TOLERANCE REGIONS FOR A MULTIVARIATE NORMAL POPULATION*

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1. Summary and introduction

Suppose X: $k \times 1$ is a random vector having a k-variate normal distribution with mean vector μ : $k \times 1$ and positive definite covariance matrix $\sum k \times k$, i.e., with density function

(1)
$$f(X) = (2\pi)^{-k/2} \sum_{k=1}^{-1/2} \exp \left\{-\frac{1}{2}(X-\mu)' \sum_{k=1}^{-1} (X-\mu)\right\}.$$

The problem treated here is to construct the tolerance region based on a sample $S \equiv (X_1, X_2, \dots, X_N)$ of size N drawn from this population, which is a multivariate generalization of the univariate case treated by Wald and Wolfowitz [19].

The tolerance region under consideration is defined as the region R(S) such that, for given $\gamma(1>\gamma>0)$ and p(1>p>0),

$$(3) P\{A(S) \ge p\} = \gamma.$$

A(S) represents the proportion of the population which R(S) includes for a particular sample S. This proportion varies from sample to sample. The requirement (3) for the tolerance region is to guarantee, with the confidence coefficient γ , that the proportion A(S) is greater than or equal to a preassigned p.

Since we are concerned with a normal population, it is natural to consider, as R(S), the ellipsoidal region, because the equiprobability surface of the multivariate normal distribution (1) is an ellipsoid. Moreover the population tolerance region defined by

(4)
$$R_0 \equiv \{X: (X-\mu)' \sum^{-1} (X-\mu) \leq \chi_k^2(q)\} \quad (q=1-p)$$

has the smallest volume among regions which include proportion p of

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the population, where $\chi_k^2(q)$ is the upper 100 q% point of the chi-square variate with k degrees of freedom.

The following three cases are considered separately:

- (i) μ is unknown, \sum is known, (section 2),
- (ii) \sum is unknown, μ is known, (section 4),
- (iii) both μ and Σ are unknown, (section 5).

For these cases, μ or \sum or both must be replaced by its respective estimate obtained from the sample S. We use the usual unbiased estimates,

$$\bar{X} = \frac{1}{N} \sum_{\alpha=1}^{N} X_{\alpha} \text{ and } L_{0} = \frac{1}{N} \sum_{\alpha=1}^{N} (X_{\alpha} - \mu)(X_{\alpha} - \mu)', \ (\mu \text{ is known})$$

or
$$L = \frac{1}{N-1} \sum_{\alpha=1}^{N} (X_{\alpha} - \bar{X})(X_{\alpha} - \bar{X})', \ (\mu \text{ is unknown})$$

Noticing that the ellipsoid obtained by replacing the unknown parameters of $(X-\mu)' \sum^{-1} (X-\mu)$ by the corresponding estimates converges in probability to the ellipsoid in the population as $N \rightarrow \infty$, we can take our tolerance region in the form

(4)
$$R(\bar{X}, C^{i}) \equiv \{X: (X - \bar{X})' \sum^{-1} (X - \bar{X}) \leq C^{i}\},\$$

or

(5)
$$R(L_0, C^2) \equiv \{X: (X-\mu)'L_0^{-1}(X-\mu) \leq C^2\},\$$

or

(6)
$$R(\bar{X}, L, C^2) \equiv \{X: (X - \bar{X})'L^{-1}(X - \bar{X}) \leq C^2\},\$$

according to the three cases under consideration, where $C^2 \equiv C_{k,N}^2$ is the constant, depending on k and N, to be determined so that the requirement (3) is satisfied. In this formulation, it is of course necessary that C^2 should tend to $\chi_k^2(q)$ as $N \to \infty$.

In the following sections, A(S) and R(S) in (2) and (3) will be written as the function of C^2 and the statistics which are used in the definition of the sample ellipsoidal region.

For cases (ii) and (iii), there is a difficulty in constructing the regions satisfying the requirement (3) exactly, which arises from the complexity of the exact density functions of some positive definite quadratic forms. In section 3, some approximations to the probability function of the quadratic form are considered, which forces us to modify the requirement (3).

In section 6, a brief discussion of simultaneous tolerance intervals

is given by an argument similar to that developed by S. N. Roy and others. After a short discussion of some distribution theory (section 7), some charts are given in order to facilitate in the practical use of the method (section 8).

2. The case when μ is unknown but Σ is known

In this case, the problem is to determine the positive constant C^2 which defines the ellipsoidal region

(4)
$$R(\bar{X}, C^2) = \{X: (X - \bar{X})' \sum^{-1} (X - \bar{X}) \leq C^2\},\$$

such that the requirement (3) is satisfied for any μ . It is easily seen that, for fixed \overline{X} , the variable

$$\begin{aligned} \chi_{k}^{\prime 2} &= (X - \bar{X})' \Sigma^{-1} (X - \bar{X}) \\ &= \{ (X - \mu) - (\bar{X} - \mu) \}' \Sigma^{-1} \{ (X - \mu) - (\bar{X} - \mu) \} \end{aligned}$$

is distributed according to the noncentral chi-square distribution with k degrees of freedom with the noncentrality parameter

(7)
$$\tau^2 = (\bar{X} - \mu)' \sum^{-1} (\bar{X} - \mu).$$

Therefore the conditional probability A(S) under a particular sample S, which is now written as $A(\overline{X}, C^2)$ or $A(\tau^2, C^2)$, is evaluated from

(8)
$$A(\tau^{3}, C^{2}) \equiv P\{X \in R(X, C^{3}) \mid X\}$$
$$= 2^{-k/2} e^{-\tau^{2}/2} \sum_{r=0}^{\infty} \frac{\tau^{2r}}{r! 2^{2r} \Gamma(\frac{1}{2}k+r)} \int_{0}^{C^{2}} y^{k/2+r-1} e^{-y/2} dy.$$

For fixed C^2 , $A(\tau^2, C^2)$ varies from sample to sample; in other words, $A(\tau^2, C^2)$ is a random variable whose distribution is derived from the distribution of τ^2 . Moreover, for fixed C^2 , $A(\tau^2, C^2)$ is a continuous and strictly monotonic decreasing function of τ^2 . Therefore if, for a given γ , τ^2_{τ} is the value such that

(9)
$$P\{\tau^2 \equiv (\bar{X} - \mu)' \sum^{-1} (\bar{X} - \mu) \leq \tau_r^2\} = \gamma,$$

then we have

(10)
$$P\{A(\tau^2, C^2) \ge A(\tau_r^2, C^2)\} = \Pr\{\tau^2 \le \tau_r^2\} = \gamma,$$

since the relation $A(\tau^2, C^2) \ge A(\tau_r^2, C^2)$ is exactly equivalent to the relation $\tau^2 \le \tau_r^2$. (Fig. 1.) Hence if, for a preassigned p, we determine C_1^2

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satisfying

(11)
$$A(\tau_r^2, C_1^2) = p$$
,

which can be done uniquely, C_1^2 and therefore the region $R(\bar{X}, C_1^2)$ fulfills the required condition (3).

