Minimum Ellipsoids

By Donald D. Fisher

1. Introduction. A well-known statistical problem is to determine an ellipsoid R_s^e in E_n which contains a certain fraction of the points from a set S . Here we use the word "contains" to mean that a point $p_i \in S$ is either in the interior or on the surface of the ellipsoid R_s^e . Although the determination of R_s^e is easy computationally, the determination of the ellipsoid of minimum volume, say, which contains all the points of S is quite difficult. In this note we give a method for determining ellipsoids satisfying a certain minimum property and compare these with ones obtained by statistical methods.

2. Statistical Test Region. If the points of S tend to be correlated, an ellipsoid is an appropriate regular test region. One statistical test region is set up by making use of the F -distribution and multivariate analysis. We assume that S has a multivariate normal distribution with an unknown mean μ which we estimate by taking the mean of the points in S . Furthermore, we assume the unknown covariance matrix associated with S may be estimated by the (symmetric) matrix

$$(2.1) \quad S = \frac{1}{N-1} \begin{bmatrix} \sum (x_i - \bar{x})^2 & \sum (x_i - \bar{x})(y_i - \bar{y}) & \sum (x_i - \bar{x})(z_i - \bar{z}) & \cdots \\ \cdot & \sum (y_i - \bar{y})^2 & \sum (y_i - \bar{y})(z_i - \bar{z}) & \cdots \\ \cdot & \cdot & \sum (z_i - \bar{z})^2 & \cdots \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

where N is the number of points in S [3].

We assume a point q of unknown lineage has the same distribution as the points $p_i \in S$. Let α be the fraction of allowed false positives, i.e., the allowed fraction of unknowns which do not lie in R_s^e , but by some other test are found to be a member of S . The unknown point q belongs to S with probability $1 - \alpha$ if

$$(2.2) \quad (q - \bar{w})^T S^{-1} (q - \bar{w}) \leq \frac{N_2(N_1 + 1)(N_1 - 1)}{N_1(N_1 - N_2)} F_{N_2, N_1 - N_2}^\alpha,$$

where N_1, N_2 are the number of degrees of freedom of the denominator and numerator, respectively, associated with the F -distribution and $\bar{w}$ is the computed mean of the points $p_i \in S$. Inequality (2.2) derives from Hotelling's T^2 statistic in multivariate analysis [1]. Geometrically, (2.2) defines the interior and boundary of an ellipsoid with the mean $\bar{w}$ as center. For fixed N_1, N_2 , $F_{N_2, N_1 - N_2}^\alpha$ increases as α decreases, consequently, the size of the ellipsoid increases as α decreases. For a given F the volume of R_s^e is

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$$(2.3) \quad V_s^e = \pi \left\{ N_2(N_1 + 1)(N_1 - 1) F_{N_2, N_1 - N_2}^\alpha \left[N_1(N_1 - N_2) \prod_j \lambda_j \right]^{-1} \right\}^{1/2}.$$

In E_3 the eigenvalues λ_j of S may be computed directly by trigonometric relations [6]. In general a certain number of points from S will lie outside the above ellipsoid. As F increases more and more points of S will be contained in R_s^e .

3. "Minimum" Ellipsoid Region. C. Loewner has proved that there is a unique ellipsoid of minimum volume which contains all points of S . The problem may be stated as a minimum problem, i.e., given $p_i \in S$ with mean $\bar{w}$, determine the matrix $\mathfrak{J}$ for which

$$(3.1) \quad \det\{\mathfrak{J}^{-1}\} \equiv \prod_j \lambda_j$$

is a minimum subject to the constraints

$$(3.2) \quad (p_i - \bar{w})^T \mathfrak{J} (p_i - \bar{w}) \leq 1.$$

This formulation possesses two disadvantages [4]: (i) The volume becomes insensitive to change in all λ_j if any $\lambda_i \rightarrow 0$; (ii) $\det\{\mathfrak{J}^{-1}\}$ is not a convex function of $\mathfrak{J}$ and consequently the numerical computations for the minimum are difficult to perform.

The problem may be recast in a form which avoids these difficulties. We determine the matrix $\mathfrak{J}$ for which

$$(3.3) \quad \varphi(\mathfrak{J}) \equiv \text{trace}\{\mathfrak{J}^{-1}\} = \sum (\lambda_j)^{-1} = \sum r_j^2$$

is a minimum subject to the constraints

$$(3.4) \quad \begin{aligned} (p_i - \bar{w})^T \mathfrak{J} (p_i - \bar{w}) &\leq 1, \\ t_{ii} &\geq \sum_{j \neq i} |t_{ij}|, \end{aligned}$$

where r_j is the length of the j th semiaxis and t_{ij} is the i, j element of $\mathfrak{J}$. In [4] it is shown that $\text{trace}\{\mathfrak{J}^{-1}\}$ is a strictly convex function of $\mathfrak{J}$ and that $\mathfrak{J}^{-1}$ is a convex function of $\mathfrak{J}$. This measure of size is unique and, furthermore, there is a method (gradient projection (GP) method) for determining the associated ellipsoid R_s^v numerically [5], [7].

