# INFERENCE IN MULTIVARIATE NORMAL POPULATIONS WITH STRUCTURE
## PART 2: INFERENCE WHEN CORRELATIONS HAVE STRUCTURE

by

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## PREFACE

This report extends the results of Styan (1968) to the situation where the correlations are all equal but unknown (Section III). In Section IV we extend the results of Anderson (1966, 1968) to the case where the correlation matrix, or its inverse, can be expressed as an unknown linear combination of given matrices. We assume that the variances and mean vectors are unspecified.

Most of the literature dealing with structure for the correlation matrix where the mean vectors and variances are unspecified is recent. Bartlett & Rajalakshman (1953), Bartlett (1954), Kullback (1959), p. 304, and Kullback (1967) gave criteria for testing the hypothesis of a given correlation matrix. Anderson (1963), Lawley (1963), and Gleser (1968) considered testing all correlations equal while Kullback (1959), p. 320, Kullback (1967), and Cole (1968) presented tests for homogeneity of correlation matrices. A general discussion, summary, and some new results are given by Olkin (1967) and Aitkin, Nelson, & Reinfurt (1968). In a factor analysis context, Jöreskog (1963) simplified the estimation problem, replacing the diagonal elements in the inverse of the correlation matrix by ones. Olkin (1967) and Corsten (1968) tested equality of two correlation coefficients in a trivariate population. Votaw (1948), Halperin (1951), Olkin & Pratt (1958), and Hájek (1962) examined the case of equal variances and correlations in regression problems (cf. also Selliah (1964) and Olkin (1967) for this case with unspecified mean vectors). Han (1967, 1968) tested all variances equal given homogeneity of the correlation coefficients. Patterned correlation matrices arising in econometrics are studied by Goldberger (1964). Additional references on these and related topics will be found in Anderson, Das Gupta, & Styan (ca. 1970).

In Section III we find closed-form expressions for the maximum likelihood equations for the variances and common correlation coefficient. Again as in Section II [Styan (1968)] these cannot be solved analytically in general, and we inquire about uniqueness of the solution. We fail to prove uniqueness in all cases but study in detail the matrix $\underset{\sim}{H}$ of second derivatives of $\ell$, a decreasing linear function of the log-likelihood. Using the arithmetic mean/geometric mean and Cauchy-Schwarz inequalities we obtain various tight bounds on the solutions of the maximum likelihood equations. These bounds are tabulated extensively and some are sketched. We apply these bounds to a criterion obtained from the Marshall and Olkin (1964) strengthened form of the Kantorovich inequality. When positive the criterion implies positive definiteness of the second derivative matrix, $\underset{\sim}{H}$. As a consequence we show positive definiteness for a wide range of values of $\hat{\rho}$, the maximum likelihood estimate of the common correlation coefficient. Given $\hat{\rho}$, it follows from Section II [Styan (1968)] that the solutions for the variance estimates are uniquely determined. We also study the case where all sample correlations have the same sign and obtain other bounds.

In the case of three dimensions, uniqueness of the solution is established. Using a new algorithm developed from the Newton-Raphson process by Brown (1966), we generated and solved 7035 sets of maximum likelihood equations in 3 minutes central processor time on the CDC 6600 computer. This suggested a surprising inequality between $\hat{\rho}$ and $r$, the average sample correlation coefficient, which we prove using an interesting inequality based on the difference between the differences in the Cauchy-Schwarz and arithmetic mean/geometric mean inequalities. Representative values of the solutions for the 7035 sets were compared against the theoretical bounds, and the latter were found to be rather tight. We evaluate the asymptotic efficiencies of the sample estimates and find the average sample correlation coefficient fully efficient; the efficiency of the variances equals that of the modified estimator found in Section II [Styan (1968)]. We conclude Section III with the case where the variances are known, and so only a single parameter is to be estimated. The resulting maximum likelihood equation is a cubic. We extend the result for the two-dimensional case by Kendall & Stuart (1967) to prove that as the sample size increases, the probability that there is only one real solution and this lies in the desired interval tends to one.

In Section IV we consider the case where either the correlation matrix or its inverse is expressed as an unknown linear combination of given matrices. The nonlinear maximum likelihood equations are more complicated than those in the previous sections but again are obtained in closed form. When the inverse correlation matrix has this so-called linear structure, we find that both the principal diagonal submatrices of the second derivative matrix are positive definite. We are, however, unable to establish positive definiteness of the whole matrix which would lead to uniqueness of solution.

The notation used is the same as that in Styan (1968). Vectors are denoted by lower case letters, matrices by capital letters, and both have wavy underlining to denote bold face print. Transposition is indicated by a prime, with row vectors always appearing primed [cf. Halperin (1965)]. The generating element of a vector or matrix is given in curly brackets. When $\underset{\sim}{A}$ is a square matrix, tr $\underset{\sim}{A}$ denotes its trace, $|\underset{\sim}{A}|$ its determinant, and $ch_j\underset{\sim}{A}$ its j-th characteristic root.

The diagonal matrix formed from $\underset{\sim}{A}$ is denoted $\underset{\sim}{A}_{dg} = (a_{11}, a_{22}, \ldots, a_{pp})_{dg}$. We use $\underset{\sim}{I}$ for the identity matrix, $\underset{\sim}{e}$ for the column vector with each component unity, and $\underset{\sim}{e}_j$ for the column vector with each element zero except for the $j$-th which is unity [cf. Bodewig (1959)]. Matrix differentiation techniques follow Dwyer (1967).

As far as convenient, an estimate of a parameter is indicated by the Latin letter corresponding to the Greek letter for the parameter, and the matrix analogue of a scalar quantity is denoted by the capital letter corresponding to the lower case letter for the scalar. An exception is the scalar parameter $\rho$ (rho) which we use for correlation coefficient. We indicate the population correlation matrix by $\underset{\sim}{R}$ instead of $\underset{\sim}{P}$ (capital rho). Another exception is the population covariance matrix which we denote by $\underset{\sim}{\Sigma}$, reserving $\Sigma$ for summation. The sample analogue of $\underset{\sim}{\Sigma}$ is indicated by $\underset{\sim}{C} = \underset{\sim}{X}'\underset{\sim}{C}_e\underset{\sim}{X}/N$, where $\underset{\sim}{X}' = (\underset{\sim}{x}_1, \ldots, \underset{\sim}{x}_N)$ is the $p \times N$ matrix of observations and $\underset{\sim}{C}_e = \underset{\sim}{I} - \underset{\sim}{e}\underset{\sim}{e}'/p$ is the centering matrix of order $p$ [cf. Sharpe & Styan (1965)].

If $\underset{\sim}{x}$ is a random vector, $E(\underset{\sim}{x})$ denotes its expected value and $V(\underset{\sim}{x})$ its covariance matrix. If $\underset{\sim}{y}$ is another random vector, the covariance matrix between $\underset{\sim}{x}$ and $\underset{\sim}{y}$, $E(\underset{\sim}{x}\underset{\sim}{y}') - E(\underset{\sim}{x})E(\underset{\sim}{y}')$, is denoted $\text{cov}(\underset{\sim}{x}, \underset{\sim}{y})$. $L$ is the joint likelihood and $\ell$ is a decreasing linear function of $\log L$ [cf. (2.1.8) in Styan (1968)]. The end of a proof is indicated by (qed). The symbol § denotes section number and cf. means compare or see, while ca. stands for circa or about.

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## III. INFERENCE WHEN THE CORRELATIONS ARE EQUAL BUT UNKNOWN

### 3.1 Maximum Likelihood Estimates.

The problem we now consider is the same as that described in §2.1 but with

$$(3.1.1) \qquad \underset{\sim}{R} = (1-\rho)\underset{\sim}{I} + \rho\underset{\sim}{e}\underset{\sim}{e}',$$

where $\rho$ is unknown. We will use the same notation and many of the results derived in Section II of Styan (1968).

We will estimate the unknown variances and unknown common correlation coefficient by the method of maximum likelihood. We study the problem in terms of

$$(3.1.2) \qquad \underset{\sim}{\lambda} = \underset{\sim}{D}\underset{\sim}{\sigma}^{(-1)},$$

where, as in (2.3.12)*, the elements of $\underset{\sim}{\lambda}$ are ratios of sample to population standard deviations. Following §2.1, and using (2.3.4) and (2.7.1), maximizing the likelihood is equivalent to minimizing

$$(3.1.3) \qquad \ell = \underset{\sim}{\lambda}'(\underset{\sim}{R}^{-1}*\underset{\sim}{R})\underset{\sim}{\lambda} - 2\underset{\sim}{e}'\underset{\sim}{\lambda}^{(\ell)} + \log|\underset{\sim}{R}| + 2\log|\underset{\sim}{D}|,$$

which we achieve by differentiation with respect to $\underset{\sim}{\lambda}$ and $\rho$. $\underset{\sim}{R}$ is the sample correlation matrix. Differentiating (3.1.3) with respect to $\underset{\sim}{\lambda}$ gives

$$(3.1.4) \qquad \frac{\partial\ell}{\partial\underset{\sim}{\lambda}} = 2[(\underset{\sim}{R}^{-1}*\underset{\sim}{R})\underset{\sim}{\lambda} - \underset{\sim}{\lambda}^{(-1)}],$$

similar to (2.3.6). As in (2.9.2), we have that

$$(3.1.5) \qquad \underset{\sim}{R}^{-1} = \frac{1}{1-\rho}\left[\underset{\sim}{I} - \frac{\rho}{1+\rho(p-1)}\underset{\sim}{e}\underset{\sim}{e}'\right], \quad -\frac{1}{p-1} < \rho < 1.$$

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*Equations, theorems, etc. with leading symbol 2 or A are in Styan (1968).

To ease the notation we will write

$$(3.1.6) \qquad q = p - 1,$$

and as in (2.9.10),

$$(3.1.7) \qquad \alpha = (1-\rho)(1+\rho[p-1]) = 1 + \rho(p-2) - \rho^2(p-1)$$
$$= (1-\rho)(1+\rho q) = 1 + \rho(q-1) - \rho^2 q.$$

Thus

$$(3.1.8) \qquad \underset{\sim}{R}^{-1} * \underset{\sim}{R} = \frac{1}{1-\rho}\, \underset{\sim}{I} - \frac{\rho}{\alpha}\, \underset{\sim}{R},$$

which differentiated with respect to $\rho$ yields

$$(3.1.9) \qquad \frac{\partial}{\partial\rho}(\underset{\sim}{R}^{-1} * \underset{\sim}{R}) = \frac{1}{(1-\rho)^2}\, \underset{\sim}{I} - \frac{1+\rho^2 q}{\alpha^2}\, \underset{\sim}{R}.$$

Since $|\underset{\sim}{R}| = (1-\rho)^q(1+\rho q)$, we may write the part of $\ell$ involving $\rho$ as

$$(3.1.10) \qquad \ell_\rho = \underset{\sim}{\lambda}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R})\underset{\sim}{\lambda} + q \log (1-\rho) + \log (1+\rho q)$$

so that

$$(3.1.11) \qquad \frac{\partial \ell}{\partial \rho} = \frac{\underset{\sim}{\lambda}'\underset{\sim}{\lambda}}{(1-\rho)^2} - \frac{1+\rho^2 q}{\alpha^2}\, \underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda} - \frac{\rho p q}{\alpha}.$$

Setting (3.1.4) and (3.1.11) equal to zero yields the following:

THEOREM 3.1.1. <u>The maximum likelihood equations for the variances and common correlation coefficient in a</u> p-<u>dimensional normal population are</u>

$$(3.1.12) \qquad (\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R})\hat{\underset{\sim}{\lambda}} = \frac{1}{1-\hat{\rho}}\, \hat{\underset{\sim}{\lambda}} - \frac{\hat{\rho}}{\hat{\alpha}}\, \underset{\sim}{R}\hat{\underset{\sim}{\lambda}} = \hat{\underset{\sim}{\lambda}}^{(-1)}$$

and

$$(3.1.13)\qquad (1+\hat{\rho}q)^2\hat{\lambda}'\hat{\lambda} - (1+\hat{\rho}^2q)\hat{\lambda}'R\hat{\lambda} = \hat{\alpha}\hat{\rho}pq.$$

$\hat{R}$ and $R$ are the maximum likelihood estimate and sample correlation matrices, $\hat{\lambda}^{(-1)}$ is the Hadamard inverse of $\hat{\lambda}$ which contains ratios of sample to maximum likelihood estimate standard deviations, and $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$, where $\hat{\rho}$ is the maximum likelihood estimate correlation coefficient and $q = p-1$.

Equation (3.1.12) is the same as (2.9.4) except that we have replaced $\rho$ with $\hat{\rho}$. Equation (3.1.13) is new and may not hold in §2.9 with $\rho$ instead of $\hat{\rho}$.

Premultiplying (3.1.12) by $\hat{\alpha}(1+\hat{\rho}q)\hat{\lambda}'$ and subtracting (3.1.13) leads to

$$(3.1.14)\qquad \hat{\lambda}'R\hat{\lambda} = p(1+\hat{\rho}q).$$

Substituting this in (3.1.13) gives

$$(3.1.15)\qquad \hat{\lambda}'\hat{\lambda} = p,$$

which substituted in (3.1.14) yields

$$(3.1.16)\qquad \hat{\rho} = \frac{1}{pq}\,\hat{\lambda}'(R-I)\hat{\lambda}.$$

If $\hat{\lambda} = e$, then $\hat{\rho}$ would be $r$, the average sample correlation coefficient.

Aitkin, Nelson, & Reinfurt (1968) independently obtained (3.1.12) through (3.1.16) in scalar notation; Han (1967) gave (3.1.12) and (3.1.13) only. As observed by these writers, (3.1.12) through (3.1.16) cannot in general be solved analytically (cf. §2.3). When $R$ has constant row sums, however, a closed form solution is immediate. This occurs if and only if $\tilde{R}^{-1}*\tilde{R}$ has constant row sums. Unless $p = 2$ this is possible only with probability zero. We obtain, as in (2.3.14),

$$(3.1.17) \qquad (\hat{\tilde{R}}^{-1}*\tilde{R})\tilde{e} = \mu^2\tilde{e},$$

say, and $\hat{\tilde{\lambda}}^{(-1)} = \mu\tilde{e}$. Since $\hat{\tilde{\lambda}}'\hat{\tilde{\lambda}} = p$, we have $\mu^2 = 1$. Thus $\hat{\tilde{\lambda}} = \tilde{e}$ and $\hat{\rho} = r$. Also $\tilde{R}\tilde{e} = (1+rq)\tilde{e}$, so that the average of the correlation coefficients in any row of $\tilde{R}$ is also $r$. When $p = 2$, the sample covariance matrix $\tilde{C} = \hat{\tilde{\Sigma}}$ and (3.1.17) is always true.

If $\hat{\rho} = 0$, then from (3.1.12), $\hat{\tilde{\lambda}} = \hat{\tilde{\lambda}}^{(-1)}$. Since $\hat{\tilde{\lambda}}'\hat{\tilde{\lambda}} = p$, we obtain $\hat{\tilde{\lambda}} = \tilde{e}$. From (3.1.16), $\tilde{e}'(\tilde{R}-\tilde{I})\tilde{e} = 0$, so that $r = 0$. In this case, however, we do not necessarily have $(\tilde{R}-\tilde{I})\tilde{e} = \tilde{0}$. We will study later whether $r = 0$ always implies $\hat{\rho} = 0$.

We now show that (3.1.12) and (3.1.13) have at least one solution. We will study later the question of whether there is only one.

LEMMA 3.1.1. <u>For any positive definite correlation matrix</u> $\tilde{R}$ <u>of order</u> $p$ <u>and any</u> $p \times 1$ <u>vector</u> $\tilde{u}$,

$$(3.1.18) \qquad \tilde{u}'\tilde{R}\tilde{u} < p\tilde{u}'\tilde{u}.$$

<u>Proof</u>. By definition $\tilde{u}'\tilde{R}\tilde{u}/\tilde{u}'\tilde{u} \leq ch_1(\tilde{R})$, the largest characteristic root of $\tilde{R}$. Since $\mathrm{tr}\,\tilde{R} = p$ and $\tilde{R}$ is positive definite, $ch_1(\tilde{R}) < p$. Hence the result. We note that if $\tilde{R}$ is positive semi-definite equality occurs in (3.1.18) when $\tilde{R} = \tilde{v}\tilde{v}'$, where $\tilde{v}'\tilde{v} = ch_1(\tilde{R}) = p$, $\tilde{v}$ is proportional to $\tilde{u}$, and has each component plus or minus one. (qed)

THEOREM 3.1.2. <u>The maximum likelihood equations in Theorem 3.1.1 admit at least one real solution which is consistent.</u>

Proof. Using Theorem 2.3.2 it suffices to show that $\ell_\rho \to +\infty$ when $\rho \to -1/q$ or when $\rho \to 1$. Apart from terms which remain finite as $\rho \to -1/q$, we have from (3.1.8) and (3.1.10) that $\ell_\rho$ is

$$(3.1.19) \qquad \underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda}/p(1+\rho q) + \log (1+\rho q) = \log (e^{k\theta}/\theta),$$

where $k = \underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda}/p > 0$ and $\theta = 1/(1+\rho q)$. Thus $\ell_\rho \to +\infty$ as $\theta \to +\infty$. When $\rho \to 1$ we find the corresponding expression for $\ell_\rho$ to be

$$(3.1.20) \qquad \frac{\underset{\sim}{\lambda}'\underset{\sim}{\lambda}}{1-\rho} [1 - \frac{\underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda}}{p\underset{\sim}{\lambda}'\underset{\sim}{\lambda}}] + q \log (1-\rho) = \log (e^{k\theta}/\theta^q),$$

where now $k = \underset{\sim}{\lambda}'\underset{\sim}{\lambda}(1-\underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda}/p\underset{\sim}{\lambda}'\underset{\sim}{\lambda}) > 0$ from Lemma 3.1.1, and $\theta = 1/(1-\rho)$. Thus $\ell_\rho \to +\infty$ as $\theta \to +\infty$, as before. Consistency follows from Chanda (1954). (qed)

We examine the range for any $\hat{\rho}$ which satisfies (3.1.12) and (3.1.13).

THEOREM 3.1.3. For any solution $\hat{\rho}$ to the maximum likelihood equations in Theorem 3.1.1,

$$(3.1.21) \qquad -\frac{1}{q} < \frac{1}{q} \, ch_p(\underset{\sim}{R}-\underset{\sim}{I}) \leq \hat{\rho} \leq \frac{1}{q} \, ch_1(\underset{\sim}{R}-\underset{\sim}{I}) < 1$$

and $\hat{\underset{\sim}{R}}$ positive definite, where $q = p-1$.

Proof. By definition of characteristic root (cf. Rao (1965), p. 50), we have from (3.1.14) and (3.1.15) that $0 < ch_p(\underset{\sim}{R}) \leq \hat{\underset{\sim}{\lambda}}'\underset{\sim}{R}\hat{\underset{\sim}{\lambda}}/\hat{\underset{\sim}{\lambda}}'\hat{\underset{\sim}{\lambda}} = 1 + \hat{\rho}q \leq ch_1(\underset{\sim}{R}) < p$, using positive definiteness of $\underset{\sim}{R}$ and Lemma 3.1.1. Subtracting $\underset{\sim}{I}$ or 1 throughout and dividing by $q$ gives (3.1.21). Since $\hat{\underset{\sim}{R}}$ has roots $1 - \hat{\rho}$ and $1 + \hat{\rho}q$ it is positive definite. (qed)

It follows from a result of Brauer and Perron (cf. Marcus & Minc (1964), p. 145), that for any positive definite matrix $\underset{\sim}{A}$ of order p, $ch_1(\underset{\sim}{A}) \leq \max_i \sum_{j=1}^{p} |a_{ij}|$. Applying this to (3.1.21) yields

$$(3.1.22) \qquad -\frac{1}{q} \min\left(1, \max_i \sum_{\substack{j=1 \\ j\neq i}}^{p} |r_{ij}|\right) < \hat{\rho} < \max_i \frac{1}{q} \sum_{\substack{j=1 \\ j\neq i}}^{p} |r_{ij}|.$$

We have given bounds for $\hat{\rho}$. In §3.3 we will give bounds for $\hat{\lambda}_i^2$; $i = 1,\ldots, p$, in terms of $\hat{\rho}$ and in §3.4 we will present tables and charts for special cases.

It follows then from Theorem 2.3.2 that for any value $\hat{\rho}$ satisfying (3.1.12) and (3.1.13), the corresponding values for $\underset{\sim}{\hat{\lambda}}$ (and so $\underset{\sim}{\hat{\sigma}}^{(2)}$) are uniquely determined. We will study later the question of uniqueness of $\hat{\rho}$; if there is more than one value of $\hat{\rho}$ we take that which provides the absolute minimum of (3.1.3). We thus take the solution minimizing

$$(3.1.23) \qquad q \log(1-\hat{\rho}) + \log(1+\hat{\rho}q) - 2\underset{\sim}{e}'\underset{\sim}{\hat{\lambda}}^{(\ell)}.$$

Equations (3.1.12) and (3.1.13) admit a consistent solution since regularity conditions I-IV of §2.3 are satisfied [cf. Chanda (1954)] and so the usual asymptotic theory applies.

THEOREM 3.1.4. <u>The limiting distribution of</u> $\sqrt{N}\,(\underset{\sim}{\hat{\sigma}}^{(2)'} - \underset{\sim}{\sigma}^{(2)'}, \hat{\rho}-\rho)$ <u>is multivariate normal with mean</u> $\underset{\sim}{0}'$ <u>and covariance matrix</u>

$$(3.1.24) \qquad 2\begin{pmatrix} \underset{\sim}{\Delta}^2\left(\frac{2\alpha}{2\alpha+p\rho^2}\underset{\sim}{I} + \rho^2\underset{\sim}{e}\underset{\sim}{e}'\left[\frac{1}{2\alpha+p\rho^2} + \frac{q}{p}\right]\right)\underset{\sim}{\Delta}^2, & (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)} \\ (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)'}, & \alpha^2/pq \end{pmatrix}.$$

**Proof.** It suffices to establish (3.1.24). From (2.3.19) we see that the covariance matrix in question is the inverse of

$$(3.1.25)\qquad \tfrac{1}{2}E\left(\frac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\gamma} \partial \underset{\sim}{\gamma}'}\right),$$

where $\underset{\sim}{\gamma}' = (\underset{\sim}{\sigma}^{(2)'}, \rho)$ and $\ell_\mu$ is as given by (2.3.20). We first show that

$$(3.1.26)\qquad E\left(\frac{\partial \ell_\mu}{\partial \underset{\sim}{\gamma}}\right) = \underset{\sim}{0}.$$

From (3.1.11)

$$(3.1.27)\qquad \frac{\partial \ell_\mu}{\partial \rho} = \frac{\underset{\sim}{\sigma}^{(-1)'} \underset{\sim}{D}_\mu^2 \underset{\sim}{\sigma}^{(-1)}}{(1-\rho)^2} - \frac{(1+\rho^2 q)}{\alpha^2}\, \underset{\sim}{\sigma}^{(-1)'} \underset{\sim}{C}_\mu \underset{\sim}{\sigma}^{(-1)} - \frac{\rho p q}{\alpha},$$

where $\underset{\sim}{C}_\mu = \underset{\sim}{D}_\mu \underset{\sim}{R}_\mu \underset{\sim}{D}_\mu$ as in (2.1.6). Since $E(\underset{\sim}{C}_\mu) = \underset{\sim}{\Delta R \Delta}$, we obtain

$$(3.1.28)\qquad E\left(\frac{\partial \ell_\mu}{\partial \rho}\right) = \frac{p}{(1-\rho)^2} - \frac{p(1+\rho^2 q)}{\alpha(1-\rho)} - \frac{\rho p q}{\alpha} = 0.$$

Combining (3.1.28) with (2.3.24) establishes (3.1.26).