 τ_r^2 is calculated from

(12)
$$\tau_r^2 = \frac{1}{N} \chi_k^2(\delta), \text{ where } \delta = 1 - \gamma,$$

since $N\tau^2$ has the central chi-square distribution with k degrees of freedom. The charts for computing C_1^2 by (11) will be prepared in section 8 for k=2 and k=3. It is noted that C_1^2 depends on N and tends to $\chi_k^2(1-p)$ as $N\to\infty$.

The above argument is summarized as follows:

The γ tolerance ellipsoidal region, which contains, with probability 7, at least a proportion p of the k-variate normal population with known Σ , is the region defined by

(13)
$$R(\bar{X}, C_{1}^{2}) \equiv \{X: (X - \bar{X})' \sum^{-1} (X - \bar{X}) \leq C_{1}^{2}\},\$$

where C_{i}^{z} is given from (11) for $\tau_{\tau}^{z} = \frac{1}{N} \chi_{k}^{z} (1-\tau)$.

3. The approximation to the probability function of the positive definite quadratic form

Consider the positive definite quadratic form

(14)
$$Q_k = \frac{1}{a_1} y_1^2 + \frac{1}{a_2} y_2^2 + \cdots + \frac{1}{a_k} y_k^2,$$

where y_1, \dots, y_k are normally and independently distributed about zero

with unit variance and $0 < a_1 \le a_3 \le \cdots \le a_k$. The exact and approximate distributions of Q_k have been discussed by many authors, for example, Geisser [1], Gurland ([3], [4]), Grad and Solomon [2], Laurent [6], Pachares [8], Robbins [10] and Solomon [18]. Recently, Shah and Khatri [17] have discussed the case when y_i , $i=1, \cdots, k$, are noncentral normal variates.

Unfortunately, the existing results are not appropriate for the purpose of this paper. Consider the problem of finding a function h(a) of a_1, \dots, a_k but independent of y's such that

(15)
$$P\{y_1^2 + \cdots + y_k^2 \leq h(a)t\}$$

gives a good approximation to or a close lower bound of the exact value of $P(Q_k \leq t)$. Moreover it is desired to make the form of h(a) as simple as possible.

Since $y_1^2 + \cdots + y_k^2$ is a chi-square variable with k degrees of freedom, let us put $\chi_k^2 \equiv y_1^2 + \cdots + y_k^2$. Then the inequalities

(16)
$$P\{\chi_k^2 \leq a_1 t\} \leq P(Q_k \leq t) \leq P\{\chi_k^2 \leq (\prod_{i=1}^k a_i)^{1/k} t\}$$

hold for any positive a's and for any t. The first inequality is obvious and the second inequality is the result obtained by Okamoto [7]. The equality signs hold if and only if all the a_i are equal. From the point of view of the approximation, the lower bound is very poor but, on the other hand, the upper bound gives quite close values to $P(Q_k \leq t)$ for all t unless the variation of a_i 's is too large, as seen below. Therefore, starting with $(\prod_{i=1}^{k} a_i)^{1/k}$, we seek a desirable h(a). Noticing that among the elementary symmetric functions, $S_1(=\sum a_i), S_2, \dots, S_k(=\prod_{i=1}^{k} a_i)$ of a_1, a_2, \dots, a_k , we have the Maclaurin inequalities [5],

(17)
$$\frac{S_1}{\binom{k}{1}} \ge \left[\frac{S_2}{\binom{k}{2}}\right]^{1/2} \ge \cdots \ge \left[\frac{S_{k-1}}{\binom{k}{k-1}}\right]^{1/(k-1)} \ge S_k^{1/k} ,$$

we try to determine the positive integral values of ν and i in

(18)
$$h(a) = S_{k}^{1/k} \left(\frac{S_{k}^{1/k}}{\left[\frac{S_{\nu}}{\binom{k}{\nu}}\right]^{1/\nu}} \right)^{i} \qquad i = 1, 2, \dots; 1 \leq \nu \leq k-1.$$

In Tables 1 and 2 numerical results are given for k=2 and 3 respectively. The entries in tables are the values of the following expressions:

(a) k=2: (I) Exact: $P(Q_2 \le t) = P\left\{\frac{1}{1+u}y_1^2 + \frac{u}{1+u}y_2^2 \le \frac{a_1t}{1+u}\right\}$,

where $u = \frac{a_1}{a_3}$ $(1 \ge u \ge 0)$.

(II)
$$h(a) = \sqrt{a_1 a_2}$$
: $P\{\chi_2^2 \le h(a)t\} = P\{\chi_2^2 \le \frac{1+u}{\sqrt{u}}, \frac{a_1 t}{1+u}\}$
(III) $h(a) = \sqrt{a_1 a_2} \left(\frac{\sqrt{a_1 a_2}}{\frac{a_1 + a_2}{2}}\right) = \left[\frac{1}{2} \left(\frac{1}{a_1} + \frac{1}{a_2}\right)\right]^{-1}$:
 $P\{\chi_2^2 \le h(a)t\} = P\{\chi_2^2 \le 2\frac{a_1 t}{1+u}\}$

(IV)
$$h(a) = \sqrt{a_1 a_2} \left(\frac{\sqrt{a_1 a_2}}{\frac{a_1 + a_2}{2}} \right)^2 : P\{\chi_2^2 \leq h(a)t\} = P\left\{ \chi_2^2 \leq \frac{4\sqrt{u}}{1+u} \frac{a_1 t}{1+u} \right\}$$

