The Annals of Statistics
1985, Vol. 13, No. 1, 95–115

BOOTSTRAP TESTS AND CONFIDENCE REGIONS FOR FUNCTIONS OF A COVARIANCE MATRIX[1]

BY RUDOLF BERAN AND MUNI S. SRIVASTAVA

University of California, Berkeley and University of Toronto

Bootstrap tests and confidence regions for functions of the population covariance matrix have the desired asymptotic levels, provided model restrictions, such as multiple eigenvalues in the covariance matrix, are taken into account in designing the bootstrap algorithm.

1. Introduction. An important part of standard multivariate analysis deals with tests and confidence regions for functions of the covariance matrix. Familiar examples include principal component analysis and tests of structural hypotheses about the population covariance matrix. The classical theoretical development for such procedures rests upon the assumption that the data is normally distributed. Without strict normality, the asymptotic distribution theory for many multivariate test statistics and confidence regions becomes more complex and sometimes leads to untabulated limit distributions. Likelihood ratio tests about the covariance matrix and confidence regions in principal component analyses offer immediate examples of this phenomenon. As a result, nonnormal model asymptotic theory has been applied sparingly in the practice of multivariate analysis, despite the evident nonnormality of much data.

Nonparametric bootstrap methods offer an attractive alternative approach. Recent studies by several authors suggest that bootstrap procedures can compete successfully, both in theoretical performance and in practical feasibility, with more traditional procedures based on asymptotic approximations (cf. Efron, 1979; Bickel and Freedman, 1981; Freedman, 1981; Singh, 1981; Beran 1982, 1984). While these studies have concentrated on certain, mostly univariate, classes of examples, the potential value of bootstrap methods in nonnormal model multivariate analysis seems clear.

Bootstrap procedures for eigenvalues, eigenvectors, and other interesting functions of a covariance matrix are the subject of this paper. Specific topics include: bootstrap confidence regions for differentiable functions of the population covariance matrix; bootstrap confidence regions and tests for eigenvalues and eigenvectors in both simple and multiple eigenvalue situations; bootstrap critical values for normal model likelihood ratio and other test statistics used to test structural hypotheses about the population covariance matrix. The bootstrap

Received October 1983; revised May 1984.

[1] This research was supported in part by a grant from the Natural Sciences and Engineering Research Council of Canada and in part by National Science Foundation grant MCS 80-02698.

AMS 1980 *subject classifications.* 62G05, 62E20.

Key words and phrases. Bootstrap procedures, covariance matrix, eigenvalues, eigenvectors, confidence regions, tests, multivariate analysis.

tests and confidence regions have the desired asymptotic levels if model restrictions, such as multiple eigenvalues, are taken into account in designing the bootstrap algorithm.

2. Bootstrapping the sample covariance matrix. Under natural assumptions, the nonparametric bootstrap distribution for the sample covariance matrix converges to the actual distribution, as sample size increases. This fact, to be proved in this section, is basic to further analysis of bootstrap tests and confidence regions concerning the population covariance matrix.

Suppose the observations $\{x_i;\ 1 \le i \le n\}$ are i.i.d. $p \times 1$ random vectors. Suppose F, the unknown cdf of $x_i = (x_{i1}, x_{i2}, \cdots, x_{ip})'$ has mean vector μ_F and covariance matrix $\Sigma_F = \{\sigma_{F,ij}\}$. Let $\bar{x}_n = n^{-1} \sum_{i=1}^n x_i$ be the sample mean, let

$$S_n = \{s_{n,ij}\} = (n-1)^{-1} \sum_{i=1}^n (x_i - \bar{x}_n)(x_i - \bar{x}_n)' \tag{2.1}$$

be the sample covariance matrix, and let

$$J_n(F) = \mathscr{L}[n^{1/2}(S_n - \Sigma_F) \mid F] \tag{2.2}$$

be the distribution of the centered sample covariance matrix.

For any $p \times p$ symmetric matrix $A = \{a_{ij}\}$, let uvec(A) denote the $p(p+1)/2$ dimensional column vector $\{\{a_{ij};\ 1 \le i \le j\};\ 1 \le j \le p\}$ formed from the elements in the upper trianglar half of A, including the diagonal elements. Suppose $Z_F = \{z_{F,ij}\}$ is a symmetric $p \times p$ random matrix such that $\mathscr{L}[\text{uvec}(Z_F)]$ is normal with mean vector zero and covariance matrix Ω_F; the components of Ω_F are determined by the requirement

$$\begin{aligned} \text{Cov}(z_{F,ij}, z_{F,k\ell}) = \text{Cov}_F[(x_{1i} - \mu_F)(x_{1j} - \mu_F), (x_{1k} - \mu_F)(x_{1\ell} - \mu_F)] \\ 1 \le i, j, k, \ell, \le p. \end{aligned} \tag{2.3}$$

If F has finite fourth moments, the distributions $\{J_n(F);\ n \ge 1\}$ converge weakly to $\mathscr{L}(Z_F)$.

Let $\hat{F}_n$ be the sample cdf based on the $\{x_i;\ 1 \le i \le n\}$. The nonparametric bootstrap estimate of $J_n(F)$ is the functional estimate $J_n(\hat{F}_n)$, which can be interpreted as follows: Let the $\{x_i^*;\ 1 \le i \le n\}$ be i.i.d. random vectors whose cdf is the realized $\hat{F}_n$, and let S_n^* be the sample covariance matrix of the $\{x_i^*\}$. Then $J_n(\hat{F}_n)$ is the distribution of $n^{1/2}(S_n^* - \Sigma_{\hat{F}_n})$. In practice, $J_n(\hat{F}_n)$ can be approximated by Monte Carlo methods. An alternative, more traditional estimate for $J_n(F)$ is the normal distribution on R^{p^2} with mean zero and estimated covariance structure. Theorem 1 below implies that both of these distributional estimates coverge to $J_n(F)$ as n increases.

In proving convergence of bootstrap estimates, we will rely on a triangular array approach previously described in Beran (1984).

DEFINITION. A sequence of cdf's $\{F_n;\ n \ge 1\}$ on R^p belongs to the class $\mathscr{C}(F)$ if and only if $\{F_n\}$ converges weakly to the cdf F and

$$\lim_{n\to\infty} E[\textstyle\prod_{j=1}^p x_{ij}^{r_j} \mid F_n] = E[\prod_{j=1}^p x_{ij}^{r_j} \mid F] \tag{2.4}$$

for every set of nonnegative integers such that $\sum_{j=1}^p r_j = 4$.

THEOREM 1. *Suppose F has finite fourth moments. If $\{F_n;\ n \geq 1\}$ is any sequence of cdf's in $\mathscr{C}(F)$, the sequence of distributions $\{J_n(F_n);\ n \geq 1\}$ converges weakly to the $\mathscr{N}(0, \Omega_F)$ distribution. Hence*

$$J_n(\hat{F}_n) \Rightarrow \mathscr{N}(0, \Omega_F) \tag{2.5}$$

with probability one.

PROOF. By the strong law of large numbers, $P_F[\{\hat{F}_n\} \in \mathscr{C}(F)] = 1$. Let $\{F_n\}$ be any sequence in $\mathscr{C}(F)$. Since $S_n = n(n-1)^{-1}\Sigma_{\hat{F}_n}$, it is enough to show that $\mathscr{L}[n^{1/2}(\Sigma_{\hat{F}_n} - \Sigma_{F_n}) \mid F_n] \Rightarrow \mathscr{L}(Z_F)$ in order to prove the theorem. Note that, if

$$Z_{n,i} = (x_i - \mu_{F_n})(x_i - \mu_{F_n})' - \Sigma_{F_n}, \tag{2.6}$$

then

$$n^{1/2}(\Sigma_{\hat{F}_n} - \Sigma_{F_n}) = n^{-1/2} \textstyle\sum_{i=1}^n Z_{n,i} - n^{1/2}(\bar{x}_n - \mu_{F_n})(\bar{x}_n - \mu_{F_n})'. \tag{2.7}$$

Let a be any constant column vector of dimension $p(p+1)/2$. By the Lindeberg central limit theorem for a triangular array,

$$\mathscr{L}[a'\operatorname{uvec}(n^{-1/2} \textstyle\sum_{i=1}^n Z_{n,i}) \mid F_n] \Rightarrow \mathscr{N}(0, a'\Omega_F a),$$

which is $\mathscr{L}[a'\operatorname{uvec}(Z_F)]$, provided

$$\lim_{n\to\infty} E_{F_n}[a'\operatorname{uvec}(Z_{n,1})]^2 = a'\Omega_F a < \infty \tag{2.8}$$

and

$$\lim_{n\to\infty} E_{F_n}\{[a'\operatorname{uvec}(Z_{n,1})]^2 I[\,|\,a'\operatorname{uvec}(Z_{n,1})\,| > n^{1/2}\delta]\} = 0 \tag{2.9}$$

for every positive δ. Let G_n be the cdf of $a'\operatorname{uvec}(Z_{n,1})$ under F_n and let G be the cdf of $a'\operatorname{uvec}[(x_1 - \mu_F)(x_1 - \mu_F)' - \Sigma_F]$ under F. The assumption $\{F_n\} \in \mathscr{C}(F)$ implies $G_n \Rightarrow G$ and

$$\lim_{n\to\infty} \int y^2\, dG_n(y) = \int y^2\, dG(y) = a'\Omega_F a.$$

Properties (2.8) and (2.9) follow immediately. Hence $\mathscr{L}[n^{-1/2} \sum_{i=1}^n Z_{n,i} \mid F_n] \Rightarrow \mathscr{L}(Z_F)$.

By another application of the Lindeberg central limit theorem,

$$\mathscr{L}[n^{1/2}(\bar{x}_n - \mu_{F_n}) \mid F_n] \Rightarrow \mathscr{N}(0, \Sigma_F)$$

(cf. example 3 in Beran, 1984). Thus, the second term on the right side of (2.7) converges in probability to zero. The theorem follows.