As in (2.3.25), we may therefore write

$$(3.1.29)\qquad E\left(\frac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\gamma} \partial \underset{\sim}{\gamma}'}\right) = E\begin{bmatrix} \dfrac{\partial \underset{\sim}{\lambda}_\mu}{\partial \underset{\sim}{\sigma}^{(2)'}}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{bmatrix} \begin{bmatrix} \dfrac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\lambda}_\mu \partial \underset{\sim}{\lambda}_\mu'}, & \dfrac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\lambda}_\mu \partial \rho} \\ \dfrac{\partial^2 \ell_\mu}{\partial \rho\, \partial \underset{\sim}{\lambda}_\mu'}, & \dfrac{\partial^2 \ell_\mu}{\partial \rho^2} \end{bmatrix} \begin{bmatrix} \dfrac{\partial \underset{\sim}{\lambda}_\mu}{\partial \underset{\sim}{\sigma}^{(2)'}}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{bmatrix}$$

where $\underset{\sim}{\lambda}_\mu = \underset{\sim}{D}_\mu \underset{\sim}{\Delta}^{-1}$. Substituting $\partial \underset{\sim}{\lambda}_\mu / \partial \underset{\sim}{\sigma}^{(2)'} = -\tfrac{1}{2} \underset{\sim}{\Lambda}_\mu \underset{\sim}{\Delta}^{-2}$, where $\underset{\sim}{\Lambda}_\mu$ is the diagonal matrix formed from $\underset{\sim}{\lambda}_\mu$, (3.1.29) becomes

$$(3.1.30)\qquad E\left(\frac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\gamma} \partial \underset{\sim}{\gamma}'}\right) = \begin{pmatrix} -\tfrac{1}{2}\underset{\sim}{\Delta}^{-2}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{pmatrix} E\begin{bmatrix} \underset{\sim}{\Lambda}_\mu \dfrac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\lambda}_\mu \partial \underset{\sim}{\lambda}_\mu'} \underset{\sim}{\Lambda}_\mu, & \underset{\sim}{\Lambda}_\mu \dfrac{\partial^2 \ell_\mu}{\partial \underset{\sim}{\lambda}_\mu \partial \rho} \\ \dfrac{\partial^2 \ell_\mu}{\partial \rho\, \partial \underset{\sim}{\lambda}_\mu'} \underset{\sim}{\Lambda}_\mu, & \dfrac{\partial^2 \ell_\mu}{\partial \rho^2} \end{bmatrix} \begin{pmatrix} -\tfrac{1}{2}\underset{\sim}{\Delta}^{-2}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{pmatrix}.$$

From (3.1.4) we find that

$$(3.1.31)\qquad \frac{\partial^2 \ell}{\partial \underset{\sim}{\lambda} \partial \underset{\sim}{\lambda}'} = 2(\underset{\sim}{R}^{-1} * \underset{\sim}{R} + \underset{\sim}{\Lambda}^{-2}),$$

similar to (2.3.18). Using (3.1.9), we have further that

$$(3.1.32)\qquad \frac{\partial^2 \ell}{\partial \underset{\sim}{\lambda} \partial \rho} = 2[\frac{1}{(1-\rho)^2} \underset{\sim}{I} - \frac{1+\rho^2 q}{\alpha^2} \underset{\sim}{R}]\underset{\sim}{\lambda}.$$

Finally from (3.1.11) we obtain

$$(3.1.33)\qquad \frac{\partial^2 \ell}{\partial \rho^2} = \frac{2\underset{\sim}{\lambda}'\underset{\sim}{\lambda}}{(1-\rho)^3} + \frac{2}{\alpha^3}(q-1-3\rho q-\rho^3 q^2)\underset{\sim}{\lambda}'\underset{\sim}{R}\underset{\sim}{\lambda} - \frac{pq(1+\rho^2 q)}{\alpha^2} .$$

Hence

$$(3.1.34)\qquad E(\frac{\partial^2 \ell}{\partial \underset{\sim}{\gamma} \partial \underset{\sim}{\gamma}'}\mu) = \begin{pmatrix} \underset{\sim}{\Lambda}^{-2}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{pmatrix} \underset{\sim}{G} \begin{pmatrix} \underset{\sim}{\Lambda}^{-2}, & \underset{\sim}{0} \\ \underset{\sim}{0}', & 1 \end{pmatrix}$$

where

$$(3.1.35)\qquad \underset{\sim}{G} = \begin{pmatrix} \frac{1}{2}(\underset{\sim}{R}^{-1} * \underset{\sim}{R} + \underset{\sim}{I}), & -\rho q\underset{\sim}{e}/\alpha \\ -\rho q\underset{\sim}{e}'/\alpha, & pq(1+\rho^2 q)/\alpha^2 \end{pmatrix} .$$

We can invert (3.1.34) provided $\underset{\sim}{G}$ is nonsingular. We evaluate $|\underset{\sim}{G}|$ and then $\underset{\sim}{G}^{-1}$ by the so-called Frobenius-Schur method (cf. Bodewig (1959), p. 217 and Rao (1965), pp. 28-29). From Table 2.9.1 we recall that

$$(3.1.36)\qquad 2(\underset{\sim}{R}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})^{-1} = \frac{2\alpha}{2\alpha + p\rho^2}(\underset{\sim}{I} + \frac{\rho^2}{2\alpha}\underset{\sim}{e}\underset{\sim}{e}'),$$

so that $pq(1+\rho^2 q) - 2\rho^2 q^2 \underset{\sim}{e}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})^{-1}\underset{\sim}{e} = pq$. Hence $|\underset{\sim}{G}| = |\frac{1}{2}(\underset{\sim}{R}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})|pq/\alpha^2 > 0$ so that $\underset{\sim}{G}$ is nonsingular. The element in the bottom right-hand corner of $\underset{\sim}{G}^{-1}$ is therefore $\alpha^2/pq$. Above it we have

$$(3.1.37) \qquad -\frac{2\alpha}{2\alpha+p\rho^2}(\underset{\sim}{I} + \frac{\rho^2}{2\alpha}\underset{\sim}{ee}')(-\rho q/\alpha)(\alpha^2/pq)\underset{\sim}{e} = \alpha\rho\underset{\sim}{e}/p.$$

Thus the upper left-hand corner of $\underset{\sim}{G}^{-1}$ is

$$(3.1.38) \qquad \frac{2\alpha}{2\alpha+p\rho^2}(\underset{\sim}{I} + \frac{\rho^2}{2\alpha}\underset{\sim}{ee}') + (\alpha\rho/p)(pq/\alpha^2)(\alpha\rho/p)\underset{\sim}{ee}'$$

$$= \frac{2\alpha}{2\alpha+p\rho^2}\underset{\sim}{I} + \rho^2\underset{\sim}{ee}'(\frac{1}{2\alpha+p\rho^2} + \frac{q}{p}).$$

Hence

$$(3.1.39) \left[\tfrac{1}{2}E(\frac{\partial^2 \ell}{\partial\underset{\sim}{\gamma}\partial\underset{\sim}{\gamma}'}\mu)\right]^{-1} = 2\begin{pmatrix}\underset{\sim}{\Delta}^2, & \underset{\sim}{0}\\ \underset{\sim}{0}', & 1\end{pmatrix}\begin{bmatrix}\frac{2\alpha}{2\alpha+p\rho^2}\underset{\sim}{I} + \rho^2\underset{\sim}{ee}'(\frac{1}{2\alpha+p\rho^2} + \frac{q}{p}), & \alpha\rho\underset{\sim}{e}/p\\ \alpha\rho\underset{\sim}{e}'/p, & \alpha^2/pq\end{bmatrix}\begin{pmatrix}\underset{\sim}{\Delta}^2, & \underset{\sim}{0}\\ \underset{\sim}{0}', & 1\end{pmatrix}$$

which is (3.1.24). (qed)

### 3.2 Matrix of Second Derivatives at Solutions of the Maximum Likelihood Equations.

We now study the question of uniqueness of solution of the maximum likelihood equations by examining the matrix of second derivatives of $\ell$ given by (3.1.31) through (3.1.33), when its elements satisfy (3.1.12) and (3.1.13).

If the solution maximizes the likelihood, then the matrix

$$(3.2.1) \qquad \begin{bmatrix}\frac{\partial^2\ell}{\partial\underset{\sim}{\lambda}\partial\underset{\sim}{\lambda}'}, & \frac{\partial^2\ell}{\partial\underset{\sim}{\lambda}\partial\rho}\\ \frac{\partial^2\ell}{\partial\rho\partial\underset{\sim}{\lambda}'}, & \frac{\partial^2\ell}{\partial\rho^2}\end{bmatrix}_{\underset{\sim}{\lambda}=\hat{\underset{\sim}{\lambda}},\ \rho=\hat{\rho}} = \underset{\sim}{H},$$

say, is positive definite. If this is so <u>whenever</u> (3.1.12) and (3.1.13) are satisfied, then the solution must be unique, using Theorem 3.1.2

(cf. Theorem 2.3.2). For if $\ell$ has two (or more) relative minima then it must have at least one relative maximum, which would make $\underset{\sim}{H}$ negative definite.

Since the regularity conditions I-IV of Section 2.3 are satisfied here, it follows from Chanda (1954) that the second derivative matrix $\underset{\sim}{H}$, evaluated at a consistent solution, will be positive definite with probability tending to unity as the sample size N approaches infinity.

It seems, however, that $\underset{\sim}{H}$ may be positive definite for any fixed sample size in parallel to our result in Section II. This would lead to the much more powerful conclusion that the likelihood equations admit a unique solution, even for small samples. It follows from Theorem 2.3.2 that for a particular solution $\hat{\rho}$ the corresponding value of $\underset{\sim}{\hat{\sigma}}^{(2)}$ is uniquely determined.

In his doctoral dissertation, Han (1967) extensively studied the maximum likelihood estimation problem when the correlations are all equal but unknown, and the variances are unspecified. He did not, however, examine the question of uniqueness of solution but concentrated on solving the likelihood equations by the Newton-Raphson process. He obtained in closed form an estimate for the variances which is asymptotically normal and efficient. We consider this in Section 3.5.

We now study in detail the question of positive definiteness of the second derivative matrix $\underset{\sim}{H}$ in (3.2.1) for fixed sample size N. Two different versions arise according as $\hat{\rho} = 0$ ($\underset{\sim}{H}_0$, say) or $\hat{\rho} \neq 0$ ($\underset{\sim}{H}_1$, say). We easily establish $\underset{\sim}{H}_0$ positive definite but have difficulty in finding the same result for $\underset{\sim}{H}_1$. We show, however, that $\underset{\sim}{H}_1$ is positive definite for a wide range of values of positive $\hat{\rho}$ and arbitrary $p \geq 4$ and in all cases when $p = 3$ (cf. §3.4.3).

3.2.1 Case of $\hat{\rho} = 0$.

When $\hat{\rho} = 0$ we found in §3.1 that $\hat{\lambda} = e$ and $e'(R-I)e = 0$. This solution maximizes the likelihood when from (3.1.31) through (3.1.33),

$$(3.2.2) \qquad H_o = \begin{bmatrix} 4I, & 2(I-R)e \\ 2e'(I-R), & pq \end{bmatrix}$$

is positive definite.

It suffices to show $|H_o| > 0$. Using the Frobenius-Schur method, we obtain

$$(3.2.3) \qquad \begin{aligned} |H_o| &= 2^{2p}(pq - e'(I-R)^2 e) \\ &= 2^{2p}(p^2 - e'R^2 e) > 2^{2p}(p^2 - pe'Re) = 0, \end{aligned}$$

from Lemma 3.1.1 with $u = R^{\frac{1}{2}}e$, since $e'Re = p$. Hence the solution $\hat{\rho} = 0$, $\hat{\lambda} = e$ maximizes the likelihood.

We note that $e'(R-I)e = 0$ does not necessarily imply that $(R-I)e = 0$.

3.2.2 Case of $\hat{\rho} \neq 0$.

When $\hat{\rho} \neq 0$, we obtain from (3.1.12) that

$$(3.2.4) \qquad R\hat{\lambda} = \frac{1+\hat{\rho}q}{\hat{\rho}} [\hat{\lambda} - (1-\hat{\rho})\hat{\lambda}^{(-1)}].$$

Substituting this in (3.1.32), and (3.1.14) and (3.1.15) in (3.1.33), and using (3.1.31) gives

$$(3.2.5) \qquad \underset{\sim}{H}_1 = \begin{bmatrix} 2(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2}), & \frac{2}{\hat{\alpha}\hat{\rho}}[(1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)} - \hat{\underset{\sim}{\lambda}}] \\ \frac{2}{\hat{\alpha}\hat{\rho}}[(1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)} - \hat{\underset{\sim}{\lambda}}]', & pq(1+\hat{\rho}^2 q)/\hat{\alpha}^2 \end{bmatrix}.$$

From Theorems 2.3.2, 3.1.3, and A.2.1, it follows that the leading $p \times p$ submatrix of $\underset{\sim}{H}_1$ is positive definite. Thus for any particular solution $\hat{\rho}$, the vector $\hat{\underset{\sim}{\lambda}}$ (and hence $\hat{\underset{\sim}{\sigma}}^{(2)} = \underset{\sim}{D}^2 \hat{\underset{\sim}{\lambda}}^{(-2)}$) is uniquely determined. To show that only one value is possible for $\hat{\rho}$ (given $\underset{\sim}{R}$ and $\underset{\sim}{D}$), it suffices to show that the determinant of (3.2.5) is positive. We have

$$(3.2.6) \qquad |\underset{\sim}{H}_1| = \frac{2^{2p}}{\hat{\rho}^2\hat{\alpha}^2} \begin{vmatrix} \frac{1}{2}(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2}), & \hat{\underset{\sim}{\lambda}} - (1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)} \\ \hat{\underset{\sim}{\lambda}}' - (1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)'}, & pq\hat{\rho}^2(1+\hat{\rho}^2 q) \end{vmatrix}.$$

We have not been able to prove that (3.2.6) is positive in general. Before considering special cases, we have the following:

THEOREM 3.2.1. <u>A necessary and sufficient condition for $\underset{\sim}{H}_1$ to be positive definite is that any one of the following inequalities is satisfied, in which case they are all satisfied</u>:

$$(3.2.7) \qquad p(1+\hat{\rho}^2 q) > 2\hat{\underset{\sim}{\lambda}}'(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})^{-1}\hat{\underset{\sim}{\lambda}},$$

$$(3.2.8) \qquad \hat{\underset{\sim}{\lambda}}'[\hat{\underset{\sim}{R}} * \underset{\sim}{R} - 2(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})^{-1}]\hat{\underset{\sim}{\lambda}} > 0,$$

$$(3.2.9) \qquad \hat{\underset{\sim}{\lambda}}^{(2)'}[\hat{\underset{\sim}{Q}} * \underset{\sim}{R} - 2(\hat{\underset{\sim}{Q}}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})^{-1}]\hat{\underset{\sim}{\lambda}}^{(2)} > 0,$$

<u>where</u> $\hat{\underset{\sim}{Q}} = \hat{\underset{\sim}{\Lambda}}^{-1}\hat{\underset{\sim}{R}}\hat{\underset{\sim}{\Lambda}}^{-1}$,

$$(3.2.10) \qquad \sum_{i=1}^{q} (\underset{\sim}{u}_i' \hat{\underset{\sim}{\lambda}}^{(2)})^2 / w_i < pq\hat{\rho}^2.$$

<u>where</u> $\frac{1}{2}(\hat{\underset{\sim}{Q}}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})\underset{\sim}{u}_i = w_i \underset{\sim}{u}_i$ ; $i=1,\ldots, q$,

(3.2.11) $\quad p^2(1+\hat{\rho}q)^2 > 2\hat{\lambda}'R(\hat{R}^{-1}*R + \hat{\Lambda}^{-2})^{-1}R\hat{\lambda}$,

(3.2.12) $\quad \hat{\lambda}'R[\hat{\lambda}\hat{\lambda}' - 2(\hat{R}^{-1}*R + \hat{\Lambda}^{-2})^{-1}]R\hat{\lambda} > 0$,

(3.2.13) $\quad |\tfrac{1}{2}(\hat{R}^{-1}*R + \hat{\Lambda}^{-2}) - \hat{\lambda}\hat{\lambda}'/p(1+\hat{\rho}^2q)| > 0$.

Proof. It suffices to show that (3.2.7) through (3.2.13) are equivalent to $|H_1| > 0$.

In (3.2.6) we add $(1+\hat{\rho}^2q)\hat{\lambda}'$ times the first $p$ rows to the last row, and then add the first $p$ columns times $(1+\hat{\rho}^2q)\hat{\lambda}$ to the last column to yield

$$(3.2.14) \qquad |H_1| = \frac{2^{2p}}{\hat{\rho}^2\hat{\alpha}^2} \begin{vmatrix} \tfrac{1}{2}(\hat{R}^{-1}*R + \hat{\Lambda}^{-2}), & \hat{\lambda} \\ \hat{\lambda}', & p(1+\hat{\rho}^2q) \end{vmatrix} .$$

Expanding (3.2.14) by the Frobenius-Schur method leads directly to (3.2.7) and (3.2.13). From (3.1.14) and (3.1.15) we have that

$$(3.2.15) \qquad \begin{aligned} \hat{\lambda}'(\hat{R}*R)\hat{\lambda} &= \hat{\lambda}'[(1-\hat{\rho})I + \hat{\rho}R]\hat{\lambda} \\ &= p(1-\hat{\rho}) + \hat{\rho}p(1+\hat{\rho}q) \\ &= p(1+\hat{\rho}^2q). \end{aligned}$$

Substituting this in (3.2.7) gives (3.2.8) immediately. Factoring out $\hat{\Lambda}$ on both sides of the part in square brackets leads to (3.2.9). We note that if $\hat{Q} = R$ then (3.2.9) would be satisfied as a consequence of Theorem 2.5.1. However, $\hat{Q} = R$ implies $\hat{\Sigma} = DRD = C$ and this is only so when there is no structure specified on $\Sigma$. We notice, though, that (3.1.12) may be written as $(\hat{Q}^{-1}*R)e = e$, while we have from Appendix A* that for any $R$, $(R^{-1}*R)e = e$, with $R^{-1}*R$ having minimum

*Appendix A appeared in Styan (1968).

characteristic root unity. Since $\hat{Q}^{-1}*R$ has a characteristic root of unity with corresponding vector $e$, we may write

$$(3.2.16)\quad \tfrac{1}{2}(\hat{Q}^{-1}*R + I) = ee'/p + \sum_{i=1}^{q} u_i u_i' w_i,$$

where $u_i'u_j = \delta_{ij}$, and $u_i'e = 0$. The $w_i$ are the characteristic roots (other than unity) and the $u_i$ the normalized characteristic vectors (other than $e/\sqrt{p}$) of $\tfrac{1}{2}(\hat{Q}^{-1}*R + I)$. We note that $\hat{Q}^{-1}*R$ has the same characteristic vectors with corresponding roots $2w_i - 1$. Hence

$$(3.2.17)\quad 2\hat{\lambda}^{(2)\prime}(\hat{Q}^{-1}*R + I)^{-1}\hat{\lambda}^{(2)} = p + \sum_{i=1}^{q} (u_i'\hat{\lambda}^{(2)})^2/w_i.$$

Substituting this in (3.2.7) leads directly to (3.2.10).

It remains to derive (3.2.11) and (3.2.12). In (3.2.6) we add the first p columns times $\hat{\rho}(1+\hat{\rho}q)\hat{\lambda}$ to the last column, and then add $\hat{\rho}(1+\hat{\rho}q)\hat{\lambda}'$ times the first p rows to the last row and obtain using (3.2.4)

$$(3.2.18)\quad |H_1| = \frac{2^{2p}}{(1-\hat{\rho})^2(1+\hat{\rho}q)^4}\begin{vmatrix} \tfrac{1}{2}(\hat{R}^{-1}*R + \hat{\Lambda}^{-2}), & R\hat{\lambda} \\ \hat{\lambda}'R, & p^2(1+\hat{\rho}q)^2 \end{vmatrix}.$$

Expansion by the Frobenius-Schur method leads to (3.2.11), while (3.2.12) follows by substitution of (3.1.14). (qed)

We have expanded $|H_1|$ in various ways based on the Frobenius-Schur principle. Another approach is to reduce $|H_1|$ to a determinant of one less order by elementary row and column operations.

With $\hat{Q} = \hat{\Lambda}^{-1}\hat{R}\hat{\Lambda}^{-1}$, as in (3.2.9), we may write (3.2.14) as

$$(3.2.19)\quad |H_1| = \frac{2^{2p}}{\hat{\rho}^2\hat{\alpha}^2}|\hat{\Lambda}^{-2}|\cdot\begin{vmatrix} \tfrac{1}{2}(\hat{Q}^{-1}*R + I), & \hat{\lambda}^{(2)} \\ \hat{\lambda}^{(2)\prime}, & p(1+\hat{\rho}^2 q) \end{vmatrix}.$$

We add columns 2 through p to column 1 and then rows 2 through p to row 1. Recalling from (3.1.12) and (3.1.15) that $(\hat{\underset{\sim}{Q}}^{-1}*\underset{\sim}{R})\underset{\sim}{e} = \underset{\sim}{e}$ and $\underset{\sim}{e}'\hat{\underset{\sim}{\lambda}}^{(2)} = p$, we obtain for the determinant in (3.2.19),

$$(3.2.20) \quad \begin{vmatrix} p, & \underset{\sim}{e}', & p \\ \underset{\sim}{e}, & \underset{\sim}{G}_1, & \hat{\underset{\sim}{\lambda}}_1^{(2)} \\ p, & \hat{\underset{\sim}{\lambda}}_1^{(2)'}, & p(1+\hat{\rho}^2 q) \end{vmatrix},$$

where $\underset{\sim}{G}_1 = \frac{1}{2}(\underset{\sim}{0}, \underset{\sim}{I}_q)(\hat{\underset{\sim}{Q}}^{-1}*\underset{\sim}{R} + \underset{\sim}{I})(\underset{\sim}{0}, \underset{\sim}{I}_q)'$ and $\hat{\underset{\sim}{\lambda}}_1 = (\underset{\sim}{0}, \underset{\sim}{I}_q)\hat{\underset{\sim}{\lambda}}$. We now subtract column 1 from column p + 1, and from columns 2 through p (after division by p), to give

$$(3.2.21) \quad \begin{vmatrix} p, & \underset{\sim}{0}', & 0 \\ \underset{\sim}{e}, & \underset{\sim}{G}_1-\underset{\sim}{e}\underset{\sim}{e}'/p, & \hat{\underset{\sim}{\lambda}}_1^{(2)}-\underset{\sim}{e} \\ p, & \hat{\underset{\sim}{\lambda}}_1^{(2)'}-\underset{\sim}{e}', & pq\hat{\rho}^2 \end{vmatrix}.$$

Substituting back into (3.2.19) yields

$$(3.2.22) \quad |\underset{\sim}{H}_1| = \frac{2^{2p}|\hat{\underset{\sim}{\Lambda}}^{-2}|p}{\hat{\rho}^2\hat{\alpha}^2} \begin{vmatrix} \underset{\sim}{G}_1-\underset{\sim}{e}\underset{\sim}{e}'/p, & \hat{\underset{\sim}{\lambda}}_1^{(2)}-\underset{\sim}{e} \\ \hat{\underset{\sim}{\lambda}}_1^{(2)'}-\underset{\sim}{e}, & pq\hat{\rho}^2 \end{vmatrix}$$

$$= \frac{2^{2p}p}{\hat{\rho}^2\hat{\alpha}^2\hat{\lambda}_1^2} \begin{vmatrix} \underset{\sim}{A}_1-\hat{\underset{\sim}{\lambda}}_1^{(-1)}\hat{\underset{\sim}{\lambda}}_1^{(-1)'}/p, & \hat{\underset{\sim}{\lambda}}_1-\hat{\underset{\sim}{\lambda}}_1^{(-1)} \\ \hat{\underset{\sim}{\lambda}}_1'-\hat{\underset{\sim}{\lambda}}_1^{(-1)'}, & pq\hat{\rho}^2 \end{vmatrix},$$

where $\hat{\lambda}_1 = \underset{\sim}{e}_1'\hat{\underset{\sim}{\lambda}}$ and

$$(3.2.23) \quad \underset{\sim}{A}_1 = \frac{1}{2}(\underset{\sim}{0}, \underset{\sim}{I}_q)(\hat{\underset{\sim}{R}}^{-1}*\underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})(\underset{\sim}{0}, \underset{\sim}{I}_q)'.$$

Our choice of eliminating the first row and column was quite arbitrary; (3.2.22) is equally valid with the definitions of $\underset{\sim}{G}_1$, $\hat{\underset{\sim}{\lambda}}_1$,

$\underset{\sim}{A}_1$, and $\hat{\underset{\sim}{\lambda}}_1$ modified for any other row and column. We will find (3.2.22) useful for computing $|\underset{\sim}{H}_1|$. We note that the method of reduction establishes positive definiteness of $\underset{\sim}{G}_1 - \underset{\sim}{e}\underset{\sim}{e}'/p$ and $\underset{\sim}{A}_1 - \hat{\underset{\sim}{\lambda}}_1^{(-1)}\hat{\underset{\sim}{\lambda}}_1^{(-1)'}/p$. Expansion of (3.2.22) by the Frobenius-Schur method leads only to expressions even less tractable than those considered in Theorem 3.2.1.

The inequalities (3.2.7) through (3.2.13) lead to various conditions which are sufficient, but may not be necessary to assure $|\underset{\sim}{H}_1| > 0$. Any sufficient inequality will not be useful if it is not satisfied when $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r$. We develop one sufficient condition which does hold in this special case. Let us write

(3.2.24) $$\underset{\sim}{A} = \tfrac{1}{2}(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2}),$$

in keeping with (3.2.23), and

(3.2.25) $$\underset{\sim}{\gamma} = \hat{\underset{\sim}{\lambda}}/\sqrt{p}.$$

Expanding (3.2.14) by the Frobenius-Schur method we obtain

(3.2.26) $$|\underset{\sim}{H}_1| = 2^{2p}|\underset{\sim}{A}|p(1+\hat{\rho}^2 q - \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma})/\hat{\rho}^2\hat{\alpha}^2,$$

Clearly $1+\hat{\rho}^2 q - \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} > 0$ is equivalent to (3.2.7). We study this inequality. From the Cauchy-Schwarz and Kantorovich Inequalities (cf. e.g., Marcus & Minc (1964), pp. 61, 110, & 117), we have

(3.2.27) $$(\underset{\sim}{\gamma}'\underset{\sim}{\gamma})^2 \leq (\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma})(\underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma}) \leq \frac{(M+m)^2}{4Mm}(\underset{\sim}{\gamma}'\underset{\sim}{\gamma})^2,$$

where $0 < m \leq ch(\underset{\sim}{A}) \leq M$. Substituting (3.2.24) and (3.2.25) in (3.1.12) and (3.1.15) gives $\underset{\sim}{\gamma}'\underset{\sim}{\gamma} = \underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma} = 1$. Thus (3.2.27) simplifies to

$$(3.2.28) \qquad 1 \leq \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} \leq (M+m)^2/4Mm.$$

Equality on the left-hand side is attained if and only if $\underset{\sim}{\gamma}$ is a characteristic vector of $\underset{\sim}{A}$. This is so only in the special case $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r$. Then

$$(3.2.29) \qquad |\underset{\sim}{H}_1| = 2^{2p}|\tfrac{1}{2}(\underset{\sim}{\bar{R}}^{-1}*\underset{\sim}{R} + \underset{\sim}{I})|pq/a^2,$$

where $\underset{\sim}{\bar{R}} = (1-r)\underset{\sim}{I} + r\underset{\sim}{e}\underset{\sim}{e}'$, as in (2.9.7), and $a = (1-r)(1+rq)$. Since (3.2.29)is positive, the solution $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r$, provides at least a local maximum of the likelihood when $\underset{\sim}{R}$ has constant row sums.

