Minimax Estimation of a Multivariate Normal Mean with Unknown Covariance Matrix\*

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### ABSTRACT

Let x be a p-variate (p>3) vector, normally distributed with unknown mean  $\theta$  and unknown covariance matrix  $\Sigma$ . Let W:p×p be distributed independently of x, and let W have a Wishart distribution with n degrees of freedom and parameter  $\Sigma$ . It is desired to estimate  $\theta$  under the quadratic loss  $(\delta-\theta)$ 'Q $(\delta-\theta)$ , where Q is a known positive definite matrix. Under the condition that a lower bound for the smallest characteristic root of Q  $\Sigma$  is known, a family of minimax estimators is developed.

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### 1. INTRODUCTION

Let  $x:p\times 1$  be a normally distributed random vector with unknown mean  $\theta$  and unknown covariance matrix  $\Sigma$ . Assume that we have an independent estimator  $\hat{\Sigma} = n^{-1} W$  of  $\Sigma$ , where  $W: p\times p$  has a Wishart distribution with n degrees of freedom and parameter  $\Sigma = n^{-1}E(W)$ . In the usual notation,

$$\mathbf{x} \sim \mathbf{N}(\theta, \Sigma)$$
 ,  $\mathbf{W} \sim \mathcal{Y}_{\mathbf{p}}(\mathbf{n}, \Sigma)$ . (1)

We wish to estimate  $\theta$  with an estimator  $\delta(x,W)$  subject to the quadratic loss function

$$L(\delta, \theta, \Sigma) = (\delta - \theta) 'Q(\delta - \theta) / tr(Q\Sigma)$$
 (2)

Here, Q is a known pxp positive definite matrix, and tr(A) denotes the trace of the matrix A. Note that  $tr(Q\Sigma)$  is just a normalizing constant, chosen to give the estimator  $\delta_0(x,W)=x$  constant risk. It is well known that  $\delta_0$  is a minimax estimator for this problem.

The limiting case of this problem where  $\Sigma$  is completely known (corresponding here to  $n = \infty$ ) has recently received a good deal of attention. [See Berger [1] for references.] The problem with  $\Sigma$  unknown and  $Q = \Sigma^{-1}$  (which is <u>not</u> a special case for our problem because  $Q = \Sigma^{-1}$  cannot be known) has also been studied by James and Stein [5], Lin and Tsai [6], Bock [2], and Efron and Morris [3,4], among others. However, the assumption that  $Q = \Sigma^{-1}$  is rather artificial (it seems to be motivated only by invariance arguments), and does not seem to be of practical importance. A possibly more reasonable assumption to make relating Q and  $\Sigma$  is

that something is known about the characteristic roots of Q $\Sigma$ . [Note that if Q =  $\Sigma^{-1}$ , all of the characteristic roots of Q $\Sigma$  are equal to 1.] In the present paper, we assume that there exists a known constant K > 0 such that

$$\operatorname{ch}_{\mathbf{p}}(Q\Sigma) \geq K$$
, all  $\Sigma > 0$ , (3)

where

$$\operatorname{ch}_{1}(A) \geq \operatorname{ch}_{2}(A) \geq \dots \geq \operatorname{ch}_{p}(A)$$

denote the ordered characteristic roots of the  $p \times p$  symmetric matrix A. We consider estimators of the form

$$\delta_h(x, W) = (I_p - h(x'W^{-1}x)Q^{-1}W^{-1})x,$$
 (4)

where h(u) is an absolutely continuous function on  $[0,\infty)$ . Our main result, which is proven in Section 2, is the following.

THEOREM 1. If (3) holds, then any estimator of the form (4) for which

- (i) <u>u h(u) is nondecreasing in u</u>,
- (ii)  $0 \le h(u) \le 2(p-2)(n-p)Ku/(n-1)$ , all  $u \ge 0$ , dominates  $\delta_0(x, W) = x$  in risk, and hence is minimax.