3. Bootstrap confidence regions for functions of Σ_F. By bootstrapping appropriately chosen pivots, we can construct confidence regions for Σ_F or functions of Σ_F whose coverage probabilities are asymptotically equal to a specified level $1 - \alpha$. For our purposes, a pivot is any function of the observations and of the parameter of interest whose distribution can be estimated consistently. For instance, suppose a confidence region for $g(\Sigma_F)$ is desired, where g is a $k \times 1$ vector-valued function of $\operatorname{uvec}(\Sigma_F)$ which is continuously differentiable and has first derivative matrix $\dot{g}$, of dimensions $k \times p(p+1)/2$. Let u be a real-valued continuous function on R^k such that $\{z \in R^k: u(z) = c\}$ has Lebesgue measure zero for every c. Let $J_{n,g}(F) = \mathscr{L}[u(n^{1/2}[g(S_n) - g(\Sigma_F)]) \mid F]$ and let $J_{n,g}(x, F)$ be the corresponding cdf. For $\alpha \in (0, 1)$, let

$$\begin{aligned} c_{n,g,L}(\alpha, F) &= \inf\{x: J_{n,g}(x, F) \geq 1 - \alpha\} \\ c_{n,g,u}(\alpha, F) &= \sup\{x: J_{n,g}(x, F) \leq 1 - \alpha\}. \end{aligned} \tag{3.1}$$

Suppose $c_{n,g}(\alpha, \hat{F}_n)$ is a random variable such that

$$c_{n,g,L}(\alpha, \hat{F}_n) \leq c_{n,g}(\alpha, \hat{F}_n) \leq c_{n,g,u}(\alpha, \hat{F}_n). \tag{3.2}$$

In other words, $c_{n,g}(\alpha, \hat{F}_n)$ is an upper α-point of the bootstrap distribution $J_{n,g}(\hat{F}_n)$. A bootstrap confidence region for $g(\Sigma_F)$, based on the pivot $u(n^{1/2}[g(S_n) - g(\Sigma_F)])$ and having ostensible level $1 - \alpha$, is

$$D_{n,g}(\alpha) = \{g(\Sigma_F): u(n^{1/2}[g(S_n) - g(\Sigma_F)]) \leq c_{n,g}(\alpha, \hat{F}_n)\}. \tag{3.3}$$

In the examples to be considered, the function u has the additional property that $u(bz) = bu(z)$ for every z in R^k and every positive b. Then

$$D_{n,g}(\alpha) = \{g(\Sigma_F): u[g(S_n) - g(\Sigma_F)] \leq c^*_{n,g}(\alpha)\}, \tag{3.4}$$

where $c^*_{n,g}(\alpha)$ is an upper α-point of the distribution of $u[g(S^*_n) - g(\Sigma_{\hat{F}_n})]$ when $\hat{F}_n$ is fixed at its realized value and S^*_n is the bootstrap sample covariance matrix defined in Section 2.

COROLLARY 1. *Suppose F has finite fourth moments and g is continuously differentiable over its domain with first derivative matrix $\dot{g}$. Then*

$$J_{n,g}(\hat{F}_n) \Rightarrow \mathscr{L}(u[\dot{g}(\Sigma_F)\text{uvec}(Z_F)]) \tag{3.5}$$

with probability one. Consequently, if $\dot{g}(\Sigma_F)$ is nonzero,

$$\lim_{n\to\infty} P_F[g(\Sigma_F) \in D_{n,g}(\alpha)] = 1 - \alpha. \tag{3.6}$$

PROOF. For every sequence of cdf's $\{F_n\} \in \mathscr{C}(F)$,

$$\mathscr{L}[u(n^{1/2}[g(S_n) - g(\Sigma_{F_n})]) \mid F_n] \Rightarrow \mathscr{L}(u[\dot{g}(\Sigma_F)\text{uvec}(Z_F)])$$

because of Theorem 1, the assumptions on g, and continuity of u. This implies (3.5) as in the proof of Theorem 1. The limit law on the right side of (3.5) is continuous, because the set $\{z \in R^k: u(z) = c\}$ has Lebesgue measure zero for every c. Hence

$$\lim_{n\to\infty} P_F[u(n^{1/2}[g(S_n) - g(\Sigma_F)]) \leq c_{n,g}(\alpha, \hat{F}_n)] = 1 - \alpha, \tag{3.7}$$

which is equivalent to (3.6); see Theorem 1 in Beran (1984) for details.

As immediate applications of Corollary 1, consider the following examples:

(a) Let $g(\Sigma_F)$ be the correlation coefficient $\rho_{F,ij} = \sigma_{F,ij}/(\sigma_{F,ii}\sigma_{F,jj})$. Then $g(S_n)$ is the sample correlation coefficient $r_{n,ij}$ and bootstrap confidence regions based on the pivot $|r_{n,ij} - \rho_{F,ij}|$ have the intended asymptotic level. Also covered by Corollary 1 is Fisher's transformation of $\rho_{F,ij}$: $g(\Sigma_F) = \log[(1 + \rho_{F,ij})/(1 - \rho_{F,ij})]$.

(b) Suppose the random vector x_i is partitioned into two subvectors y_i and t_i of dimensions $p_1 \times 1$ and $p_2 \times 1$ respectively. Correspondingly Σ_F is partitioned into the submatrices $\{\Sigma_{F,ij};\ 1 \le i, j \le 2\}$. Let $g(\Sigma_F)$ be the regression coefficients $\beta_F = \Sigma_{F,22}^{-1}\Sigma_{F,21}$ which define the best linear predictor of y_i given t_i. The least squares estimate of β_F is $b_n = g(S_n)$. By Corollary 1, the Lévy distance between the bootstrap distribution of $n^{1/2}(b_n - \beta_F)$ and the actual distribution converges to zero, with probability one. Moreover, if $|\cdot|$ is any norm on $R^{p_2 \times p_1}$, bootstrap confidence regions based on the pivot $|b_n - \beta_F|$ have the intended asymptotic level. An earlier, somewhat different, analysis of this regression example appeared in Freedman (1981) for $p_1 = 1$.

3.1 *Confidence regions for eigenvalues* (*simple roots*). Suppose F is such that Σ_F has simple eigenvalues $\lambda_1(\Sigma_F) > \lambda_2(\Sigma_F) > \cdots > \lambda_p(\Sigma_F) > 0$. The vector $\lambda(\Sigma_F) = (\lambda_1(\Sigma_F), \lambda_2(\Sigma_F), \cdots, \lambda_p(\Sigma_F))'$ is then a continuously differentiable function of $\mathrm{uvec}(\Sigma_F)$ (Kato, 1982, especially Section 6 of Chapter 2). The ordered sample eigenvalues are $\ell_n = (\ell_{n,1}, \cdots, \ell_{n,p})'$, where $\ell_{n,i} = \lambda_i(S_n)$. To construct a simultaneous confidence region for the $\{\lambda_i(\Sigma_F)\}$, consider the pivot

$$\max_{1\le i\le p} |\log(\ell_{n,i}) - \log(\lambda_i(\Sigma_F))| \tag{3.8}$$

where $|\cdot|$ denotes absolute value. The logarithmic transformation stabilizes variance in the normal model asymptotics for sample eigenvalues. The bootstrap confidence region $D_{n,g}(\alpha)$ corresponding to (3.8) is

$$\begin{aligned}\{\lambda_i(\Sigma_F)\colon \ell_{n,i}A_n^{-1} \le \lambda_i(\Sigma_F) \le \ell_{n,i}A_n \text{ simultaneously for } 1 \le i \le p \\ \text{and } \lambda_1(\Sigma_F) > \lambda_2(\Sigma_F) > \cdots > \lambda_p(\Sigma_F) > 0\}\end{aligned} \tag{3.9}$$

where

$$A_n = \exp[c_{n,g}^*(\alpha)] \tag{3.10}$$

and $c_{n,g}^*(\alpha)$ is an upper α-point of the bootstrap distribution for the pivot (3.8). By Corollary 1, the asymptotic level of the confidence region (3.9) is $1 - \alpha$. Here $u(z) = \max_{1\le i\le p} |z_i|$ for $z \in R^p$.

EXAMPLE 1. Mardia, Kent, and Bibby (1979) reported test scores for 88 college students, each of whom took two closed-book and three open-book tests. Diaconis and Efron (1983) bootstrapped the principal components of this data with two questions in mind: Which averages of the test scores best discriminate among students? How trustworthy are the averages suggested by the estimated principal components? It is interesting to re-examine these and related questions with the help of the more formal bootstrap confidence regions studied in this section.

The eigenvalues of the sample covariance matrix are: 687.0, 202.1, 103.7, 84.6, 32.2. Simultaneous confidence regions for the five eigenvalues were constructed from pivot (3.8) in two ways: by the bootstrap method (3.9), using 200 samples in the Monte Carlo approximation; and by combining normal model asymptotics for the individual sample eigenvalues through the Bonferroni inequality. The

TABLE 1

90% simultaneous confidence intervals for the eigenvalues $\{\lambda_i\}$. *The bootstrap critical value* $c^*_{n,g}(\alpha) = 0.4527$ ($A_n = 1.5726$) *was obtained from a Monte Carlo sample of size* 200.

		λ_1	λ_2	λ_3	λ_4	λ_5
Bootstrap	L	436.9	128.5	66.0	53.8	20.4
	U	1080.3	317.8	163.1	133.0	50.6
Bonferroni	L	483.7	142.3	73.1	59.6	22.6
	U	975.7	287.0	147.3	120.2	45.7

TABLE 2

95% simultaneous confidence intervals for the eigenvalues $\{\lambda_i\}$. *The bootstrap critical value* $c^*_{n,g}(\alpha) = 0.4870$ ($A_n = 1.6273$) *was obtained from a Monte Carlo sample of size* 200.

		λ_1	λ_2	λ_3	λ_4	λ_5
Bootstrap	L	422.2	124.2	63.8	52.0	19.8
	U	1118.0	329.0	168.9	137.8	52.3
Bonferroni	L	466.2	137.1	70.4	57.4	21.8
	U	1012.4	297.8	152.9	124.7	47.4

upper (U) and lower (L) endpoint of the 90% and 95% simultaneous confidence intervals are reported in Tables 1 and 2.

According to the bootstrap confidence intervals, the largest and smallest eigenvalues differ substantially from the other three eigenvalues, which could be clustered together. The Bonferroni intervals are somewhat narrower than the corresponding bootstrap intervals. Since both intervals are based on the same pivot, possible explanations include slight nonnormality of the data (though it passes two tests of multivariate normality) and differing rates of convergence (both methods are asymptotic.)