When $r = 0$, (3.2.29) becomes

$$(3.2.30) \qquad |\underset{\sim}{H}_1| = 2^{2p}pq.$$

This equals (3.2.3), however, only when $\underset{\sim}{e}'(\underset{\sim}{R}-\underset{\sim}{I})^2\underset{\sim}{e} = 0$, that is, $(\underset{\sim}{R}-\underset{\sim}{I})\underset{\sim}{e} = \underset{\sim}{0}$. Our development in this section has assumed (3.2.4) which does not apply when $\hat{\rho} = 0$. This restriction implies $\underset{\sim}{R}\underset{\sim}{e} = (1+qr)\underset{\sim}{e}$ when $\hat{\rho} \neq 0$. Thus when $\underset{\sim}{e}'\underset{\sim}{R}\underset{\sim}{e} = p$ we need not necessarily have $\underset{\sim}{R}\underset{\sim}{e} = \underset{\sim}{e}$ for the solution to be $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r = 0$.

From (3.2.28) we immediately see that

$$(3.2.31) \qquad \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} - 1 \geq 0,$$

while a reversal of this would have established (3.2.26) positive. We note that (3.2.31) follows directly from (3.2.17). Moreover from (3.2.28),

$$(3.2.32) \qquad 0 \leq \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} - 1 \leq (M-m)^2/4Mm.$$

This suggests that the inequality

$$(3.2.33) \quad (M-m)^2 \leq 4Mm\hat{\rho}^2q$$

might be sufficient to establish $|\underset{\sim}{H}_1| > 0$. When $p = 2$, however, (3.2.33) does not hold for all $r$ in $(-1, 1)$. To see this we find from (3.1.8) and (3.2.24) that

$$(3.2.34) \quad \text{tr } \underset{\sim}{A} = \tfrac{1}{2}(p + \text{tr } \hat{\underset{\sim}{\Lambda}}^{-2}) + \hat{\rho}^2qp/2\hat{\alpha}.$$

When $p = 2$, $\hat{\underset{\sim}{\Lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r$, $\hat{\alpha} = 1-r^2$. Substituting we find $\text{tr } \underset{\sim}{A} = 2 + r^2/1-r^2$. But $\underset{\sim}{A}$ has only 2 roots when $p = 2$ and one of these is 1. Hence the other is $1/1-r^2$. Thus $(M-m)^2 = (r^2/1-r^2)^2$ and $4Mm\hat{\rho}^2q = 4r^2/1-r^2$. Hence (3.2.33) holds if and only if $r^2 \leq 4(1-r^2)$, that is for $r$ in $(-2/\sqrt{5}\ , 2/\sqrt{5})$. This interval lies wholly within $(-1, 1)$ so (3.2.33) is not of use in establishing $|\underset{\sim}{H}_1| > 0$.

Marshall & Olkin (1964) strengthened the Kantorovich Inequality. With $\underset{\sim}{\gamma}'\underset{\sim}{\gamma} = 1$, as in our case, they proved that

$$(3.2.35) \quad \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} \leq (M + m - \underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma})/Mm.$$

Substituting $\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma} = 1$ we obtain in contrast to (3.2.32),

$$(3.2.36) \quad 0 \leq \underset{\sim}{\gamma}'\underset{\sim}{A}^{-1}\underset{\sim}{\gamma} - 1 \leq (M-1)(1-m)/Mm.$$

This shows immediately that

$$(3.2.37) \quad ch_p(\underset{\sim}{A}) \leq 1 \leq ch_1(\underset{\sim}{A}).$$

By definition of characteristic root, however, we also have (cf. Rao (1965), p. 50), that $ch_p(\underset{\sim}{A}) \leq \underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma}/\underset{\sim}{\gamma}'\underset{\sim}{\gamma} \leq ch_1(\underset{\sim}{A})$. Since $\underset{\sim}{\gamma}'\underset{\sim}{A}\underset{\sim}{\gamma} = \underset{\sim}{\gamma}'\underset{\sim}{\gamma} = 1$ we obtain (3.2.37).

We see that (3.2.36) is stronger than (3.2.32) by noting that

(3.2.38) $$\frac{(M-m)^2}{4Mm} - \frac{(M-1)(1-m)}{Mm} = \frac{[(M-1) + (m-1)]^2}{4Mm} \geq 0.$$

This leads to the following:

THEOREM 3.2.2. *A sufficient condition for $\underset{\sim}{H}_1$ to be positive is that*

(3.2.39) $$(M-1)(1-m) \leq \hat{\rho}^2 qMm,$$

*where* $0 < m \leq ch[\frac{1}{2}(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})] \leq M$. *The inequality (3.2.39) is satisfied for the special case of* $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$, $\hat{\rho} = r \neq 0$ *when* $\underset{\sim}{R}$ *has constant row sums.*

*Proof.* We have only to prove the second part. When $\underset{\sim}{R}$ has constant row sums, $\underset{\sim}{A} = \frac{1}{2}(\overline{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \underset{\sim}{I})$, and from Corollary A.2.1 we have that

(3.2.40) $$\frac{1}{2}(1 + \frac{1}{1+rq}) \leq ch(\underset{\sim}{A}) \leq \frac{1}{2}(1 + \frac{1}{1-r})$$

when $r > 0$. The inequality (3.2.40) is reversed when $r < 0$. Either way we obtain

(3.2.41) $$4(M-1)(1-m) = r^2 q/a,$$

(3.2.42) $$4Mm = (2+rq)(2-r)/a,$$

where we write $M$, $m$ for the bounds in (3.2.40). Hence (3.2.39) is satisfied whenever

(3.2.43) $$(2+rq)(2-r) \geq 1.$$

That is whenever $r$ lies between the roots of the quadratic $qr^2 - 2(q-1)r - 3 = 0$,

(3.2.44) $$-\frac{1}{q} - (\sqrt{1 + \frac{1}{q} + \frac{1}{q^2}} - 1),\ 1 + (\sqrt{\frac{1}{q^2} + \frac{1}{q} + 1} - \frac{1}{q}).$$

Thus (3.2.43) holds for all $r$ in $(-\frac{1}{q}, 1)$ and the theorem is proved. (qed)

COROLLARY 3.2.1. <u>A sufficient condition for $\underset{\sim}{H}_1$ to be positive definite is that (3.2.39) holds with</u>

$$(3.2.45) \quad 2m = \frac{1}{1+\hat{\rho}q} + \frac{1}{\hat{\lambda}_M^2} \quad , \quad 2M = \frac{1}{1-\hat{\rho}} + \frac{1}{\hat{\lambda}_m^2} \; ; \; \hat{\rho} > 0,$$

$$(3.2.46) \quad 2m = \frac{1}{1-\hat{\rho}} + \frac{1}{\hat{\lambda}_M^2} \quad , \quad 2M = \frac{1}{1+\hat{\rho}q} + \frac{1}{\hat{\lambda}_m^2} \; ; \; \hat{\rho} < 0,$$

<u>where</u> $\hat{\lambda}_m^2 \leq \hat{\lambda}_i^2 \leq \hat{\lambda}_M^2$ ; $i = 1,\ldots, p$.

<u>Proof</u>. Since $ch_1(\underset{\sim}{U}) + ch_1(\underset{\sim}{V}) \geq ch(\underset{\sim}{U} + \underset{\sim}{V})$ whenever $\underset{\sim}{U}$ and $\underset{\sim}{V}$ are symmetric (cf. Marcus & Minc (1965), p. 208 for a more general result), we have

$$(3.2.47) \quad 2\, ch[\tfrac{1}{2}(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})] \leq ch_1(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R}) + \hat{\lambda}_m^{-2} \; .$$

By Corollary A.2.1, we find using (2.9.3) that

$$(3.2.48) \quad ch_1(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R}) \leq ch_1(\hat{\underset{\sim}{R}}^{-1})$$

which is $1/(1-\hat{\rho})$ when $\hat{\rho} > 0$. This proves the right-hand side of (3.2.45). The left-hand side and (3.2.46) follow similarly. (qed)

We evaluate various bounds $\hat{\lambda}_m^2$ and $\hat{\lambda}_M^2$ in §3.3 and apply them to Corollary 3.2.1 in §3.4. We conclude this section by proving $|\underset{\sim}{H}_1| > 0$ for a particular value of $\hat{\rho}$.

THEOREM 3.2.3. <u>When</u> $\hat{\rho} = 1/(1 + \sqrt{p})$ <u>the matrix $\underset{\sim}{H}_1$ is positive definite</u>.

Proof. We establish (3.2.13), which using (3.1.8) may be written as the determinant of

$$(3.2.49)\qquad \tfrac{1}{2}\left(\frac{1}{1-\hat{\rho}}\,\underset{\sim}{I} - \frac{2}{(1+\hat{\rho}^2 q)p}\,\hat{\underset{\sim}{\lambda}}\hat{\underset{\sim}{\lambda}}'\right) + \tfrac{1}{2}\hat{\underset{\sim}{\Lambda}}^{-1}[(\underset{\sim}{I} - \frac{\hat{\rho}}{\hat{\alpha}}\,\hat{\underset{\sim}{\lambda}}\hat{\underset{\sim}{\lambda}}')*\underset{\sim}{R}]\hat{\underset{\sim}{\Lambda}}^{-1}$$

being positive. The first matrix in parentheses has $q$ equal roots of $1/1-\hat{\rho}$ and a simple root of

$$(3.2.50)\qquad \frac{1}{1-\hat{\rho}} - \frac{2p}{(1+\hat{\rho}^2 q)p} = \frac{\hat{\rho}^2 q+2\hat{\rho}-1}{(1-\hat{\rho})(1+\hat{\rho}^2 q)}\;.$$

The second matrix in parentheses has $q$ equal roots of unity and a simple root of

$$(3.2.51)\qquad 1 - p\hat{\rho}/\hat{\alpha} = -(\hat{\rho}^2 q + 2\hat{\rho} - 1)/\hat{\alpha}.$$

When $\hat{\rho} = 1/(1 + \sqrt{p})$, (3.2.50) and (3.2.51) are zero. Otherwise they differ in sign for $\hat{\rho}$ in $(-\frac{1}{q}, 1)$. While $\hat{\underset{\sim}{\lambda}}$ is a characteristic vector of the first parenthesized matrix corresponding to (3.2.50) it is not a characteristic vector for the remainder of (3.2.49). Hence $\underset{\sim}{H}_1$ is positive definite. (qed)

In Theorem 3.1.3 we gave bounds for $\hat{\rho}$. We now develop bounds for $\hat{\lambda}_i^2$ ; $i = 1,\ldots, p$ in terms of $\hat{\rho}$. While of interest in themselves, these bounds will enable us to compute the quantities in Corollary 3.2.1 and thus obtain further information about the positive definiteness of $\underset{\sim}{H}_1$.

## 3.3 Bounds for Solutions of the Maximum Likelihood Equations.

In Theorem 3.1.3 we proved that any $\hat{\rho}$ satisfying the maximum likelihood equations (3.1.12) and (3.1.13) must lie between $-\frac{1}{q}$ and 1, where $q = p - 1$. We now obtain bounds for the components of $\hat{\underset{\sim}{\lambda}}^{(2)}$, i.e., the ratios of sample to maximum likelihood estimate variances, in terms of $\hat{\rho}$. Tables and charts to illustrate these bounds will be presented in the next section.

The maximum likelihood equation (3.1.12) may be written in scalar notation as

$$(3.3.1) \qquad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 = \hat{\rho}\hat{\lambda}_i \sum_{j \neq i} \hat{\lambda}_j r_{ij} + \hat{\alpha} \; ; \; i = 1, \ldots, p.$$

We obtain bounds for $\hat{\lambda}_i$ and $\hat{\lambda}_i^2$ by applying the following inequalities to (3.3.1). From the Cauchy-Schwarz inequality we have

$$(3.3.2) \qquad (\underset{\sim}{e}'\underset{\sim}{\hat{\lambda}})^2 \leq \underset{\sim}{e}'\underset{\sim}{e} \cdot \underset{\sim}{\hat{\lambda}}'\underset{\sim}{\hat{\lambda}} = p^2,$$

from (3.1.15). Thus

$$(3.3.3) \qquad \sum_{j=1}^{p} \hat{\lambda}_j \leq p.$$

We also apply the arithmetic mean/geometric mean inequality

$$(3.3.4) \qquad \hat{\lambda}_i\hat{\lambda}_j \leq \tfrac{1}{2}(\hat{\lambda}_i^2 + \hat{\lambda}_j^2).$$

Two cases arise according as $\hat{\rho} > 0$ or $\hat{\rho} < 0$.

### 3.3.1 <u>Case of</u> $0 < \hat{\rho} < 1$.

When $\hat{\rho} > 0$ applying (3.3.3) to (3.3.1) gives, since $r_{ij} < 1$ $(i \neq j)$,

$$(3.3.5) \qquad (1 + \hat{\rho}(q-1))\hat{\lambda}_i^2 < \hat{\rho}\hat{\lambda}_i(p-\hat{\lambda}_i) + \hat{\alpha} \; ; \; i = 1, \ldots, p.$$

Thus $\hat{\lambda}_i$ must lie between the roots of the quadratic equation

$$(3.3.6) \qquad (1 + \hat{\rho}q)\hat{\lambda}_i^2 - \hat{\rho}p\hat{\lambda}_i - \hat{\alpha} = 0,$$

which are

$$(3.3.7) \qquad \frac{\hat{\rho}p \pm \sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)}}{2(1+\hat{\rho}q)} \quad .$$

One root of (3.3.7) is negative since $4\hat{\alpha}(1+\hat{\rho}q) > 0$. We will study only the other root, which is positive, and which provides an upper bound for $\hat{\lambda}_i$ , $i = 1,\ldots, p$.

Since $r_{ij} > -1$ $(i \neq j)$, applying (3.3.3) to (3.3.1) also yields

$$(3.3.8) \qquad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 > - \hat{\rho}\hat{\lambda}_i(p-\hat{\lambda}_i) + \hat{\alpha} \quad ; \; i = 1,\ldots, p.$$

Thus $\hat{\lambda}_i$ must lie outside the roots of the quadratic equation

$$(3.3.9) \qquad [1 + \hat{\rho}(q-2)]\hat{\lambda}_i^2 + \hat{\rho}p\hat{\lambda}_i - \hat{\alpha} = 0,$$

which are

$$(3.3.10) \qquad \frac{-\hat{\rho}p \pm \sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}[1+\hat{\rho}(q-2)]}}{2[1 + \hat{\rho}(q-2)]} \quad .$$

One root of (3.3.10) is negative and of no interest. The other root is positive and provides a lower bound for $\hat{\lambda}_i$ , $i = 1,\ldots, p$. We thus have the following:

THEOREM 3.3.1. <u>The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when</u> $0 < \hat{\rho} < 1$, $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$, $q = p - 1$,

$$(3.3.11) \qquad \frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}[1+\hat{\rho}(q-2)]} - \hat{\rho}p}{2[1+\hat{\rho}(q-2)]} < \hat{\lambda}_i < \frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} + \hat{\rho}p}{2(1+\hat{\rho}q)} \; ;$$

$$i = 1,\ldots, p.$$

As $\hat{\rho}$ tends to 0, the bounds in (3.3.11) both tend to 1. As $\hat{\rho}$ approaches 1, however, the bounds tend to 0 and 1 respectively. Tables and charts of (3.3.11) follow in §3.4.

Additional bounds for $\hat{\lambda}_i$, independent of p, follow from (3.3.11). We may write the upper bound as

$$(3.3.12)\quad \sqrt{\frac{\hat{\rho}^2}{4(\hat{\rho}+\frac{1-\hat{\rho}}{p})^2} + 1 - \hat{\rho}} \quad + \quad \frac{\hat{\rho}}{2(\hat{\rho}+\frac{1-\hat{\rho}}{p})} .$$

As p increases, (3.3.12) increases monotonically to $\frac{1}{2}(\sqrt{5-4\hat{\rho}} + 1)$. Similarly the left-hand side of (3.3.11) decreases monotonically to $\frac{1}{2}(\sqrt{5-4\hat{\rho}} - 1)$. To see the monotonicity for the lower bound we note that $\sqrt{a^2+x} - a$ expanded as a Taylor series gives $O(x/a)$, and $x > 0$ in our case. Hence we have the following:

COROLLARY 3.3.1. <u>For any value of p, the solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when</u> $0 < \hat{\rho} < 1$,

$$(3.3.13)\quad 0 < \tfrac{1}{2}(3 - 2\hat{\rho} - \sqrt{5-4\hat{\rho}}) < \hat{\lambda}_i^2 < \tfrac{1}{2}(3 - 2\hat{\rho} + \sqrt{5-4\hat{\rho}}),$$

$$(3.3.14)\quad \hat{\lambda}_i^2 < \tfrac{1}{2}(3 + \sqrt{5}) \;;\; i = 1,\ldots, p.$$

As $\hat{\rho}$ approaches 0 the bounds in (3.3.13) tend to .3820 and 2.6180 respectively, correct to four decimal places. As $\hat{\rho}$ approaches 1, however, the bounds tend to 0 and 1 respectively. Thus for any value of $p \geq 3$ and $0 < \hat{\rho} < 1$, $\hat{\lambda}_i^2$ is at most 2.6180 to four decimal places. Tables and a plot follow in §3.4.

The application of (3.3.4) to (3.3.1) yields bounds which are weaker than those in Theorem 3.3.1 and Corollary 3.3.1. Since $-1 < r_{ij} < 1$ $(i \neq j)$, we obtain

$$(3.3.15)\quad -\tfrac{1}{2}\hat{\rho} \sum_{j\neq i} (\hat{\lambda}_i^2 + \hat{\lambda}_j^2) < [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 - \hat{\alpha} < \tfrac{1}{2}\hat{\rho} \sum_{j\neq i} (\hat{\lambda}_i^2 + \hat{\lambda}_j^2);\; i=1,\ldots, p.$$

Using (3.1.15) we reduce (3.3.15) to

$$(3.3.16)\qquad 1 - \frac{q\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} < \hat{\lambda}_i^2 < 1 + \frac{q\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} \ ; \ i = 1,\ldots, p,$$

where

$$(3.3.17)\qquad t = \tfrac{1}{2}(q-1) = \tfrac{1}{2}p - 1.$$

We now show that the bounds (3.3.16) are weaker than (3.3.11). For the upper bound this is so provided

$$(3.3.18)\qquad 4(1+\hat{\rho}q)^2 + \frac{4q\hat{\rho}\hat{\alpha}(1+\hat{\rho}q)}{1+t\hat{\rho}} > \left(\sqrt{\hat{\rho}^2p^2+4\hat{\alpha}(1+\hat{\rho}q)} + \hat{\rho}p\right)^2.$$

Using $2(1+\hat{\rho}q) = 2(1+t\hat{\rho}) + \hat{\rho}p$, we write (3.3.18) as

$$(3.3.19)\qquad 4(1+\hat{\rho}q)^2 + 4q\hat{\rho}\hat{\alpha} + \frac{2pq\hat{\rho}^2\hat{\alpha}}{1+t\hat{\rho}} > 2\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q) + 2\hat{\rho}p\sqrt{\hat{\rho}^2p^2+4\hat{\alpha}(1+\hat{\rho}q)} .$$

Cancelling terms and dividing through by $2p\hat{\rho}$ gives

$$(3.3.20)\qquad 2(1+t\hat{\rho}) + \frac{q\hat{\rho}\hat{\alpha}}{1+t\hat{\rho}} > \sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} .$$

Squaring both sides yields

$$(3.3.21)\qquad \frac{q^2\hat{\rho}^2\hat{\alpha}^2}{(1+t\hat{\rho})^2} > \hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q) - 4(1+t\hat{\rho})^2 - 4q\hat{\rho}\hat{\alpha} = \hat{\rho}^2p^2+4(\hat{\alpha}-(1+t\hat{\rho})^2)=0,$$

establishing (3.3.18). For the lower bound we will find

$$(3.3.22)\qquad \left(\sqrt{\hat{\rho}^2p^2+ 4\hat{\alpha}(1+\hat{\rho}u)} - \hat{\rho}p\right)^2 > 4(1+\hat{\rho}u)^2 - \frac{4q\hat{\rho}(1+\hat{\rho})(1+\hat{\rho}u)^2}{1+3t\hat{\rho}}$$

where

$$(3.3.23)\qquad u = q-2 = p-3.$$

Using $2(1+\hat{\rho}u) = 2(1+3t\hat{\rho}) - \hat{\rho}p$, we write (3.3.22) as

$$(3.3.24)\qquad 2\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u) -2\hat{\rho}p\sqrt{\hat{\rho}^2p^2+4\hat{\alpha}(1+\hat{\rho}u)} > 4(1+\hat{\rho}u)^2- 4q\hat{\rho}(1+\hat{\rho})(1+\hat{\rho}u) + \frac{2pq\hat{\rho}^2(1+\hat{\rho})(1+\hat{\rho}u)}{1+3t\hat{\rho}} .$$

Cancelling terms and dividing through by $2p\hat{\rho}$ gives

$$(3.3.25) \quad 2(1+3t\hat{\rho}) - \frac{q\hat{\rho}(1+\hat{\rho})(1+\hat{\rho}u)}{1+3t\hat{\rho}} > \sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u)} \; .$$

Squaring both sides yields

$$(3.3.26) \quad \frac{q^2\hat{\rho}^2(1+\hat{\rho})^2(1+\hat{\rho}u)^2}{(1+3t\hat{\rho})^2} > \hat{\rho}^2p^2 + 4(1+\hat{\rho}u)[\hat{\alpha} + q\hat{\rho}(1+\hat{\rho})]$$

$$- 4(1+\hat{\rho}u)^2 - \hat{\rho}^2p^2 - 4p\hat{\rho}(1+\hat{\rho}u)$$

$$= 4(1+\hat{\rho}u)(2\hat{\rho}t + \hat{\rho}q - \hat{\rho}u - \hat{\rho}p) = 0,$$

establishing (3.3.22).

As $\hat{\rho}$ approaches 0, the bounds (3.3.16) both tend to 1 as do (3.3.11). As $\hat{\rho}$ approaches 1, however, the bounds (3.3.16) tend to $-t/(1+3t)$ and 1 respectively, while (3.3.11) tend to 0 and 1. The bounds in Corollary 3.3.1 are paralleled by

$$(3.3.27) \quad \max(0, (1-2\hat{\rho})/3) < \lambda_i^2 < 3 - 2\hat{\rho} < 3,$$

by letting $p$ tend to $\infty$ in (3.3.16). It follows that (3.3.27) is weaker than (3.3.13) and (3.3.14).