It is clearly of interest to determine what happens to estimators of the form (4) when the bound (3) can be violated. In Section 3 it is shown that when (3) does not hold, no estimator of the form (4) can be minimax. [Bock [2] has previously shown that for  $Q = I_p$ , no estimator of the form  $h(x^*W^{-1}x)x$  can be minimax.] It is conjectured that members of a certain family (see (36)) of estimators closely resembling the estimators (4) in form may be minimax, but no proof of this result is given.

$$\Delta(\theta, \Sigma) = tr(Q\Sigma)E[L(\delta_h, \theta, \Sigma) - L(\delta_0, \theta, \Sigma)].$$
 (5)

Clearly if  $\Delta(\theta,\Sigma)\leq 0$ , all  $\theta$ , all  $\Sigma$  satisfying (3), then  $\delta_h$  is minimax for our problem.

Using the fact that a'Qa - b'Qb = (a-b)'Q(a+b), the fact that  $\delta_0(x,W) = x$ , and (4), we obtain

$$\Delta(\theta, \Sigma) = E[h^{2}(x' W^{-1}x)x' W^{-1}Q^{-1}W^{-1}x] - 2E[h(x' W^{-1}x)x'W^{-1}(x-\theta)]. \quad (6)$$

Note that for any functions g(x,W) for which Eg(x,W) exists, we may write

$$E[g(x,W)] = E_{W} \{E_{x|W}[g(x,W)]\} = E_{W} \{E_{x}[g(x,W)]\},$$
 (7)

where  $E_{x|W}[g(x,W)]$  denotes expectation over the conditional distribution of x given W, and  $E_{W}$  and  $E_{X}$  denote expectations over the marginal distributions of W and x respectively. The last equality in (7) holds since x and W are statistically independent. Further, using integration by parts term by term in the elements of x (with W treated as a fixed matrix), it can be shown (see Berger [1]) that

$$E_{x}[h(x^{\dagger}W^{-1}x)x^{\dagger}W^{-1}(x-\theta)] = E_{x}[h(x^{\dagger}W^{-1}x) trW^{-1}] + 2E_{x}[h^{(1)}(x^{\dagger}W^{-1}x) x^{\dagger}W^{-1}\Sigma W^{-1}x], \quad (8)$$

where  $h^{(1)}(u) = dh(u)/du$ . [Note: We are assuming that h(u) is differentiable; if not, a similar argument, using Riemann integration, produces a corresponding result; see Berger [1].]

From (6), (7). and (8), we have

$$\Delta(\theta, \Sigma) = E[h^{2}(x'W^{-1}x)x'W^{-1}Q^{-1}W^{-1}x - 2h(x'W^{-1}x)trW^{-1}\Sigma - 4h^{(1)}(x'W^{-1}x)$$

$$x'W^{-1}\Sigma W^{-1}x]. \qquad (9)$$

We now find a canonical representation for (9). Make the change of variables

$$y = \Sigma^{-1/2}x$$
,  $V = \Sigma^{-1/2}W\Sigma^{-1/2}$ , where  $\Sigma^{1/2}$  is any square root of  $\Sigma$ . Then

$$y \sim N(n, I_p), \quad V \sim \mathcal{Y}_p(n, I_p),$$
 (11)

where  $\eta = \Sigma^{-1/2}\theta$ . Further, y and V are statistically independent. From (9) and (10), with

$$Q^* = \Sigma^{1/2} Q\Sigma^{1/2},$$

and using arguments and notation analagous to that used to obtain (7), we have

$$\Delta(\theta, \Sigma) = E_{y} E_{V}[h^{2}(y'V^{-1}y) y'V^{-1}(Q^{*})^{-1}V^{-1}y - 2h(y'V^{-1}y)trV^{-1}$$

$$-4h^{(1)}(y'V^{-1}y)y'V^{-2}y] .$$
(12)

Let  $\Gamma_y$  be pxp orthogonal with first row equal to  $(y'y)^{-1/2}y'$ . Let  $U = \Gamma_y V \Gamma_y'$ ,  $Q_y^* = \Gamma_y Q^* \Gamma_y'$ . (13)