TABLE 1. $P(Q_k \leq t)$ and $P\{\chi_k^3 \leq h(a)t\}$ for k=2.

u	$a_1t/(1+u)$	0.2	0.4	0.6	0.8	1.0	1.5	2.0	3.0	4.0	5.0
0.7	: (I)	0.1836	0.3331	0.4548	0.5540	0.6350	0.7781	0.8646	0.9490	0.9806	0.9925
	(11)	0.1839	0.3339	0.4564	0.5564	0.6379	0.7821	0.8689	0.9525	0.9828	0.9938
	(皿)	0.1813	0.3297	0.4512	0.5507	0.6321	0.7769	0.8647	0.9503	0.9817	0.9933
	(IV)	1	1		•	0.6263	0.7716	0.8603	0.9478	0.9805	0.9927
0.5	(I)	0.1900	0.3422	0.4644	0.5628	0.6423	0.7811	0.8642	0.9460	0.9777	0.9906
	, (I)	0.1911	0.3458	0.4708	0.5720	0.6537	0.7963	0.8801	0.9585	0.9856	0.9950
	(Ш)	0.1813	0.3297	0.4512	0.5507	0.6321	0.7769	0.8647	0.9503	0.9817	0.9933
	(IV)				, i	0.6105	0.7569	0.8483	0.9409	0.9770	0.9910
0.3	(1)	0.2066	0.3649	0.4873	0.5824	0.6583	0.7862	0.8619	0.9391	0.9719	0.9867
	(11)	0.2113	0.3779	0.5094	0.6130	0.6948	0.8314	0.9068	0.9716	0.9913	0.9974
	(Ⅲ)	0.1813	0.3297	0.4512	0.5507	0.6321	0.7769	0.8647	0.9503	0.9817	0.9933
	(IV)		,			0.5526	0.7175	0.7999	0.9202	0.9656	0.9852

(b) k=3:

(I) Exact:
$$P\{Q_3 \le t\} = P\{\frac{w}{u+w+uw}y_1^2 + \frac{u}{u+w+uw}y_2^2 + \frac{uw}{u+w+uw}y_3^2 - \frac{wa_1t}{u+w+uw}\}$$
,

where $u = \frac{a_1}{a_3}$ and $w = \frac{a_2}{a_3}$ $(1 \ge w \ge u \ge 0)$.

$\sqrt{wa_1t/(u+w+uw)}$													
1	10		0.2	0.4	0.6	0.8	1.0	1.6	2.0	2.4	3.0	4.0	5.0
	0.7	(1)	0.1052	0.2499	0.38830	.5093	0.61070	.81300	.88760	. 9330 0	. 9695 0	.9919().9979
		(II)	0.1055	0.2509	0.39040	0.5124	0.61460	.81810	.89230	.93700	.97230	.99320).9983
		(III)	0.1036	0.2470	0.38510	.5064	0.60840	.81300	.88840	.93420	.97070	.9926().9982
0.7		(IV)	1			 	0.60110	.80690	.88370	.93080	.96880	.99200).9980
	0.9	(I)	0.1051	0.2497	0.38810	.5091	0.61040	.81320	.88770	.93320	.96960	.9919).9979
		(II)	0.1052	0.2503	0.3896 0	.5115	0.61360	.81730	.89170	.93660	.97200	.9931).9983
		(Ⅲ)	0.1036	0.2470	0.38510	.5064	0.60840	.81300	.88840	.93420	.97070	. 9926 ().9982
		(IV)			Ì	(0.60360	.80900	.88530	. 9320 0	.96940	. 9922 ().9980
		(1)	0.1084	0.2556	0.39460	.5149	0.61490	.81300	.88590	.9307.0	.9673.0	.9907).9973
	0.6	(I)	0.1093	0.2589	0.40110	.5246	0.62710	.82810	.89980	.94240	.97530	.9941 ().9986
	0.0	(III)	0.1036	0.2470	0.38510	.5064	0.60840	.81300	.88840	.93420	.97070	.9926).9982
		(IV)	.		i	ļ	0.58580	.79400	.8736 0	. 9 234 0	.96440	.9904 ().9975
	0.8	(T)	0.1090	1 9565	2060.0	E164	61640	01070	9960.0	0202.0	0667.0	0001	0070
		(I) (П)	0.1005	2506	0.35000	52561	0.01040	8200,0	00000 0	04290	. 9057 0	00420	1.9970
0.5			0 10360) 2470	0.40210	5064	0.02020 0.60840	.02500 81300	. 50050 8884 0	034200	07070	0026(1.0092
			0.1000	.2470	1		0.59150	7988.0	8774.0	9262.0	96610	99100	1 9977
				· · · · · · · · · · · · · · · · · · ·	·								
		(1)	0.11060	0.2598	0.39980	.5201	0.61940	.81420	.88540	.92910	.96520	.9891().9965
	1.0	(II)	0.1116	0.2637	0.40760	0.53190	0.63450	.83390	.90420	.94540	.97690	.9947().9988
		(III) (III)	0.10360).2470	0.38510	.5064	0.60840	.81300	.88840	.93420	.97070	.9926().9982
		(1V)	, İ		÷ •		J.5895 U	.79710	.87610	.92520	.98550	.99080).9976
		(I)	0.11770	0.2714	0.41060	.5281	0.62420	.81210	.88200	.92630	.96390	.9884).9962
	0.4	(II)	0.1208).2823	0.43220	.5592	0.66200	.85480	.91940	.95580	.98230	.9963 ().9992
		(Ⅲ)	0.1036	0.2470	0.38510	.5064	0.60840	.81300	.88840	.93420	.9707 _, 0	.9926).9982
		(IV)					0.53430	.74770	.83590	.89450	.94640	.9832).9948
	0.6	(I)	0.1188	0.2743	0.41520	.5334	0.62940	.81450	.88230	.92410	.96310	.9866).9952
		(I)	0.1215).2839	0.4343 0	.5615	0.66440	.85650	. 9206 0	.95660	.9828'0	.9964).9993
		(Ⅲ)	0.1036).2470	0.38510	.5064	0.60840	.81300	.88840	. 9 3420	.9707 0	.9926).9982
		(IV)			Ì	0	0.55850	.76990	.85430	.90910	.95560	.9870).9963
0.3	0.8	(I)	0.1218).2804	0.42300	.5413	0.63630	.81610	.88140	.92250	.95900	.9848 ().9941
		(Π)	0.1254).2916	0.44400	.5725	0.67520	.86440	.9262.0	.96030	.98460	.9969 ().9994
		(Щ)	0.1036).2470	0.38510	.5064	0.60840	.81300	.8884.0	.93420	.97070	.99260).9982
		(IV)		Í		6	0.56570	.77640	.8596 0	.91280	.95800	.9879),9966
		(I)	0 12570	2860	1 43060	54860	64230	8166.0	8795.0	91080	9565.0	0833	0054
	1.0	(Π)	0.1301	.3011	. 45660	5857).68830	.8735.0	9325.0	9644	0,0000	9975) 9995
		(III)	0.1036	2470	0.38510	.5064).6084.0	.8130.0	88840	9342.0	97070	99261) 9982
		(IV)				1).56350	.7744.0	85800	.91160	.95730	.9877).9965
		(<u> </u>		<u> </u>	1							