We obtain a further set of bounds by using (3.1.14) in (3.3.1). We will use the following:

LEMMA 3.3.1. <u>For any symmetric matrix</u> $\underset{\sim}{A} = \{a_{ij}\}$ <u>of order</u> $p = q + 1$,

$$(3.3.28) \quad \sum_{\substack{j=1 \\ j\neq i}}^{p} a_{ij} = \sum_{j=1}^{q} \sum_{k=j+1}^{p} a_{kj} - \sum_{\substack{j=1 \\ j\neq i}}^{q} \sum_{\substack{k=j+1 \\ k\neq i}}^{p} a_{kj}.$$

<u>Proof</u>. The right-hand side of (3.3.28) may be written

$$(3.3.29)\quad \sum_{j=1}^{q}\Big(\sum_{k=j+1}^{p} a_{kj} - \sum_{\substack{k=j+1\\ j\neq i}}^{p} a_{kj}\Big) + \sum_{k=i+1}^{p} a_{ki} = \sum_{j=1}^{q} a_{ij}\epsilon_{ij} + \sum_{k=i+1}^{p} a_{ki},$$

where $\epsilon_{ij} = 1$ if $i \geq j + 1$, and zero otherwise. Thus (3.3.29) becomes

$$(3.3.30)\quad \sum_{j=1}^{i-1} a_{ij} + \sum_{k=i+1}^{p} a_{ik} = \sum_{\substack{j=1\\ j\neq i}}^{p} a_{ij}. \qquad \text{(qed)}$$

Applying Lemma 3.3.1 to (3.3.1) yields

$$(3.3.31)\quad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 - \hat{\alpha} = \hat{\rho}\Big(\tfrac{1}{2}pq\hat{\rho} - \sum_{\substack{j=1\\ j\neq i}}^{q} \sum_{\substack{k=j+1\\ k\neq i}}^{p} \hat{\lambda}_j\hat{\lambda}_k r_{jk}\Big),$$

using (3.1.14). Since $-r_{jk} < 1$ $(j \neq k)$, we obtain

$$(3.3.32)\quad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 - \hat{\alpha} - \tfrac{1}{2}pq\hat{\rho}^2 < \hat{\rho} \sum_{\substack{j=1\\ j\neq i}}^{q} \sum_{\substack{k=j+1\\ k\neq i}}^{p} \hat{\lambda}_j\hat{\lambda}_k .$$

Applying the Cauchy-Schwarz and arithmetic mean/geometric mean inequalities to (3.3.32) leads to the same new set of bounds in contrast to our earlier results of Theorem 3.3.1 and (3.3.16). We introduce the $q \times 1$ vector

$$(3.3.33)\quad \hat{\underset{\sim}{\theta}}_i = (\hat{\lambda}_1, \ldots, \hat{\lambda}_{i-1}, \hat{\lambda}_{i+1}, \ldots, \hat{\lambda}_p)' \; ; \; i = 1, \ldots, p.$$

The right-hand side of (3.3.32) is $\frac{1}{2}\hat{\rho}$ times the sum of the off-diagonal elements in $\hat{\underset{\sim}{\theta}}_i\hat{\underset{\sim}{\theta}}_i'$,

$$(3.3.34)\quad \underset{\sim}{e}'(\hat{\underset{\sim}{\theta}}_i\hat{\underset{\sim}{\theta}}_i')\underset{\sim}{e} - \operatorname{tr} \hat{\underset{\sim}{\theta}}_i\hat{\underset{\sim}{\theta}}_i'.$$

Using (3.1.15), $\operatorname{tr} \hat{\underset{\sim}{\theta}}_i\hat{\underset{\sim}{\theta}}_i' = \hat{\underset{\sim}{\theta}}_i'\hat{\underset{\sim}{\theta}}_i = p - \hat{\lambda}_i^2$, while analogous to (3.3.2),

$$(3.3.35)\quad (\underset{\sim}{e}'\hat{\underset{\sim}{\theta}}_i)^2 \leq \underset{\sim}{e}'\underset{\sim}{e}\cdot\hat{\underset{\sim}{\theta}}_i'\hat{\underset{\sim}{\theta}}_i = q(p-\hat{\lambda}_i^2).$$

Thus (3.3.34) is at most $(q-1)(p-\hat{\lambda}_i^2)$. Substituting in (3.3.32) yields

$$(3.3.36) \qquad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 - \hat{\alpha} - \tfrac{1}{2}pq\hat{\rho}^2 < t\hat{\rho}(p-\hat{\lambda}_i^2),$$

using (3.3.17). On the other hand we have from (3.3.4) that the right-hand side of (3.3.32) is at most $\frac{1}{2}\hat{\rho}$ times

$$(3.3.37) \qquad \sum_{\substack{j=1 \\ j\neq i}}^{q} \sum_{\substack{k=j+1 \\ k\neq i}}^{p} (\hat{\lambda}_j^2 + \hat{\lambda}_k^2),$$

which is $\frac{1}{2}$ the sum of the off-diagonal elements of $\underset{\sim}{e}\hat{\underset{\sim}{\theta}}_i^{(2)\prime} + \hat{\underset{\sim}{\theta}}_i^{(2)}\underset{\sim}{e}' = \underset{\sim}{B}$, say. Since $\underset{\sim}{e}'\underset{\sim}{B}\underset{\sim}{e} = 2\underset{\sim}{e}'\underset{\sim}{e}\cdot\underset{\sim}{e}'\hat{\underset{\sim}{\theta}}_i^{(2)} = 2q(p-\hat{\lambda}_i^2)$ and $\operatorname{tr} \underset{\sim}{B} = 2\underset{\sim}{e}'\hat{\underset{\sim}{\theta}}_i^{(2)} = 2(p-\hat{\lambda}_i^2)$ we find that (3.3.37) equals $(q-1)(p-\hat{\lambda}_i^2)$. Substitution in (3.3.32) yields (3.3.36) once more. This leads to the following:

THEOREM 3.3.2. <u>The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when</u> $0 < \hat{\rho} < 1$, $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$,

$$(3.3.38) \qquad 1 - \frac{tq\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < \hat{\lambda}_i^2 < 1 + \frac{tq\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} \quad ; i=1,\ldots, p.$$

<u>Proof</u>. We may write (3.3.38) as

$$(3.3.39) \qquad (1+2t\hat{\rho})\hat{\lambda}_i^2 < 1 + 2t\hat{\rho} - q\hat{\rho}^2 + \tfrac{1}{2}pq\hat{\rho}^2 + t\hat{\rho}(p-\hat{\lambda}_i^2),$$

which simplifies directly to the right-hand side of (3.3.38). Since $r_{jk} > -1$ $(j \neq k)$ we have that the left-hand side of (3.3.32), and thus that also of (3.3.36) is greater than minus the respective right-hand side. This reverses the inequality in (3.3.39) with the last term becoming $-t\hat{\rho}(p-\hat{\lambda}_i^2)$. Simplifying completes the proof. (qed)

As $\hat{\rho}$ approaches 0 both bounds in (3.3.38) tend to 1. As $\hat{\rho}$ approaches 1, however, the bounds tend to 1 and $1 + (2tq/1+3t)$ respectively, in contrast to those in (3.3.11) which tend to 0 and 1 and those in (3.3.16) which tend to $-t/1+3t$ and 1 respectively. As p tends to $\infty$ the bounds in (3.3.38) explode. As indicated by the tables and charts in §3.4 the bounds (3.3.38) and (3.3.11) overlap in general. We do, however, have the following:

THEOREM 3.3.3. *The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when* $0 < \hat{\rho} < 1$, $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$,

$$(3.3.40) \qquad \hat{\lambda}_i^2 < \left[\frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} + \hat{\rho}p}{2(1+\hat{\rho}q)}\right]^2 < 1 + \frac{tq\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}}, \quad p = 4, 5, \ldots$$

$$(3.3.41) \qquad \left[\frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u)} - \hat{\rho}p}{2(1+\hat{\rho}u)}\right]^2 < 1 - \frac{tq\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < \hat{\lambda}_i^2, \quad p = 3, 4,$$

*for* $i = 1, \ldots, p$, *where* $u = p-3 = q-2$, $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$.

*Proof.* To show (3.3.40) it suffices to prove the upper bound in (3.3.16) less than that in (3.3.38),

$$(3.3.42) \qquad 1 + \frac{q\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < 1 + \frac{tq\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}},$$

which holds provided

$$(3.3.43) \qquad t(t+3)\hat{\rho}^2 + (t-1)^2\hat{\rho} + t-1 > 0.$$

When $p = 4$, $t = \frac{1}{2}p-1 = 1$ and (3.3.43) is satisfied. For $p = 5, 6, \ldots$, $t > 1$, and (3.3.43) is always satisfied if its discriminant is negative,

$$(3.3.44) \qquad (t-1)^4 - 4t(t-1)(t+3) < 0.$$

Substituting $t = \frac{1}{2}p-1$ in (3.3.44) we see after some algebra that we need

$$(3.3.45) \quad \tfrac{1}{2}p^2 - 10p + 16 < 0,$$

which is so provided $p$ lies between the roots $10 \pm \sqrt{68}$ which are about 1.8 and 18.2. Thus (3.3.40) is established for $p = 4, 5, \ldots, 18$. For $p = 19, 20, \ldots,$ (3.3.43) has real roots, the larger of which is

$$(3.3.46) \quad \frac{-(t-1)^2 + \sqrt{(t-1)^4 - 4t(t-1)(t+3)}}{2t(t+3)},$$

which is negative. Thus (3.3.43) holds with $\hat{\rho} > 0$ and (3.3.40) is established for $p = 4, 5, \ldots.$

We prove (3.3.41) first for $p = 3$. Then $u = 0$ and so we need

$$(3.3.47) \quad \left[\frac{\sqrt{9\hat{\rho}^2 + 4\hat{\alpha}} - 3\hat{\rho}}{2}\right]^2 < 1 - \frac{\hat{\rho}(1-\hat{\rho})}{1+\frac{1}{2}\hat{\rho}}.$$

Since $9\hat{\rho}^2 + 4\hat{\alpha} = (\hat{\rho}+2)^2$, (3.3.47) reduces to

$$(3.3.48) \quad \tfrac{1}{2}\hat{\rho}^2 - \hat{\rho} - 1 < 0.$$

The roots are $1 \pm \sqrt{3}$ or $-.7, 2.7$ approximately. Thus (3.3.41) holds when $p = 3$. For $p = 4$, we want

$$(3.3.49) \quad \left[\frac{\sqrt{4\hat{\rho}^2 + \hat{\alpha}(1+\hat{\rho})} - 2\hat{\rho}}{1+\hat{\rho}}\right]^2 < 1 - \frac{3\hat{\rho}(1-\hat{\rho})}{1+\hat{\rho}},$$

which after considerable algebra reduces to

$$(3.3.50) \quad 2 + 3\hat{\rho} - 3\hat{\rho}^2 < 2\sqrt{4\hat{\rho}^2 + \hat{\alpha}(1+\hat{\rho})}.$$

Squaring both sides and cancelling common terms leads to

$$(3.3.51) \quad 3\hat{\rho}^2 - 2\hat{\rho} - 5 < 0.$$

The roots are $-1$ and $5/3$ which establishes (3.3.41) also for $p = 4$. (qed)

We have therefore shown that for $p = 4, 5, \ldots$ the upper bound (3.3.11) and for $p = 3, 4$ the lower bound (3.3.38) are preferred. Let us now compare the upper bounds (3.3.11) and (3.3.38) when $p = 3$. We see that (3.3.11) is stronger when

$$(3.3.52) \qquad \left[ \frac{\sqrt{9\hat{\rho}^2 + 4\hat{\alpha}(1+2\hat{\rho})} + 3\hat{\rho}}{2(1+2\hat{\rho})} \right]^2 < 1 + \frac{\hat{\rho}(1+\hat{\rho})}{1+1\frac{1}{2}\hat{\rho}} .$$

Expanding the left-hand side and cancelling some terms yields

$$(3.3.53) \qquad 3\sqrt{9\hat{\rho}^2 + 4\hat{\alpha}(1+2\hat{\rho})} < \frac{2(1+2\hat{\rho})^2(4+5\hat{\rho})}{2+3\hat{\rho}} - 9\hat{\rho}.$$

Squaring both sides yields the cubic

$$(3.3.54) \qquad 25\hat{\rho}^3 + 39\hat{\rho}^2 - 10 > 0.$$

This cubic has its local maximum at $\hat{\rho} = -78/75$ and local minimum at $\hat{\rho} = 0$. Hence there is only one positive root, which equals .4463 to four places of decimals. Thus (3.3.38) is stronger for $\hat{\rho}$ below this root while (3.3.11) is stronger above.

The lower bounds (3.3.11) and (3.3.38) tend to 0 and 1 respectively as $\hat{\rho}$ approaches 1, but (3.3.38) explodes as $p$ becomes large. We see that the lower bound (3.3.38) is positive only if

$$(3.3.55) \qquad 1 + t\hat{\rho} > tq\hat{\rho}(1-\hat{\rho}),$$

or for $\hat{\rho}$ outside the roots of the quadratic $tq\hat{\rho}^2 - 2t^2\hat{\rho} + 1 = 0$, which are

$$(3.3.56) \qquad \frac{t \pm \sqrt{t^2 - q/t}}{q} .$$

As $p$ becomes large so does $t = \frac{1}{2}p-1$ and (3.3.56) approaches 0 and 1.

For $p = 10$, for example, $t = 4$ and (3.3.56) is .032 and .857 to three places of decimals. Values of (3.3.56) are tabulated in §3.4. We summarize our results in the following:

TABLE 3.3.1.

Preferred bounds for $\hat{\lambda}_i^2$ ; $i = 1,\dots, p$, when $0 < \hat{\rho} < 1$.

| p | Lower Bound | Upper Bound |
|---|---|---|
| 3 | (3.3.38) | (3.3.38) $0 < \hat{\rho} \leq .4463$<br>(3.3.11) $.4463 \leq \hat{\rho} < 1$ |
| 4 | (3.3.38) | (3.3.11) |
| $\geq 5$ | (3.3.38) for $\hat{\rho}$ near 0 or 1<br>(3.3.11) otherwise | (3.3.11) |

We close this section by giving bounds for the average of $q = p-1$ $\hat{\lambda}_i$'s. These are obtained by applying (3.1.15) to (3.3.11) and (3.3.38).

THEOREM 3.3.4. *The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when* $0 < \hat{\rho} < 1$, $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$,

$$(3.3.57)\quad 1 - \frac{\hat{\rho}p\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} - 2\hat{\rho}(1-2\hat{\rho}t^2+\hat{\rho}^2q)}{2q(1+\hat{\rho}q)^2} < \overline{\lambda}_j^2$$

$$< 1 + \frac{\hat{\rho}p\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u)} - 2\hat{\rho}(1+\hat{\rho}t(p+2)-\hat{\rho}^2qu)}{2q(1+\hat{\rho}u)^2},$$

$$(3.3.58)\quad 1 - \frac{t\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} < \overline{\lambda}_j^2 < 1 + \frac{t\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}},$$

*for* $j = 1,\dots, p$, *where* $u = q-2 = p-3$, $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$, *and*

$$(3.3.59)\quad \overline{\lambda}_j^2 = \frac{1}{q}\sum_{i\neq j} \hat{\lambda}_i^2.$$

For $p = 4, 5, \ldots$ (3.3.57) provides the stronger lower bound while for $p = 3, 4$ (3.3.58) gives the stronger upper bound.

Proof. Substituting (3.1.15) in (3.3.11) and (3.3.38) yields(3.3.57) and (3.3.58) respectively after some algebraic manipulation. The proof of the theorem is completed using Theorem 3.3.3. (qed)

Another set of bounds for $\bar{\lambda}_j^2$ are obtained by applying (3.1.15) to (3.3.16),

$$(3.3.60) \quad 1 - \frac{\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < \bar{\lambda}_j^2 < 1 + \frac{\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} \; ; \; j = 1, \ldots, p.$$

While of a much simpler form than (3.3.57), the bounds (3.3.60) are weaker, as shown by the discussion comparing (3.3.16) with (3.3.11).

3.3.2 Case of $-1/q < \hat{\rho} < 0$.

Many of our results for $\hat{\rho} > 0$ carry over immediately to the case of $\hat{\rho} < 0$, but with the signs reversed. Some results, however, become vacuous when $\hat{\rho} < 0$.

Applying (3.3.3) to (3.3.1) we obtain

$$(3.3.61) \quad [1+\hat{\rho}(q-1)]\hat{\lambda}_i^2 > \hat{\rho}\hat{\lambda}_i(p-\hat{\lambda}_i) + \hat{\alpha} \; ; \; i = 1, \ldots, p,$$

cf. (3.3.5), and so $\hat{\lambda}_i$ must lie outside the roots of (3.3.6). The positive root given in (3.3.7) now provides a lower bound for $\hat{\lambda}_i$, $i = 1, \ldots, p$. Similarly the positive root in (3.3.10) gives an upper bound. We combine these bounds as the following:

THEOREM 3.3.5. The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when $-1/q < \hat{\rho} < 0$,

$$(3.3.62)\quad \frac{\sqrt{\hat\rho^2 p^2 + 4\hat\alpha(1+\hat\rho q)} + \hat\rho p}{2(1+\hat\rho q)} < \hat\lambda_i < \frac{\sqrt{\hat\rho^2 p^2 + 4\hat\alpha(1+\hat\rho u)} - \hat\rho p}{2(1+\hat\rho u)},$$

for $i = 1,\ldots, p$, where $u = p-3 = q-2$ and $\hat\alpha = (1-\hat\rho)(1+\hat\rho q)$.

As $\hat\rho$ approaches 0 we saw in §3.3.1 that the bounds in (3.3.62) both tend to 1. As $\hat\rho$ approaches $-1/q$, however, the bounds tend to 0 and $\frac{1}{2}p$ respectively. Since $-1/q$ tends to 0 as $p$ goes to $\infty$, we have no counterpart to Corollary 3.3.1 for $\hat\rho < 0$.

Applying (3.3.4) to (3.3.1) again yields a weaker set of bounds than we obtained with (3.3.3). Parallel to (3.3.16) we find

$$(3.3.63)\quad 1 + \frac{q\hat\rho(1-\hat\rho)}{1+t\hat\rho} < \hat\lambda_i^2 < 1 - \frac{q\hat\rho(1+\hat\rho)}{1+3t\hat\rho}\ ;\ i = 1,\ldots, p.$$

The upper bound in (3.3.63) is only valid for

$$(3.3.64)\quad -1/3t < \hat\rho < 0.$$

For $p = 3$ and 4, (3.3.64) is always satisfied since then $3t \leq q$. But for $p \geq 5$, $3t > q$ and so $-1/3t > -1/q$ and the valid range is restricted to (3.3.64). As $\hat\rho$ approaches 0 we saw in §3.3.1 that the bounds (3.3.63) both tend to 1. As $\hat\rho \to -1/q$ the lower bound in (3.3.63) tends to $-1$, while the upper bound tends to 3 for $p = 3$. When $p \geq 4$ the upper bound explodes as $\hat\rho \to -1/3t \geq -1/q$.

Applying Lemma 3.3.1 to (3.3.1) yields as counterpart to Theorem 3.3.2:

THEOREM 3.3.6. The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when $-1/q < \hat\rho < 0$, $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$,

$$(3.3.65)\quad \hat\lambda_i^2 < 1 - \frac{tq\hat\rho(1-\hat\rho)}{1+t\hat\rho}\ ;\ i = 1,\ldots, p,$$

and with $\max(-1/3t, -1/q) < \hat{\rho} < 0$,

$$(3.3.66) \quad 1 + \frac{tq\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} < \hat{\lambda}_i^2 \ ; \ i = 1,\ldots, p.$$

As already observed, $\max(-1/3t, -1/q) = -1/q$ for $p = 3, 4$ and $= -1/3t$ for $p \geq 5$. As $\hat{\rho}$ approaches 0 the bounds (3.3.65) and (3.3.66) both tend to 1 as shown for (3.3.38). As $\hat{\rho}$ approaches $-1/q$ the upper bound (3.3.65) tends to $q$, while the lower bound tends to 0 for $p = 3$. When $p \geq 4$ the lower bound explodes as $\hat{\rho} \to -1/3t \geq -1/q$. As $p \to \infty$ both bounds diverge. We will see in §3.4 that the upper bound (3.3.62) is stronger than (3.3.65) for $p \geq 5$ through $\hat{\rho}$ just above $-1/q$.

We have the following slightly stronger counterpart to Theorem 3.3.3:

THEOREM 3.3.7. The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when $-1/q < \hat{\rho} < 0$, $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$,

$$(3.3.67) \quad \hat{\lambda}_i^2 < 1 - \frac{tq\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < \left[\frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u)} - \hat{\rho}p}{2(1+\hat{\rho}u)}\right]^2, \ p = 3, 4,$$

$$(3.3.68) \quad \left[\frac{\sqrt{9\hat{\rho}^2 + 4\hat{\alpha}(1+2\hat{\rho})} + 3\hat{\rho}}{2(1+2\hat{\rho})}\right]^2 < 1 + \frac{\hat{\rho}(1+\hat{\rho})}{1+1\frac{1}{2}\hat{\rho}} < \hat{\lambda}_i^2 \ (p = 3),$$

and with $-1/3t < \hat{\rho} < 0$,

$$(3.3.69) \quad 1 + \frac{tq\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} < \left[\frac{\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} + \hat{\rho}p}{2(1+\hat{\rho}q)}\right]^2 < \hat{\lambda}_i^2, \ p = 4, 5,\ldots,$$

for $i = 1,\ldots, p$, where $u = p-3 = q-2$ and $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$.

Proof. It suffices to establish (3.3.68), since (3.3.67) and (3.3.69) follow immediately from Theorem 3.3.3. To prove (3.3.68) we require

(3.3.52) which now holds provided the cubic [from (3.3.54)]

$$(3.3.70) \quad 25\hat{\rho}^3 + 35\hat{\rho}^2 - 10 < 0.$$

Since the cubic is negative between its local maximum and minimum (3.3.68) follows. (qed)

We summarize our results in the following:

TABLE 3.3.2.

Preferred bounds for $\hat{\lambda}_i^2$ ; $i = 1,\ldots, p$ when $-1/q < \hat{\rho} < 0$.

| p | Lower Bound | Upper Bound |
|---|---|---|
| 3 | (3.3.66) | (3.3.65) |
| 4 | (3.3.62) | (3.3.65) |
| ≥ 5 | (3.3.62) | (3.3.62) for $\hat{\rho}$ nearer 0 |
| | | (3.3.65) for $\hat{\rho}$ nearer $-1/q$ |

We conclude with bounds for the average of $q = p-1$ $\hat{\lambda}_i$'s. The counterpart of Theorem 3.3.4 is:

THEOREM 3.3.8. The solutions of the maximum likelihood equations (3.1.12) and (3.1.13) satisfy, when $-1/q < \hat{\rho} < 0$, $\hat{\alpha} = (1-\hat{\rho})(1+\hat{\rho}q)$,

$$(3.3.71) \quad 1 + \frac{\hat{\rho}p\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}u)} - 2\hat{\rho}(1+\hat{\rho}t(p+2) - \hat{\rho}^2qu)}{2q(1+\hat{\rho}u)^2}$$

$$< \overline{\lambda}_j^2 < 1 - \frac{\hat{\rho}p\sqrt{\hat{\rho}^2p^2 + 4\hat{\alpha}(1+\hat{\rho}q)} - 2\hat{\rho}(1-2\hat{\rho}t^2+\hat{\rho}^2q)}{2q(1+\hat{\rho}q)^2},$$

$$(3.3.72) \quad 1 + \frac{t\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} < \overline{\lambda}_j^2 ,$$

where $u = p-3 = q-2$ and $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$

and with max $(-1/3t, -1/q) < \hat{\rho} < 0$,

$$(3.3.73) \quad \overline{\lambda}_j^2 < 1 - \frac{t\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}},$$

for $j = 1, \ldots, p$, where $\overline{\lambda}_j^2 = (\Sigma_{i \neq j} \lambda_i^2)/q$. For $p = 3$, (3.3.73) is the stronger upper bound, while for $p \geq 4$, (3.3.71) provides the stronger upper bound. For $p = 3, 4$ (3.3.72) is the stronger lower bound.

We notice that (3.3.73) only gives an upper bound for $\hat{\rho} > \max(-1/3t, -1/q)$. Thus for $p \geq 5$, (3.3.73) gives no upper bound for $-1/q < \hat{\rho} \leq -1/3t$. Another set of bounds for $\overline{\lambda}_j^2$ are obtained in parallel to (3.3.63),

$$(3.3.74) \quad 1 + \frac{\hat{\rho}(1+\hat{\rho})}{1+3t\hat{\rho}} < \overline{\lambda}_j^2 < 1 - \frac{\hat{\rho}(1-\hat{\rho})}{1+t\hat{\rho}} \; ; \; j = 1, \ldots, p.$$

These are of a much simpler form than (3.3.71) though weaker. Moreover the upper bound is not valid for $-1/q < \hat{\rho} \leq -1/3t$, $p \geq 5$.

## 3.4 Selected Values of the Bounds, with Applications to the Determinant of Second Derivatives. Special Cases.

We now evaluate numerically the bounds obtained in §3.3. We present tables and charts of these values and examine their relative strengths. We also apply these results to Corollary 3.2.1, in an attempt to prove positive the determinant $|\underset{\sim}{H}_1|$ of second derivatives, where $\underset{\sim}{H}_1$ is defined by (3.2.5). This would show that the maximum likelihood equations (3.1.12) and (3.1.13) admit a unique real solution. By computation we find our bounds tight enough to show $|\underset{\sim}{H}_1| > 0$ for a wide range of positive values of $\hat{\rho}$ when $p \geq 4$; when $\hat{\rho}$ is negative our bounds are inadequate for use in Corollary 3.2.1. We examine the case $p = 3$ in detail and prove analytically that $|\underset{\sim}{H}_1| > 0$ for $\hat{\rho} \geq -.2465$ (to four decimal places). We found $|\underset{\sim}{H}_1| > 0$ for the remaining range of $\hat{\rho}$, analytically when two $\hat{\lambda}_i$'s are equal, and by numerical evaluation otherwise. We establish a surprising inequality that $\hat{\rho}$ and $r$, the average sample correlation coefficient, satisfy. We obtain further bounds on $\hat{\lambda}_i^2$ when all sample correlation coefficients have the same sign, and in that case find $|\underset{\sim}{H}_1| > 0$ whenever $\hat{\rho} > 0$, $p \geq 3$ and $\hat{\rho} < 0$, $p = 3$.

### 3.4.1 Bounds Independent of $p$.

In Corollary 3.3.1 we obtained bounds for $\hat{\lambda}_i^2$ with $\hat{\rho} \geq 0$, independent of the value of $p$. Since $\hat{\rho}$ must be larger than $-1/(p-1)$, no such bounds are possible with $\hat{\rho} < 0$. The bounds (3.3.13) are tabulated in Table 3.4.1 for $\hat{\rho} = 0\ (.01)1$ and sketched in Figure 3.4.1 in §3.4.2. We notice that the bounds almost form straight lines from .3820 and 2.6180 at $\hat{\rho} = 0$ to 0 and 1 at $\hat{\rho} = 1$ (values to four decimal places). In §3.4.2 we calculate comparative bounds from Table 3.3.1 for a wide range of $p$.

### 3.4.2 Tables and Charts for Selected Values when $p \geq 4$.

We now present numerical values for the bounds obtained in §3.3 as indicated in Tables 3.3.1 and 3.3.2. We study here the cases where $p \geq 4$ reserving $p = 3$ for a more exhaustive study in §3.4.3.