Indeed, if there is even slight nonnormality then $z_{\alpha/2}$, the upper $\alpha/2$ point of a standard normal distribution, used in the Bonferroni bounds should be changed to $(k_4 + 2\lambda^2)^{1/2} z_{\alpha/2}/(2\lambda^2)^{1/2}$ where k_4 and λ^2 are estimated from the sample; see Fujikoshi (1980) for the definition of k_4. This change widens the Bonferroni intervals. The percentage points for the Bonferroni intervals might also be recalculated using an Edgeworth expansion (cf. Fujikoshi 1980, page 48).

Before deciding how many principal components are needed to summarize a set of multivariate data, it is helpful to estimate the cumulative eigenvalue ratios:

$$\rho_j(\Sigma_F) = \sum_{i=1}^{j} \lambda_i(\Sigma_F)/\sum_{i=1}^{p} \lambda_i(\Sigma_F); \quad 1 \le j \le p-1 \tag{3.11}$$

by the corresponding sample quantities $r_{n,j} = \rho_j(S_n)$; $1 \le j \le p - 1$. To construct a simultaneous lower confidence bound for the $\{\rho_j(\Sigma_F)\}$, consider the pivot

$$\max_{1 \le j \le p-1}(r_{n,j} - \rho_j(\Sigma_F)). \tag{3.12}$$

Since the vector of the $\{\rho_j(\Sigma_F)\}$ is a continuously differentiable function of $\text{uvec}(\Sigma_F)$, Corollary 1 applies. The bootstrap confidence region induced by (3.12) and having asymptotic level $1 - \alpha$ is

$$\{\rho_j(\Sigma_F)\colon \rho_j(\Sigma_F) > r_{n,j} - c_n^*(\alpha) \text{ simultaneously for } 1 \le j \le p - 1\}, \tag{3.13}$$

where $c_n^*(\alpha)$ is an upper α-point of the bootstrap distribution for (3.12).

EXAMPLE 1 (continued). Applied to the test score data, the bootstrap procedure just discussed yields the simultaneous lower confidence bounds for the $\{\rho_j\}$ which are recorded in Table 3. In effect, the raw estimates $\{r_{n,j}\}$ of the cumulated standardized eigenvalues are reduced by .0744, so as to take their variability into proper account at the 95% level. Thus, projection of the test-score data onto the subspace spanned by the first eigenvector of S_n, or even the subspace spanned by the first two eigenvectors, yields only a moderately accurate representation of the data.

3.2 *Confidence regions for eigenvalues* (*multiple roots*). The bootstrap confidence regions constructed in Section 3.1 were derived on the assumption that the eigenvalues of Σ_F have multiplicity one. Without this assumption, the bootstrap estimate $J_{n,\lambda}(\hat{F}_n)$ of

$$J_{n,\lambda}(F) = \mathscr{L}[n^{1/2}(\ell_n - \lambda(\Sigma_F)) \mid F] \tag{3.14}$$

need not converge to $J_{n,\lambda}(F)$. The following extreme case illustrates the problem.

Suppose F is absolutely continuous, has finite fourth moments, and is such that the eigenvalues of Σ_F are all equal to $\nu(\Sigma_F)$. With probability one, the ordered sample eigenvalues $\{\ell_{n,i};\ 1 \le i \le p\}$ are distinct and positive (Okamoto, 1973). Let $P_{n,i}$ be the sample eigenprojection associated with the sample eigenvalue $\ell_{n,i}$. Let Z_F be the symmetric random matrix defined in Section 2.

COROLLARY 2. *Under the model of the preceding paragraph, the Lévy distance between the bootstrap distribution $J_{n,\lambda}(\hat{F}_n)$ and $\mathscr{L}[\mathrm{tr}(Z_F P_{n,1}), \cdots, \mathrm{tr}(Z_F P_{n,p})]$, the latter being computed with respect to the distribution of Z_F, converges to zero with probability one.*

PROOF. Let $\{F_n\}$ be any sequence of cdf's in $\mathscr{S}(F)$ such that the eigenvalues of Σ_{F_n} have multiplicity one, for every $n \ge p$. Let $P_i(\Sigma_{F_n})$ be the eigenprojection associated with the eigenvalue $\lambda_i(\Sigma_{F_n})$. By Kato (1982),

$$\ell_{n,i} = \lambda_i(\Sigma_{F_n}) + \mathrm{tr}[(S_n - \Sigma_{F_n})P_i(\Sigma_{F_n})] + o(\| S_n - \Sigma_{F_n} \|), \tag{3.15}$$

where $\| \cdot \|$ is the Euclidean matrix norm. The elements of $P_i(\Sigma_{F_n})$ are bounded

TABLE 3

95% simultaneous lower confidence bounds for the cumulated standardized eigenvalues $\{\rho_j\}$. The bootstrap critical value $c_{n,s}^*(\alpha) = .0744$ was obtained from a Monte Carlo sample of size 200.

	ρ_1	ρ_2	ρ_3	ρ_4
Lower bound	0.5447	0.7269	0.8204	0.8967

in absolute value by one. Hence, by Theorem 1 and (3.15), the Lévy distance between $J_{n,\lambda}(F_n)$ and $\mathscr{L}[\mathrm{tr}(Z_F P_1(\Sigma_{F_n})), \cdots, \mathrm{tr}(Z_F P_p(\Sigma_{F_n}))]$ converges to zero as n increases. The corollary follows from this because, with probability one, $\{\hat{F}_n\}$ belongs to $\mathscr{C}(F)$ and the eigenvalues of $\Sigma_{\hat{F}_n}$ are distinct for every $n \geq p$.

Davis (1977), extending Anderson's (1963) normal model asymptotics for spectral decompositions, showed that the actual distribution $J_{n,\lambda}(F)$ converges weakly to $\mathscr{L}[\lambda_1(Z_F), \cdots, \lambda_p(Z_F)]$. Thus, the bootstrap distribution $J_{n,\lambda}(\hat{F}_n)$ does *not* converge to the actual distribution $J_{n,\lambda}(F)$ in the equal roots case. It is possible to construct another bootstrap estimate for $J_{n,\lambda}(F)$ which works when the eigenvalues of Σ_F are not all different (see Corollary 4 of Section 4.2). However, that construction presupposes knowledge of the eigenvalue multiplicities, a situation arising more naturally in testing theory than in confidence region theory.

A different approach is needed to obtain theoretically valid bootstrap confidence regions for the ordered eigenvalues $\{\lambda_i(\Sigma_F)\}$ when no asumptions are made about eigenvalue multiplicities. Let the $\{\beta_i(\Sigma_F);\ 1 \leq i \leq p\}$ be the p elementary symmetric polynomials in the variables $\{\lambda_i(\Sigma_F);\ 1 \leq i \leq p\}$:

$$
\begin{aligned}
\beta_1(\Sigma_F) &= \textstyle\sum_{j=1}^{p} \lambda_j(\Sigma_F) \\
\beta_2(\Sigma_F) &= \textstyle\sum_{j<k}^{p} \lambda_j(\Sigma_F)\lambda_k(\Sigma_F) \\
&\ \ \vdots \\
\beta_p(\Sigma_F) &= \textstyle\prod_{j=1}^{p} \lambda_j(\Sigma_F).
\end{aligned}
\tag{3.16}
$$

Since the eigenvalues are roots of the characteristic polynomial, each $\beta_i(\Sigma_F)$ is a continuously differentiable function of the elements of uvec(Σ_F). Let the $\{b_{n,i}\}$ be the sample estimates $b_{n,i} = \beta_i(S_n);\ 1 \leq i \leq p$. By bootstrapping the pivot

$$
\max_{1\leq i\leq p} |\log(b_{n,i}) - \log(\beta_i(\Sigma_F))| \tag{3.17}
$$

and arguing as in the first paragraph of Section 3.1, we obtain a simultaneous confidence region for the $\{\beta_i(\Sigma_F)\}$, of asymptotic level $1 - \alpha$. This region can be reinterpreted as a confidence region for the ordered eigenvalues $\{\lambda_i(\Sigma_F)\}$, because the mapping (3.16) from ordered eigenvalues to elementary symmetric polynomials is one-to-one.

Though the eigenvalue confidence region so obtained has the correct asymptotic level *whatever* the eigenvalue multiplicities may be, its shape in eigenvalue space is relatively strange, even when $p = 2$. For applications where distinctness of the eigenvalues is a reasonable assumption, confidence regions like the one decribed in Section 3.1 may be preferred.

3.3 *Bootstrap distributions for eigenvalues versus Edgeworth expansions.* When F is standard bivariate normal with strictly positive correlation ρ, means zero and variances one, the eigenvalues of Σ_F are $\lambda_1 = 1 + \rho$ and $\lambda_2 = 1 - \rho$. The marginal cdf of $w_i = (n/2)^{1/2}(\ell_{n,i} - \lambda_i)/\lambda_i$, $i = 1, 2$, has an Edgeworth expansion (Fujikoshi, 1980):

$$\begin{aligned} P[w_i \le x] &= \Phi(x) - n^{1/2}[a_{1i}\sigma_i^{-1}\Phi^{(1)}(x) + a_{3i}\sigma_i^{-3}\Phi^{(3)}(x)] \\ &\quad + n^{-1}[(b_{2i} + 2^{-1}a_{1i}^2)\sigma_i^{-2}\Phi^{(2)}(x) + (b_{4i} + a_{1i} + a_{3i})\sigma_i^{-4}\Phi^{(4)}(x) \\ &\qquad + 2^{-1}a_{3i}^2\sigma_i^{-6}\Phi^{(6)}(x)] + o(n^{-1}) \end{aligned} \tag{3.18}$$

where $\Phi^{(j)}(x)$ is the jth derivative of the standard normal cdf $\Phi(x)$ and