TABLE 2. $P(Q_k \leq t)$ and $P\{\chi_k^2 \leq h(a)t\}$ for k=3.

$$(II) \quad h(a) = (a_{1}a_{3}a_{3})^{1/3} : P\{\chi_{3}^{2} \leq h(a)t\} = P\{\chi_{3}^{2} \leq \frac{u+w+uw}{(uw)^{2/3}} \cdot \frac{wa_{1}t}{u+w+uw}\}$$

$$(III) \quad h(a) = (a_{1}a_{2}a_{3})^{1/3} \left[\frac{(a_{1}a_{2}a_{3})^{1/3}}{\sqrt{1/3}\sqrt{a_{1}a_{2}+a_{2}a_{3}+a_{3}a_{1}}} \right]^{2} = \left[\frac{1}{3} \left(\frac{1}{a_{1}} + \frac{1}{a_{2}} + \frac{1}{a_{3}} \right) \right]^{-1} :$$

$$P\{\chi_{3}^{2} \leq h(a)t\} = P\{\chi_{3}^{2} \leq 3 \cdot \frac{wa_{1}t}{u+w+uw}\}$$

$$(IV) \quad h(a) = (a_{1}a_{2}a_{3})^{1/3} \cdot \left[\frac{(a_{1}a_{2}a_{3})^{1/3}}{(1/3)(a_{1}+a_{2}+a_{3})} \right]^{2} = \frac{9a_{1}a_{2}a_{3}}{(a_{1}+a_{2}+a_{3})^{3}} :$$

$$P\{\chi_{3}^{2} \leq h(a)t\} = P\{\chi_{3}^{2} \leq 9 \cdot \frac{u+w+uw}{(1+u+w)^{2}} \cdot \frac{wa_{1}t}{u+w+uw}\}.$$

As seen in the following sections, we are concerned with the upper part of the range of $P(Q_k \leq t) (\geq p=0.8 \text{ or } 0.9, \text{ say})$, and we are looking for an h(a), such that $P\{X_k^2 \leq h(a)t\}$ is smaller than, but not so rough or approximately equal to $P(Q_k \leq t)$. From this point of view and from the inspection of Tables 1 and 2, it is seen that

(19)
$$h(a) = (a_1 \cdots a_k)^{1/k} \left[\frac{(a_1 \cdots a_k)^{1/k}}{\frac{1}{k} (a_1 + \cdots + a_k)} \right]^2 \quad (k = 2, 3)$$

satisfies our requirements unless $u=a_1/a_k$ is too small. A similar examination could be carried out for $k \ge 4$, if necessary, but this would be quite laborious.

Now we shall return to the problem of the construction of the tolerance region.

4. The case when μ is known but Σ is unknown

Using the unbiased estimate L_0 of Σ , we want to determine the value of C^2 so that the ellipsoidal region

(5)
$$R(L_0, C^2) \equiv \{X: (X-\mu)' L_0^{-1} (X-\mu) \leq C^2\}$$

has the required property. However, the exact treatment is very complicated in this case and some modification or approximation will be used.

It is well known in the theory of matrices that for two positive definite matrices \sum and L_0 (L_0 is positive definite with probability one), there exists a nonsingular matrix T such that

(20)
$$T \sum T' = I$$
 and $TL_0 T' = D_{\lambda 0} \equiv \operatorname{diag}(\lambda_{01}, \dots, \lambda_{0k})$,

where $0 < \lambda_{01} \leq \lambda_{02} \leq \cdots \leq \lambda_{0k} < \infty$ are the roots of the determinantal equa-

tion $|L_0 - \lambda_0 \sum| = 0$. Using this matrix *T*, make the transformation

(21)
$$Y=T(X-\mu)$$
 and $T(X_{\alpha}-\mu)=Y_{\alpha}, \alpha=1, \cdots, N$.

Then

(22)
$$(X-\mu)'L_0^{-1}(X-\mu) = Y'D_{\lambda_0}^{-1}Y$$
$$= \frac{1}{\lambda_{01}}y_1^2 + \frac{1}{\lambda_{02}}y_2^2 + \cdots + \frac{1}{\lambda_{0k}}y_k^2,$$

where y_1, \dots, y_k are now mutually independent and are normally distributed with 0 mean and unit variance.

Consider the explicit evaluation of

(23)

$$A(S) \equiv A(L_{0}, C^{2}) = P_{r} \{ X \in R(L_{0}, C^{2}) | L_{0} \}$$

$$= P_{r} \{ \frac{1}{\lambda_{01}} y_{1}^{2} + \frac{1}{\lambda_{02}} y_{2}^{2} + \cdots + \frac{1}{\lambda_{0k}} y_{k}^{2} \leq C^{2} | \lambda_{0} = (\lambda_{01}, \cdots, \lambda_{0k}) \}$$

$$\equiv A(\lambda_{0}, C^{2}) .$$

This is of the same form as $P(Q_k \leq t)$ of the last section, and the complexity of the λ_{0t} 's in the exact or approximate expressions of $A(\lambda_0, C^2)$ is such that an evaluation of $P\{A(\lambda_0, C^2) \geq p\}$ is untractable. In order to solve our problem, even if approximate, let us consider the replacement of $A(\lambda_0, C^2)$ by $B(h(\lambda_0), C^2)$, which is an abbreviated notation of the form

(24)
$$P\{y_1^2 + \cdots + y_k^2 \leq h(\lambda_0)C^2 \mid \lambda_0\} = P\{\chi_k^2 \leq h(\lambda_0)C^2 \mid \lambda_0\},\$$

and let us assume for a moment that we can find a $h(\lambda_0)$ such that for any fixed λ_0 , $A(\lambda_0, C^2)$ is closely bounded below by $B(h(\lambda_0), C^2)$ for all C^2 or at least for all C^2 which gives $A(\lambda_0, C^2)$ the value greater than or equal to a preassigned p. In this case we can determine the tolerance region with the confidence coefficient greater than or equal to a given 7 based on $B(h(\lambda_0), C^2)$.