In Table 3.4.2 we give values for the upper bound of $\hat{\lambda}_i^2$ from (3.3.11) for $\hat{\rho} = .025(.025).25(.05).75(.025).975$ and $p = 4(1)10(5)50$. We notice that $p$ must exceed 20 for the upper bound to be larger than 2. In

TABLE 3.4.1. Bounds for $\hat{\lambda}_i^2$ independent of p, as given by Corollary 3.3.1; $\hat{\rho}$ = 0(.01)1.

| $\hat{\rho}$ | Bounds Lower | Bounds Upper |
|---|---|---|
| 0.00 | .3820 | 2.6180 |
| .01 | .3764 | 2.6036 |
| .02 | .3709 | 2.5891 |
| .03 | .3655 | 2.5745 |
| .04 | .3600 | 2.5600 |
| .05 | .3546 | 2.5454 |
| .06 | .3491 | 2.5309 |
| .07 | .3437 | 2.5163 |
| .08 | .3383 | 2.5017 |
| .09 | .3330 | 2.4870 |
| .10 | .3276 | 2.4724 |
| .11 | .3223 | 2.4577 |
| .12 | .3170 | 2.4430 |
| .13 | .3117 | 2.4283 |
| .14 | .3064 | 2.4136 |
| .15 | .3012 | 2.3988 |
| .16 | .2960 | 2.3840 |
| .17 | .2908 | 2.3692 |
| .18 | .2856 | 2.3544 |
| .19 | .2804 | 2.3396 |
| .20 | .2753 | 2.3247 |
| .21 | .2702 | 2.3098 |
| .22 | .2651 | 2.2949 |
| .23 | .2600 | 2.2800 |
| .24 | .2550 | 2.2650 |
| .25 | .2500 | 2.2500 |
| .26 | .2450 | 2.2350 |
| .27 | .2401 | 2.2199 |
| .28 | .2351 | 2.2049 |
| .29 | .2302 | 2.1898 |
| .30 | .2253 | 2.1747 |
| .31 | .2205 | 2.1595 |
| .32 | .2156 | 2.1444 |
| .33 | .2108 | 2.1292 |
| .34 | .2061 | 2.1139 |
| .35 | .2013 | 2.0987 |
| .36 | .1966 | 2.0834 |
| .37 | .1919 | 2.0681 |
| .38 | .1873 | 2.0527 |
| .39 | .1826 | 2.0374 |
| .40 | .1780 | 2.0220 |
| .41 | .1735 | 2.0065 |
| .42 | .1690 | 1.9910 |
| .43 | .1645 | 1.9755 |
| .44 | .1600 | 1.9600 |
| .45 | .1556 | 1.9444 |
| .46 | .1512 | 1.9288 |
| .47 | .1468 | 1.9132 |
| .48 | .1425 | 1.8975 |
| .49 | .1382 | 1.8818 |
| .50 | .1340 | 1.8660 |
| .51 | .1298 | 1.8502 |
| .52 | .1256 | 1.8344 |
| .53 | .1215 | 1.8185 |
| .54 | .1174 | 1.8026 |
| .55 | .1133 | 1.7867 |
| .56 | .1093 | 1.7707 |
| .57 | .1054 | 1.7546 |
| .58 | .1015 | 1.7385 |
| .59 | .0976 | 1.7224 |
| .60 | .0938 | 1.7062 |
| .61 | .0900 | 1.6900 |
| .62 | .0863 | 1.6737 |
| .63 | .0826 | 1.6574 |
| .64 | .0790 | 1.6410 |
| .65 | .0754 | 1.6246 |
| .66 | .0719 | 1.6081 |
| .67 | .0684 | 1.5916 |
| .68 | .0650 | 1.5750 |
| .69 | .0617 | 1.5583 |
| .70 | .0584 | 1.5416 |
| .71 | .0552 | 1.5248 |
| .72 | .0520 | 1.5080 |
| .73 | .0489 | 1.4911 |
| .74 | .0459 | 1.4741 |
| .75 | .0429 | 1.4571 |
| .76 | .0400 | 1.4400 |
| .77 | .0372 | 1.4228 |
| .78 | .0344 | 1.4056 |
| .79 | .0318 | 1.3882 |
| .80 | .0292 | 1.3708 |
| .81 | .0267 | 1.3533 |
| .82 | .0243 | 1.3357 |
| .83 | .0219 | 1.3181 |
| .84 | .0197 | 1.3003 |
| .85 | .0175 | 1.2825 |
| .86 | .0155 | 1.2645 |
| .87 | .0136 | 1.2464 |
| .88 | .0117 | 1.2283 |
| .89 | .0100 | 1.2100 |
| .90 | .0084 | 1.1916 |
| .91 | .0069 | 1.1731 |
| .92 | .0055 | 1.1545 |
| .93 | .0043 | 1.1357 |
| .94 | .0032 | 1.1168 |
| .95 | .0023 | 1.0977 |
| .96 | .0015 | 1.0785 |
| .97 | .0008 | 1.0592 |
| .98 | .0004 | 1.0396 |
| .99 | .0001 | 1.0199 |
| 1.00 | 0.0000 | 1.0000 |

TABLE 3.4.2. <u>Upper bounds for</u> $\hat{\lambda}_i^2$ <u>from (3.3.11)</u>; $\hat{\rho}$ = .025(.025).250(.050).750(.025).975, p = 4(1)10(5)50.

| $\hat{\rho}$ | p=4 | 5 | 6 | 7 | 8 | 9 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 45 | 50 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| .025 | 1.07 | 1.09 | 1.12 | 1.14 | 1.16 | 1.18 | 1.20 | 1.29 | 1.37 | 1.44 | 1.51 | 1.57 | 1.62 | 1.67 | 1.71 |
| .050 | 1.14 | 1.18 | 1.21 | 1.25 | 1.29 | 1.32 | 1.35 | 1.49 | 1.60 | 1.69 | 1.76 | 1.83 | 1.88 | 1.93 | 1.97 |
| .075 | 1.19 | 1.25 | 1.30 | 1.34 | 1.39 | 1.43 | 1.47 | 1.62 | 1.74 | 1.83 | 1.90 | 1.96 | 2.01 | 2.05 | 2.08 |
| .100 | 1.24 | 1.31 | 1.37 | 1.42 | 1.47 | 1.52 | 1.56 | 1.72 | 1.83 | 1.92 | 1.96 | 2.03 | 2.08 | 2.11 | 2.14 |
| .125 | 1.29 | 1.36 | 1.43 | 1.48 | 1.54 | 1.58 | 1.62 | 1.79 | 1.89 | 1.97 | 2.03 | 2.08 | 2.11 | 2.14 | 2.17 |
| .150 | 1.33 | 1.41 | 1.47 | 1.53 | 1.59 | 1.63 | 1.68 | 1.83 | 1.93 | 2.00 | 2.06 | 2.10 | 2.13 | 2.15 | 2.17 |
| .175 | 1.36 | 1.44 | 1.51 | 1.57 | 1.63 | 1.67 | 1.72 | 1.86 | 1.96 | 2.02 | 2.07 | 2.10 | 2.13 | 2.15 | 2.17 |
| .200 | 1.39 | 1.47 | 1.55 | 1.61 | 1.66 | 1.70 | 1.74 | 1.88 | 1.97 | 2.03 | 2.07 | 2.10 | 2.13 | 2.15 | 2.16 |
| .225 | 1.41 | 1.50 | 1.57 | 1.63 | 1.68 | 1.72 | 1.76 | 1.89 | 1.97 | 2.03 | 2.06 | 2.09 | 2.11 | 2.13 | 2.15 |
| .250 | 1.43 | 1.54 | 1.59 | 1.65 | 1.70 | 1.74 | 1.77 | 1.90 | 1.97 | 2.02 | 2.05 | 2.06 | 2.10 | 2.11 | 2.13 |
| .300 | 1.46 | 1.55 | 1.61 | 1.67 | 1.71 | 1.75 | 1.78 | 1.89 | 1.95 | 1.99 | 2.02 | 2.04 | 2.05 | 2.07 | 2.08 |
| .350 | 1.48 | 1.56 | 1.62 | 1.67 | 1.71 | 1.75 | 1.77 | 1.87 | 1.92 | 1.95 | 1.97 | 1.99 | 2.00 | 2.01 | 2.02 |
| .400 | 1.49 | 1.56 | 1.62 | 1.66 | 1.70 | 1.73 | 1.75 | 1.83 | 1.87 | 1.90 | 1.92 | 1.93 | 1.94 | 1.95 | 1.96 |
| .450 | 1.48 | 1.55 | 1.60 | 1.64 | 1.67 | 1.70 | 1.72 | 1.79 | 1.82 | 1.84 | 1.86 | 1.87 | 1.88 | 1.89 | 1.89 |
| .500 | 1.47 | 1.53 | 1.58 | 1.61 | 1.64 | 1.66 | 1.68 | 1.73 | 1.77 | 1.78 | 1.80 | 1.81 | 1.81 | 1.82 | 1.82 |
| .550 | 1.45 | 1.50 | 1.54 | 1.57 | 1.60 | 1.61 | 1.63 | 1.68 | 1.70 | 1.72 | 1.73 | 1.74 | 1.74 | 1.75 | 1.75 |
| .600 | 1.42 | 1.47 | 1.50 | 1.53 | 1.55 | 1.56 | 1.58 | 1.62 | 1.64 | 1.65 | 1.66 | 1.67 | 1.67 | 1.68 | 1.68 |
| .650 | 1.39 | 1.43 | 1.46 | 1.48 | 1.50 | 1.51 | 1.52 | 1.55 | 1.57 | 1.58 | 1.59 | 1.59 | 1.60 | 1.60 | 1.60 |
| .700 | 1.35 | 1.38 | 1.41 | 1.42 | 1.44 | 1.45 | 1.46 | 1.48 | 1.50 | 1.51 | 1.51 | 1.52 | 1.52 | 1.52 | 1.52 |
| .750 | 1.30 | 1.33 | 1.35 | 1.37 | 1.38 | 1.38 | 1.39 | 1.41 | 1.42 | 1.43 | 1.43 | 1.44 | 1.44 | 1.44 | 1.44 |
| .775 | 1.28 | 1.30 | 1.32 | 1.33 | 1.34 | 1.35 | 1.36 | 1.38 | 1.39 | 1.39 | 1.39 | 1.40 | 1.40 | 1.40 | 1.40 |
| .800 | 1.25 | 1.28 | 1.29 | 1.30 | 1.31 | 1.32 | 1.32 | 1.34 | 1.35 | 1.35 | 1.35 | 1.36 | 1.36 | 1.36 | 1.36 |
| .825 | 1.23 | 1.25 | 1.26 | 1.27 | 1.27 | 1.28 | 1.29 | 1.30 | 1.31 | 1.31 | 1.31 | 1.31 | 1.32 | 1.32 | 1.32 |
| .850 | 1.20 | 1.21 | 1.23 | 1.23 | 1.24 | 1.24 | 1.25 | 1.26 | 1.26 | 1.27 | 1.27 | 1.27 | 1.27 | 1.27 | 1.28 |
| .875 | 1.17 | 1.18 | 1.19 | 1.20 | 1.20 | 1.21 | 1.21 | 1.22 | 1.22 | 1.23 | 1.23 | 1.23 | 1.23 | 1.23 | 1.23 |
| .900 | 1.14 | 1.15 | 1.16 | 1.16 | 1.16 | 1.17 | 1.17 | 1.18 | 1.18 | 1.18 | 1.18 | 1.19 | 1.19 | 1.19 | 1.19 |
| .925 | 1.11 | 1.11 | 1.12 | 1.12 | 1.13 | 1.13 | 1.13 | 1.13 | 1.14 | 1.14 | 1.14 | 1.14 | 1.14 | 1.14 | 1.14 |
| .950 | 1.07 | 1.08 | 1.08 | 1.08 | 1.08 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.09 | 1.10 | 1.10 | 1.10 |
| .975 | 1.04 | 1.04 | 1.04 | 1.04 | 1.04 | 1.04 | 1.04 | 1.05 | 1.05 | 1.05 | 1.05 | 1.05 | 1.05 | 1.05 | 1.05 |

Table 3.4.3 we present values for lower bounds of $\hat{\lambda}_i^2$ from (3.3.11) and (3.3.38) for $\hat{\rho} = .01(.01).10(.05).95$ and $p = 4(1)10, 25, 50$. For $p = 4$ only (3.3.38) is given (cf. Theorem 3.3.3). For $p = 5(1)10$ we present both bounds and indicate where they cross by a dividing line. We note that as $p$ increases from 5 to 10 the range for which (3.3.11) is stronger increases from $\hat{\rho} \leq .50$ to $\hat{\rho} \leq .85$. For $p = 25$ and 50 only (3.3.11) is given. As $p$ increases the range of values of (3.3.38) which are negative also increases and we present this at the bottom of Table 3.4.3 for $p \geq 6$. We sketch the upper and lower bounds from Tables 3.4.2 and 3.4.3 for $p = 4$ and 25 in Figure 3.4.1, together with the bounds independent of $p$ from Table 3.4.1. We notice that the convergence of (3.3.11) is rather fast, the more so for the lower bound.

For $\hat{\rho} < 0$ we tabulate the bounds against $\hat{\rho}$ subdivided into fiftieths of $-1/q$, the lower limit of $\hat{\rho}$. For $\hat{\rho}q$ held fixed at $-k$, say, the lower bound (3.3.62) converges to a limit as $p \to \infty$. We have

$$(3.4.1) \qquad \frac{\sqrt{\frac{k^2p^2}{q^2} + 4(1 + \frac{k}{q})(1 - k)^2} - \frac{kp}{q}}{2(1-k)} < \hat{\lambda}_i .$$

As $p \to \infty$, $p/q \to 1$ and we obtain in the limit

$$(3.4.2) \qquad \frac{\sqrt{k^2 + 4(1-k)^2} - k}{2(1-k)} < \hat{\lambda}_i .$$

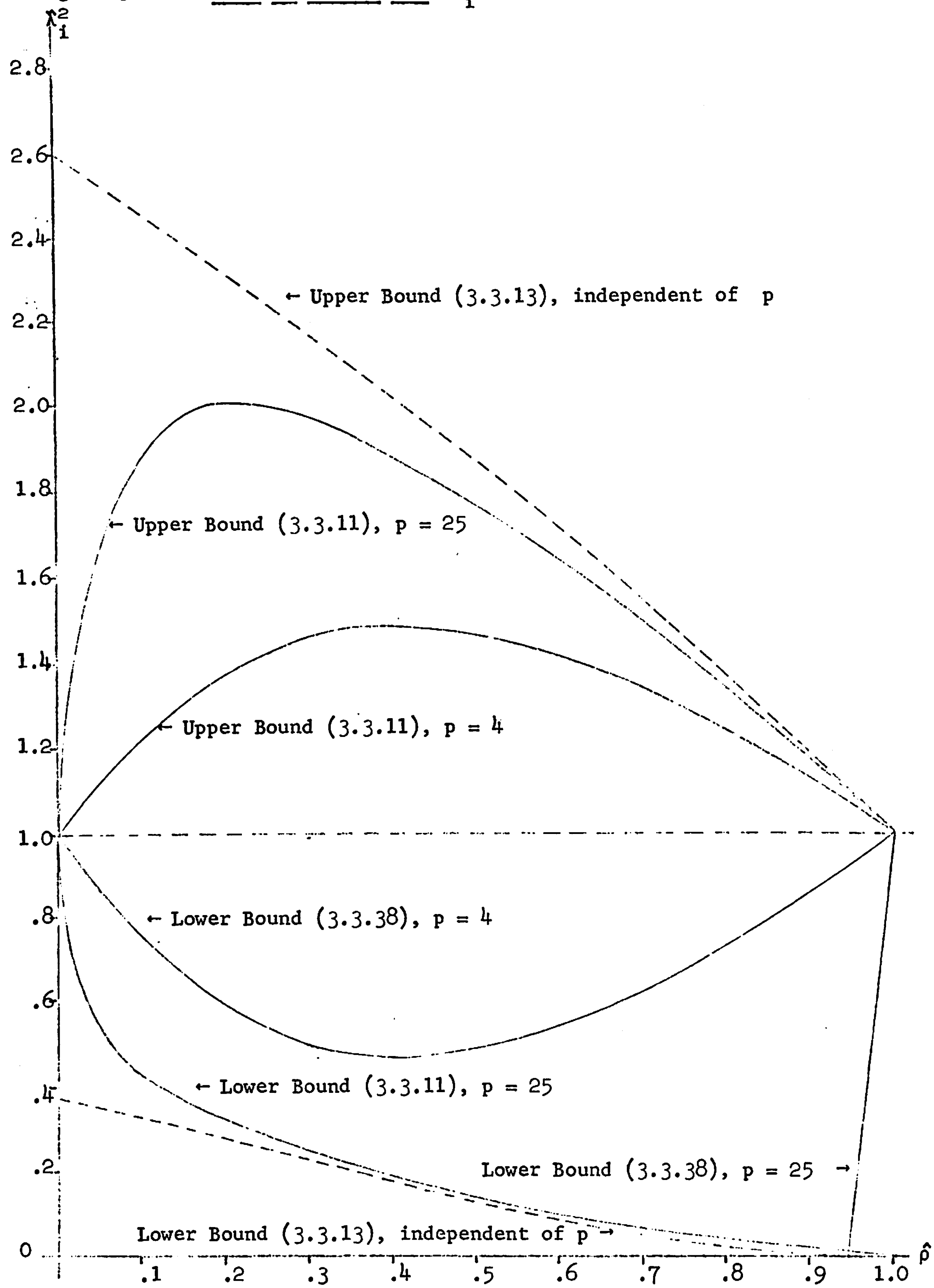
Squaring both sides yields

$$(3.4.3) \qquad \frac{3k^2 - 4k + 2 - k\sqrt{k^2 + 4(1-k)^2}}{2(1-k)^2} < \hat{\lambda}_i^2 .$$

TABLE 3.4.3. Lower bounds for $\hat{\lambda}_i^2$ from (3.3.11/38); $\hat{\rho}$ = .01(.01).10(.05).95, p = 4(1)10,25,50.

| p | 4 | 5 | | 6 | | 7 | | 8 | | 9 | | 10 | | 25 | 50 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\hat{\rho}$ | (38) | (38) | (11) | (38) | (11) | (38) | (11) | (38) | (11) | (38) | (11) | (38) | (11) | (11) | (11) |
| .01 | .97 | .94 | .96 | .90 | .95 | .86 | .94 | .80 | .94 | .73 | .93 | .66 | .92 | .82 | .72 |
| .02 | .94 | .89 | .93 | .81 | .91 | .72 | .89 | .61 | .88 | .49 | .87 | .35 | .85 | .71 | .60 |
| .03 | .92 | .83 | .89 | .73 | .87 | .59 | .85 | .44 | .83 | .26 | .81 | .06 | .80 | .64 | .54 |
| .04 | .89 | .78 | .86 | .64 | .83 | .48 | .81 | .28 | .79 | .06 | .77 | -.19 | .75 | .59 | .50 |
| .05 | .86 | .73 | .83 | .57 | .80 | .37 | .77 | .13 | .75 | -.13 | .73 | -.42 | .71 | .55 | .47 |
| .06 | .84 | .69 | .80 | .50 | .77 | .26 | .74 | -.00 | .71 | -.31 | .69 | -.64 | .67 | .52 | .45 |
| .07 | .82 | .65 | .77 | .43 | .74 | .17 | .71 | -.13 | .68 | -.46 | .66 | -.83 | .64 | .50 | .43 |
| .08 | .80 | .61 | .75 | .37 | .71 | .08 | .68 | -.25 | .66 | -.61 | .63 | -1.01 | .61 | .47 | .41 |
| .09 | .77 | .57 | .72 | .31 | .69 | -.00 | .66 | -.35 | .63 | -.74 | .61 | -1.17 | .59 | .46 | .40 |
| .10 | .75 | .53 | .70 | .25 | .66 | -.08 | .63 | -.45 | .61 | -.87 | .58 | -1.31 | .56 | .44 | .39 |
| .15 | .67 | .38 | .60 | .02 | .56 | -.39 | .53 | -.85 | .51 | -1.34 | .49 | -1.87 | .47 | .38 | .34 |
| .20 | .60 | .26 | .52 | -.14 | .48 | -.60 | .45 | -1.10 | .43 | -1.64 | .42 | -2.20 | .40 | .33 | .30 |
| .25 | .55 | .18 | .44 | -.25 | .41 | -.73 | .39 | -1.25 | .37 | -1.80 | .36 | -2.37 | .35 | .29 | .27 |
| .30 | .52 | .13 | .38 | -.31 | .36 | -.80 | .34 | -1.32 | .32 | -1.87 | .31 | -2.44 | .30 | .26 | .24 |
| .35 | .49 | .10 | .33 | -.34 | .31 | -.82 | .29 | -1.33 | .28 | -1.86 | .27 | -2.41 | .26 | .23 | .21 |
| .40 | .49 | .10 | .28 | -.33 | .26 | -.80 | .25 | -1.29 | .24 | -1.80 | .23 | -2.32 | .23 | .20 | .19 |
| .45 | .49 | .11 | .24 | -.30 | .22 | -.75 | .21 | -1.21 | .20 | -1.69 | .20 | -2.18 | .19 | .17 | .16 |
| .50 | .50 | .14 | .20 | -.25 | .18 | -.67 | .18 | -1.10 | .17 | -1.55 | .17 | -2.00 | .16 | .15 | .14 |
| .55 | .52 | .19 | .16 | -.18 | .15 | -.56 | .15 | -.96 | .14 | -1.37 | .14 | -1.78 | .14 | .12 | .12 |
| .60 | .55 | .24 | .13 | -.09 | .12 | -.44 | .12 | -.80 | .11 | -1.17 | .11 | -1.54 | .11 | .10 | .10 |
| .65 | .59 | .31 | .10 | .01 | .10 | -.30 | .09 | -.62 | .09 | -.95 | .09 | -1.28 | .09 | .08 | .08 |
| .70 | .63 | .39 | .08 | .12 | .07 | -.15 | .07 | -.42 | .07 | -.70 | .07 | -.99 | .07 | .06 | .06 |
| .75 | .68 | .47 | .05 | .25 | .05 | .02 | .05 | -.21 | .05 | -.45 | .05 | -.69 | .05 | .04 | .04 |
| .80 | .73 | .56 | .04 | .36 | .03 | .20 | .03 | .01 | .03 | -.18 | .03 | -.37 | .03 | .03 | .03 |
| .85 | .79 | .66 | .02 | .53 | .02 | .39 | .02 | .25 | .02 | .10 | .02 | -.04 | .02 | .02 | .02 |
| .90 | .86 | .77 | .01 | .68 | .01 | .58 | .01 | .49 | .01 | .39 | .01 | .30 | .01 | .01 | .01 |
| .95 | .93 | .88 | .00 | .84 | .00 | .79 | .00 | .74 | .00 | .69 | .00 | .64 | .00 | .00 | .00 |
| (38) NEGATIVE BETWEEN | | | | .1551 | | .0896 | | .0597 | | .0429 | | .032 | | .004 | .001 |
| AND | | | | .6449 | | .7437 | | .7974 | | .8521 | | .857 | | .955 | .979 |

Figure 3.4.1. Plot of bounds for $\hat{\lambda}_i^2$; $0 < \hat{\rho} < 1$.



As $\hat{\rho} \to 0$, $k \to 0$ and the bounds tend to 1. As $\hat{\rho} \to -1/q$, $k \to 1$ and the bounds tend to 0, as observed below Theorem 3.3.5. In Table 3.4.4 we give values of the limiting bound (3.4.3) as well as the bounds from (3.3.62) for $p = 4$ and 5, with $\hat{\rho}q = -49/50(1/50)-1/50$. The convergence is very fast; differences between (3.4.3) and the bounds from (3.3.62) for $p = 4$ are all below .02. We notice that the lower bounds increase to their limiting values. In Figure 3.4.2 we sketch (3.4.3). We present values of the upper bounds from (3.3.62) and (3.3.65) for $p = 4(1)8$ in Table 3.4.5. When $p = 4$ only (3.3.65) is tabulated (cf. Theorem 3.3.7). Table 3.4.6 continues the tabulation for $p = 9, 10, 25, 50$ and in both tables $\hat{\rho} = -29/30q(1/30q) - 1/30q$. We notice that (3.3.65) is the stronger bound nearer $-1/q$ in a range decreasing from $\hat{\rho} \leq -20/30q$ when $p = 4$ to $\hat{\rho} \leq -27/30q$ when $p = 50$. For $\hat{\rho}$ near $-1/q$ the bound from (3.3.62) may exceed $p$; in such cases we tabulate the value $p$ instead in Tables 3.4.5 and 3.4.6. The crossing points of (3.3.62) and (3.3.65) are indicated by dividing lines. The upper bounds for $p = 4$ and 6 are plotted in Figure 3.4.2. As with the lower bound, when $\hat{\rho}q$ is held fixed at $-k$, say, the upper bound (3.3.62) converges to a limit as $p \to \infty$. We obtain similarly to (3.4.3),

$$(3.4.4) \qquad \lambda_i^2 < \frac{3k^2 - 4k + 2 + k\sqrt{k^2 + 4(1-k)^2}}{2(1-k)^2}$$

Values of (3.4.4) are tabulated in Table 3.4.6. It is clear that convergence to (3.4.4) is much slower than to (3.4.3). Figure 3.4.2 includes a plot of (3.4.4).