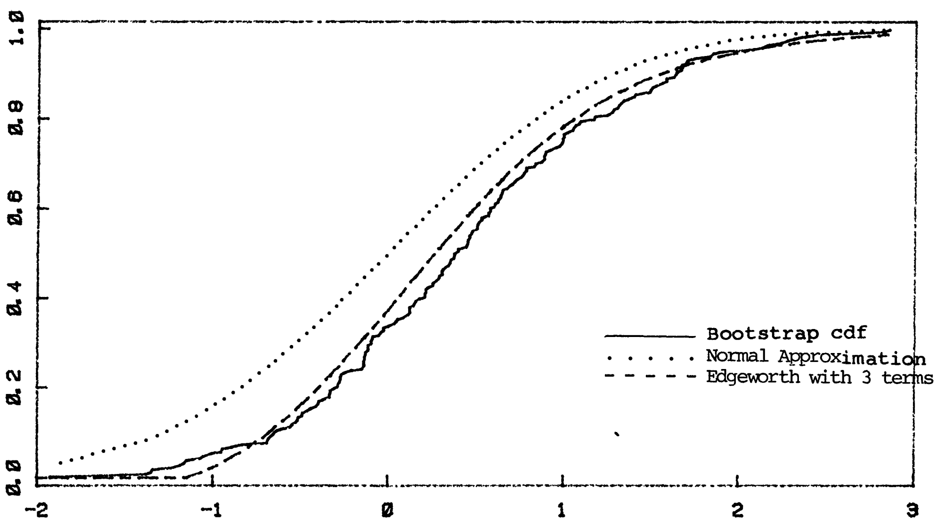
$$\begin{aligned} &\sigma_i^2 = 2\lambda_i^2, \quad a_{1i} = \textstyle\sum_{j\neq i} \lambda_i\lambda_j(\lambda_i - \lambda_j)^{-1}, \quad a_{3i} = 4/3\lambda_i^3 \\ &b_{2i} = -\textstyle\sum_{j\neq i} \lambda_i^2\lambda_j^2(\lambda_i - \lambda_j)^{-2}, \quad b_{4i} = 2\lambda_i^4. \end{aligned} \tag{3.19}$$

The parameters in the expansion (3.18) can be estimated from the sample eigenvalues $\ell_{n,1}$ and $\ell_{n,2}$. How well does the nonparametric bootstrap cdf for w_i compare with Edgeworth cdf estimates of various orders? Asymptotic theory in related situations indicates that, for moderate sample sizes, the difference beween the bootstrap cdf and the two-term Edgeworth estimate should be small; both of these estimates should be less biased than the normal cdf approximation; and higher order Edgeworth estimates should differ little from the bootstrap or two-term Edgeworth estimate (Beran, 1982; Singh, 1981). The same conclusions are indicated when F is nonnormal, though in this case the Edgeworth expansion becomes rather complicated.

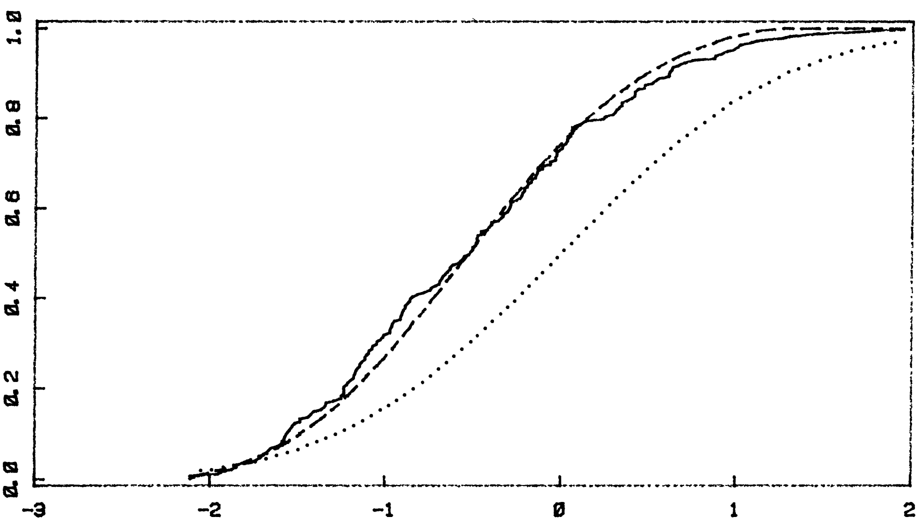
To test these surmises, random samples of size 30 were generated from the bivariate normal distributions with $\rho = 0.1, 0.5, 0.9$, means zero and variances one. The bootstrap cdf (approximated in a Monte Carlo simulation using 200 samples from $\hat{F}_n$) and Edgeworth cdf estimates with one, two, or three terms were computed for each of the three samples. Figure 1 compares the bootstrap cdf with the three-term Edgeworth estimate and with the simple normal approximation (the first term in (3.18)). The two-term Edgeworth estimates are not plotted, because they are nearly identical to the three-term estimates. The agreement between the bootstrap cdf and the three-term Edgeworth estimates is remarkable, as is the bias in the normal approximation when $\rho = 0.1$.

How well do the bootstrap cdf and the Edgeworth cdf estimates of various orders approximate the actual cdf of w_i? The theory in Beran (1982) indicates that the bootstrap cdf and the Edgeworth estimates of two or more terms are locally asymptotically minimax among *all* estimates for the actual cdf. Moreover, the bias in the normal cdf estimate causes it to be suboptimal, except for very special choices of F where the bias vanishes.

3.4 *Confidence cones for eigenvectors.* Suppose F is such that the eigenvalues of Σ_F have multiplicity one. Let $\gamma_i(\Sigma_F)$ be a $p \times 1$ eigenvector of unit length associated with the ith eigenvalue $\lambda_i(\Sigma_F)$; the sign of $\gamma_i(\Sigma_F)$ may be chosen arbitrarily. A sample eigenvector associated with the ith sample eigenvalue $\ell_{n,i}$ is



Largest sample eigenvalue with $\rho = 0.1$.



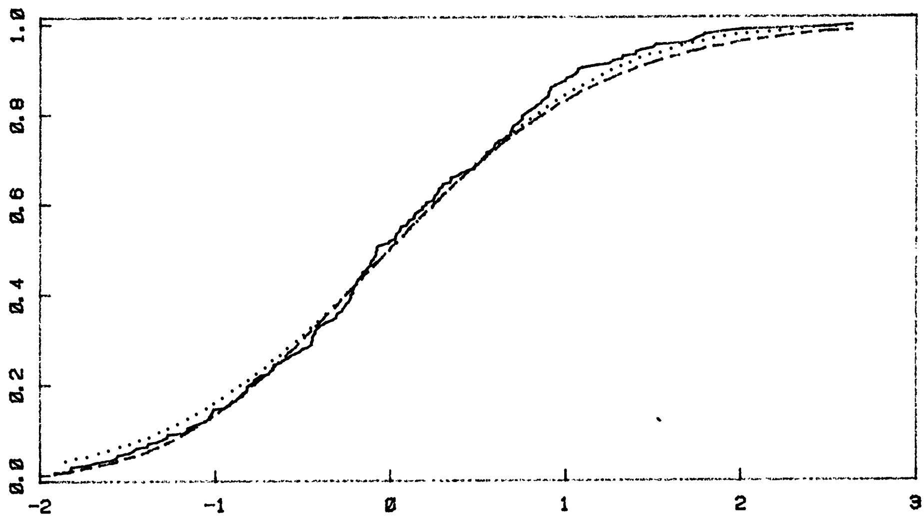
Smallest sample eigenvalue with $\rho = 0.1$.

FIG. 1. *Comparison of the bootstrap, normal approximation, and estimated three-term Edgeworth expansion for the cdfs of the centered sample eigenvalues in a bivariate normal sample of size* 30. *The bootstrap Monte Carlo used* 200 *samples.*

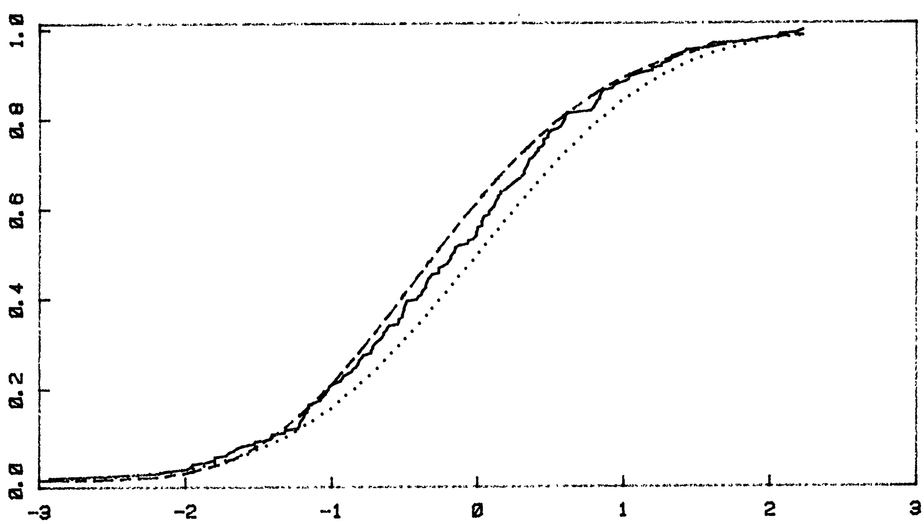
$c_{n,i} = \gamma_i(S_n)$. To construct a confidence cone for $\gamma_i(\Sigma_F)$, consider the pivot

$$1 - |c_{n,i}'\gamma_i(\Sigma_F)| \tag{3.20}$$

whose nonnormal model asymptotics have been studied by Davis (1977). Let $c_n^*(\alpha)$ be an upper α-point of the bootstrap distribution for (3.20). The bootstrap



Largest sample eigenvalue with $\rho = 0.5$.



Smallest sample eigenvalue with $\rho = 0.5$.