Then, given y,  $U \sim \mathcal{H}_p(n, I_p)$ , so that U and y are statistically independent. Partition U as

$$U = \begin{pmatrix} u_{11} & u_{21}^{\dagger} \\ u_{21} & U_{22} \end{pmatrix}, \quad u_{11}: 1 \times 1, \ U_{22}: (p-1) \times (p-1),$$

and let

$$s = u_{11} - u_{21}^{\dagger} U_{22}^{-1} u_{21}^{\dagger}, \quad t = U_{22}^{-1/2}$$
 (14)

where  $U_{22}^{1/2}$  is any square root of  $U_{22}$ . It is well known that s, t, and  $U_{22}$  are statistically independent, with

$$s \sim \chi_{n-p+1}^2$$
,  $t \sim N(0, I_{p-1})$ ,  $U_{22} \sim \mathcal{W}_{p-1}(n, I_{p-1})$ . (15)

Further,  $V^{-1} = \Gamma_y U^{-1} \Gamma_y$  and

$$U^{-1} = s^{-1} \begin{pmatrix} 1 & -t'U_{22}^{-1/2} \\ -U_{22}^{-1/2}t & U_{22}^{-1/2} (sI_{p-1} + tt')U_{22}^{-1/2} \end{pmatrix} ,$$
 (16)

so that

$$y'V^{-1}y = s^{-1}y'y$$
,  $y'V^{-2}y = s^{-2}y'y(1+t'U_{22}^{-1}t)$ , (17)

$$trV^{-1} = trU^{-1} = s^{-1} (1+t^{\prime}U_{22}^{-1}t) + trU_{22}^{-1},$$
 (18)

and

$$y^{\dagger}V^{-1}(Q^{*})^{-1}V^{-1}y = s^{-2}y^{\dagger}y(1,-t^{\dagger}U_{22}^{-1/2})(Q_{y}^{*})^{-1}(1,-t^{\dagger}U_{22}^{-1/2})^{\dagger}.$$
 (19)

Under the distributional assumptions given in (15), it is known that  $E\left(U_{22}^{-1}\right) = (n-p)^{-1}I_{p-1}, \text{ so that}$ 

$$EtrU_{22}^{-1} = tr EU_{22}^{-1} = (n-p)^{-1}(p-1).$$
 (20)

For any constant matrix A,

$$E[(1,-t'U_{22}^{-1/2})A(1,-t'U_{22}^{-1/2})']$$

$$= E_{U_{22}}E_{t} \left\{ tr \left[ A \begin{pmatrix} 1 & -t'U_{22}^{-1/2} \\ -U_{22}^{-1/2}t & U_{22}^{-1/2}tt'U_{22}^{-1/2} \end{pmatrix} \right] \right\}$$

$$= E_{U_{22}}tr \left[ A \begin{pmatrix} 1 & 0 \\ 0 & U_{22}^{-1} \end{pmatrix} \right]$$

$$= tr \left[ A \begin{pmatrix} 1 & 0 \\ 0 & (n-p)^{-1}I_{p-1} \end{pmatrix} \right]. \tag{21}$$

Taking  $A = I_p$ , the result (21) allows us to verify that

$$E(1 + t \cdot U_{22}^{-1}t) = (n-p)^{-1}(n-1).$$
(22)

Taking A =  $(Q_y^*)^{-1}$ , the result (21) yields

$$E[(1,-t,U_{22}^{-1/2})(Q_y^*)^{-1}(1,-t,U_{22}^{-1/2})']$$

$$= tr(Q_y^*)^{-1}\begin{pmatrix} 1 & 0 \\ 0 & (n-p)^{-1}I_{p-1} \end{pmatrix}.$$
(23)