(25)
$$B(h(\lambda_0), C^2) = \frac{1}{2^{k/2} \Gamma\left(\frac{1}{2}k\right)} \int_0^{h(\lambda_0) C^2} y^{k/2-1} e^{-y/2} dy.$$

This varies from sample to sample, in other words, varies by sampling fluctuations in λ_0 or $h(\lambda_0)$. For a fixed C^2 , $B(h(\lambda_0), C^2)$ is a continuous and strictly increasing function of $h(\lambda_0)$. Therefore, if we determine h_r such that

$$(26) P\{h(\lambda_0) \ge h_r\} = r,$$

and then determine C_2^2 satisfying

 $B(h_r, C_2) = p$,

i.e.,

(27)
$$C_{2}^{2} = \chi_{k}^{2}(q)/h_{r}$$
, where $q = 1 - p$,

we have

$$P\{B(h(\lambda_0), C_2^2) \ge B(h_r, C_2^2)\} = P\{B(h(\lambda_0), C_2^2) \ge p\}$$

= $P\{h(\lambda_0) \ge h_r\} = \gamma$.

Since

(28)
$$P\{A(\lambda_0, C_2^2) \ge p\} \ge P\{B(h(\lambda_0), C_2^2) \ge p\} = \gamma,$$

the ellipsoidal region determined by C_2^2 thus obtained, i.e.,

(29) $R(L_0, C_2^2) \equiv \{X: (X-\mu)'L_0^{-1}(X-\mu) \leq C_2^2\},$

is the tolerance ellipsoidal region with the confidence coefficient $\geq r$.

Now we shall consider the assumption made on the function $h(\lambda_0)$. Unfortunately the author has not succeeded in finding such a $h(\lambda_0)$ except the ones which give rough lower bounds of $A(\lambda_0, C^2)$ and hence result in significantly larger regions than exact one. For example, λ_{01} , the smallest characteristic root of $L_0 \sum^{-1}$, causes a great loss. However, if we allow $h(\lambda_0)$ to be reasonable such that even if $B(h(\lambda_0), C^2)$ is greater than $A(\lambda_0, C^2)$ for some range of C^2 , the excess is so small that $B(h(\lambda_0), C^2)$ can be regarded as a good approximation to $A(\lambda_0, C^2)$ for these C^2 , we could find such a function and treat the problem. In fact, we have prepared in the last section (with the replacement of a_i 's there by λ_{0i} 's)

(30)
$$h(\lambda_0) = (\lambda_{01} \cdots \lambda_{0k})^{1/k} \left[\frac{(\lambda_{01} \cdots \lambda_{0k})^{1/k}}{\frac{1}{k} (\lambda_{01} + \cdots + \lambda_{0k})} \right]^2 \quad (k=2, 3)$$

as a reasonable function for our aim.* If $h(\lambda_0)$ like (30) are necessary for $k \ge 4$, similar trials as the cases of k=2 and 3 will be done. Using

^{*} In the last section, (30) has desired properties unless $u = \lambda_{01}/\lambda_{0k}$ is too small. But each of $\lambda_{01}, \dots, \lambda_{0k}$, the roots of $L_0 \sum^{-1}$ tends to 1 in probability as $N \rightarrow \infty$ and so for a sufficiently large sample, it is expected with high probability that u is not too small. For k=2, the following data are obtained.

N	21	31	41	51	61	81	101
$P(u \ge 0.3)$	0.96742	0.99412	0.99894	0.99981	0.99997	1.00000	1.00000
<i>P</i> (<i>u</i> ≩0.2)	0.99720	0.99985	0.999999	1.00000	1.00000	1.00000	1.00000

these $h(\lambda_0)$'s, we can go through from (25) to (29) without any change except the replacement of $i \geq i$ in the middle of (28) by $i \geq i$ which is the notation for the statement, "greater than or approximately equal to".

The above arguments are summarized as follows:

The region $R(L_o, C_2^*)$ in (29) is a tolerance region that contains at least proportion p of a k-variate normal population with known mean μ and unknown covariance matrix, $\sum C_2^*$ is given by $C_2^* = \chi_k^*(q)/h_r$, (q = 1-p), and h_r is the lower (1-r) point of the distribution of $h(\lambda_o)$, which is a function of $\lambda_{o_1}, \dots, \lambda_{o_k}$, the characteristic roots of $L_o \sum^{-1}$, chosen properly for the problem. If $h(\lambda_o)$ can be chosen (though it failed to be found here) so that $B(h(\lambda_o), C^2) \leq A(\lambda_o, C^2)$ holds for all λ_o and C^2 , the confidence coefficient of the region is $\geq r$. If $h(\lambda_o)$ is a function like (30), the confidence coefficient of the region is $\geq r$.

It is noted that, for $h(\lambda_0)$ in (30), $C_2^2 \rightarrow \chi_k^2(q)$ as $N \rightarrow \infty$ since each of $\lambda_{01}, \dots, \lambda_{0k}$ tends to 1 in probability and hence $\lim_{q \to \infty} h_q = 1$.