TABLE 3.4.4. Lower bounds for $\hat{\lambda}_i^2$ from (3.3.62) for $p = 4$ and 5 and limiting values (3.4.3); $\hat{\rho}q = \frac{-49}{50}(\frac{1}{50})\frac{-1}{50}$ .

| $\hat{\rho}q$ | p=4 $\hat{\rho}$ | p=4 Bound | p=5 $\hat{\rho}$ | p=5 Bound | (3.4.3) |
|---|---|---|---|---|---|
| -49/50 | -.3267 | .0004 | -.2450 | .0004 | .0004 |
| -48/50 | -.3200 | .0017 | -.2400 | .0017 | .0017 |
| -47/50 | -.3133 | .0039 | -.2350 | .0040 | .0040 |
| -46/50 | -.3067 | .0072 | -.2300 | .0072 | .0074 |
| -45/50 | -.3000 | .0115 | -.2250 | .0116 | .0120 |
| -44/50 | -.2933 | .0170 | -.2200 | .0172 | .0179 |
| -43/50 | -.2867 | .0238 | -.2150 | .0241 | .0252 |
| -42/50 | -.2800 | .0318 | -.2100 | .0322 | .0339 |
| -41/50 | -.2733 | .0412 | -.2050 | .0417 | .0440 |
| -40/50 | -.2667 | .0519 | -.2000 | .0527 | .0557 |
| -39/50 | -.2600 | .0640 | -.1950 | .0650 | .0690 |
| -38/50 | -.2533 | .0775 | -.1900 | .0788 | .0837 |
| -37/50 | -.2467 | .0925 | -.1850 | .0940 | .1000 |
| -36/50 | -.2400 | .1088 | -.1800 | .1107 | .1177 |
| -35/50 | -.2333 | .1266 | -.1750 | .1287 | .1368 |
| -34/50 | -.2267 | .1456 | -.1700 | .1480 | .1573 |
| -33/50 | -.2200 | .1659 | -.1650 | .1686 | .1789 |
| -32/50 | -.2133 | .1873 | -.1600 | .1904 | .2017 |
| -31/50 | -.2067 | .2099 | -.1550 | .2132 | .2254 |
| -30/50 | -.2000 | .2335 | -.1500 | .2371 | .2500 |
| -29/50 | -.1933 | .2580 | -.1450 | .2618 | .2754 |
| -28/50 | -.1867 | .2834 | -.1400 | .2873 | .3013 |
| -27/50 | -.1800 | .3094 | -.1350 | .3135 | .3278 |
| -26/50 | -.1733 | .3360 | -.1300 | .3402 | .3548 |
| -25/50 | -.1667 | .3632 | -.1250 | .3674 | .3820 |
| -24/50 | -.1600 | .3907 | -.1200 | .3949 | .4094 |
| -23/50 | -.1533 | .4185 | -.1150 | .4227 | .4369 |
| -22/50 | -.1467 | .4466 | -.1100 | .4507 | .4645 |
| -21/50 | -.1400 | .4747 | -.1050 | .4787 | .4920 |
| -20/50 | -.1333 | .5029 | -.1000 | .5068 | .5195 |
| -19/50 | -.1267 | .5311 | -.0950 | .5348 | .5468 |
| -18/50 | -.1200 | .5592 | -.0900 | .5626 | .5739 |
| -17/50 | -.1133 | .5871 | -.0850 | .5903 | .6007 |
| -16/50 | -.1067 | .6147 | -.0800 | .6177 | .6273 |
| -15/50 | -.1000 | .6421 | -.0750 | .6448 | .6535 |
| -14/50 | -.0933 | .6692 | -.0700 | .6716 | .6794 |
| -13/50 | -.0867 | .6959 | -.0650 | .6981 | .7050 |
| -12/50 | -.0800 | .7222 | -.0600 | .7241 | .7302 |
| -11/50 | -.0733 | .7481 | -.0550 | .7497 | .7549 |
| -10/50 | -.0667 | .7735 | -.0500 | .7749 | .7793 |
| -9/50 | -.0600 | .7985 | -.0450 | .7996 | .8033 |
| -8/50 | -.0533 | .8229 | -.0400 | .8239 | .8268 |
| -7/50 | -.0467 | .8469 | -.0350 | .8477 | .8499 |
| -6/50 | -.0400 | .8704 | -.0300 | .8709 | .8726 |
| -5/50 | -.0333 | .8933 | -.0250 | .8937 | .8949 |
| -4/50 | -.0267 | .9157 | -.0200 | .9160 | .9167 |
| -3/50 | -.0200 | .9376 | -.0150 | .9377 | .9382 |
| -2/50 | -.0133 | .9589 | -.0100 | .9590 | .9592 |
| -1/50 | -.0067 | .9797 | -.0050 | .9797 | .9798 |

Figure 3.4.2. Plot of bounds for $\hat{\lambda}_i^2$; $-1/q < \hat{\rho} < 0$.

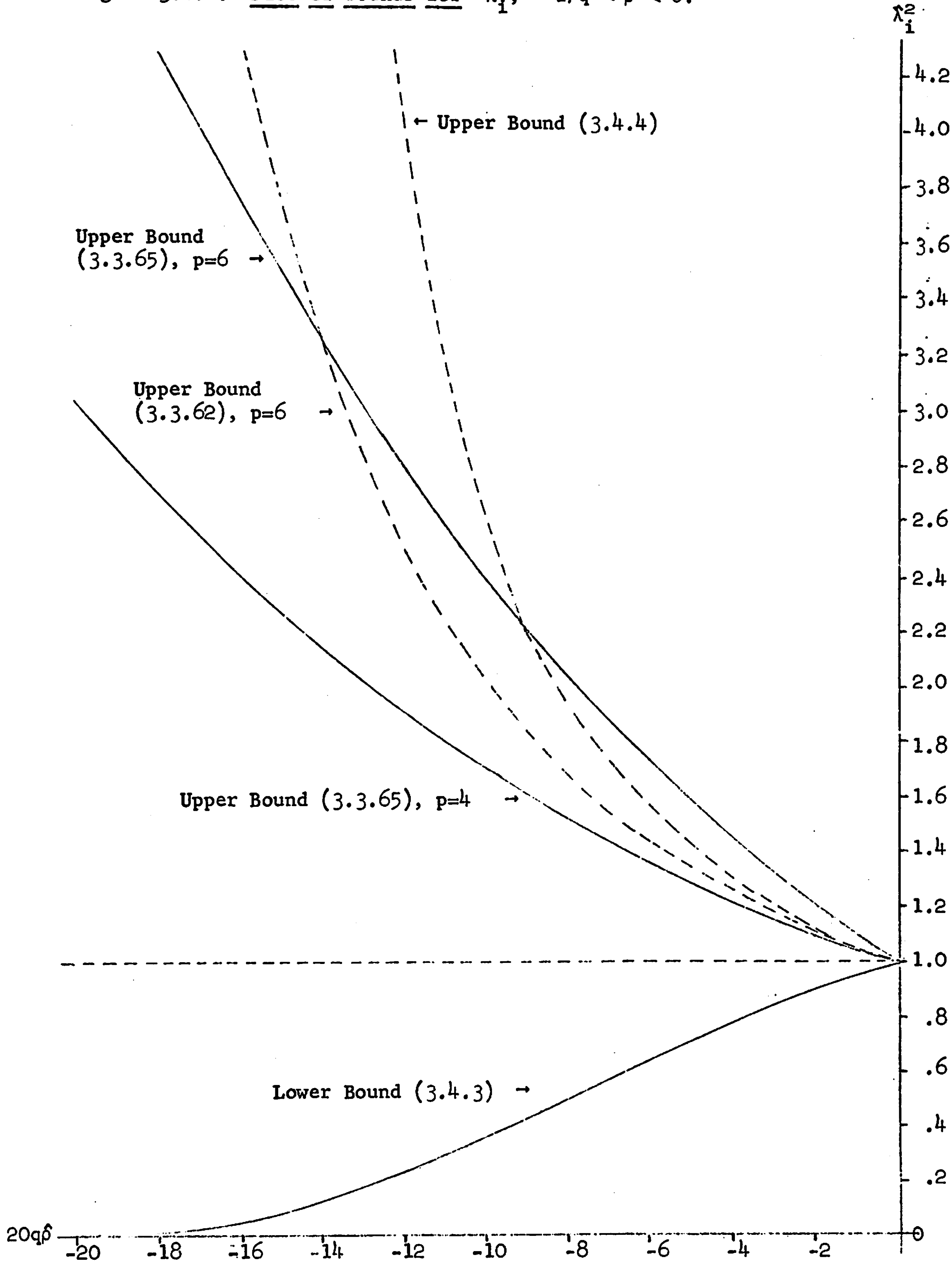


TABLE 3.4.5. Upper bounds for $\hat{\lambda}_i^2$ from (3.3.62/65); $\hat{\rho}$ = -29/30q(1/30q)-1/30q, p = 4(1)8.

| p=4 | | p=5 | | | p=6 | | | p=7 | | | p=8 | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\hat{\rho}$ | (65) | $\hat{\rho}$ | (65) | (62) | $\hat{\rho}$ | (65) | (62) | $\hat{\rho}$ | (65) | (62) | $\hat{\rho}$ | (65) | (62) |
| -.322 | 2.89 | -.242 | 3.82 | 5.00 | -.193 | 4.76 | 6.00 | -.161 | 5.70 | 7.00 | -.138 | 6.63 | 8.00 |
| -.311 | 2.78 | -.233 | 3.66 | 5.00 | -.187 | 4.53 | 6.00 | -.156 | 5.41 | 7.00 | -.133 | 6.29 | 8.00 |
| -.300 | 2.67 | -.225 | 3.50 | 4.62 | -.180 | 4.32 | 6.00 | -.150 | 5.14 | 7.00 | -.129 | 5.96 | 8.00 |
| -.289 | 2.57 | -.217 | 3.34 | 4.21 | -.173 | 4.11 | 5.33 | -.144 | 4.88 | 6.44 | -.124 | 5.65 | 7.53 |
| -.278 | 2.47 | -.208 | 3.20 | 3.85 | -.167 | 3.92 | 4.75 | -.139 | 4.63 | 5.61 | -.119 | 5.35 | 6.42 |
| -.267 | 2.38 | -.200 | 3.06 | 3.53 | -.160 | 3.73 | 4.25 | -.133 | 4.40 | 4.92 | -.114 | 5.07 | 5.54 |
| -.256 | 2.29 | -.192 | 2.92 | 3.25 | -.153 | 3.55 | 3.83 | -.128 | 4.18 | 4.36 | -.110 | 4.80 | 4.83 |
| -.244 | 2.21 | -.183 | 2.80 | 3.01 | -.147 | 3.38 | 2.48 | -.122 | 3.96 | 3.88 | -.105 | 4.54 | 4.24 |
| -.233 | 2.13 | -.175 | 2.67 | 2.79 | -.140 | 3.22 | 3.17 | -.117 | 3.76 | 3.49 | -.100 | 4.30 | 3.76 |
| -.222 | 2.05 | -.167 | 2.56 | 2.60 | -.133 | 3.06 | 2.90 | -.111 | 3.56 | 3.15 | -.095 | 4.07 | 3.37 |
| -.211 | 1.97 | -.158 | 2.44 | 2.43 | -.127 | 2.91 | 2.67 | -.106 | 3.38 | 2.87 | -.090 | 3.84 | 3.03 |
| -.200 | 1.90 | -.150 | 2.34 | 2.27 | -.120 | 2.77 | 2.47 | -.100 | 3.20 | 2.62 | -.086 | 3.63 | 2.75 |
| -.189 | 1.83 | -.142 | 2.23 | 2.13 | -.113 | 2.63 | 2.29 | -.094 | 3.03 | 2.41 | -.081 | 3.43 | 2.51 |
| -.178 | 1.76 | -.133 | 2.13 | 2.01 | -.107 | 2.50 | 2.13 | -.089 | 2.87 | 2.23 | -.076 | 3.23 | 2.31 |
| -.167 | 1.70 | -.125 | 2.04 | 1.90 | -.100 | 2.37 | 2.00 | -.083 | 2.71 | 2.07 | -.071 | 3.05 | 2.13 |
| -.156 | 1.64 | -.117 | 1.95 | 1.80 | -.093 | 2.25 | 1.87 | -.078 | 2.56 | 1.93 | -.067 | 2.87 | 1.98 |
| -.144 | 1.58 | -.108 | 1.86 | 1.70 | -.087 | 2.14 | 1.77 | -.072 | 2.42 | 1.81 | -.062 | 2.70 | 1.85 |
| -.133 | 1.52 | -.100 | 1.78 | 1.62 | -.080 | 2.03 | 1.67 | -.067 | 2.28 | 1.70 | -.057 | 2.53 | 1.73 |
| -.122 | 1.47 | -.092 | 1.70 | 1.54 | -.073 | 1.92 | 1.58 | -.061 | 2.15 | 1.61 | -.052 | 2.37 | 1.63 |
| -.111 | 1.42 | -.083 | 1.62 | 1.47 | -.067 | 1.82 | 1.50 | -.056 | 2.02 | 1.52 | -.048 | 2.22 | 1.54 |
| -.100 | 1.37 | -.075 | 1.55 | 1.41 | -.060 | 1.72 | 1.43 | -.050 | 1.90 | 1.44 | -.043 | 2.08 | 1.46 |
| -.089 | 1.32 | -.067 | 1.47 | 1.35 | -.053 | 1.63 | 1.36 | -.044 | 1.78 | 1.38 | -.038 | 1.94 | 1.36 |
| -.078 | 1.27 | -.058 | 1.41 | 1.29 | -.047 | 1.54 | 1.31 | -.039 | 1.67 | 1.31 | -.033 | 1.80 | 1.32 |
| -.067 | 1.23 | -.050 | 1.34 | 1.24 | -.040 | 1.45 | 1.25 | -.033 | 1.56 | 1.26 | -.029 | 1.67 | 1.26 |
| -.056 | 1.19 | -.042 | 1.28 | 1.20 | -.033 | 1.37 | 1.20 | -.028 | 1.46 | 1.20 | -.024 | 1.55 | 1.21 |
| -.044 | 1.15 | -.033 | 1.22 | 1.15 | -.027 | 1.29 | 1.15 | -.022 | 1.36 | 1.16 | -.019 | 1.43 | 1.16 |
| -.033 | 1.11 | -.025 | 1.16 | 1.11 | -.020 | 1.21 | 1.11 | -.017 | 1.27 | 1.11 | -.014 | 1.32 | 1.11 |
| -.022 | 1.07 | -.017 | 1.10 | 1.07 | -.013 | 1.14 | 1.07 | -.011 | 1.17 | 1.07 | -.010 | 1.21 | 1.07 |
| -.011 | 1.03 | -.008 | 1.05 | 1.03 | -.007 | 1.07 | 1.03 | -.006 | 1.08 | 1.03 | -.005 | 1.10 | 1.03 |

TABLE 3.4.6. Upper bounds for $\hat{\lambda}_i^2$ from (3.3.62/65), (3.4.4); $\hat{\rho}$ = -29/30q(1/30q)-1/30q, p = 9,10,25,50.

| p=9 | | | p=10 | | | p=25 | | | p=50 | | | Limit |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ρ | (65) | (62) | ρ | (65) | (62) | ρ | (65) | (62) | ρ | (65) | (62) | (3.4.4) |
| -.121 | 7.57 | 9.00 | -.107 | 8.51 | 10.00 | -.0403 | 22.54 | 25.00 | -.0197 | 45.93 | 50.00 | 843.00 |
| -.117 | 7.17 | 9.00 | -.104 | 8.04 | 10.00 | -.0389 | 21.17 | 25.00 | -.0190 | 43.05 | 50.00 | 197.99 |
| -.112 | 6.78 | 9.00 | -.100 | 7.60 | 10.00 | -.0375 | 19.88 | 25.00 | -.0184 | 40.34 | 46.59 | 82.99 |
| -.108 | 6.42 | 8.58 | -.096 | 7.18 | 9.61 | -.0361 | 18.66 | 20.61 | -.0177 | 37.78 | 29.06 | 44.23 |
| -.104 | 6.07 | 7.20 | -.093 | 6.78 | 7.93 | -.0347 | 17.51 | 14.94 | -.0170 | 35.37 | 19.61 | 26.96 |
| -.100 | 5.74 | 6.11 | -.089 | 6.41 | 6.64 | -.0333 | 16.42 | 11.26 | -.0163 | 33.09 | 14.00 | 17.94 |
| -.096 | 5.42 | 5.25 | -.085 | 6.05 | 5.64 | -.0319 | 15.38 | 8.76 | -.0156 | 30.93 | 10.45 | 12.72 |
| -.092 | 5.13 | 4.56 | -.081 | 5.71 | 4.85 | -.0306 | 14.40 | 7.01 | -.0150 | 28.88 | 8.09 | 9.46 |
| -.087 | 4.84 | 4.00 | -.078 | 5.38 | 4.21 | -.0292 | 13.47 | 5.73 | -.0143 | 26.93 | 6.45 | 7.31 |
| -.083 | 4.57 | 3.55 | -.074 | 5.07 | 3.70 | -.0278 | 12.58 | 4.79 | -.0136 | 25.08 | 5.27 | 5.83 |
| -.079 | 4.31 | 3.17 | -.070 | 4.77 | 3.29 | -.0264 | 11.73 | 4.07 | -.0129 | 23.32 | 4.40 | 4.77 |
| -.075 | 4.06 | 2.86 | -.067 | 4.49 | 2.95 | -.0250 | 10.93 | 3.52 | -.0122 | 21.64 | 3.75 | 4.00 |
| -.071 | 3.82 | 2.59 | -.063 | 4.22 | 2.66 | -.0236 | 10.16 | 3.06 | -.0116 | 20.04 | 3.24 | 3.42 |
| -.067 | 3.60 | 2.37 | -.059 | 3.96 | 2.42 | -.0222 | 9.42 | 2.73 | -.0109 | 18.51 | 2.85 | 2.97 |
| -.063 | 3.38 | 2.18 | -.056 | 3.71 | 2.22 | -.0208 | 8.72 | 2.45 | -.0102 | 17.05 | 2.53 | 2.62 |
| -.058 | 3.17 | 2.01 | -.052 | 3.48 | 2.04 | -.0194 | 8.05 | 2.21 | -.0095 | 15.66 | 2.27 | 2.34 |
| -.054 | 2.97 | 1.87 | -.048 | 3.25 | 1.90 | -.0181 | 7.40 | 2.02 | -.0088 | 14.32 | 2.07 | 2.11 |
| -.050 | 2.78 | 1.75 | -.044 | 3.03 | 1.77 | -.0167 | 6.79 | 1.86 | -.0082 | 13.04 | 1.89 | 1.92 |
| -.046 | 2.60 | 1.64 | -.041 | 2.82 | 1.66 | -.0153 | 6.19 | 1.72 | -.0075 | 11.81 | 1.75 | 1.77 |
| -.042 | 2.42 | 1.55 | -.037 | 2.62 | 1.56 | -.0139 | 5.63 | 1.61 | -.0068 | 10.63 | 1.62 | 1.64 |
| -.037 | 2.25 | 1.46 | -.033 | 2.43 | 1.47 | -.0125 | 5.08 | 1.51 | -.0061 | 9.49 | 1.52 | 1.53 |
| -.033 | 2.09 | 1.39 | -.030 | 2.25 | 1.39 | -.0111 | 4.55 | 1.42 | -.0054 | 8.40 | 1.43 | 1.44 |
| -.029 | 1.94 | 1.32 | -.026 | 2.07 | 1.33 | -.0097 | 4.05 | 1.34 | -.0048 | 7.35 | 1.35 | 1.35 |
| -.025 | 1.79 | 1.26 | -.022 | 1.90 | 1.26 | -.0083 | 3.56 | 1.28 | -.0041 | 6.34 | 1.28 | 1.28 |
| -.021 | 1.64 | 1.21 | -.019 | 1.73 | 1.21 | -.0069 | 3.10 | 1.22 | -.0034 | 5.37 | 1.22 | 1.22 |
| -.017 | 1.50 | 1.16 | -.015 | 1.58 | 1.16 | -.0056 | 2.65 | 1.16 | -.0027 | 4.43 | 1.16 | 1.17 |
| -.012 | 1.37 | 1.11 | -.011 | 1.42 | 1.11 | -.0042 | 2.21 | 1.12 | -.0020 | 3.53 | 1.12 | 1.12 |
| -.008 | 1.24 | 1.07 | -.007 | 1.28 | 1.07 | -.0028 | 1.79 | 1.07 | -.0014 | 2.66 | 1.07 | 1.07 |
| -.004 | 1.12 | 1.03 | -.004 | 1.14 | 1.03 | -.0014 | 1.39 | 1.03 | -.0007 | 1.81 | 1.04 | 1.04 |

Comparison of Figures 3.4.1 and 3.4.2 indicates that the bounds for positive $\hat{\rho}$ are much tighter than those for negative $\hat{\rho}$, with a sharp divergence of the upper bound for $\hat{\rho}$ negative nearing $-1/q$. We now apply these bounds to Corollary 3.2.1 in an attempt to prove $|\underset{\sim}{H}_1| > 0$. We find that the bounds are tight enough to establish

$$(3.4.5) \qquad \hat{\rho}^2 qMm - (M-1)(1-m) = d,$$

say, positive and thus $|\underset{\sim}{H}_1| > 0$, for most positive $\hat{\rho}$ but no negative $\hat{\rho}$, $p \geq 4$. In Table 3.4.7 we give values of $d$ for $\hat{\rho} = .10(.01).40$ and $p = 4(1)15$. Table 3.4.8 continues the tabulation for $p = 20(5)50(10)100$. We used (3.2.45) and (3.2.46) in computing (3.4.5), with $\hat{\lambda}^2_M$ from (3.3.11) and $\hat{\lambda}^2_m$ the larger of the lower bounds from (3.3.11) and (3.3.38). We have not tabulated $d$ for $\hat{\rho} < .10$ since we found all values negative and for $\hat{\rho} > .40$ since we found all values positive and increasing in $\hat{\rho}$. The region of interest is where $d = 0$ and this is sketched in the two tables. For $p = 4$, we find $|\underset{\sim}{H}_1| > 0$ for $\hat{\rho} \geq .30$ while for $p = 5$ we need $\hat{\rho} \geq .37$. Then as $p$ increases the range of positive $d$ also increases to $\hat{\rho} \geq .13$ for $p = 100$. All values correct to two decimal places. The reason for the "jump" between $p = 4$ and $5$ is the increased strength of the bound (3.3.38) when $p = 4$ (cf. Theorem 3.3.3).

We can also apply the above bounds on $\hat{\lambda}^2_i$ to sufficient conditions for $|\underset{\sim}{H}_1| > 0$ other than $d > 0$. It suffices for (3.2.13) that

$$(3.4.6) \qquad \tfrac{1}{2}\mathrm{ch}_p(\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2}) > 1/(1+\hat{\rho}^2 q).$$

Substituting $m$ from Corollary 3.2.1 into the left-hand side of (3.4.6) yields

TABLE 3.4.7. Values of (3.4.5); $\hat{\rho}$ = .10(.01).40, p = 4(1)15. (Positive entries imply $|\underset{\sim}{H}_1| > 0$.)

| $\hat{\rho}$ | p=4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| .10 | -.02 | -.03 | -.05 | -.06 | -.08 | -.09 | -.11 | -.12 | -.13 | -.15 | -.16 | -.17 |
| .11 | -.02 | -.04 | -.05 | -.07 | -.09 | -.10 | -.12 | -.13 | -.15 | -.16 | -.17 | -.18 |
| .12 | -.02 | -.04 | -.06 | -.08 | -.10 | -.11 | -.13 | -.14 | -.15 | -.17 | -.18 | -.19 |
| .13 | -.02 | -.05 | -.07 | -.08 | -.10 | -.12 | -.13 | -.15 | -.16 | -.17 | -.18 | -.19 |
| .14 | -.03 | -.05 | -.07 | -.09 | -.11 | -.13 | -.14 | -.15 | -.17 | -.18 | -.19 | -.20 |
| .15 | -.03 | -.05 | -.08 | -.10 | -.11 | -.13 | -.15 | -.16 | -.17 | -.18 | -.19 | -.20 |
| .16 | -.03 | -.06 | -.08 | -.10 | -.12 | -.14 | -.15 | -.16 | -.17 | -.18 | -.19 | -.20 |
| .17 | -.03 | -.06 | -.08 | -.11 | -.12 | -.14 | -.15 | -.16 | -.17 | -.18 | -.19 | -.19 |
| .18 | -.03 | -.07 | -.09 | -.11 | -.13 | -.14 | -.15 | -.16 | -.17 | -.18 | -.18 | -.18 |
| .19 | -.03 | -.07 | -.09 | -.11 | -.13 | -.14 | -.15 | -.16 | -.17 | -.17 | -.17 | -.17 |
| .20 | -.03 | -.07 | -.09 | -.11 | -.13 | -.14 | -.15 | -.16 | -.16 | -.16 | -.16 | -.16 |
| .21 | -.03 | -.07 | -.09 | -.11 | -.13 | -.14 | -.14 | -.15 | -.15 | -.15 | -.15 | -.14 |
| .22 | -.03 | -.07 | -.10 | -.11 | -.12 | -.13 | -.14 | -.14 | -.14 | -.14 | -.13 | -.12 |
| .23 | -.03 | -.07 | -.09 | -.11 | -.12 | -.13 | -.13 | -.13 | -.13 | -.12 | -.11 | -.10 |
| .24 | -.03 | -.07 | -.09 | -.11 | -.12 | -.12 | -.12 | -.12 | -.11 | -.10 | -.09 | -.07 |
| .25 | -.02 | -.07 | -.09 | -.10 | -.11 | -.11 | -.11 | -.10 | -.09 | -.08 | -.06 | -.04 |
| .26 | -.02 | -.07 | -.09 | -.10 | -.10 | -.10 | -.09 | -.08 | -.07 | -.05 | -.03 | -.01 |
| .27 | -.01 | -.07 | -.08 | -.09 | -.09 | -.08 | -.07 | -.06 | -.04 | -.02 | .00 | .03 |
| .28 | -.01 | -.07 | -.08 | -.08 | -.08 | -.07 | -.05 | -.03 | -.01 | .01 | .04 | .07 |
| .29 | -.00 | -.06 | -.07 | -.07 | -.06 | -.05 | -.03 | -.00 | .02 | .05 | .09 | .12 |
| .30 | .00 | -.06 | -.06 | -.06 | -.04 | -.03 | -.00 | .03 | .06 | .10 | .13 | .17 |
| .31 | .01 | -.05 | -.05 | -.04 | -.03 | -.00 | .03 | .06 | .10 | .14 | .19 | .23 |
| .32 | .02 | -.05 | -.04 | -.03 | -.00 | .03 | .06 | .10 | .15 | .19 | .24 | .30 |
| .33 | .03 | -.04 | -.03 | -.01 | .02 | .06 | .10 | .15 | .20 | .25 | .31 | .37 |
| .34 | .04 | -.03 | -.01 | .01 | .05 | .09 | .14 | .19 | .25 | .31 | .38 | .44 |
| .35 | .05 | -.02 | .01 | .04 | .08 | .13 | .19 | .25 | .31 | .38 | .45 | .53 |
| .36 | .07 | -.00 | .02 | .06 | .11 | .17 | .24 | .31 | .38 | .46 | .54 | .62 |
| .37 | .08 | .01 | .05 | .09 | .15 | .22 | .29 | .37 | .45 | .54 | .63 | .72 |
| .38 | .09 | .03 | .07 | .13 | .19 | .27 | .35 | .44 | .53 | .63 | .73 | .83 |
| .39 | .11 | .05 | .10 | .16 | .24 | .33 | .42 | .52 | .62 | .72 | .83 | .94 |
| .40 | .13 | .07 | .13 | .20 | .29 | .39 | .49 | .60 | .71 | .83 | .95 | 1.07 |

