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WITH SINGULAR COVARIANCE MATRIX

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ABSTRACT

The problem of estimating the mean of a p-variate normal distribution has been of considerable interest to the statisticians since the pioneering work of Stein who showed that the maximum likelihood estimator (MLE) is inadmissible with respect to a quadratic loss function when $p \ge 3$. Certain families of estimators have been shown in the literature to dominate the MLE. In this paper we consider the case in which the covariance matrix of the normal distribution is singular. An application of the given result arises in a problem of estimating the mean of a multinomial distribution.

Key Words: Multivariate Normal Distribution; Quadratic Loss; Minimax; Admissible; Multinomial Distribution.

AMS Classification: 62F10

*The author's work was supported by the Office of Naval Research under Contract N00014-75-C-0451. 1. <u>Introduction</u>. Let X be a K-component (K \geq 3) random vector distributed according to a multivariate normal distribution N(μ , Σ) with mean μ and covariance Σ . For estimating μ let the loss function be given by

(1.1)
$$L(\delta;\mu,\Sigma) = (\delta-\mu)'A(\delta-\mu)$$

where $\delta = \delta(X)$ denotes any estimator of μ , and A is a given symmetric positive (semi-positive) definite matrix. The maximum likelihood estimator (MLE) is the vector X and is known to be minimax. On the other hand, for A = I and $\Sigma = \sigma^2 I$, where I denotes the identity matrix, Stein (1955) showed that the MLE is inadmissible with respect to the given loss function. Since the pioneering work of Stein, the given problem has been examined by various authors. They have considered certain families of estimators which are shown to dominate the MLE. They are therefore minimax. The papers of Alam (1977) and Efron and Morris (1973, 1976) may be cited for reference. A list of other papers may be seen in the bibliography given in the two papers.

In the papers cited above, the minimax estimators are given for the case in which the covariance Σ is a non-singular matrix. In this paper we consider the case in which Σ is singular. Two cases may be considered: (i) Σ is known and (ii) Σ is unknown, but an estimate S/m is given, where S is distributed independent of X according to a Wishart distribution $W(S;\Sigma,m)$. Let $\phi: [0,\infty) \rightarrow [0,1]$. If Σ is non-singular, consider a class of estimators, given by

(1)

(1.2)
$$\delta(X) = \phi(X'\Sigma^{-1}X)X \text{ for case (i), and}$$

(1.3)
$$\eta(X) = \phi(X'S^{-1}X)X$$
 for case (ii).

The author has shown (Alam (1977), Theorems 2.1 and 2.2*) that δ and η dominate the MLE for a certain class of functions ϕ . In the following section we shall extend the given result to the case in which Σ is singular. For this case, the estimators are given by substituting Σ^{-1} for Σ^{-1} in (1.2) and S^{-1} for S^{-1} in (1.3), where Σ^{-1} and S^{-1} are generalized inverse of Σ and S, respectively, satisfying the relations $\Sigma\Sigma^{-}\Sigma = \Sigma$ and $SS^{-}S = S$.

An application of the given result arises in the problem of estimating the mean of a multinomial distribution M(n,p), where $p = (p_1, \ldots, p_k)'$ denotes the cell probabilites and n represents the total of cell frequencies. To see this, let $X \stackrel{d}{\sim} M(n,p)$ where $\stackrel{d}{\sim}$ means "distributed as". The vector X/n is the maximum likelihood estimator of p, its covariance is a singular matrix and it is asymptotically normally distributed for large n.

2. <u>Main results</u>. First let Σ be known. Consider the estimator δ , given by (1.2), with the substitution of Σ^- for Σ^{-1} , where Σ^- is a generalized inverse of Σ . Let X = QY, where $Y \stackrel{d}{\sim} N(v,I)$, $QQ' = \Sigma$ and $\mu = Qv$. Since $\Sigma\Sigma^-\Sigma = \Sigma$ or $QQ'\Sigma^-QQ' = QQ'$, we have $Q'\Sigma^-QQ' = Q'$. Therefore

 $(2.1) \qquad Q'\Sigma QQ'\Sigma Q = Q'\Sigma Q.$

(2)

That is, Q'E Q is an idempotent matrix. Also

(2.2) Rank
$$Q'\Sigma Q = Rank \Sigma = l$$
, say.

Since DADE D = DE DAD, or

 $Q(Q'A\Sigma\Sigma^{-}Q - Q'\Sigma^{-}\SigmaAQ)Q' = 0$

we have

$$(2.3) \qquad Q'AQQ'\Sigma Q = Q'\Sigma QQ'AQ.$$

That is, the matrices Q'AQ and Q' Σ Q commute. Therefore, there exists an orthogonal matrix P, say, which diagonalizes simultaneously the two matrices. Since Q' Σ Q is idempotent, we have

$$P'Q\Sigma^{-}QP = I_{\ell}$$
$$P'Q'AOP = D$$

where I_{g} denotes a K×K diagonal matrix with l elements on the diagonal, each equal to 1 and the remaining elements equal to zero, and D denotes a diagonal matrix of rank r, where

 $r = Rank Q'AQ \leq Rank Q = Rank QQ' = \ell$.