If in (12) we make the change of variables (13) and (14), and take account of the identities (17), (18), and (19), then by taking our expected values in the order  $E_y E_t E_t$ , and using (20), (22), and (23), we obtain

$$\Delta(\theta, \Sigma) = (n-p)^{-1} E_{y}^{2} E_{s} [h^{2}(s^{-1}y'y)s^{-2}y'y \tau(y, Q') -2h(s^{-1}y'y)s^{-1}(n-1)-2h(s^{-1}y'y)(p-1) -4h^{(1)}(s^{-1}y'y)s^{-2}y'y(n-1)], \qquad (24)$$

where

$$\tau(y,Q^*) = tr(Q_y^*)^{-1} \begin{pmatrix} n-p & 0 \\ 0 & I_{p-1} \end{pmatrix}$$

$$= (n-p-1)(y'y)^{-1}y'(Q^*)^{-1}y + tr(Q^*)^{-1}.$$
(25)

Finally, integrating by parts in s, we can show that

$$E_s^{h(s^{-1}y \cdot y)} = (n-p-1)E_s^{[s^{-1}h(s^{-1}y \cdot y)]} - 2E_s^{[s^{-2}y \cdot yh^{(1)}(s^{-1}y \cdot y)]}, (26)$$

which, when substituted in (24), yields the expression

$$\Delta(\theta, \Sigma) = (n-p)^{-1} E_y E_s [h^2 (s^{-1}y'y)s^{-2}y'y\tau(y, Q^*) - 2p(n-p)s^{-1}h(s^{-1}y'y) - 4(n-p)h^{(1)}(s^{-1}y'y)s^{-2}y'y], \qquad (27)$$

where

$$y \sim N(\eta, I_p)$$
,  $s \sim \chi^2_{n-p+1}$ 

y and s are independent,  $\eta = \Sigma^{-1/2}\theta$ ,  $Q^* = \Sigma^{1/2}Q\Sigma^{1/2}$ , and  $\tau(y,Q^*)$  is given by (25). The expression (27) is the desired cononical form.

Now, we are ready to complete the proof of Theorem 1.

Let

$$r(u) = uh(u), (28)$$

and note that

$$h^{(1)}(u) = \frac{r^{(1)}(u)}{u} - \frac{r(u)}{u^2},$$
 (29)

where  $r^{(1)}(u) = dr(u)/du$ . Substituting in (27), we obtain

$$\Delta(\theta, \Sigma) = (n-p)^{-1} E_{y} \{ (y'y)^{-1} E_{s} [r^{2} (s^{-1}y'y)_{\tau}(y, Q^{*}) - 2(p-2)(n-p)r(s^{-1}y'y) - 4(n-p)s^{-1}r^{(1)}(s^{-1}y'y)] \}$$

$$\leq (n-p)^{-1} E_{y} E_{s} \left[ \frac{r(s^{-1}y^{r}y)}{y^{1}y} (\tau(y, Q^{*})r(s^{-1}y'y) - 2(p-2)(n-p)) \right],$$
(70)

since, by assumption (i) of Theorem 1, r(u) is nondecreasing in u. Note from (3) and (25) that

$$\tau(y,Q^*) \leq (n-1) \operatorname{ch}_1[(Q^*)^{-1}] \leq (n-1) \left[\operatorname{ch}_p(Q\Sigma)\right]^{-1} \leq (n-1) K^{-1}.$$
(31)

Thus, applying assumption (ii) of Theorem 1, (30), and (31), we conclude that for all satisfying (3),

$$\Delta(\theta, \Sigma) \leq 0$$
, all  $\theta$ .

This completes the proof of Theorem 1.1.

We remark that our proof actually demonstrates the following.

## THEOREM 2. Let an estimator $\delta_h(x,W)$ of the form (4) satisfy

- (i) <u>u h(u) is nondecreasing in u</u>,
- (ii)  $0 \le h(u) \le 2(p-2)(n-p)Lu$ , all  $u \ge 0$ ,

where L > 0 is a given constant. Then if  $\Sigma$  satisfies

$$\underline{(n-p-1)(\operatorname{ch}_{p}(Q\Sigma))^{-1} + \operatorname{tr}(Q\Sigma)^{-1}} \leq \underline{L}^{-1},$$
(32)

we have

 $\Delta(\theta, \Sigma) \leq 0$ , all  $\theta$ ,

### and $\delta_h(x,W)$ is minimax.

Although Theorem 2 is more general than Theorem 1, the additional generality is unlikely to be of practical importance.

