{\Lambda} = \operatorname{diag}(\tilde{l}_1, \dots, \tilde{l}_{p-r}), \ \tilde{l}_1 \geq \dots \geq \tilde{l}_{p-r} \geq 0, \ \tilde{H} \in \mathcal{V}_{p-r,p-r}$. Let

$$\mathcal{L}_r^+ = \{l = (l_1, \dots, l_r) \mid l_1 \ge \dots \ge l_r > 0\}$$

and

$$\partial \mathcal{L}_r^+ = \{ l = (l_1, \dots, l_r) \mid l_1 \ge \dots \ge l_r > 0, l_1^2 + \dots + l_r^2 = 1 \}.$$

From Lemma 2.3, Corollary 2.1, and Remark 2.3, the integral (3.2) is separated into two parts as

$$I_{r,p}(i) = c_p \sum_{(q,\bar{q})} \int_{\partial \mathcal{L}_r^+} \det(l_k^{q_j})_{1 \leq k,j \leq r} d\mu_r(l) \cdot \int_{\partial \mathcal{L}_{p-r}^+} \det(\tilde{l}_k^{\bar{q}_j})_{1 \leq k,j \leq p-r} d\mu_{p-r}(\tilde{l}),$$

where the summation $\sum_{(q,\bar{q})}$ is over

$$(3.3) (q_1, \ldots, q_r, \bar{q}_1, \ldots, \bar{q}_{p-r}) \in Q_{r,p}(-i - r + p(p+1)/2),$$

and the constant is

(3.4)
$$c_{p} = \frac{1}{2^{r}} 2^{r(r-1)/4 + p(p-r)/2} \int_{\mathcal{V}_{r,p}} dH_{r,p}(H_{1})$$

$$\times \frac{1}{2^{p-r}} 2^{(p-r)(p-r-1)/4} \int_{\mathcal{V}_{p-r,p-r}} dH_{p-r,p-r}(\tilde{H})$$

$$= \frac{2^{p(p-1)/4} \pi^{p(p+1)/4}}{\prod_{k=1}^{p} \Gamma(k/2)}.$$

Note that (3.4) does not depend on r.

Then, the mixed volume defined by i) of Theorem A.1 is

$$\binom{p(p+1)/2}{i} V_{p(p+1)/2-i,i} = \frac{1}{i(p(p+1)/2-i)} \sum_{r} I_{r,p}(i),$$

where the summation \sum_{r} is over

$$(3.5) r \in R_p(i) = \{r \mid 0 \le i - (p-r)(p-r+1)/2 \le r(p-r)\},$$

since $\operatorname{tr}_{m'}(\Lambda^{-1} \otimes Y) = \operatorname{tr}_{m'}(\Lambda^{-1} \otimes \tilde{\Lambda}) = 0$ for m' > r(p-r). Now, by ii) of Theorem A.1, we obtain the following theorem.

Theorem 3.1. The weight $w_{p(p+1)/2-i}$ of (1.6) is given by

$$(3.6) w_{p(p+1)/2-i} = \binom{p(p+1)/2}{i} \frac{V_{p(p+1)/2-i,i}}{\omega_i \omega_{p(p+1)/2-i}} = \frac{1}{i(p(p+1)/2-i)} \Gamma\left(\frac{i}{2}+1\right) \Gamma\left(\frac{p(p+1)/2-i}{2}+1\right) \frac{2^{p(p-1)/4}}{\prod_{k=1}^{p}(k/2)} \times \sum_{r} \sum_{(q,\bar{q})} \int_{\partial \mathcal{L}_{r}^{+}} \det(l_k^{q_j})_{1 \leq k,j \leq r} d\mu_r(l) \times \int_{\partial \mathcal{L}_{p-r}^{+}} \det(\tilde{l}_k^{\bar{q}_j})_{1 \leq k,j \leq p-r} d\mu_{p-r}(\tilde{l}),$$

where the summations \sum_r and $\sum_{(q,\bar{q})}$ are over (3.5) and (3.3), respectively.