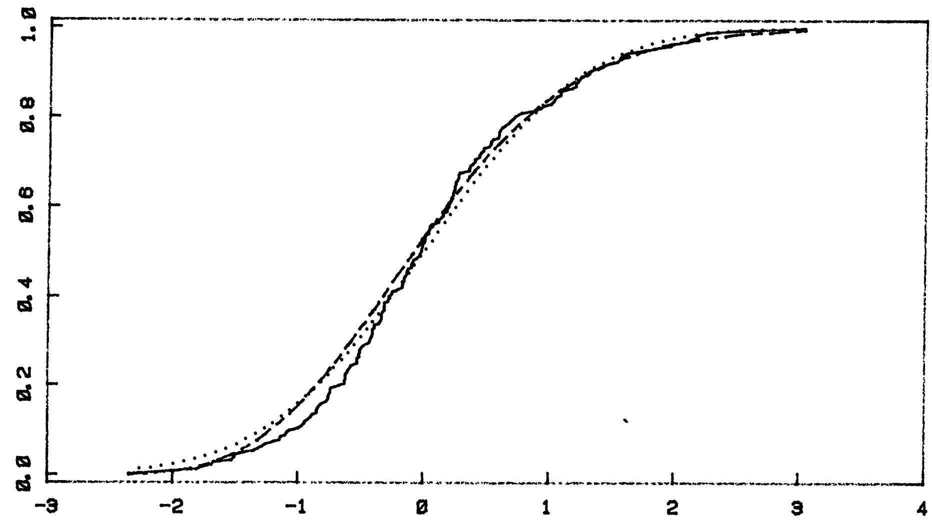
FIG. 1. *(continued)*

confidence cone generated by (3.20) is

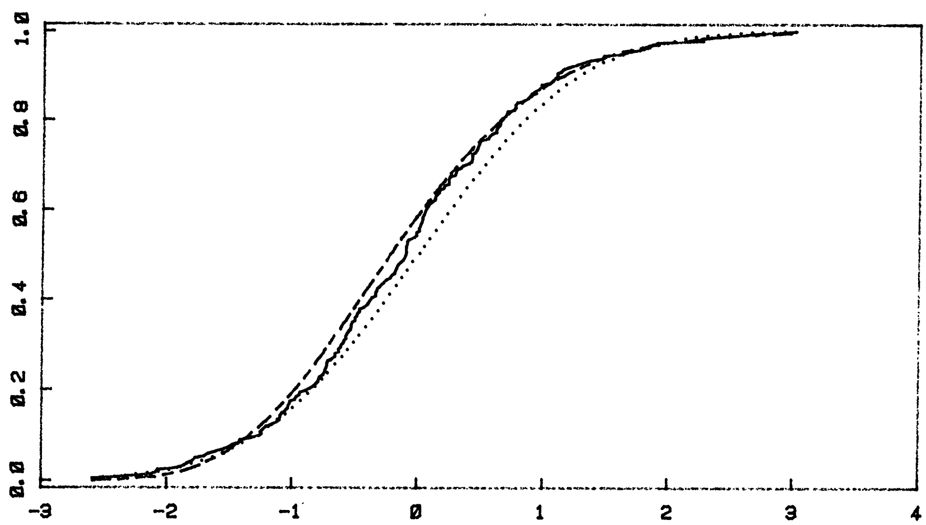
$$\{\gamma_i(\Sigma_F): |c'_{n,i}\gamma_i(\Sigma_F)| \geq d_n^*(\alpha),\ |\gamma_i(\Sigma_F)| = 1\}, \tag{3.21}$$

where $d_n^*(\alpha) = 1 - c_n^*(\alpha)$. In practice, $d_n^*(\alpha)$ could be calculated as a *lower* α-point of the bootstrap distribution for $|c'_{n,i}\gamma_i(\Sigma_F)|$.

To see that confidence cone (3.21) has asymptotic level $1 - \alpha$, let $P_i(\Sigma_F) = \gamma_i(\Sigma_F)\gamma_i'(\Sigma_F)$ be the eigenprojection corresponding to $\lambda_i(\Sigma_F)$ and let $P_{n,i} = c_{n,i}c'_{n,i}$



Largest sample eigenvalue with $\rho = 0.9$.



Smallest sample eigenvalue with $\rho = 0.9$.

FIG. 1. (*continued*)

be the ith sample eigenprojection. By algebraic manipulation,

$$1 - |c'_{n,i}\gamma_i(\Sigma_F)| = 1 - [1 - 2^{-1} \| P_{n,i} - P_i(\Sigma_F) \|^2]^{1/2} \tag{3.22}$$

where $\| \cdot \|$ is the Euclidean matrix norm. Since $P_i(\Sigma_F)$ is a continuously differentiable function of $\text{uvec}(\Sigma_F)$ (Kato, 1982), Corollary 1 can be applied with $g = P_i$. Consequently, the bootstrap distribution of $n[1 - |c'_{n,i}\gamma_i(\Sigma_F)|]$ converges with probability one to the same continuous limit distribution as does the actual distribution of $n[1 - |c'_{n,i}\gamma_i(\Sigma_F)|]$. Hence, confidence cone (3.21) has asymptotic level α.

Simultaneous confidence cones of asymptotic level $1 - \alpha$ can be constructed by bootstrapping the pivot

$$\max_{1\le i\le p}[1 - |c'_{n,i}\gamma_i(\Sigma_F)|]. \tag{3.23}$$

Unfortunately, the simultaneous confidence cones so obtained tend to be very wide in practice, because the distribution of $|c'_{n,i}\gamma_i(\Sigma_F)|$ may vary substantially with i.

EXAMPLE 1 (continued). For the test score data discussed in Section 3.1, the first three sample eigenvectors are

$$\begin{aligned} c_{n,1} &= (0.505, 0.386, 0.346, 0.451, 0.535) \\ c_{n,2} &= (0.749, 0.207, -0.075, -0.301, -0.548) \\ c_{n,3} &= (-0.300, 0.416, 0.145, 0.547, -0.600). \end{aligned} \tag{3.24}$$

The critical values $d_n^*(\alpha)$ defining the 95% bootstrap confidence cones for $\gamma_1(\Sigma_F)$, $\gamma_2(\Sigma_F)$ and $\gamma_3(\Sigma_F)$ are 0.985, 0.915, and 0.310 respectively. The confidence cone for $\gamma_i(\Sigma_F)$ widens substantially as i increases.

As might be expected, the 95% confidence cone for $\gamma_1(\Sigma_F)$ contains the vector $5^{1/2}(1/5, 1/5, 1/5, 1/5, 1/5)'$, which corresponds to the average test score for each student. On general grounds, a natural candidate for $\gamma_2(\Sigma_F)$ is the vector $(6/5)^{1/2}(1/2, 1/2, -1/3, -1/3, -1/3)$; the associated principal component is the difference between the average closed-book score and the average open-book score for each student. However, this vector lies well outside the 95% confidence cone for $\gamma_2(\Sigma_F)$. On the other hand, the modified comparison-of-averages vector $(1/2, 1/2, 0, -1/2, -1/2)$, which ignores the first open-book test, very nearly lies within the same confidence cone.

From this analysis and the earlier examination of the cumulated eigenvalue ratios, we draw the following conclusions: The average score is a rough summary of a student's performance in the five tests. Finer distinctions among students can be made by calculating the difference between the average of the two closed book tests and the average of the second and third open book tests.

When the eigenvalues of Σ_F are not simple, it is still possible to devise bootstrap confidence regions for eigenvectors which have the desired asymptotic level. Suppose $\lambda_{i-1}(\Sigma_F) > \lambda_i(\Sigma_F) = \cdots = \lambda_{i+q_i-1}(\Sigma_F) > \lambda_{i+q_i}(\Sigma_F)$. Let $\Gamma_i(\Sigma_F)$ be a $p \times q_i$ matrix whose columns are orthonormal eigenvectors corresponding to this eigenvalue of multiplicity q_i. Let $C_{n,i}$ be a $p \times q_i$ matrix whose columns are orthonormal eigenvectors associated with the sample eigenvalues $\ell_{n,i} \ge \ell_{n,i+1} \ge \cdots \ge \ell_{n,i+q_i-1}$. The eigenprojections corresponding to $\Gamma_i(\Sigma_F)$ and $C_{n,i}$ are $P_i(\Sigma_F) = \Gamma_i(\Sigma_F)\Gamma_i'(\Sigma_F)$ and $P_{n,i} = C_{n,i}C'_{n,i}$ respectively. The pivot (3.20) generalizes to

$$q_i^{1/2} - \|C'_{n,i}\Gamma_i(\Sigma_F)\| = q_i^{1/2} - [q_i - 2^{-1}\|P_{n,i} - P_i(\Sigma_F)\|^2]^{1/2}, \tag{3.25}$$

where $\|\cdot\|$ is the Euclidean matrix norm. Because the eigenprojection $P_i(\Sigma_F)$ is still continuously differentiable, the earlier analysis for $q_i = 1$ may be extended to general q_i. The confidence region of asymptotic level $1 - \alpha$ for $\Gamma_i(\Sigma_F)$ is

$$\{\Gamma_i(\Sigma_F)\colon \| C'_{n,i}\Gamma_i(\Sigma_F) \| \geq d_n^*(\alpha);\ \Gamma_i'(\Sigma_F)\Gamma_i(\Sigma_F) = I_{q_i}\}, \tag{3.26}$$

where $d_n^*(\alpha)$ is a lower α-point of the bootstrap distribution for $\| C'_{n,i}\Gamma_i(\Sigma_F) \|$.

4. Bootstrap tests about Σ_F. A bootstrap confidence region for $g(\Sigma_F)$ can be inverted in the usual way to test hypotheses about the value of $g(\Sigma_F)$. It is also possible, and sometimes simpler, to construct bootstrap tests directly from a test statistic (cf. Beran, 1984). This second approach to testing structural hypotheses about Σ_F is the subject of this section.

Consider the following framework. Let π be a continuous projection, not the identity map, which takes any nonsingular $p \times p$ covariance matrix into a $p \times p$ covariance matrix. Suppose $T_n = nh(S_n)$ is a test statistic for the null hypothesis

(4.1) H_0: the $\{x_i;\ i \geq 1\}$ are independent identically distributed $p \times 1$ random vectors with unknown cdf F_0, which has finite fourth moments; F_0 is such that $\Sigma_{F_0} = \pi(\Sigma_{F_0})$.

The function h defining the test statistic T_n is twice continuously differentiable at $\text{uvec}(\Sigma_{F_0})$, with h and the first derivative of h vanishing there for every possible choice of Σ_{F_0} satisfying the hypothesis H_0. The test rejects H_0 if T_n is sufficiently large. As will be seen later in the section, this formulation includes likelihood ratio and other multisided tests concerning the structure of Σ_F.