3. THE CASE WHERE  $\Sigma$  IS COMPLETELY UNRESTRICTED

When  $\Sigma$  is unrestricted, and (3) need not hold, then  $\delta_0(x,W)$  is essentially the only estimator of the form (4) that can be minimax.

THEOREM 3. When  $\Sigma$  is unrestricted, no estimator of the form  $\delta_h(x,W) = \frac{(I_p - h(x \cdot W^{-1}x)Q^{-1}W^{-1})x}{(I_p - h(x \cdot W^{-1}x)Q^{-1}W^{-1})x} \frac{\partial_{\mu}(x,W)}{\partial_{\mu}(x,W)} = \frac{\partial_{\mu}(x,W)}{\partial_{\mu}$ 

$$\tau(y,Q^*) \ge tr(Q^*)^{-1},$$
 for all y. (33)

Now from (33) and (27),

$$\Delta(\theta, \Sigma) \ge \operatorname{tr}(Q^*)^{-1} E[h^2(s^{-1}y^{\dagger}y)s^{-2}y^{\dagger}y]$$

$$-2(n-p)E[ps^{-1}h(s^{-1}y^{\dagger}y)-2h^{(1)}(s^{-1}y^{\dagger}y)s^{-2}y^{\dagger}y] \qquad (34)$$

where the expected values in (34) are easily shown to depend only on  $\theta^{\dagger} \Sigma^{-1} \theta$ . Thus, if we choose a sequence  $\{(\theta_i, \Sigma_i)\}$  of parameter values such that  $\theta_i^{\dagger} \Sigma_i^{-1} \theta_i = c$ , all i, and

$$\operatorname{tr}(Q^*)^{-1} = \operatorname{tr}(\Sigma_i)^{-1}Q^{-1} \rightarrow \infty$$
, as  $i \rightarrow \infty$ ,

we see that unless

$$E[h^{2}(s^{-1}y^{\dagger}y)s^{-2}y^{\dagger}y] = 0$$
, all  $\theta^{\dagger}\Sigma^{-1}\theta = c$ , (35)

we will have  $\Delta(\theta_i, \Sigma_i) \to \infty$ . Thus, for some parameter points  $\Delta(\theta, \Sigma)$  will be positive (indeed, infinitely large), and hence  $\delta_h(x, W)$  cannot be minimax. On the other hand, it is easy to show that (35) holds if and only if h(u) = 0 for almost all  $u \ge 0$ . This completes the proof.

Estimators of the form (4) do not perform well when any linear combination of the elements of x has low variability (implying that  $\operatorname{ch}_{\mathbf{p}}(\Sigma)$  is small). To find a class of minimax estimators when  $\Sigma$  is unrestricted, we might think of modifying members of the class (4) to produce new estimators of the form

$$\delta_{h}^{*}(x,W) = (I_{p} - ch_{p}(n^{-1}QW)h(x'W^{-1}x)Q^{-1}W^{-1})x.$$
(36)

Assuming that  $\operatorname{ch}_p(n^{-1}QW)$  and  $\operatorname{ch}_p(Q\Sigma)$  are close in value (which should be true at least when n is large), any member of the class (36) will behave like the minimax estimator x when  $\operatorname{ch}_p(\Sigma)$  is small, and will behave like  $\delta_{\operatorname{ch}_p}(Q\Sigma)h$  otherwise. Thus, we have good intuitive reasons for conjecturing that a member of the class (36) of estimators is minimax provided that (i) uh(u) is nondecreasing in u, and (ii)  $0 \le h(u) \le 2(p-2)u$ , all  $u \ge 0$ . Unfortunately, we have not yet been able to prove this conjecture. One can follow the steps used in Section 2, but unlike the result (24) obtained for the class (4), integration over t and  $U_{22}$  does not lead to any simplification. This lack of simplification is due to

the fact that  $ch_p(n^{-1}QW)$ , after the change of variables from (x,W) to  $(y,s,t,U_{22})$ , is a complicated and nonlinear function of y, s, t, and  $U_{22}$ .

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