It is easy to verify that (3.6) coincides with the previous result in Kuriki (1993). Corresponding formula in Kuriki (1993) is

$$(3.7) w_{p(p+1)/2-i} = d_p \sum_{r} \sum_{(q,\bar{q})} \int_{\mathcal{L}_r^+} e^{-(l_1^2 + \dots + l_r^2)/2} \det(l_k^{q_j})_{1 \le k, j \le r} \prod_{k=1}^r dl_k$$

$$\times \int_{\mathcal{L}_{p-r}^+} e^{-(\bar{l}_1^2 + \dots + \bar{l}_{p-r}^2)/2} \det(\bar{l}_k^{\bar{q}_j})_{1 \le k, j \le p-r} \prod_{k=1}^{p-r} d\tilde{l}_k$$

where

$$d_p = \frac{1}{2^{p/2} \prod_{k=1}^p \Gamma(k/2)},$$

and the ranges of the summations \sum_r and $\sum_{(q,\bar{q})}$ are the same as in (3.6). Letting $l_1^2 + \cdots + l_r^2 = R^2$ and $\tilde{l}_1^2 + \cdots + \tilde{l}_{p-r}^2 = \tilde{R}^2$, we have $\prod_{k=1}^r dl_k = R^{r-1} dR d\mu_r(l)$ and $\prod_{k=1}^{p-r} d\tilde{l}_k = \tilde{R}^{p-r-1} d\tilde{R} d\mu_{p-r}(\tilde{l})$. By integrating with respect to R and \tilde{R} using

$$\int_0^\infty R^\alpha e^{-R^2/2} dR = 2^{(\alpha-1)/2} \Gamma\left(\frac{\alpha+1}{2}\right),$$

we see that (3.7) coincides with (3.6).

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Appendix : $ar{\chi}^2$ distribution for piecewise smooth cone alternatives

Let x be a random vector distributed according to the p dimensional normal distribution $N_p(\mu, I_p)$. Let K be a convex cone in \mathbb{R}^p . The dual cone of K is denoted by

$$K^* = \{y \mid \langle y, x \rangle \leq 0, \forall x \in K\},\$$

where $\langle \, , \, \rangle$ is the inner product. Then, for the problems of testing

$$H_0: \mu = 0$$
 against $H_1: \mu \in K$

and of testing

$$H_1: \mu \in K$$
 against $H_2: \mu \in \mathbb{R}^p$,

the likelihood ratio test statistics based on the observation x are given by $||x_K||^2$ and $||x_{K^*}||^2$, respectively, where x_K and x_{K^*} are the orthogonal projections onto K and K^* . We summarize here the results on the distributions for $||x_K||^2$ and $||x_{K^*}||^2$ under H_0 as well as relevant definitions from Section 2.3 of Takemura and Kuriki (1997).

For each point s on the boundary ∂K of the convex cone K, the normal cone N(K,s) is defined as

$$N(K, s) = \{ y \mid \langle y, z - s \rangle \leq 0, \forall z \in K \}$$

(Section 2.2 of Schneider (1993)). According to the dimension of the normal cone, we have a partition of the boundary

$$\partial K = D_1(\partial K) \cup \cdots \cup D_p(\partial K),$$

where

$$D_m(\partial K) = \{ s \in \partial K \mid \dim N(K, s) = m \}, \quad m = 1, \dots, p.$$

We make the following assumption on the convex cone K. We call such K piecewise smooth cone. As a special case, when $D_m(\partial K) = \emptyset$ for $m = 2, \ldots, p-1$, we call such K smooth cone.

ASSUMPTION A.1. $D_m(\partial K)$ is a p-m dimensional C^2 -manifold consisting of a finite number of relatively open connected components. Furthermore N(K,s) is continuous in s on $D_m(\partial K)$ in the sense of Lemma 1.2 of Takemura and Kuriki (1997).