The asymptotic distribution under H_0 of the test statistic T_n may be found by Taylor expansion of $h(S_n)$ about $h(\Sigma_{F_0})$ and by reference to Theorem 1. Let $\ddot{h}$ denote the second derivative of h, and let $z_{F_0} = \text{uvec}(Z_{F_0})$. Then

$$\mathscr{L}[T_n \mid F_0] \Rightarrow \mathscr{L}[z'_{F_0}\ddot{h}(\Sigma_{F_0})z_{F_0}] \tag{4.2}$$

as n tends to infinity. Approximate critical values for the test under discussion can be obtained by computing the upper quantiles of the limiting distribution on the right side of (4.2), after first estimating the unknown cdf F_0 by the empirical cdf $\hat{F}_n$. Substantial algebraic calculations are required in this approach.

Alternatively and more simply, we can construct a bootstrap estimate for the null distribution $\mathscr{L}[T_n \mid F_0]$ as follows. Let

$$V_{n,F} = [\pi(\Sigma_F)]^{1/2}\Sigma_F^{-1/2}S_n\Sigma_F^{-1/2}[\pi(\Sigma_F)]^{1/2} \tag{4.3}$$

and let $K_{n,h}(F) = \mathscr{L}[nh(V_{n,F}) \mid F]$. The bootstrap estimate for the null distribution of T_n is defined to be $K_{n,h}(\hat{F}_n)$. Let $d_{n,h}(\alpha, \hat{F}_n)$ be an upper α-point of $K_{n,h}(\hat{F}_n)$.

COROLLARY 3. *Under the null hypothesis* H_0,

$$K_{n,h}(\hat{F}_n) \Rightarrow \mathscr{L}[z'_{F_0}\ddot{h}(\Sigma_{F_0})z_{F_0}] \tag{4.4}$$

with probability one. Hence, the test which rejects H_0 whenever $T_n > d_{n,h}(\alpha, \hat{F}_n)$ has asymptotic size α, provided $\ddot{h}(\Sigma_{F_0})$ is nonzero.

PROOF. Suppose the $\{x_i\}$ are i.i.d. with cdf F_0 which satisfies the constraint

(4.1). Let $\{F_n;\, n \geq 1\}$ be any sequence of cdf's in $\mathscr{S}(F_0)$. Both $\{\Sigma_{F_n}\}$ and $\{\pi(\Sigma_{F_n})\}$ converge to Σ_{F_0} as n increases. Thus, by Theorem 1,

$$\mathscr{L}[n^{1/2}(V_{n,F_n} - \pi(\Sigma_{F_n})) \mid F_n] \Rightarrow \mathscr{L}[Z_{F_0}]. \tag{4.5}$$

From this, the vanishing of h and $\dot{h}$ at $\pi(\Sigma_{F_n})$, and the continuity of $\ddot{h}$ at Σ_{F_0},

$$K_{n,h}(F_n) \Rightarrow \mathscr{L}[z'_{F_0}\ddot{h}(\Sigma_{F_0})z_{F_0}] \tag{4.6}$$

as n increases. Equation (4.4) follows because $P_{F_0}[\{\hat{F}_n\} \in \mathscr{S}(F_0)] = 1$. The other assertion in Corollary 3 is also an immediate consequence, the limit law on the right side of (4.6) being continuous (cf. the proof of Theorem 1 in Beran, 1984).

In practice, the bootstrap null distribution can be constructed as follows. Let

$$y_i = [\pi(\Sigma_{\hat{F}_n})]^{1/2}\Sigma_{\hat{F}_n}^{-1/2}x_i, \quad 1 \leq i \leq n. \tag{4.7}$$

Let the $\{y_i^*;\, 1 \leq i \leq n\}$ be i.i.d. random vectors whose cdf is the realized empirical cdf of the $\{y_i;\, 1 \leq i \leq n\}$. Let $S^*_{n,y}$ be the sample covariance matrix of the $\{y_i^*\}$. Then $K_{n,h}(\hat{F}_n)$ is the distribution of $nh(S^*_{n,y})$ and can be approximated by Monte Carlo methods.

From the proof of Corollary 3, it is evident that factorizations of Σ_F other than the symmetric square root factorization can be used to construct consistent bootstrap null distribution estimates.

When the map π is a linear projection (see Section 4.1 for an example), equation (4.7) is equivalent to $y_i = [\pi(S_n)]^{1/2}S_n^{-1/2}x_i$. The sample covariance matrix $S_{n,y}$ of the $\{y_i;\, 1 \leq i \leq n\}$ now satisfies the relation $S_{n,y} = \pi(S_{n,y})$, a sample analog of the null hypothesis constraint $\Sigma_{F_0} = \pi(\Sigma_{F_0})$. The bootstrap algorithm discussed in Corollary 3 was motivated by this consideration.

4.1. *Testing for specified eigenvectors.* Let B be a $p \times r$ matrix whose columns are orthonormal. Suppose the null hypothesis asserts that the columns of B are eigenvectors of the unknown covariance matrix of the data. Let C be any $p \times (p - r)$ matrix such that $\Gamma = (B \vdots C)$ is orthogonal. Let the $\{x_i;\, 1 \leq i \leq n\}$ be the images under Γ' of the original sample random vectors. The null hypothesis states that Σ_{F_0}, the covariance matrix of the $\{x_i\}$, has the form

$$\Sigma_{F_0} = \begin{pmatrix} \operatorname{diag}\{\sigma_{F_0,ii};\, 1 \leq i \leq r\} & 0 \\ 0 & \Sigma_{F_0,22} \end{pmatrix}, \tag{4.8}$$

where $\Sigma_{F_0,22}$ is an arbitrary covariance matrix of dimension $(p - r) \times (p - r)$. The normal model likelihood ratio test rejects this hypothesis if

$$h(S_n) = \textstyle\sum_{i=1}^{r} \log(s_{n,ii}) + \log[\det(S_{n,22})] - \log[\det(S_n)] \tag{4.9}$$

is too large (Mallows, 1961), The test does not depend upon the choice of C (Srivastava, 1983).

The null hypotheses for the transformed observation vectors $\{x_i\}$ is of the form (4.1). Let Σ be any $p \times p$ covariance matrix, partitioned into four submatrices of the dimensions indicated in (4.8). Then π is the linear projection of Σ which zeroes the submatrices Σ_{12}, Σ_{21} and the off-diagonal elements of Σ_{11}. The function

h defined by (4.9) is twice continously differentiable at $\pi(\Sigma)$, with both h and the first derivative of h vanishing there. Thus, by Corollary 3, the bootstrap test based on $nh(S_n)$ has asymptotic size α.

4.2. *Testing hypotheses about eigenvalue multiplicities.* Sometimes a null hypothesis concerning the structure of Σ_F implies or is equivalent to a hypothesis about the multiplicities of the eigenvalues of Σ_F. Natural test statistics for such eigenvalue hypotheses are often expressible as smooth functions of the sample eigenvalues. Let $\lambda(\Sigma_F)$ be the $p \times 1$ vector of ordered eigenvalues $\lambda_1(\Sigma_F) \geq \lambda_2(\Sigma_F) \geq \cdots \geq \lambda_p(\Sigma_F) > 0$ of Σ_F; let $\Gamma(\Sigma_F)$ be an orthogonal matrix whose columns are eigenvectors of Σ_F; and let $\Delta(\Sigma_F) = \text{diag}\{\lambda_i(\Sigma_F); 1 \leq i \leq p\}$. Suppose $T_n^* = nh^*(\ell_n)$, a function of the sample eigenvalues $\ell_{n,1} \geq \ell_{n,2} \geq \cdots \geq \ell_{n,p}$, is a test statistic for the null hypothesis

H_0^*: the $\{x_i; i \geq 1\}$ are i.i.d. with unknown cdf F_0 which has finite fourth moments; Σ_{F_0} has eigenvalue matrix

$$\Delta(\Sigma_{F_0}) = \begin{bmatrix} \nu_1(\Sigma_{F_0})I_{q_1} & & & 0 \\ & \nu_2(\Sigma_{F_0})I_{q_2} & & \\ & & \ddots & \\ 0 & & & \nu_r(\Sigma_{F_0})I_{q_r} \end{bmatrix} \tag{4.10}$$

where $\nu_1(\Sigma_{F_0}) > \nu_2(\Sigma_{F_0}) > \cdots > \nu_r(\Sigma_{F_0}) > 0$ and $\sum_{i=1}^r q_i = p$.

Suppose further that the function h^* defining the test statistic T_n^* is twice continuously differentiable at $\lambda(\Sigma_{F_0})$, with both h^* and its first derivative vanishing there for every possible choice of Σ_{F_0} satisfying the hypothesis H_0^*. The test rejects H_0^* if T_n^* is sufficiently large. Examples of such tests are discussed in Section 4.3.

Davis (1977), extending Anderson's (1963) normal model asymptotics for spectral decompositions, showed that, as n increases,

$$\mathscr{L}[n^{1/2}[\ell_n - \lambda(\Sigma_{F_0})] \mid F_0] \Rightarrow \mathscr{L}[\lambda(U_{11}(F_0, \Gamma)), \cdots, \lambda(U_{rr}(F_0, \Gamma))], \tag{4.11}$$

where $U_{ii}(F_0, \Gamma)$ is the ith diagonal block, of dimension $q_i \times q_i$, in the random matrix

$$U(F_0, \Gamma) = \Gamma'(\Sigma_{F_0})Z_{F_0}\Gamma(\Sigma_{F_0}). \tag{4.12}$$

Here Z_{F_0} is the $p \times p$ symmetric random matrix defined in Corollary 1. Let w_{F_0} be a $p \times 1$ random vector which has the distribution on the right side of (4.11). Note that $\mathscr{L}(w_{F_0})$ does not depend upon the particular choice of $\Gamma(\Sigma_{F_0})$, because the left side of (4.11) does not; and that $\mathscr{L}(w_{F_0})$ is continuous. From (4.11) and the properties of h^*,

$$\mathscr{L}[T_n^* \mid F_0] \Rightarrow \mathscr{L}[w'_{F_0}\ddot{h}^*(\lambda(\Sigma_{F_0}))w_{F_0}], \tag{4.13}$$

$\ddot{h}^*$ being the second derivative matrix of h^*.