5. The case when both μ and Σ are unknown

It is ordinary in practical applications that both μ and \sum are unknown and must be estimated from a sample. Using \overline{X} and L, the region to be determined is (6), i.e.,

$$R(\bar{X}, L, C^{i}) \equiv \{X: (X - \bar{X})'L^{-1}(X - \bar{X}) \leq C^{i}\}.$$

In the canonical form, this can be expressed with standard normal variates as

(32)
$$R(\overline{Y}, \lambda, C^2) \equiv \{Y \colon (Y - \overline{Y})' D_{\lambda}^{-1} (Y - \overline{Y}) \leq C^2\},$$

where Y, Y_{α} 's are N(O, I)-variates, $\overline{Y} = \frac{1}{N} \sum_{\alpha=1}^{N} Y_{\alpha}, D_{\lambda} = \operatorname{diag}(\lambda_{1}, \dots, \lambda_{k}),$

with $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_k < \infty$ and the λ_i 's are the roots of the determinantal equation in λ

$$|L-\lambda \Sigma|=0.$$

Then

(31)
$$F(u) = 2^{N-1} \frac{u^{(N-1)/2}}{(1+u)^{N-1}} \quad (1 \ge u \ge 0) .$$

 $[\]longrightarrow$ Entries are easily calculated from the cumulative distribution function F(u) of u,

For k=3, the comparable data has not been calculated because of the complexity of the cumulative distribution function of $\lambda_{01}/\lambda_{03}$.

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$$(34) \qquad A(S) = A(\bar{Y}, \lambda, C^{2}) = P\{Y \in R(\bar{Y}, \lambda, C^{2}) \mid \bar{Y}, \lambda\}$$
$$= P\{\frac{1}{\lambda_{1}}(Y_{1} - \bar{Y}_{1})^{2} + \cdots + \frac{1}{\lambda_{k}}(Y_{k} - \bar{Y}_{k})^{2} \leq C^{2} \mid \bar{Y}, \lambda\}.$$

Now set

(37)

(35)
$$G(p, C^2) = P\{A(\overline{Y}, \lambda, C^2) \geq p\}$$

and denote its conditional probability for a particular value of \overline{Y} by $G(p, C^* | \overline{Y})$. Then

$$G(p, C^{2}) = E_{\overline{Y}} \{G(p, C^{2} | \overline{Y})\}$$
$$= N^{k/2} (2\pi)^{-1/2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} G(p, C^{2} | \overline{Y}) \exp\left\{-\frac{1}{2}N\overline{Y}'\overline{Y}\right\} d\overline{Y}_{1} \cdots d\overline{Y}_{k}.$$

We consider the approximation of $G(p, C^2)$ by expanding $G(p, C^2 | \bar{Y})$ in a Taylor series and taking expectations. Since \bar{Y} is distributed symmetrically about O and each principal axis of the ellipsoid under consideration is parallel to the corresponding y-axis of coordinates, it is clear that $G(p, C^2 | \bar{Y})$ is an even function of each component of \bar{Y} . Hence, in the expansion of $G(p, C^2 | \bar{Y})$ in a power series of components of \bar{Y} , only even powers will occur. Accordingly the Taylor expansion about O is

(36)

$$G(p, C^{2} | \overline{Y}) = G(p, C^{2} | O) + \frac{1}{2!} \sum_{i=1}^{k} \overline{Y}_{i}^{2} \frac{\partial^{2}G}{\partial \overline{Y}_{i}^{2}} + \frac{1}{4!} \left\{ \sum_{i=1}^{k} \overline{Y}_{i}^{4} \frac{\partial^{4}G}{\partial \overline{Y}_{i}^{4}} + 3 \sum_{i \neq j}^{k} \overline{Y}_{i}^{2} \overline{Y}_{j}^{2} \frac{\partial^{4}G}{\partial \overline{Y}_{i}^{2} \partial \overline{Y}_{j}^{2}} + \cdots, \right\}$$

where all the derivatives are evaluated at $\overline{Y}=O$. Taking expectations, we obtain

$$G(p, C^{2}) = G(p, C^{2}|O) + \frac{1}{2N} \sum_{i=1}^{k} \frac{\partial^{2}G}{\partial \overline{Y}_{i}^{2}} + \frac{1}{8N^{2}} \left\{ \sum_{i=1}^{k} \frac{\partial^{4}G}{\partial \overline{Y}_{i}^{4}} + \sum_{i\neq j}^{k} \frac{\partial^{4}G}{\partial \overline{Y}_{i}^{2}\partial \overline{Y}_{j}^{2}} \right\} + \cdots,$$

since \overline{Y} has the distribution $N(O, \frac{1}{N}I)$. On comparing (36) with (37), we see that if in (36) we set $\overline{Y}_i = \frac{1}{\sqrt{N}}$ $(i=1, \dots, k)$ (36) becomes identical with (37) except for terms involving the second and higher powers of 1/N. Then for moderately large N we have the approximation

(38)
$$G(p, C^2) \simeq G\left(p, C^2 \middle| \frac{1}{\sqrt{N}} e\right),$$

where e is the column vector whose components are all unity.

Thus for moderate N, we need only consider

(39)
$$A\left(\frac{1}{\sqrt{N}}-e, \lambda, C^{2}\right) = P\left\{\frac{1}{\lambda_{1}}\left(y_{1}-\frac{1}{\sqrt{N}}\right)^{2}+\cdots+\frac{1}{\lambda_{k}}\left(y_{k}-\frac{1}{\sqrt{N}}\right)^{2}\leq C^{2}|\lambda\right\}$$

instead of $A(\overline{Y}, \lambda, C^2)$ in (34) and consider the determination of C^2 satisfying this requirement. However, there is the similar complicated situation as in the last section in the explicit evaluation of (39), which is due to variations in $\lambda = (\lambda_1, \dots, \lambda_k)$. This forces us to make the analogous modification of (39) as made for $A(\lambda_0, C^2)$, i.e., to replace (39) by

(40)
$$B(h'(\lambda), C^2) = P\left\{ \left(y_1 - \frac{1}{\sqrt{N}} \right)^2 + \cdots + \left(y_k - \frac{1}{\sqrt{N}} \right)^2 \leq h'(\lambda) C^2 | \lambda \right\}$$
$$= P\left\{ \chi'_k \leq h'(\lambda) C^2 | \lambda \right\},$$

where χ_k^2 is a noncentral chi-square variate with k degrees of freedom and with noncentrality parameter

(41)
$$\varphi^{2} = \left(\frac{1}{\sqrt{N}} e\right)' \left(\frac{1}{\sqrt{N}} e\right) = \frac{k}{N}$$

and $h'(\lambda)$ is a function of $\lambda_1, \dots, \lambda_k$ chosen in a manner similar to that of the last section. The only point of difference from the last section is that χ_k^2 here is noncentral instead of central. However, since we are considering the case of large N, the effect of noncentrality, $\varphi^2 = k/N$, on the selection of $h'(\lambda)$ will be so small that we can safely take $h'(\lambda)$ of the same form as $h(\lambda_0)$ in the central case. Especially, for k=2 and 3, we could use

(42)
$$h'(\lambda) = (\lambda_1 \cdots \lambda_k)^{1/k} \left[\frac{(\lambda_1 \cdots \lambda_k)^{1/k}}{\frac{1}{k} (\lambda_1 + \cdots + \lambda_k)} \right]^2 \quad (k=2, 3).$$

If we have a close lower bound of $A\left(\frac{1}{\sqrt{N}}e, \lambda, C^2\right)$ for all λ and C^2 , we

of course use it as $B(h'(\lambda), C^{2})$.