TABLE 3.4.8. Values of (3.4.5); $\hat{\rho}$ = .10(.01).40; p = 20(5)50(10)100. (Positive entries imply $|\underset{\sim}{H}_1| > 0$.)

| $\hat{\rho}$ | p=20 | 25 | 30 | 35 | 40 | 45 | 50 | 60 | 70 | 80 | 90 | 100 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| .10 | -.21 | -.25 | -.27 | -.28 | -.29 | -.29 | -.29 | -.28 | -.27 | -.24 | -.22 | -.19 |
| .11 | -.22 | -.25 | -.27 | -.27 | -.28 | -.27 | -.27 | -.25 | -.22 | -.19 | -.15 | -.11 |
| .12 | -.23 | -.25 | -.26 | -.26 | -.26 | -.25 | -.24 | -.20 | -.16 | -.12 | -.07 | -.02 |
| .13 | -.23 | -.24 | -.25 | -.24 | -.23 | -.22 | -.20 | -.15 | -.10 | -.04 | .02 | .08 |
| .14 | -.22 | -.23 | -.23 | -.22 | -.20 | -.18 | -.15 | -.09 | -.02 | .05 | .13 | .20 |
| .15 | -.22 | -.22 | -.21 | -.19 | -.16 | -.13 | -.10 | -.02 | .07 | .15 | .25 | .34 |
| .16 | -.21 | -.20 | -.18 | -.15 | -.12 | -.08 | -.03 | .06 | .17 | .27 | .38 | .49 |
| .17 | -.19 | -.18 | -.15 | -.11 | -.06 | -.01 | .04 | .16 | .28 | .40 | .53 | .66 |
| .18 | -.18 | -.15 | -.11 | -.06 | -.00 | .06 | .12 | .26 | .40 | .55 | .70 | .85 |
| .19 | -.16 | -.12 | -.06 | -.00 | .07 | .14 | .21 | .37 | .54 | .71 | .88 | 1.06 |
| .20 | -.13 | -.08 | -.01 | .06 | .14 | .23 | .32 | .50 | .69 | .89 | 1.09 | 1.29 |
| .21 | -.10 | -.04 | .04 | .13 | .23 | .33 | .43 | .64 | .86 | 1.08 | 1.31 | 1.54 |
| .22 | -.07 | .01 | .11 | .21 | .32 | .44 | .55 | .80 | 1.04 | 1.30 | 1.55 | 1.81 |
| .23 | -.03 | .07 | .18 | .30 | .42 | .56 | .69 | .96 | 1.25 | 1.53 | 1.82 | 2.11 |
| .24 | .02 | .13 | .26 | .40 | .54 | .69 | .84 | 1.15 | 1.46 | 1.78 | 2.11 | 2.43 |
| .25 | .06 | .20 | .34 | .50 | .66 | .83 | 1.00 | 1.35 | 1.70 | 2.06 | 2.42 | 2.78 |
| .26 | .12 | .27 | .44 | .62 | .80 | .99 | 1.18 | 1.57 | 1.96 | 2.36 | 2.76 | 3.16 |
| .27 | .18 | .35 | .54 | .74 | .95 | 1.16 | 1.37 | 1.80 | 2.24 | 2.68 | 3.13 | 3.58 |
| .28 | .25 | .45 | .66 | .88 | 1.11 | 1.34 | 1.58 | 2.06 | 2.55 | 3.04 | 3.53 | 4.02 |
| .29 | .32 | .54 | .78 | 1.03 | 1.29 | 1.55 | 1.81 | 2.34 | 2.88 | 3.42 | 3.96 | 4.50 |
| .30 | .40 | .65 | .92 | 1.19 | 1.48 | 1.76 | 2.05 | 2.64 | 3.23 | 3.83 | 4.42 | 5.02 |
| .31 | .49 | .77 | 1.07 | 1.37 | 1.68 | 2.00 | 2.32 | 2.96 | 3.61 | 4.27 | 4.92 | 5.58 |
| .32 | .58 | .90 | 1.23 | 1.56 | 1.91 | 2.25 | 2.61 | 3.31 | 4.03 | 4.75 | 5.47 | 6.19 |
| .33 | .69 | 1.04 | 1.40 | 1.77 | 2.15 | 2.53 | 2.91 | 3.69 | 4.47 | 5.26 | 6.05 | 6.84 |
| .34 | .80 | 1.19 | 1.58 | 1.99 | 2.41 | 2.83 | 3.25 | 4.10 | 4.95 | 5.81 | 6.68 | 7.54 |
| .35 | .92 | 1.35 | 1.79 | 2.24 | 2.69 | 3.15 | 3.61 | 4.54 | 5.47 | 6.41 | 7.35 | 8.29 |
| .36 | 1.06 | 1.52 | 2.01 | 2.50 | 2.99 | 3.49 | 4.00 | 5.01 | 6.03 | 7.05 | 8.08 | 9.11 |
| .37 | 1.20 | 1.71 | 2.24 | 2.78 | 3.32 | 3.87 | 4.42 | 5.52 | 6.63 | 7.75 | 8.86 | 9.98 |
| .38 | 1.36 | 1.92 | 2.50 | 3.08 | 3.67 | 4.27 | 4.87 | 6.07 | 7.28 | 8.49 | 9.70 | 10.92 |
| .39 | 1.53 | 2.14 | 2.77 | 3.41 | 4.05 | 4.70 | 5.35 | 6.66 | 7.97 | 9.29 | 10.61 | 11.93 |
| .40 | 1.71 | 2.36 | 3.07 | 3.76 | 4.46 | 5.17 | 5.88 | 7.30 | 8.72 | 10.15 | 11.59 | 13.02 |

$$(3.4.7)\qquad \frac{1}{1+\hat\rho q} + \frac{1}{\hat\lambda_M^2} > \frac{2}{1+\hat\rho^2 q} \quad ; \ \hat\rho > 0,$$

$$(3.4.8)\qquad \frac{1}{1-\hat\rho} + \frac{1}{\hat\lambda_M^2} > \frac{2}{1+\hat\rho^2 q} \quad ; \ \hat\rho < 0.$$

Making $\hat\lambda_M^2$ the subject yields

$$(3.4.9)\qquad \hat\lambda_M^2 < \frac{(1+\hat\rho^2 q)(1+\hat\rho q)}{1+\hat\rho q(2-\hat\rho)} \quad ; \quad \frac{1}{1+\sqrt{p}} \le \hat\rho$$

$$(3.4.10)\qquad \hat\lambda_M^2 < \frac{(1-\hat\rho)(1+\hat\rho^2 q)}{1-2\hat\rho-\hat\rho^2 q} \quad ; \quad \hat\rho \le 1 - \sqrt{\frac{p}{q}} \ .$$

Since $\hat\lambda_M^2 \ge 1$ the bounds are restricted to the indicated regions for $\hat\rho$. It follows that $|\underset{\sim}{H}_1| > 0$ whenever all $\hat\lambda_i^2$ , $i = 1,\ldots, p$ , are bounded above as in (3.4.9) and (3.4.10). For $p \ge 4$ we find by numerical computation that (3.4.9) exceeds the corresponding bound from (3.3.11) for a range of $\hat\rho$ totally included in the range for which we found $d > 0$. Furthermore $1/(1+\sqrt{p})$ is only just less than the lower bound on $\hat\rho$ for which $d > 0$. Hence we do not present a tabulation of (3.4.9). As $\hat\rho \to -1/q$, the bound in (3.4.10) tends to $1 + 1/q$. Thus for fairly large $p$ we can infer that $|\underset{\sim}{H}_1| > 0$ only for a very narrow range of values of $\hat\lambda_i^2$. We recall from Tables 3.4.5 and 3.4.6 that the corresponding upper bounds for $\hat\lambda_i^2$ are much higher than (3.4.10). In Table 3.4.9 we give values of (3.4.10) for $p = 4, 5, 6, 8, 10$ and $\hat\rho = 1 - \sqrt{p/q}\,(29 + \sqrt{p/q})/30$, $(\sqrt{p/q}(1 - \sqrt{p/q})/30)$, $1 - \sqrt{p/q}(1 + 29\sqrt{p/q})/30$. We notice that even at $p = 4$ we would need all $\hat\lambda_i^2$ to be less than at most $1\frac{1}{3}$.

We find (3.2.6) positive provided

TABLE 3.4.9. Values of upper bounds for $\hat{\lambda}_i^2$ sufficient for $|\underset{\sim}{H}_1| > 0$ from (3.4.10);

$\hat{\rho} = 1 - \sqrt{p/q}(29 + \sqrt{p/q})/30,\ (\sqrt{p/q}(1 - \sqrt{p/q})/30),\ 1 - \sqrt{p/q}(1 + 29\sqrt{p/q})/30,\ p=4,5,6,8,10.$

| p=4 | | p=5 | | p=6 | | p=7 | | p=8 | |
|---|---|---|---|---|---|---|---|---|---|
| $\hat{\rho}$ | (3.4.10) | $\hat{\rho}$ | (3.4.10) | $\hat{\rho}$ | (3.4.10) | $\hat{\rho}$ | (3.4.10) | $\hat{\rho}$ | (3.4.10) |
| -.1607 | 1.0053 | -.1224 | 1.0041 | -.0989 | 1.0033 | -.0715 | 1.0024 | -.0560 | 1.0019 |
| -.1666 | 1.0111 | -.1268 | 1.0084 | -.1024 | 1.0068 | -.0740 | 1.0049 | -.0579 | 1.0039 |
| -.1726 | 1.0171 | -.1312 | 1.0131 | -.1059 | 1.0105 | -.0764 | 1.0076 | -.0598 | 1.0060 |
| -.1785 | 1.0236 | -.1356 | 1.0180 | -.1094 | 1.0145 | -.0789 | 1.0105 | -.0617 | 1.0082 |
| -.1845 | 1.0304 | -.1400 | 1.0232 | -.1129 | 1.0187 | -.0813 | 1.0135 | -.0636 | 1.0106 |
| -.1904 | 1.0376 | -.1444 | 1.0286 | -.1164 | 1.0231 | -.0838 | 1.0167 | -.0655 | 1.0130 |
| -.1964 | 1.0452 | -.1488 | 1.0344 | -.1198 | 1.0277 | -.0863 | 1.0200 | -.0674 | 1.0157 |
| -.2023 | 1.0532 | -.1532 | 1.0404 | -.1233 | 1.0326 | -.0887 | 1.0235 | -.0693 | 1.0184 |
| -.2083 | 1.0615 | -.1576 | 1.0467 | -.1268 | 1.0377 | -.0912 | 1.0272 | -.0712 | 1.0212 |
| -.2142 | 1.0702 | -.1620 | 1.0533 | -.1303 | 1.0430 | -.0936 | 1.0310 | -.0731 | 1.0242 |
| -.2202 | 1.0794 | -.1664 | 1.0602 | -.1338 | 1.0485 | -.0961 | 1.0350 | -.0750 | 1.0273 |
| -.2262 | 1.0889 | -.1708 | 1.0674 | -.1373 | 1.0543 | -.0986 | 1.0391 | -.0769 | 1.0306 |
| -.2321 | 1.0988 | -.1752 | 1.0749 | -.1408 | 1.0603 | -.1010 | 1.0434 | -.0788 | 1.0339 |
| -.2381 | 1.1091 | -.1796 | 1.0826 | -.1442 | 1.0665 | -.1035 | 1.0479 | -.0807 | 1.0374 |
| -.2440 | 1.1198 | -.1840 | 1.0907 | -.1477 | 1.0730 | -.1060 | 1.0525 | -.0826 | 1.0410 |
| -.2500 | 1.1309 | -.1884 | 1.0991 | -.1512 | 1.0797 | -.1084 | 1.0573 | -.0845 | 1.0448 |
| -.2559 | 1.1424 | -.1928 | 1.1078 | -.1547 | 1.0867 | -.1109 | 1.0623 | -.0864 | 1.0486 |
| -.2619 | 1.1544 | -.1972 | 1.1167 | -.1582 | 1.0939 | -.1133 | 1.0675 | -.0883 | 1.0526 |
| -.2678 | 1.1668 | -.2016 | 1.1260 | -.1617 | 1.1013 | -.1158 | 1.0728 | -.0902 | 1.0568 |
| -.2738 | 1.1796 | -.2060 | 1.1356 | -.1651 | 1.1090 | -.1183 | 1.0782 | -.0921 | 1.0610 |
| -.2797 | 1.1928 | -.2104 | 1.1456 | -.1686 | 1.1169 | -.1207 | 1.0839 | -.0940 | 1.0654 |
| -.2857 | 1.2066 | -.2148 | 1.1558 | -.1721 | 1.1251 | -.1232 | 1.0897 | -.0959 | 1.0700 |
| -.2917 | 1.2207 | -.2192 | 1.1664 | -.1756 | 1.1335 | -.1256 | 1.0957 | -.0978 | 1.0746 |
| -.2976 | 1.2353 | -.2236 | 1.1773 | -.1791 | 1.1422 | -.1281 | 1.1019 | -.0997 | 1.0794 |
| -.3036 | 1.2504 | -.2280 | 1.1885 | -.1826 | 1.1512 | -.1306 | 1.1083 | -.1016 | 1.0844 |
| -.3095 | 1.2660 | -.2324 | 1.2001 | -.1861 | 1.1604 | -.1330 | 1.1148 | -.1035 | 1.0894 |
| -.3155 | 1.2821 | -.2368 | 1.2121 | -.1895 | 1.1699 | -.1355 | 1.1216 | -.1054 | 1.0946 |
| -.3214 | 1.2987 | -.2412 | 1.2243 | -.1930 | 1.1797 | -.1379 | 1.1285 | -.1073 | 1.1000 |
| -.3274 | 1.3157 | -.2456 | 1.2370 | -.1965 | 1.1897 | -.1404 | 1.1356 | -.1092 | 1.1055 |

$$(3.4.11)\quad pq\hat{\rho}^2(1+\hat{\rho}^2 q) > 2(\hat{\underset{\sim}{\lambda}} - (1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)})'\hat{\underset{\sim}{\Lambda}}^2(\hat{\underset{\sim}{\lambda}} - (1+\hat{\rho}^2 q)\hat{\underset{\sim}{\lambda}}^{(-1)}),$$

which reduces to

$$(3.4.12)\quad p(1 + \hat{\rho}^2 q)(2-\hat{\rho}^2 q) > 2 \sum_{i=1}^{4} \hat{\lambda}_i^4.$$

Similarly it is sufficient for (3.2.11) that

$$(3.4.13)\quad p^2(1 + \hat{\rho} q)^2 > 2\hat{\underset{\sim}{\lambda}}'\underset{\sim}{R}\hat{\underset{\sim}{\Lambda}}^2\underset{\sim}{R}\hat{\underset{\sim}{\lambda}}.$$

Substituting (3.2.4) into the right-hand side yields

$$(3.4.14)\quad p[2 + \hat{\rho}^2(p-2)] > 2 \sum_{i=1}^{p} \hat{\lambda}_i^4 .$$

The left-hand side of (3.4.12) exceeds that of (3.4.14) for $\hat{\rho} \leq 1/q$; otherwise that of (3.4.12) is the smaller. We find an upper bound for $\Sigma\hat{\lambda}_i^4$ using (3.2.35). We obtain

$$(3.4.15)\quad \sum_{i=1}^{p} \hat{\lambda}_i^4 \leq p(\hat{\lambda}_M^2 + \hat{\lambda}_m^2 - \hat{\lambda}_M^2\hat{\lambda}_m^2).$$

Hence we have as sufficient for $|\underset{\sim}{H}_1| > 0$. that

$$(3.4.16)\quad (1+\hat{\rho}^2 q)(2-\hat{\rho}^2 q) > 2(\hat{\lambda}_M^2 + \hat{\lambda}_m^2 - \hat{\lambda}_M^2\hat{\lambda}_m^2)\ ;\ - 1/q < \hat{\rho} \leq 1/q,$$

$$(3.4.17)\quad 2 + \hat{\rho}^2(p-2) > 2(\hat{\lambda}_M^2 + \hat{\lambda}_m^2 - \hat{\lambda}_M^2\hat{\lambda}_m^2)\ ;\ 1/q \leq \hat{\rho} < 1.$$

We found, however, by numerical evaluation that (3.4.16) and (3.4.17) are weaker than that of Corollary 3.2.1 for all $\hat{\rho}$.

### 3.4.3 Case of $p = 3$.

From §3.3 (cf. Tables 3.3.1 and 3.3.2) we have the bounds

$$(3.4.18)\quad 1 + \frac{\hat\rho(1+\hat\rho)}{1+3\hat\rho/2} < \hat\lambda_i^2 < 1 - \frac{\hat\rho(1-\hat\rho)}{1+\frac{1}{2}\hat\rho}\ ;\ -\tfrac{1}{2} < \hat\rho \le 0,$$

$$(3.4.19)\quad 1 - \frac{\hat\rho(1-\hat\rho)}{1+\frac{1}{2}\hat\rho} < \hat\lambda_i^2\ ;\ 0 \le \hat\rho < 1\ ,$$

$$(3.4.20)\quad \hat\lambda_i^2 < (1 + \frac{\hat\rho(1+\hat\rho)}{1+3\hat\rho/2}\ ,\ \left[\frac{\sqrt{9\hat\rho^2 + 4\hat\alpha(1+2\hat\rho)}\ + 3\hat\rho}{2(1+2\hat\rho)}\right]^2\ )\ ;\ 0 \le \hat\rho < 1.$$

The first upper bound in (3.4.20) is stronger for $\hat\rho$ below the positive root of the cubic equation (3.3.54), which we found to be .4463 to four decimal places. Above this root the second upper bound is stronger. This is illustrated in Table 3.4.10 and Figure 3.4.3 which contain values and a plot of (3.4.18) through (3.4.20) respectively.

We apply the above bounds to prove $|\underset{\sim}{H}_1| > 0$ for all positive $\hat\rho$ and about half the range of values for negative $\hat\rho$.

THEOREM 3.4.1. <u>The matrix $\underset{\sim}{H}_1$ of second derivatives at solutions of the maximum likelihood equations (3.1.12) and (3.1.13) is positive definite for $p = 3$ and $\hat\rho \ge -.2465$, to four decimal places.</u>

<u>Proof</u>. It suffices to prove (3.4.5) positive with

$$(3.4.21)\quad \hat\lambda_m^2 = 1 - \frac{\hat\rho(1-\hat\rho)}{1+\frac{1}{2}\hat\rho}\ ;\ \hat\lambda_M^2 = 1 + \frac{\hat\rho(1+\hat\rho)}{1+3\hat\rho/2}\ ,$$

for $\hat\rho > 0$ and reversed when $\hat\rho < 0$. From (3.2.45) we have when $\hat\rho > 0$

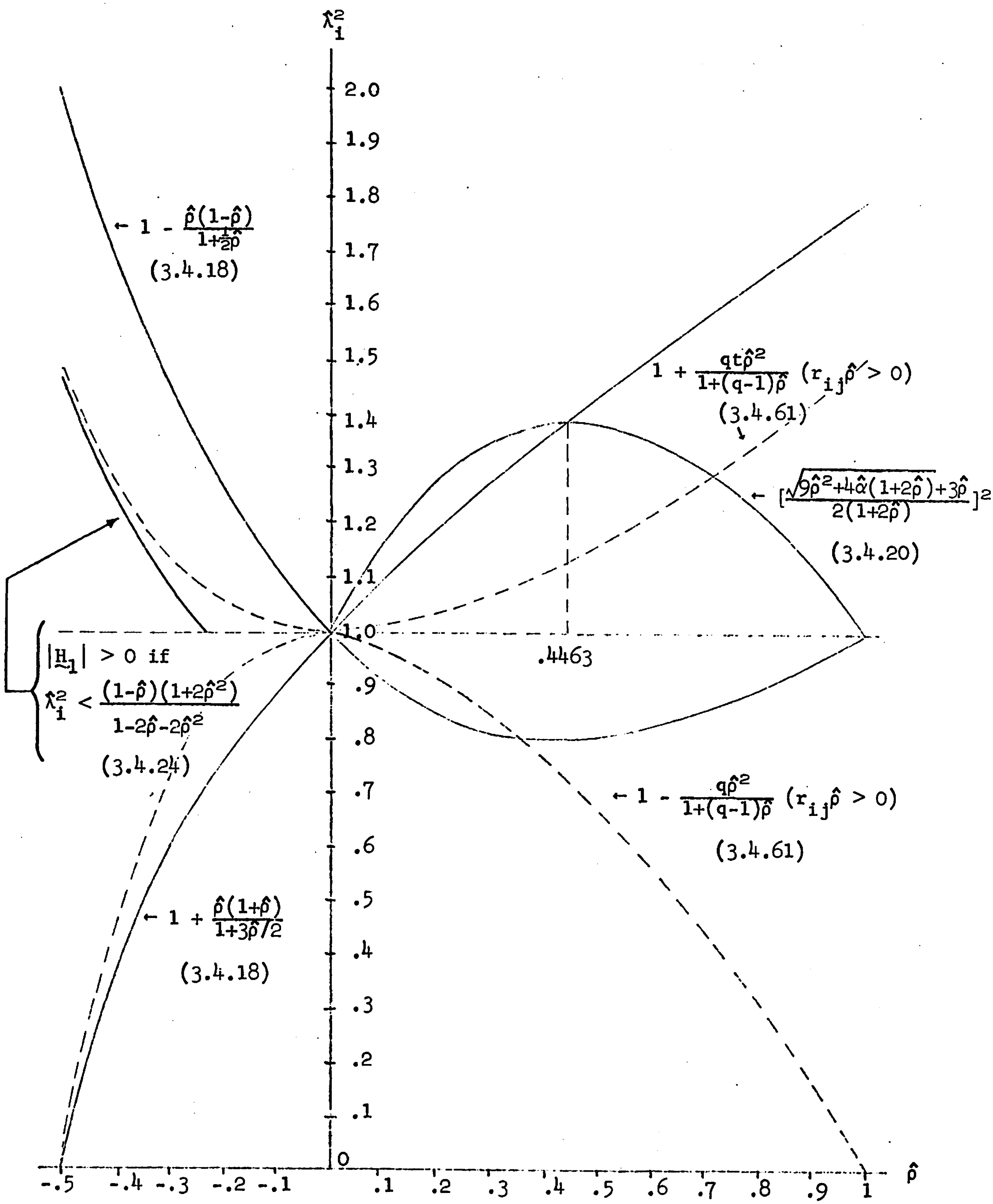
$$(3.4.22)\quad m = \frac{1+\hat\rho}{(1+2\hat\rho)(1+\frac{1}{2}\hat\rho)}\ ;\ M = \frac{1-\frac{1}{2}\hat\rho+\hat\rho^2/4}{(1-\hat\rho)(1-\frac{1}{2}\hat\rho+\hat\rho^2)}\ ,$$

and reversed when $\hat\rho < 0$. Substituting (3.4.10), we find that (3.4.5) is positive provided

TABLE 3.4.10. Bounds for $\hat{\lambda}_i^2$ when p = 3 from (3.4.18-20/24); $\hat{\rho}$ = -.475(.025).975.

| $\hat{\rho}$ | (18/19) | (18/20) | (24/20) | $\hat{\rho}$ | (19) | (20) | |
|---|---|---|---|---|---|---|---|
| -.475 | .1326 | 1.9189 | 1.4283 | .275 | .8247 | 1.2482 | 1.3415 |
| -.450 | .2385 | 1.8419 | 1.3627 | .300 | .8174 | 1.2690 | 1.3547 |
| -.425 | .3259 | 1.7690 | 1.3030 | .325 | .8113 | 1.2895 | 1.3655 |
| -.400 | .4000 | 1.7000 | 1.2486 | .350 | .8064 | 1.3098 | 1.3740 |
| -.375 | .4643 | 1.6346 | 1.1995 | .375 | .8026 | 1.3300 | 1.3803 |
| -.350 | .5211 | 1.5727 | 1.1552 | .400 | .8000 | 1.3500 | 1.3844 |
| -.325 | .5720 | 1.5142 | 1.1155 | .425 | .7985 | 1.3698 | 1.3865 |
| -.300 | .6182 | 1.4588 | 1.0803 | .450 | .7980 | 1.3896 | 1.3867 |
| -.275 | .6606 | 1.4065 | 1.0494 | .475 | .7985 | 1.4091 | 1.3850 |
| -.250 | .7000 | 1.3571 | 1.0227 | .500 | .8000 | 1.4286 | 1.3815 |
| -.225 | .7368 | 1.3106 | 1.0002 | .525 | .8025 | 1.4479 | 1.3763 |
| -.200 | .7714 | 1.2667 | | .550 | .8059 | 1.4671 | 1.3695 |
| -.175 | .8042 | 1.2253 | | .575 | .8102 | 1.4862 | 1.3610 |
| -.150 | .8353 | 1.1865 | | .600 | .8154 | 1.5053 | 1.3510 |
| -.125 | .8654 | 1.1500 | | .625 | .8214 | 1.5242 | 1.3395 |
| -.100 | .8941 | 1.1158 | | .650 | .8283 | 1.5430 | 1.3265 |
| -.075 | .9216 | 1.0838 | | .675 | .8360 | 1.5618 | 1.3120 |
| -.050 | .9486 | 1.0538 | | .700 | .8444 | 1.5805 | 1.2962 |
| -.025 | .9747 | 1.0259 | | .725 | .8537 | 1.5991 | 1.2790 |
| 0.000 | 1.0000 | 1.0000 | 1.0000 | .750 | .8636 | 1.6176 | 1.2604 |
| .025 | .9759 | 1.0247 | 1.0481 | .775 | .8743 | 1.6361 | 1.2405 |
| .050 | .9537 | 1.0488 | 1.0925 | .800 | .8857 | 1.6545 | 1.2193 |
| .075 | .9331 | 1.0725 | 1.1333 | .825 | .8978 | 1.6729 | 1.1967 |
| .100 | .9143 | 1.0957 | 1.1705 | .850 | .9105 | 1.6912 | 1.1728 |
| .125 | .8971 | 1.1184 | 1.2042 | .875 | .9239 | 1.7095 | 1.1475 |
| .150 | .8814 | 1.1408 | 1.2346 | .900 | .9379 | 1.7277 | 1.1209 |
| .175 | .8672 | 1.1629 | 1.2618 | .925 | .9526 | 1.7458 | 1.0929 |
| .200 | .8545 | 1.1846 | 1.2860 | .950 | .9678 | 1.7639 | 1.0635 |
| .225 | .8433 | 1.2061 | 1.3072 | .975 | .9836 | 1.7820 | 1.0325 |
| .250 | .8335 | 1.2273 | 1.3257 | | | | |

Figure 3.4.3. Bounds for $\hat{\lambda}_i^2$ when $p = 3$.