As was seen in Section 3.2, the simple bootstrap estimate $J_{n,\lambda}(\hat{F}_n)$ does not converge to $\mathscr{L}[n^{1/2}(\ell_n - \lambda(\Sigma_{F_0})) \mid F_0]$ whenever eigenvalue multiplicities exceed one. However, a more sophisticated bootstrap distribution estimate, which explicitly recognizes the multiplicities $q_1, q_2, \cdots, q_r$ specified in the hypothesis H_0^*, does converge appropriately and yields consistent bootstrap critical values for the test statistic T_n^*. The construction runs as follows:

Let

$$(4.14) \qquad \bar{\Delta}(\Sigma_F) = \begin{bmatrix} \bar{\lambda}_1(\Sigma_F)I_{q_1} & & & 0 \\ & \bar{\lambda}_2(\Sigma_F)I_{q_2} & & \\ & & \ddots & \\ 0 & & & \bar{\lambda}_r(\Sigma_F)I_{q_r} \end{bmatrix},$$

where $\bar{\lambda}_i(\Sigma_F)$ is the average of the q_i eigenvalues in the ith diagonal block of $\Delta(\Sigma_F)$, $\{\lambda_j(\Sigma_F)\colon \sum_{k=1}^{i-1} q_k + 1 \le j \le \sum_{k=1}^{i} q_k\}$. Let $\bar{\Sigma}_F = \Gamma(\Sigma_F)\bar{\Delta}(\Sigma_F)\Gamma'(\Sigma_F)$. Observe that $\bar{\Sigma}_F$ is a perturbation of Σ_F which has precisely the eigenvalue multiplicities specified in H_0^*. Let

$$(4.15) \qquad W_{n,F} = \bar{\Sigma}_F^{1/2}\Sigma_F^{-1/2}S_n\Sigma_F^{-1/2}\bar{\Sigma}_F^{1/2}$$

and let $J_{n,\lambda}^*(F) = \mathscr{L}[n^{1/2}(\lambda(W_{n,F}) - \lambda(\bar{\Sigma}_F)) \mid F]$. The bootstrap estimate for $\mathscr{L}[n^{1/2}(\ell_n - \lambda(\Sigma_{F_0})) \mid F_0]$ when F_0 satisfies hypothesis H_0^* is defined to be $J_{n,\lambda}^*(\hat{F}_n)$. The corresponding bootstrap estimate for $\mathscr{L}[T_n^* \mid F_0]$ is $K_{n,h}^*(\hat{F}_n)$, where $K_{n,h}^*(F) = \mathscr{L}[nh^*(W_{n,F}) \mid F]$.

In practice, $K_{n,h}^*(\hat{F}_n)$ can be constructed as follows. Let

$$(4.16) \qquad y_i = \bar{\Sigma}_{\hat{F}_n}^{1/2}\Sigma_{\hat{F}_n}^{-1/2}x_i, \quad 1 \le i \le n.$$

Let the $\{y_i^*; 1 \le i \le n\}$ be i.i.d. random vectors whose cdf is the realized empirical cdf of the $\{y_i; 1 \le i \le n\}$. Let $S_{n,y}^*$ be the sample covariance matrix of the $\{y_i^*\}$. Then $K_{n,h}^*(\hat{F}_n)$ is the distribution of $nh^*[\lambda(S_{n,y}^*)]$ and can be approximated by Monte Carlo methods.

This construction can be simplified algebraically because sample eigenvalues are invariant under rotations of the sample. Let $D_n = \mathrm{diag}\{\ell_{n,i}; 1 \le i \le p\}$ and let

$$(4.17) \qquad \bar{D}_n = \begin{bmatrix} \bar{\ell}_{n,1}I_{q_1} & & & 0 \\ & \bar{\ell}_{n,2}I_{q_2} & & \\ & & \ddots & \\ 0 & & & \bar{\ell}_{n,r}I_{q_r} \end{bmatrix}$$

where $\bar{\ell}_{n,i}$ is the average of the sample eigenvalues in the ith diagonal block, having dimension $q_i \times q_i$, of D_n. In place of (4.16), define

$$(4.18) \qquad y_i = \bar{D}_n^{1/2}D_n^{-1/2}C_n'x_i, \quad 1 \le i \le n$$

where $C_n = \Gamma(S_n)$; that is C_n is the sample eigenvector matrix $(c_{n,1}, c_{n,2}, \cdots, c_{n,p})$ associated with S_n. Complete the construction of $K_{n,h}^*(\hat{F}_n)$ as in the preceding paragraph.

Let $d^*_{n,h}(\alpha, \hat{F}_n)$ be an upper α point of $K^*_{n,h}(\hat{F}_n)$.

COROLLARY 4. *Under the null hypothesis* H_0^*,

$$J^*_{n,\lambda}(\hat{F}_n) \Rightarrow \mathscr{L}(w_{F_0}) \tag{4.19}$$

with probability one. Consequently

$$K^*_{n,h}(\hat{F}_n) \Rightarrow \mathscr{L}[w'_{F_0}\ddot{h}^*(\lambda(\Sigma_{F_0}))w_{F_0}] \tag{4.20}$$

with probability one and the test which rejects H_0^* *when* $T^*_n > d^*_{n,h}(\alpha, \hat{F}_n)$ *has asymptotic size* α, *provided* $\ddot{h}^*(\lambda(\Sigma_{F_0}))$ *is nonzero.*

PROOF. Let $\{F_n\}$ be any sequence of cdf's in $\mathscr{C}(F_0)$. Both $\{\Sigma_{F_n}\}$ and $\{\bar{\Sigma}_{F_n}\}$ converge to Σ_{F_0}, the former by definition of $\mathscr{C}(F_0)$ and the latter by continuity of the relevant eigenvalues and eigenprojections (Kato, 1982). Since

$$n^{1/2}(W_{n,F_n} - \bar{\Sigma}_{F_n}) = \bar{\Sigma}^{1/2}_{F_n}\Sigma^{-1/2}_{F_n}n^{1/2}(S_n - \Sigma_{F_n})\Sigma^{-1/2}_{F_n}\bar{\Sigma}^{1/2}_{F_n}, \tag{4.21}$$

it follows, with the help of Theorem 1, that

$$\mathscr{L}[n^{1/2}(W_{n,F_n} - \bar{\Sigma}_{F_n}) \mid F_n] \Rightarrow \mathscr{L}(Z_{F_0}). \tag{4.22}$$

From the variational characterization of eigenvalues,

$$|\lambda_i(W_{n,F_n}) - \lambda_i(\bar{\Sigma}_{F_n})| \le \| W_{n,F_n} - \bar{\Sigma}_{F_n} \|, \quad 1 \le i \le p. \tag{4.23}$$

In view of (4.22) and (4.23), the sequence of distributions $\{J^*_{n,\lambda}(F_n);\ n \ge 1\}$ is relatively compact.

Suppose $J^*_{n,\lambda}(F_n)$ does not converge weakly to $\mathscr{L}(w_{F_0})$ as n tends to infinity. By going to a subsequence, we can assume without loss of generality that $J^*_{n,\lambda}(F_n)$ converges weakly to a limit law J_1 which differ from $\mathscr{L}(w_{F_0})$. By going to a further subsequence, we can assume in addition that $\Gamma(\Sigma_{F_n})$ converges to Γ_1, a $p \times p$ matrix whose columns are an orthonormal set of eigenvectors for Σ_{F_0}. (Reason: the set of all $p \times p$ orthogonal matrices is compact in p^2-dimensional Euclidean space and $\lim_{n\to\infty}\lambda(\Sigma_{F_n}) = \lambda(\Sigma_{F_0})$).

Replacing Σ_{F_n} and $\bar{\Sigma}_{F_n}$ in (4.15) by their spectral representations yields

$$W_{n,F_n} = \Gamma(\Sigma_{F_n})I(\Sigma_{F_n})D_n(F_n)I(\Sigma_{F_n})\Gamma'(\Sigma_{F_n}) \tag{4.24}$$

where

$$\begin{aligned} I(\Sigma_{F_n}) &= \bar{\Delta}^{1/2}(\Sigma_{F_n})\Delta^{-1/2}(\Sigma_{F_n}) \\ D_n(F_n) &= \Gamma'(\Sigma_{F_n})S_n\Gamma(\Sigma_{F_n}). \end{aligned} \tag{4.25}$$

Observe that $\lim_{n\to\infty}I(\Sigma_{F_n}) = I_p$ because both $\Delta(\Sigma_{F_n})$ and $\bar{\Delta}(\Sigma_{F_n})$ converge to $\Delta(\Sigma_{F_0})$.

Let

$$\begin{aligned} U_n &= I(\Sigma_{F_n})n^{1/2}[D_n(F_n) - \Delta(\Sigma_{F_n})]I(\Sigma_{F_n}) \\ \bar{\Delta}_2(\Sigma_{F_n}) &= \mathrm{diag}\{\bar{\lambda}_i(\Sigma_{F_n})I_{q_i};\ 2 \le i \le r\}. \end{aligned} \tag{4.26}$$

Set $s = p - q_1$ and let $|A|$ denote the determinant of A. The characteristic polynomial for the matrix W_{n,F_n} is

$$
\begin{aligned}
&| W_{n,F_n} - \nu I_p | \\
(4.27) \qquad &= | n^{-1/2} U_n - (\nu I_p - \bar{\Delta}(\Sigma_{F_n})) | \\
&= n^{-q_1/2} \begin{vmatrix} U_{n,11} - n^{1/2}(\nu - \bar{\lambda}_1(\Sigma_{F_n})) I_{q_1} & n^{-1/2} U_{n,12} \\ U_{n,21} & n^{-1/2} U_{n,22} - (\nu I_s - \bar{\Delta}_2(\Sigma_{F_n}) \end{vmatrix}
\end{aligned}
$$

a representation suggested by the argument in Section 7 of Anderson (1963). Thus, $| W_{n,F_n} - \nu I_p | = 0$ if any only if

$$
\begin{aligned}
(4.28) \qquad &| n^{-1/2} U_{n,22} - (\nu I_s - \bar{\Delta}_2(\Sigma_{F_n})) | \\
&\cdot | U_{n,11} - n^{1/2}(\nu - \bar{\lambda}_1(\Sigma_{F_n})) I_{q_1} - E_n(\nu) | = 0,
\end{aligned}
$$

where

$$
(4.29) \qquad E_n(\nu) = n^{-1/2} U_{n,12} [n^{-1/2} U_{n,22} - (\nu I_s - \bar{\Delta}_2(\Sigma_{F_n}))]^{-1} U_{n,21}.
$$

From Theorem 1 and the convergence of $\Gamma(\Sigma_{F_n})$ to Γ_1, it follows that

$$
(4.30) \qquad \mathscr{L}(U_n | F_n) \Rightarrow \mathscr{L}[U(F_0, \Gamma_1)],
$$

the random matrix on the right side being defined in (4.12). By Skorokhod's theorem, there exist versions of the $\{U_n\}$ and of $U(F_0, \Gamma_1)$ such that U_n converges to $U(F_0, \Gamma_1)$ with probability one. To these versions correspond versions of $\{W_{n,F_n}\}$, defined by

$$
(4.31) \qquad W_{n,F_n} = \Sigma_{F_n} + n^{-1/2} \Gamma(\Sigma_{F_n}) U_n \Gamma'(\Sigma_{F_n}),
$$

such that W_{n,F_n} converges to Σ_{F_0} with probability one and therefore $\lambda(W_{n,F_n})$ converges to $\lambda(\Sigma_{F_0})$ with probability one. For the versions of $\{U_n, W_{n,F_n}\}$, $U(F_0, \Gamma_1)$ and for $1 \le i \le q_1$

$$
(4.32) \qquad \lim_{n\to\infty} | n^{-1/2} U_{n,22} - (\lambda_i(W_{n,F_n}) I_s - \bar{\Delta}_2(\Sigma_{F_n})) | = \textstyle\prod_{j=2}^{r} [\nu_1(\Sigma_{F_0}) - \nu_j(\Sigma_{F_0})]^{q_j}
$$

with probability one, the limit on the right side being strictly positive.