Using $h'(\lambda)$ chosen in this manner, we can construct a tolerance region with confidence coefficient, $\geq r$, a preassigned value. We have

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(43)
$$B(h'(\lambda), C^2) = e^{-\varphi^2/2} \sum_{j=0}^{\infty} \frac{\varphi^{2j}}{j! \, 2^{k/2+j} \Gamma\left(\frac{1}{2}k+j\right)} \int_0^{h'(\lambda)C^2} y^{k/2+j-1} e^{-y/2} dy \, .$$

As in the last section, we first calculate h'_{τ} for a given 7 such that

(44)
$$P\{h'(\lambda) \ge h'_r\} = \gamma ,$$

and then determine C_3^2 from

(45)
$$B(h'_r, C^2_3) = p$$

i.e.,

(46)
$$C_3^2 = \chi_k^{\prime 2}(q)/h_r$$
, where $q = 1 - p$.

Then, for a sufficiently large sample,

$$P\{A(\bar{Y}, \lambda, C_{3}^{2}) \ge p\} \simeq P\{A(\frac{1}{\sqrt{N}}e, \lambda, C_{3}^{2}) \ge p\}$$
$$\ge P\{B(h'(\lambda), C_{3}^{2}) \ge p\}$$
$$\triangleq P\{B(h'(\lambda), C_{3}^{2}) \ge B(h'_{\tau}, C_{3}^{2})\}$$
$$= P\{h'(\lambda) \ge h'_{\tau}\} = \gamma.$$

Accordingly the following conclusion is obtained :

For sufficiently large sample, the ellipsoidal region determined by C_3^s , $R(\overline{Y}, \lambda, C_3^s)$ and hence

(47)
$$R(\bar{X}, L, C_{s}^{2}) \equiv \{X : (X - \bar{X})'L^{-1}(X - \bar{X}) \leq C_{s}^{2}\}$$

is a tolerance region, with the confidence coefficient $\geq \gamma$, that contains at least a proportion p of a k-variate normal population with unknown mean and with unknown covariance matrix, $\sum C_s^2$ is calculated from (46), where h'_{τ} is the lower $(1-\gamma)$ point of the distribution of $h'(\lambda)$, which is a function of $\lambda_1, \dots, \lambda_k$, the characteristic roots of $L \sum^{-1}$, chosen properly for the problem.

It is easily seen that when $h'(\lambda)$ in (42) is used, $C_3^2 \rightarrow \chi_k^2(q)$ as $N \rightarrow \infty$, since $\varphi^2 \rightarrow 0$ and $h'_r \rightarrow 1$ in probability as $N \rightarrow \infty$.

6. Simultaneous tolerance intervals

The development by Roy, Bose and others in a series of papers ([11], [12], [13], [14], [15] and [16]) for obtaining simultaneous confidence intervals can be made for the tolerance statement. Denoting any nonnull k-dimensional non-stochastic vector by a, we shall consider the determination of

a set of the simultaneous tolerance intervals

(48)
$$R_a(\bar{X}, L, d^2) \equiv \{X: a'\bar{X} - [d^2a'La]^{1/2} \leq a'X \leq a'\bar{X} + [d^2a'La]^{1/2}\}$$

such that for given p and γ (1>p, γ >0),

(49) $A_{a}(\bar{X}, L, d^{2}) \equiv P \{ X \in R_{a}(\bar{X}, L, d^{2}) | \bar{X}, L \} ,$

(50)
$$P\{A_a(X, L, d^2) \ge p; \text{ for all } a\} \ge \gamma.$$

It is easily seen that the statement $A_a(\overline{X}, L, d^2) \ge p$ for all a, is equivalent to the statement $\inf A_a(\overline{X}, L, d^2) \ge p$ and since

$$\begin{split} \inf_{a} A_{a}(\bar{X}, L, d^{3}) &= \inf_{a} P\{X \in R_{a}(\bar{X}, L, d^{2}) | \bar{X}, L\} \\ &= \inf_{a} P\{\frac{|a'(X - \bar{X})|}{(a'La)^{1/2}} \leq d | \bar{X}, L\} \\ &= \inf_{a} P\{\frac{a'(X - \bar{X})(X - \bar{X})'a}{a'La} \leq d^{2} | \bar{X}, L\} \\ &\geq P\{\sup_{a} \frac{a'(X - \bar{X})(X - \bar{X})'a}{a'La} \leq d^{2} | \bar{X}, L\} \\ &= P\{(X - \bar{X})'L^{-1}(X - \bar{X}) \leq d^{2} | \bar{X}, L\} \\ &= A(\bar{X}, L, d^{2}), \end{split}$$

we have

(51)
$$P\{\inf A_a(\bar{X}, L, d^2) \ge p\} \ge P\{A(\bar{X}, L, d^2) \ge p\}.$$

Consequently, the problem of determining the value of d^3 so that the simultaneous confidence coefficient is greater than or equal to γ is the same one as in section 5. But the solution which gives the coefficient exactly equal to γ could not be obtained there, and some modification has been made, namely, $\geq \gamma$ has been replaced by $\geq \gamma$. If, with the same modification, C_3^3 is used as d^2 in (48), we can have a set of simultaneous tolerance intervals (48) for all nonnull a, each of which contains at least a proportion p of a normal population $N(a'\mu, a' \geq a)$, $(\mu, \sum$ are unknown) and these intervals have the simultaneous confidence coefficient $\geq \gamma$. When we know a priori either μ or \sum , obvious modifications of the above argument are necessary.