The risk, that is, the expected loss of δ is given by

(2.4)

$$R_{\delta} = E \left(\delta(X) - \mu \right)' A \left(\delta(X) - \mu \right)$$

$$= E \left(\phi(Y'Q'\Sigma^{-}QY)Y - \nu \right)' Q' A Q \left(\phi(Y'Q'\Sigma^{-}QY)Y - \nu \right)$$

$$= E \left(\phi(Z'I_{\varrho}Z)Z - \gamma \right)' D \left(\phi(Z'I_{\varrho}Z)Z - \gamma \right)$$

where $\gamma = P'v$ and $Z = P'Y \stackrel{d}{\sim} N(\gamma, I)$. Without loss of generality, we can assume that the first ℓ diagonal elements of I_{ℓ} are each equal to 1 and that $d_i = 0$ for $i > \ell$ where d_i denotes the ith diagonal element of D. Let $W = (Z_1, \ldots, Z_{\ell})', \gamma^* = (\gamma_1, \ldots, \gamma_{\ell})'$ and let D* be obtained from D by removing the last K- ℓ rows and columns. Then

(2.5) $R_{\delta} = E \left(\phi(W'W)W - \gamma^{*} \right) D^{*} \left(\phi(W'W)W - \gamma^{*} \right).$

Let $\alpha_1, \ldots, \alpha_k$ denote the characteristic roots of A Σ or equivalently of Q'AQ. Let $\psi(A\Sigma) = \text{trace } A\Sigma$ and $\alpha_0 = \frac{\psi(A\Sigma)}{2} / \max(\alpha_1, \ldots, \alpha_k) \leq 1$. Observe that the risk of the MLE is equal to $\psi(A\Sigma)$. Comparing (2.5) with (2.6) of [1] we obtain the following generalization of Theorem 2.1 of [1].

<u>Theorem 2.1</u>. Let $l \ge 3$. Then $R_{\delta} - \psi(A\Sigma) \le 0$ if (i) $x^{t+1}(1-\phi(x))$ is nondecreasing in x, and (ii) $0 \le x(1-\phi(x)) \le 2\alpha_0 l - 4t - 4$ for some value of $t \ge 0$.

When Σ is unknown we consider the estimator n, given by (1.3) with the substitution S⁻ for S⁻¹, where S⁻ denotes a generalized inverse of S. We obtain as above the following generalization of Theorem 2.1* of [1].

<u>Theorem 2.1*</u>. Let $\ell \ge 3$. Then $R_{\eta} - \psi(A\Sigma) \le 0$ if (i) $x^{t+1}(1-\phi(x))$ is nondecreasing in x, and (ii) $0 \le (m-n+2t+3)x(1-\phi(x)) \le 2\alpha_0\ell-4t-4$ for some value of $t \ge 0$.

(4)

3. Application. Consider the multinomial distribution M(n,p) with k cells, and let $X \stackrel{d}{\sim} M(n,p)$. The covariance matrix of X is given by $\Sigma = (\sigma_{ij})$, where $\sigma_{ij} = -np_ip_j$ (i \neq j) and $\sigma_{ii} = np_i(1-p_i)$. Clearly, Σ is singular. For estimating np_i let the loss be given by (1.1). Two cases are considered: (a) $A = n^{-1}I$ and (b) $A = n^{-1}C$, where C is a diagonal matrix whose ith diagonal element is equal to p_i^{-1} . In case (a) the loss is proportional to the sum of squared errors. Since n⁻¹C is a generalized inverse of Σ , the loss in case (b) is proportional to Mahalanobis distance function. The loss due to the MLE in case (b) leads to Pearson's Chi-square statistic, used for the goodness of fit test. Since X is asymptotically normally distributed for large values of n, Theorem 2.1 might be used to improve upon the maximum likelihood estimator X. For the application of the theorem it should be noted that $l = rank \Sigma = k-1$ and that the characteristic equation of $n^{-1}\Sigma$ is given by

(3.1)
$$(1 - \sum_{i=1}^{k} \frac{p_i^2}{p_i^{-\lambda}}) \prod_{i=1}^{k} (p_i^{-\lambda}) = 0.$$

Let λ_0 denote the largest characteristic root of $n^{-1}\Sigma$. From (3.1) we have that $p_{[k-1]} \leq \lambda_0 \leq p_{[k]}$, where $p_{[i]}$ denotes the ith smallest value amongst p_1, \ldots, p_k . Therefore, in the case (a)

$$\alpha_0 = (1 - \sum_{i=1}^{k} p_i^2) / \lambda_0^{(k-1)}.$$

(5)

In the case (b), the largest characteristic root of A₂ is equal to 1, and $\alpha_0 = 1$.

Consider the case (b). Let $\phi(x) = 1 - \frac{k-3}{x}$. Then

(3.2)
$$\delta(x) = (1 - \frac{k-3}{X'\Sigma X})X.$$

Since the diagonal matrix with the ith diagonal element equal to $(np_i)^{-1}$ is a generalized inverse of Σ , we substitute T^{-1} for Σ^- in (3.2) where T denotes a diagonal matrix whose ith diagonal element is equal to n_i , the maximum likelihood estimate of np_i . Then the risk of

(3.3)
$$\delta(x) = (1 - \frac{k-3}{X'TX}) X$$

$$= (1 - \frac{k-3}{n}) X$$

with respect to the loss (1.1) with $A = n^{-1}C$ is given by

(3.4)
$$R_{\delta} = (k-1) - \frac{(k+1)(k-3)}{n} + \frac{(k-1)(k-3)^2}{n^2}$$
$$< (k-1) = R_{\chi}$$

for n > (k-1)(k+3)/(k+1). Therefore, the MLE is inadmissible, being dominated by δ . The estimate can be further improved by letting

$$\delta(x) = (1 - \frac{v(k-3)}{x' z x}) x$$

and minimizing R_g for υ . The minimizing value of υ is given by

(6)

$$v_0 = \frac{k-3}{k-1} \left(1 + \frac{k-1}{n}\right)^{-1}$$

Remark: The choice of $\phi(x) = 1 - \frac{k-2}{x}$ in (1.2) for estimating the mean of a multivariate normal distribution with non-singular covariance matrix was originally proposed by James & Stein (1961). It should be noted, however, that the relation (3.4) establishing the inadmissibility of the MLE is not based on the asymptotic property of the multinomial distribution.

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