Comparing (4.28) with (4.32) yields the following conclusion: with probability one, the eigenvalues in the first cluster, $\{\lambda_i(W_{n,F_n});\ 1 \le i \le q_1\}$, satisfy the equation

$$
(4.33) \qquad | U_{n,11} - E_n(\lambda_i(W_{n,F_n})) - n^{1/2}(\lambda_i(W_{n,F_n}) - \bar{\lambda}_1(\Sigma_{F_n})) I_{q_1} | = 0
$$

for all sufficiently large n. In other words, $n^{1/2}[\lambda_i(W_{n,F_n}) - \bar{\lambda}_1(\Sigma_{F_n})]$ is ultimately the ith eigenvalue of $U_{n,11} - E_n(\lambda_i(W_{n,F_n}))$, for $1 \le i \le q_1$ and n sufficiently large. From (4.29), $E_n(\lambda_i(W_{n,F_n}))$ converges to zero with probability one for the special versions of $\{U_n\}$, etc. Thus $n^{1/2}[\lambda_i(W_{n,F_n}) - \bar{\lambda}_1(\Sigma_{F_n})]$ converges with probability one to the ith eigenvalue of $U_{11}(F_0, \Gamma_1)$.

Since rows and columns may be permuted freely in the determinant defining the characteristic polynomial of W_{n,F_n}, the same argument works for the other $r - 1$ clusters of eigenvalues. Consequently,

$$
(4.34) \qquad \lim_{n\to\infty} n^{1/2}[\lambda(W_{n,F_n}) - \lambda(\bar{\Sigma}_{F_n})] = (\lambda(U_{11}(F_0, \Gamma_1)), \cdots, \lambda(U_{rr}(F_0, \Gamma_1)))
$$

with probability one, for the special versions of $\{U_n\}$, etc. The implication of

(4.34), that $J^*_{n,\lambda}(F_n) \Rightarrow \mathscr{L}(w_{F_0})$ for the original random vectors involved, contradicts the assumption made at the start of this proof. The conclusions stated as Corollary 4 follow readily now.

4.3 *Testing the positive intraclass correlation model.* Under this model, the covariance matrix of each random vector observed is

$$\Sigma_{F_0} = \sigma^2_{F_0}[(1 - \rho_{F_0})I_p + \rho_{F_0}ee'] \tag{4.35}$$

where $e = (1, 1, \cdots, 1)'$, the intraclass correlation ρ_{F_0} lies between 0 and 1, and F_0 is unknown. Since the eigenvalue matrix of Σ_{F_0} has the form

$$\Delta(\Sigma_{F_0}) = \begin{pmatrix} \nu_1(\Sigma_{F_0}) & 0 \\ 0 & \nu_2(\Sigma_{F_0})I_{p-1} \end{pmatrix} \tag{4.36}$$

with $\nu_1(\Sigma_{F_0}) > \nu_2(\Sigma_{F_0})$, any level α test for (4.36) is necessarily of level α for (4.35). The normal model likelihood ratio test for the hypothesis (4.36) rejects whenever

$$h^*(\ell_n) = -\log[\textstyle\prod_{i=2}^{p} \ell_{n,i}] + (p - 1)\log[(p - 1)^{-1} \sum_{i=2}^{p} \ell_{n,i}] \tag{4.37}$$

is too large (cf. Srivastava and Khatri, 1979, page 292). Corollary 4 applies.

Corollary 3 provides another way to bootstrap T^*_n validly, because the null hypothesis (4.35) is of the form (4.1) and the functions $\lambda_1(\Sigma)$, $\sum_{i=2}^{p} \lambda_i(\Sigma)$, $\prod_{i=1}^{p} \lambda_i(\Sigma)$ are twice continuously differentiable at $\Sigma = \Sigma_{F_0}$ (Kato, 1982). On the other hand, the test based on the statistic $h^*(\ell_n) = \log[(\ell_{n,2} + \ell_{n,p})^2] - \log[4\ell_{n,2}\ell_{n,p}]$ can be handled by Corollary 4 but not by Corollary 3 when $p \geq 4$.

EXAMPLE 2. Rao (1948) reported 4-dimensional observations on 28 cork oaks. Each observation consisted of the weights of four cork borings taken from the north, south, east, and west sides of the tree trunk. Of particular interest was the following question: does the weight, and therefore thickness, of a boring depend on the direction from which it is taken? If the data follows the one-way random effects model, this question could be addressed by analysis of variance techniques rather than by more general multivariate methods.

Under the random effects model, the covariance matrix of each observation has the form (4.35) with $p = 4$; and the smallest three eigenvalues of the covariance matrix are therefore equal. The eigenvalues of the sample covariance matrix are: 984.4, 59.8, 23.9, 18.2. A refinement of the test statistic $T^*_n = nh^*(\ell_n)$ defined by (4.37) is

$$Q_n = \{n - 1 - 6^{-1}[2(p - 1) - 1 - 2(p - 1)^{-1}]\}h^*(\ell_n) \tag{4.38}$$

(Lawley, 1956). If the null hypothesis (4.36) holds *and* the data is normal, then the asymptotic distribution of Q_n is chi-squared with $2^{-1}(p - 1)p - 1 = 5$ degrees of freedom. The observed value of Q_n is 10.5. The 5% critical value for Q_n is 11.1 according to the chi-squared approximation; and 14.3 according to the bootstrap (using 200 samples in the Monte Carlo approximation). The p-value of the observed Q_n is 6% according to the chi-squared asymptotics but 9% according to the bootstrap null distribution.

One possible explanation for the discrepancy between the two critical values is nonnormality of the data, a conclusion supported by an independent analysis in Srivastava and Hui (1983). Nonnormality invalidates the chi-squared calculation of critical values, but not the bootstrap.

Acknowledgement. We wish to thank Mr. Y. M. Chan for carrying out the bootstrap calculations in the examples and for obtaining the estimated cdf plots.

REFERENCES

ANDERSON, T. W. (1963). Asymptotic theory for principal component analysis. *Ann. Math. Statist.* **34** 122–148.

BERAN, R. (1982). Estimated sampling distributions: the bootstrap and competitors. *Ann. Statist.* **10** 212–225.

BERAN, R. (1984). Bootstrap methods in statistics. *Jber. d. Dt. Math.-Verein.* **86** 14–30.

BERAN, R. (1984). Minimum distance procedures. *Handbook of Statistics*, Vol. 4 (P. R. Krishnaiah and P. K. Sen, eds.) 741–754, Elsevier Science Publishers.

BICKEL, P. J. and FREEDMAN, D. A. (1981). Some asymptotic theory for the bootstrap. *Ann. Statist.* **9** 1196–1217.

DAVIS, A. W. (1977). Asymptotic theory for principal component analysis: nonnormal case. *Austral. J. Statist.* **19** 206–212.

DIACONIS, P. and EFRON, B. (1983). Computer-intensive methods in statistics. *Scientific American* **248** 116–130.

EFRON, B. (1979). Bootstrap methods: another look at the jackknife. *Ann. Statist.* **7** 1–26.

FREEDMAN, D. (1981). Bootstrapping regression models. *Ann. Statist.* **9** 1218–1228.

FUJIKOSHI, Y. (1980). Asymptotic expansions for the distributions of the sample roots under nonnormality. *Biometrika* **67** 45–51.

KATO, T. (1982). *A Short Introduction to Perturbation Theory for Linear Operations.* Springer, New York.

LAWLEY, D. N. (1956). Tests of significance for the latent roots of covariance and correlation matrices. *Biometrika* **43** 128–136.

MALLOWS, C. L. (1961). Latent roots of random symmetric matrices. *Biometrika* **48** 133–149.

MARDIA, K. V., KENT, J. T., and BIBBY, J. M. (1979). *Multivariate Analysis.* Academic, New York.

OKAMOTO, M. (1973). Distinctness of the eigenvalues of a quadratic form in multivariate sample. *Ann. Statist.* **1** 763–765.

RAO, C. R. (1948). Tests of significance in multivariate analysis. *Bometrika* **35** 58–79.

SINGH, K. (1981). On the asymptotic accuracy of Efron's bootstrap. *Ann. Statist.* **9** 1187–1195.

SRIVASTAVA, M. S. (1983). On the likelihood ratio tests for the covariance structure in familial data and in principal components analysis. Unpublished.

SRIVASTAVA, M. S. and HUI, T. K. (1983). Multivariate generalization of Shapiro-Wilk and Vasicek's statistics for testing multivariate normality. Unpublished.

SRIVASTAVA, M. S. and KHATRI, C. G. (1979). *An Introduction to Multivariate Statistics.* North Holland, New York.

DEPARTMENT OF STATISTICS
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720

DEPARTMENT OF STATISTICS
UNIVERSITY OF TORONTO
TORONTO M5S 1A1
CANADA