7. Note on the distributions of $h(\lambda_0)$ and $h'(\lambda)$

In order to carry out the practical work when \sum is unknown, i.e., to calculate C_3^2 in (27) and C_3^2 in (46), we must evaluate h_r and h'_r for

a given γ . At the present time, we have $h(\lambda_0)$ in (30) and $h'(\lambda)$ in (42) as feasible for k=2 and 3. $h(\lambda_0)$ and $h'(\lambda)$ for $k \ge 4$ may be obtained by the same procedure as stated in section 3, i.e., in (18). In these cases they appear as functions of the elementary symmetric functions of the characteristic roots of $L_0 \sum^{-1}$ or $L \sum^{-1}$. Therefore in order to evaluate h_{τ} and h'_{τ} for a given γ , and hence in order to obtain the distribution of $h(\lambda_0)$ and $h'(\lambda)$, the joint distributions of these elementary symmetric functions are necessary. Unfortunately, the domains with positive joint densities are so complicated that we cannot evaluate the probability functions of $h(\lambda_0)$ and $h'(\lambda)$ explicitly except for k=2.

Thus let us consider in this section the evaluation of h_r and h'_r only for k=2. To treat these simultaneously, let θ_1 and θ_2 $(0 < \theta_1 \le \theta_2)$ be the roots of

$$(52) |W-\theta \Sigma| = 0,$$

where nW is a Wishart matrix with *n* degrees of freedom. For section 4, W, n, θ_i (i=1, 2) correspond to L_0 , N, λ_{0i} and for section 5, to L, N-1, λ_i , respectively and consider the distribution of the statistic

(53)
$$H(\theta) = \frac{4(\theta_1 \theta_2)^{3/2}}{(\theta_1 + \theta_2)^2}$$

The joint distribution of θ_1 and θ_2 has the density function

(54)
$$f(\theta_1, \theta_2) = \frac{n^n}{4\Gamma(n-1)} (\theta_1 \theta_2)^{(n-3)/2} e^{-n(\theta_1 + \theta_2)/2} (\theta_2 - \theta_1) \quad (0 < \theta_1 \leq \theta_2) .$$

Making the transformations

(54)
$$S_1 = \theta_1 + \theta_2$$
 and $S_2 = \theta_1 \theta_2$,

we have

(55)
$$f(S_1, S_2) = \frac{n^n}{4\Gamma(n-1)} S_2^{(n-3)/2} e^{-nS_1/2} ,$$

since $dS_1 dS_2 = (\theta_2 - \theta_1) d\theta_1 d\theta_2$. The domain is $S_1^2 - 4S_2 \ge 0$ or $\infty > \frac{S_1^2}{4} \ge S_2 \ge 0$. We transform (55) into the joint density function of H and S_1 by

$$H=4\frac{S_2^{3/2}}{S_1^2}$$
,

and after this, we integrate out S_1 . Since the domain of the joint distribution of H and S_1 is $\infty > S_1 \ge 2H \ge 0$, the density function of H is

(56)
$$f(H) = \frac{n^{(n-1)/3}}{3\Gamma(n-1)} \cdot H^{(n-4)/3} \int_{nH}^{\infty} Z^{(2n+1)/3-1} e^{-Z} dZ \quad (\infty > H \ge 0) .$$

The probability integral for H can be evaluated in the following manner.

$$\begin{split} P(H>H^*) &= \frac{n^{(n-1)/3}}{3\Gamma(n-1)} \int_{H^*}^{\infty} H^{(n-4)/3} \int_{nH}^{\infty} Z^{(2n+1)/3-1} e^{-Z} dZ dH \\ &= \frac{n^{(n-1)/3}}{3\Gamma(n-1)} \int_{nH^*}^{\infty} Z^{(2n+1)/3-1} e^{-Z} \int_{H^*}^{Z/n} H^{(n-4)/3} dH dZ \\ &= \frac{1}{\Gamma(n)} \int_{nH^*}^{\infty} Z^{n-1} e^{-Z} dZ - \frac{n^{(n-1)/3}}{\Gamma(n)} \cdot H^{*(n-1)/3} \int_{nH^*}^{\infty} Z^{(2n+1)/3-1} e^{-Z} dZ \,. \end{split}$$

Using the notation $I_a(\nu)$ for the incomplete gamma function [9],

$$[\Gamma(\nu)]^{-1}\int_{0}^{a}Z^{\nu-1}e^{-Z}dZ$$
,

we have

(57)
$$P(H \leq H^*) = 1 - P(H > H^*)$$
$$= I_{nH^*}(n) + \frac{\Gamma\{(2n+1)/3\} n^{(n-1)/3}}{\Gamma(n)} H^{*(n-1)/3}\{1 - I_{nH^*}((2n+1)/3)\}.$$

8. Charts for the practical use

To construct the tolerance ellipsoidal regions under the situations in sections 2 and 5, we have to calculate the upper q=1-p point of the noncentral chi-square distribution with k degrees of freedom and with a given value of the noncentrality parameter. Denoting the density function of the noncentral chi-square distribution by $f(\chi_k^2; \phi^2)$, i.e.,

$$f(\chi_k^{\prime 2}; \psi^2) = e^{-\phi^2/2} \sum_{j=0}^{\infty} \frac{\psi^{2j}}{j! 2^j} \frac{1}{2^{k/2+j} \Gamma'\left(\frac{1}{2} k+j\right)} (\chi_k^{\prime 2})^{k/2+j-1} e^{-\chi_k^{\prime 2}/2},$$

we give, for practical convenience, the charts of the relation between $\chi'_{k}(q)$ and ϕ^{2} satisfying

(58)
$$\int_{0}^{\chi_{k}^{\prime 2}(q)} f(\chi_{k}^{\prime 2}; \, \phi^{2}) d\chi_{k}^{\prime 2} = p ,$$

in Figs. 2a and 2b for k=2, 3 and p=0.900, 0.925, 0.950, 0.975, 0.990. Curves for the indicated range of ψ^3 are almost straight lines. For section 2, ψ^3 here corresponds to τ_7^3 there and $\chi_k'(q)$ here to C_1^2 there and for section 5, ψ^3 corresponds to $\varphi^3 = k/N$ there and $\chi_k'(q)$ to $h_r'C_3^2$ there.



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