Let $\mathfrak{J}^{-1} = \mathfrak{u} = (u_{ij})$. The gradient of $\varphi(\mathfrak{J})$ is given by

$$(3.5) \quad \begin{aligned} \frac{\partial \varphi}{\partial t_{ij}} &= -2u_i^T u_j, \quad i \neq j, \\ \frac{\partial \varphi}{\partial t_{ii}} &= -u_i^T u_i, \end{aligned}$$

where u_j is the j th column of $\mathfrak{u}$.

4. Numerical Results. The ellipsoids R_s^e and R_s^v (indicated in the tables by R_{sk}^v and R_{sk}^e , $k = 1, \dots, 11$) were determined for 11 sets of points in E_3 with 150 points in each set (denoted by S_{150}^k) and for 11 subsets of the above sets with 25 points in each subset (denoted by S_{25}^k). The data originated from vectorcardiographic studies [2] of subjects which had been assigned to specific sets based on

independent tests. The ellipsoids R_s^v were determined by 6 variables and either 153 constraints or 28 constraints, respectively. Most of the constraints turn out to be inactive since a unique ellipsoid in E_3 is determined by 3 “independent” points.

The relation of the size of R_s^e to the size of R_s^v highlights a characteristic of the F test. The larger the sample size the better the estimate of the various statistical quantities, hence the sharper the F test. For a sample size of 25 the F test allows for considerably more scatter than for a sample size of 150. Note that R_s^v contains all points of S whereas, by assumption, R_s^e contains only the fraction $1 - \alpha$ of the points of S . The actual number of points exterior to R_s^e is given in Table 4. Comparisons in Tables 1, $\cdots$, 4 are based on an F value for $\alpha = 0.05$. For the smaller sample size both the volume and sum of squares of the semiaxes for R_s^v are smaller

TABLE 1
 $r_{\max}^k/r_{\min}^k$

k	S_{25}^k		S_{150}^k	
	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$
1	1.36	2.46	1.52	2.37
2	1.78	2.03	2.23	2.14
3	2.49	2.37	3.31	2.02
4	2.70	1.83	2.59	2.09
5	1.31	1.74	1.82	2.09
6	1.84	1.57	1.60	1.64
7	1.35	1.52	1.50	1.32
8	1.68	1.53	1.31	1.40
9	1.64	2.43	1.84	1.71
10	1.64	2.13	1.58	1.66
11	2.52	3.07	1.72	2.04

TABLE 2
 $\prod_i r_i^k$

k	S_{25}^k		S_{150}^k	
	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$
1	0.00225	0.00199	0.00212	0.00088
2	0.00864	0.01575	0.02220	0.00957
3	0.03387	0.04217	0.09718	0.03374
4	0.06468	0.07890	0.16194	0.07966
5	0.38915	0.52527	0.91020	0.59686
6	0.78645	1.37867	1.66261	1.22425
7	0.92816	1.64883	2.56710	1.89610
8	1.46047	2.40659	3.76361	2.52306
9	0.61088	0.98923	3.61434	1.47622
10	0.30282	0.51189	2.49975	0.81512
11	0.08671	0.20482	1.59846	0.47684

TABLE 3
 $\sum_i (r_i^k)^2$

k	S_{25}^k		S_{150}^k	
	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$	R_{sk}^v	$R_{sk}^e, \alpha = 0.05$
1	0.05347	0.06169	0.05248	0.03516
2	0.14026	0.22163	0.29139	0.16590
3	0.41744	0.45623	0.96584	0.36674
4	0.65938	0.61913	1.16601	0.65657
5	1.64423	2.17246	3.15794	2.51408
6	2.88333	3.96950	4.52434	3.72471
7	2.94184	4.43341	5.94049	4.71656
8	4.21288	5.73125	7.45132	5.76568
9	2.34140	3.78881	7.96869	4.27550
10	1.46843	2.29726	5.93542	2.84975
11	0.75918	1.48931	4.51029	2.14763

TABLE 4

Number of Points Exterior to R_s^e

k	S_{25}^k	S_{150}^k
1	1	10
2	0	6
3	1	8
4	1	12
5	0	6
6	0	8
7	0	5
8	0	9
9	1	11
10	0	9
11	0	10

in most cases than those for R_s^e . However, the volume and sum of squares of the semiaxes for R_s^v are greater than those for R_s^e for the larger sample size.

Table 1 summarizes the ratios of the maximum semiaxis $r_{\max}$ to the minimum semiaxis $r_{\min}$. Table 2 gives the volumes (apart from a multiplicative constant) of the ellipsoids and Table 3 gives the sum of squares of the semiaxes. Note that even though the volume of R_s^v is greater than the corresponding volume R_s^e for the larger sample, the ratio $r_{\max}/r_{\min}$ for R_s^v is not always greater than the ratio $r_{\max}/r_{\min}$ for R_s^e . This is accounted for by the fact that R_s^v must orient itself differently from R_s^e in order to include an extreme point, whereas an extreme point does not influence R_s^e significantly.

GP computing time on the 7090 for 8 cases with 6 bounds and 28 active constraints was 0.8 minutes. For 12 cases with 6 bounds and 153 active constraints the total 7090 time was 2.7 minutes.

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