Let $s \in D_m(\partial K)$. In a neighborhood of s we take an orthonormal system of vectors $e_1, \ldots, e_{p-m}, N_{p-m+1}, \ldots, N_p$ where e_1, \ldots, e_{p-m} constitute an orthonormal basis for the tangent space $T_s(D_m(\partial K))$ and N_{p-m+1}, \ldots, N_p constitute an orthonormal basis for the orthogonal complement $T_s(D_m(\partial K))^{\perp}$ of $T_s(D_m(\partial K))$. Clearly $N(K,s) \subset T_s(D_m(\partial K))^{\perp}$.

Let

$$H_{ij\alpha}(s), \quad i, j = 1, \dots, p - m, \quad \alpha = p - m + 1, \dots, p,$$

be the elements of the second fundamental form of $D_m(\partial k)$ at s with respect to the chosen coordinate system. The second fundamental form with respect to the normal direction

$$v = \sum_{\alpha=n-m+1}^{p} v^{\alpha} N_{\alpha} \in T_s(D_m(\partial K))^{\perp}, \quad \|v\| = 1,$$

is

$$H_{ij}(s,v) = \sum_{\alpha=p-m+1}^{p} v^{\alpha} H_{ij\alpha}(s).$$

Let $H(s,v) = (H_{ij}(s,v))$ be $(p-m) \times (p-m)$, and let $\operatorname{tr}_j H(s,v)$ be the j-th elementary symmetric function of eigenvalues of H(s,v).

THEOREM A.1. Let K be a closed convex cone satisfying Assumption A.1. For $m=1,\ldots,p-1$, let du_{p-m-1} denote the (p-m-1 dimensional) volume element of $D_m(\partial K)\cap \partial U$, where U is the unit ball in R^p . Let dv_{m-1} denote the (m-1 dimensional) volume element of $N(K,u_{p-m-1})\cap \partial U$ with $u_{p-m-1}\in D_m(\partial K)\cap \partial U$.

i) Put $K_{(1)} = K \cap U$ and $K_{(1)}^* = K^* \cap U$. Let $V_p(\cdot)$ denote the p dimensional volume in \mathbb{R}^p . Then, for ν , $\lambda \geq 0$,

$$V_p(\nu K_{(1)} + \lambda K_{(1)}^*) = \sum_{i=0}^p \binom{p}{i} \nu^{p-i} \lambda^i V_{p-i,i}(K_{(1)}, K_{(1)}^*),$$

where

(A.1)
$$\binom{p}{i} V_{p-i,i}(K_{(1)}, K_{(1)}^*)$$

$$= \frac{1}{i(p-i)} \sum_{m=1}^{i} \int_{D_m(\partial K) \cap \partial U}$$

$$\left[\int_{N(K, u_{p-m-1}) \cap \partial U} \operatorname{tr}_{i-m} H(u_{p-m-1}, v_{m-1}) dv_{m-1} \right] du_{p-m-1}.$$

(The coefficient $V_{p-i,i}(K_{(1)}, K_{(1)}^*)$ is called mixed volume (Webster (1994)).)

ii) Let x be a p dimensional random vector distributed as $N_p(0, I_p)$. Then,

$$P(\|x_K\|^2 \le a, \|x_{K^*}\|^2 \le b) = \sum_{i=0}^p w_{p-i} G_{p-i}(a) G_i(b),$$

$$w_{p-i} = \binom{p}{i} \frac{V_{p-i,i}(K_{(1)}, K_{(1)}^*)}{\omega_i \omega_{p-i}},$$

where

$$\omega_d = \frac{\pi^{d/2}}{\Gamma(d/2+1)}$$

is the volume of the unit ball in \mathbb{R}^d .

Remark A.1. Independently of Takemura and Kuriki (1997), Lin and Lindsay (1997) obtained the weights of $\bar{\chi}^2$ distribution when the cone K is a smooth cone by using the Weyl's formula for volume of tubes (Weyl (1939)). Their results reduce to our Theorem A.1 when $D_m(\partial K) = \emptyset$ except for m = 1.

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