(3.4.23) $\quad 4 + 15\hat{\rho} - 6\hat{\rho}^2 - 4\hat{\rho}^3 > 0.$

We also obtain (3.4.23) with (3.4.22) reversed since (3.4.5) is symmetric in M and m. The cubic in (3.4.23) is positive between its two larger roots which are -.2465 and 1.4830 to four decimal places. Hence the result. (qed)

It remains to be shown that $|\underset{\sim}{H}_1| > 0$ for $-\frac{1}{2} < \hat{\rho} < -.2465$ before we can conclude uniqueness of solution of the maximum likelihood equations when $p = 3$. From (3.4.10) we have

(3.4.24) $$\hat{\lambda}_M^2 < \frac{(1-\hat{\rho})(1+2\hat{\rho}^2)}{1-2\hat{\rho}-2\hat{\rho}^2} \;;\; \hat{\rho} \leq 1 - \sqrt{\frac{3}{2}},$$

as a sufficient condition for $|\underset{\sim}{H}_1| > 0$. The values of the upper bound in (3.4.24) are well below those from (3.4.18) as tabulated in Table 3.4.10 and sketched in Figure 3.4.3. From (3.4.16), after substituting (3.4.18) we have

(3.4.25) $$(1+2\hat{\rho}^2)(1-\hat{\rho}^2) > 1 + \frac{\hat{\rho}^2(1-\hat{\rho}^2)}{(1+\frac{1}{2}\hat{\rho})(1+3\hat{\rho}/2)} \;;\; \hat{\rho} < 0,$$

as sufficient for $|\underset{\sim}{H}_1| > 0$. We can simplify (3.4.25) to

(3.4.26) $\quad 6\hat{\rho}^3 + 16\hat{\rho}^2 + \hat{\rho} - 8 > 0.$

In the region $-\frac{1}{2} < \hat{\rho} < 0$, the cubic in (3.4.26) is negative and so (3.4.18) is of no help.

We may write $|\underset{\sim}{H}_1|$ in terms of a determinant of order three using (3.2.22). Before doing this we write (3.1.12) as

$$(3.4.27)\quad \hat{\rho}\begin{bmatrix} 1 & r_{12} & r_{13} \\ r_{12} & 1 & r_{23} \\ r_{13} & r_{23} & 1 \end{bmatrix}\begin{pmatrix}\hat{\lambda}_1\\ \hat{\lambda}_2\\ \hat{\lambda}_3\end{pmatrix} = (1+2\hat{\rho})\begin{bmatrix}\hat{\lambda}_1 - (1-\hat{\rho})/\hat{\lambda}_1\\ \hat{\lambda}_2 - (1-\hat{\rho})/\hat{\lambda}_2\\ \hat{\lambda}_3 - (1-\hat{\rho})/\hat{\lambda}_3\end{bmatrix};$$

the first equation in (3.4.27) may be expanded as

$$(3.4.28)\quad \hat{\rho}(r_{12}\hat{\lambda}_1\hat{\lambda}_2 + r_{13}\hat{\lambda}_1\hat{\lambda}_3) = \hat{\lambda}_1^2(1+\hat{\rho}) - (1-\hat{\rho})(1+2\hat{\rho}).$$

From (3.1.16) we have that $3\hat{\rho} = r_{12}\hat{\lambda}_1\hat{\lambda}_2 + r_{13}\hat{\lambda}_1\hat{\lambda}_3 + r_{23}\hat{\lambda}_2\hat{\lambda}_3$. Substituting in (3.4.28) yields

$$(3.4.29)\quad \hat{\rho}r_{23}\hat{\lambda}_2\hat{\lambda}_3 = (1+\hat{\rho})(1-\hat{\lambda}_1^2) + \hat{\rho}^2$$

$$= (1+\hat{\rho})(\hat{\lambda}_2^2+\hat{\lambda}_3^2-2) + \hat{\rho}^2,$$

using (3.1.15). Similar expressions follow for $r_{12}$ and $r_{13}$. When $\hat{\rho} = 0$ we obtain immediately $\underset{\sim}{\hat{\lambda}} = \underset{\sim}{e}$ and from (3.1.16)

$$(3.4.30)\quad r_{12} + r_{13} + r_{23} = 0.$$

We do not require $r_{12} = r_{13} = r_{23} = 0$. When $\hat{\rho} \neq 0$, (3.4.29) leads to expressions with $r_{ij}$ as subject,

$$(3.4.31)\quad r_{23} = \frac{(1+\hat{\rho})(1-\hat{\lambda}_1^2) + \hat{\rho}^2}{\hat{\rho}\hat{\lambda}_2\hat{\lambda}_3}$$

$$= \frac{(1+\hat{\rho})(\hat{\lambda}_2^2+\hat{\lambda}_3^2-2) + \hat{\rho}^2}{\hat{\rho}\hat{\lambda}_2\hat{\lambda}_3},$$

for example.

Since $r_{ij}$ can be written wholly in terms of $\hat{\rho}$, $\hat{\lambda}_i^2$ and $\hat{\lambda}_j^2$, $i \neq j$, so can $|\underset{\sim}{H}_1|$. From (3.2.22) we find with $i = 2$, $j = 3$,

$$(3.4.32)\quad |\underset{\sim}{H}_1| = 192|\underset{\sim}{H}_2|/(\hat{\alpha}^2\hat{\rho}^2\hat{\lambda}_1^2\hat{\lambda}_2^2\hat{\lambda}_3^2),$$

where

$$(3.4.33)\qquad \underset{\sim}{H}_2 = -\begin{bmatrix} \frac{1}{6}+\frac{(1+\hat{\rho})\hat{\lambda}_2^2}{2\hat{\alpha}}, & -\frac{\hat{\rho}r_{23}\hat{\lambda}_2\hat{\lambda}_3}{2\hat{\alpha}}-\frac{1}{3}, & \hat{\lambda}_2^2-1 \\ \frac{\hat{\rho}r_{23}\hat{\lambda}_2\hat{\lambda}_3}{2\hat{\alpha}}-\frac{1}{3}, & \frac{1}{6}+\frac{(1+\hat{\rho})\hat{\lambda}_3^2}{2\hat{\alpha}}, & \hat{\lambda}_3^2-1 \\ \hat{\lambda}_2^2-1, & \hat{\lambda}_3^2-1, & 6\hat{\rho}^2 \end{bmatrix}$$

Substituting (3.4.31) in (3.4.33) leads to

$$(3.4.34)\qquad |\underset{\sim}{H}_2| = \frac{1}{6\hat{\alpha}}\begin{vmatrix} \hat{\alpha}+3(1+\hat{\rho})\hat{\lambda}_2^2, & (\hat{\rho}+2)^2-3(1+\hat{\rho})(\hat{\lambda}_2^2+\hat{\lambda}_3^2), & \hat{\lambda}_2^2-1 \\ (\hat{\rho}+2)^2-3(1+\hat{\rho})(\hat{\lambda}_2^2+\hat{\lambda}_3^2), & \hat{\alpha}+3(1+\hat{\rho})\hat{\lambda}_3^2, & \hat{\lambda}_3^2-1 \\ \hat{\lambda}_2^2-1, & \hat{\lambda}_3^2-1, & \hat{\rho}^2/\hat{\alpha} \end{vmatrix}.$$

We have not been able to analytically prove (3.4.34) positive directly for $\hat{\lambda}_2^2 \neq \hat{\lambda}_3^2$. When $\hat{\lambda}_2^2 = \hat{\lambda}_3^2$, however, we can do so. Substituting $\hat{\lambda}^2$ for the common value, (3.4.34) reduces to

$$(3.4.35)\qquad |\underset{\sim}{H}_2| = 3[(1+\hat{\rho})(3\hat{\lambda}^2-1)-\hat{\rho}^2]\begin{vmatrix} (1+\hat{\rho})(5-3\hat{\lambda}^2)-\hat{\rho}^2, & \hat{\lambda}^2-1 \\ 2(\hat{\lambda}^2-1), & \hat{\rho}^2/\hat{\alpha} \end{vmatrix}.$$

We will need the following:

LEMMA 3.4.1. <u>Let the quadratic</u> $ax^2+bx+c$ $(a>0)$ <u>have two real roots</u> $s$ <u>and</u> $t$. <u>Then</u> $0 \leq u \leq t$ <u>and</u> $s \leq v \leq 0$ <u>provided</u>

$$(3.4.36)\qquad au^2+bu+c,\ av^2+bv+c \leq 0.$$

<u>Proof</u>. The roots are $s = (-b-\sqrt{b^2-4ac})/2a \leq 0$ and $t = (-b+\sqrt{b^2-4ac})/2a \geq 0$. Then $s \leq v$ provided $-b-\sqrt{b^2-4ac} \leq 2av$. Since $v \leq 0$ we get $(-2av-b)^2 \leq b^2-4ac$. Cancelling yields $av^2+bv+c \leq 0$. The rest of (3.4.36) follows similarly. (qed)

The first factor in (3.4.35) is positive provided

$$(3.4.37)\qquad \hat{\rho}^2 - (\hat{\rho}+1)(3\hat{\lambda}^2-1) < 0$$

or $\hat{\rho}$ lies between its roots. The positive root exceeds 1 provided $1 - 2(3\hat{\lambda}^2-1) < 0$ or $\hat{\lambda}^2 > \frac{1}{2}$, applying Lemma 3.4.1. From Figure 3.4.3 we see that $\hat{\lambda}_i^2 < 2$, so when two $\hat{\lambda}_j^2$ are equal we must have $\hat{\lambda}^2 > (3-2)/2 = \frac{1}{2}$ (cf. Theorem 3.3.8). The negative root from (3.4.37) is less than $-\frac{1}{2}$ provided $\frac{1}{4} + \frac{1}{2}(3\hat{\lambda}^2-1) - (3\hat{\lambda}^2-1) < 0$ or $\hat{\lambda}^2 > \frac{1}{2}$, using (3.4.36) again. Hence (3.4.37) is established for $-\frac{1}{2} < \hat{\rho} < 1$. The second factor in (3.4.35) is positive provided

$$(3.4.38)\qquad 2\hat{\alpha}(\hat{\lambda}^2-1)^2 + 3\hat{\rho}^2(1+\hat{\rho})(\hat{\lambda}^2-1) + \hat{\rho}^2(\hat{\rho}^2-2\hat{\rho}-2) < 0,$$

or $\hat{\lambda}^2-1$ lies between its roots. From Theorem 3.3.8 we have

$$(3.4.39)\qquad \frac{\hat{\rho}(1-\hat{\rho})}{2+\hat{\rho}} < \hat{\lambda}^2-1 < \frac{-\hat{\rho}(1+\hat{\rho})}{2+3\hat{\rho}}\ ;\ -\tfrac{1}{2} < \hat{\rho} < 0.$$

The positive root from (3.4.38) exceeds the upper bound in (3.4.39) provided

$$(3.4.40)\qquad \frac{2\hat{\alpha}\hat{\rho}^2(1+\hat{\rho})^2}{(2+3\hat{\rho})^2} - \frac{3\hat{\rho}^3(1+\hat{\rho})^2}{2+3\hat{\rho}} + \hat{\rho}^2(\hat{\rho}^2-2\hat{\rho}-2) < 0.$$

This reduces to

$$(3.4.41)\qquad \hat{\rho}^2(1+2\hat{\rho})^2(\hat{\rho}^2+8\hat{\rho}+6)/(2+3\hat{\rho})^2 > 0,$$

or $\hat{\rho}$ outside the roots of $\hat{\rho}^2 + 8\hat{\rho} + 6 = 0$ which are $-4 \pm \sqrt{10} =$ $-7.2, -.8$, approximately. The negative root from (3.4.38) is less than the lower bound in (3.4.39) provided

$$(3.4.42)\qquad \frac{2\hat{\alpha}\hat{\rho}^2(1-\hat{\rho})^2}{(2+\hat{\rho})^2} + \frac{3\hat{\rho}^3(1-\hat{\rho}^2)}{2+\hat{\rho}} + \hat{\rho}^2(\hat{\rho}^2-2\hat{\rho}-2) < 0,$$

which reduces to

$$(3.4.43)\quad \hat{\rho}^2[2\hat{\rho}^3(\hat{\rho}-1) + (3\hat{\rho}^2 + 4\hat{\rho} + 2)]/(2+\hat{\rho})^2 > 0.$$

The first term within the square brackets is positive for $-\frac{1}{2} < \hat{\rho} < 0$ while the second is always positive, being a quadratic with complex roots.

Thus $|\underset{\sim}{H}_1| > 0$ when $\hat{\lambda}_2^2 = \hat{\lambda}_3^2$. When $\hat{\lambda}_2^2 \neq \hat{\lambda}_3^2$, (3.4.34) does not appear to be tractable analytically. We evaluated it numerically for $\hat{\rho} = -.4995(.0005)-.495(.005)-.245$, with $\hat{\lambda}_2^2$ ranging from $\hat{\lambda}_M^2$ to 1 and $\hat{\lambda}_3^2$ from $\min(\hat{\lambda}_2^2, 3-\hat{\lambda}_2^2-\hat{\lambda}_m^2)$ to $\max(\hat{\lambda}_m^2, (3-\hat{\lambda}_2^2)/2)$, dividing each interval into sixths. All values made (3.4.34) positive provided $|\underset{\sim}{R}| > 0$. We generated sample correlation matrices $\underset{\sim}{R}$ by decreasing the off-diagonal elements from (.95, .95, .95), (.95, .95, .90),... in ordered increments of .05 through (-.95, -.95, -.95), and requiring positive definiteness. For the 7035 matrices that resulted we found $|\underset{\sim}{H}_2| > 0$ in each case. Therefore, unless there is some extreme behavior of $|\underset{\sim}{H}_2|$ for $\hat{\lambda}_2^2 \neq \hat{\lambda}_3^2$ and $-1 < \hat{\rho} < -.2465$, the second derivative matrix $\underset{\sim}{H}_1$ is positive definite when its components satisfy the maximum likelihood equations (3.1.12) and (3.1.13), and so

RESULT 3.4.1. *When $p = 3$ the maximum likelihood equations in Theorem 3.1.1 admit a unique real solution, which is consistent.*

The 7035 sets of maximum likelihood equations due to the above correlation matrices, were solved iteratively using a new Fortran program written by Dennis R. Lienke, on the CDC 6600 at the University of Minnesota. The method is based on the doctoral dissertation by Brown (1966), and requires only $(m^2/2) + (3m/2)$ function evaluations per iterative step compared with $m^2 + m$ evaluations for the Newton-Raphson method, where $\underline{m}$ is the number of equations. When $m = 4$ this represents a saving of 6 evaluations in 20. The algorithm in Algol is described by Brown (1967). All 7035 sets were generated and solved in 185.108 seconds of central processor time, with about 4 to 6 iterations per set given initial guesses of 1 for $\hat{\lambda}_i^2$ and the average sample correlation coefficient r for $\hat{\rho}$. The convergence criterion used was that $|(x_r - x_{r-1})/x_r| < 10^{-4}$ for iterations r = t,t+1, t+2; $t \geq 1$, for each variable $x = \hat{\rho}, \hat{\lambda}_1, \hat{\lambda}_2, \hat{\lambda}_3$. Selected values are given in Table 3.4.11. Figure 3.4.4 gives values of $\hat{\rho}$ and $\hat{\lambda}_i^2$ selected to indicate $\hat{\lambda}_m^2$ and $\hat{\lambda}_M^2$. Our theoretical bounds closely approach these values though a stronger upper bound is needed when $\hat{\rho} > 0$.

Our numerical investigations led us to suppose that either $-\frac{1}{2} < \hat{\rho} \leq r \leq 0$ or $0 \leq r \leq \hat{\rho} < 1$. We prove this below using:

LEMMA 3.4.2. *Let* $x_i$, i = 1, 2, 3, *be three nonnegative quantities with* $\sum_{i=1}^{3} x_i^2 = 1$. *Then*

$$(3.4.44)\qquad 2\sum_{i=1}^{3} x_i^3 \geq \sum_{i=1}^{3} x_i - 3\prod_{i=1}^{3} x_i,$$

*with equality if and only if all the* $x_i$ *are equal*.

*Proof*. Let us write

$$(3.4.45)\qquad s = \sum_{i=1}^{3} x_i \ ; \quad p = \prod_{i=1}^{3} x_i \ ;$$

$$(3.4.46)\qquad 0 \leq x_1 = n \leq x_2 = d \leq x_3 = x \leq 1.$$

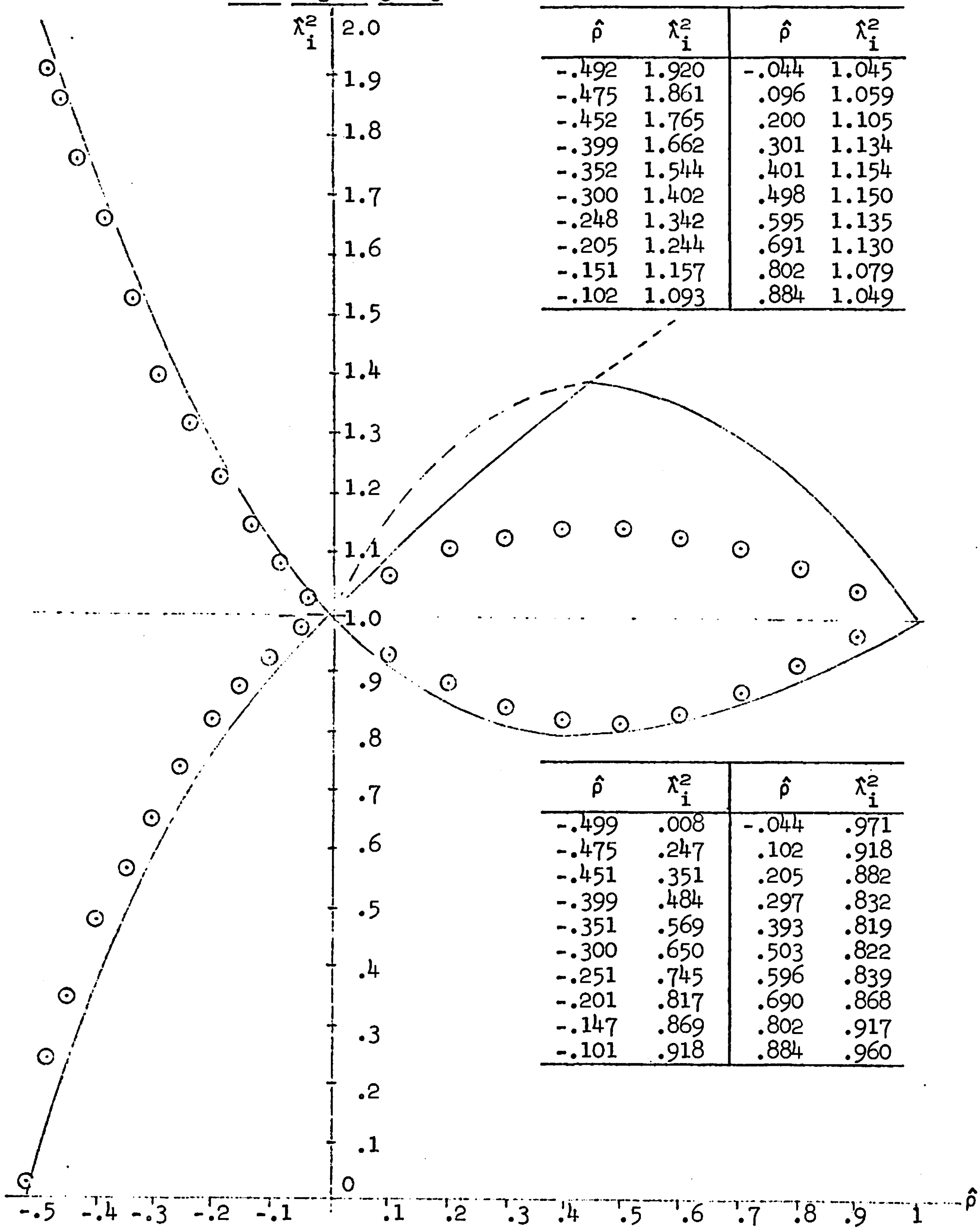
Then $s^3 = \Sigma x_i^3 + 3[n(nd + nx) + d(dn + dx) + x(xn + xd)] + 6p$, and $s^2 = 1 + 2(nd + nx + dx)$. Thus $nd + nx = \frac{1}{2}(s^2-1) - dx$, etc. Substituting yields $s^3 = \Sigma x_i^3 + 3[n(\frac{1}{2}(s^2-1) - dx) + d(\frac{1}{2}(s^2-1) - nx) + x(\frac{1}{2}(s^2-1) - nd)] + 6p = \Sigma x_i^3 + 3s(s^2-1)/2 - 3p$. Hence $\Sigma x_i^3 = s(3-s^2)/2 + 3p$ and (3.4.44) is

$$(3.4.47)\qquad s(s^2-2) \leq 9p.$$

TABLE 3.4.11. Selected values of $\hat\rho$ and $\hat\lambda_i^2$, i = 1, 2, 3 based on 7035 sample correlation matrices.

| $r_{12}$ | $r_{13}$ | $r_{23}$ | r | $\hat\rho$ | $\hat\lambda_1^2$ | $\hat\lambda_2^2$ | $\hat\lambda_3^2$ | No. of iterations |
|---|---|---|---|---|---|---|---|---|
| .95 | -.15 | -.35 | .150 | .176 | 1.077 | 1.048 | .875 | 5 |
| .90 | .50 | .45 | .617 | .624 | 1.074 | 1.054 | .872 | 4 |
| .90 | -.25 | -.55 | .033 | .041 | 1.023 | 1.011 | .965 | 6 |
| .85 | .55 | .45 | .617 | .622 | 1.073 | 1.032 | .896 | 4 |
| .85 | -.05 | -.55 | .083 | .099 | 1.057 | 1.013 | .930 | 5 |
| .80 | .80 | .35 | .650 | .657 | 1.131 | .935 | .935 | 4 |
| .80 | .20 | .20 | .400 | .412 | 1.064 | 1.064 | .872 | 5 |
| .80 | -.35 | -.65 | -.067 | -.084 | .947 | .975 | 1.076 | 6 |
| .75 | .30 | -.05 | .333 | .347 | 1.102 | 1.013 | .885 | 5 |
| .75 | -.20 | -.60 | -.017 | -.020 | .988 | .996 | 1.016 | 5 |
| .70 | .65 | .10 | .483 | .494 | 1.132 | .943 | .924 | 5 |
| .70 | .20 | -.20 | .233 | .247 | 1.087 | 1.010 | .904 | 5 |
| .70 | -.30 | -.45 | -.017 | -.019 | .992 | .994 | 1.014 | 5 |
| .65 | .55 | .10 | .433 | .441 | 1.106 | .964 | .930 | 4 |
| .65 | .15 | -.50 | .100 | .111 | 1.060 | .996 | .944 | 5 |
| .65 | -.35 | -.55 | -.083 | -.098 | .950 | .972 | 1.078 | 5 |
| .60 | .10 | -.65 | .017 | .019 | 1.012 | .998 | .989 | 5 |
| .60 | -.40 | -.50 | -.100 | -.115 | .948 | .962 | 1.090 | 5 |
| .55 | .40 | -.10 | .283 | .292 | 1.087 | .975 | .938 | 5 |
| .55 | -.00 | -.05 | .167 | .172 | 1.033 | 1.025 | .942 | 5 |
| .55 | -.45 | -.80 | -.233 | -.290 | .757 | .936 | 1.307 | 6 |
| .50 | .30 | .10 | .300 | .303 | 1.046 | 1.001 | .951 | 4 |
| .50 | -.05 | -.60 | -.050 | -.056 | .967 | 1.000 | 1.032 | 5 |
| .50 | -.60 | -.65 | -.250 | -.297 | .834 | .861 | 1.305 | 6 |
| .45 | .20 | -.15 | .167 | .171 | 1.046 | .996 | .958 | 5 |
| .45 | -.15 | -.95 | -.217 | -.286 | .673 | 1.059 | 1.268 | 6 |
| .40 | .40 | -.10 | .233 | .238 | 1.065 | .968 | .966 | 5 |
| .40 | .05 | -.05 | .133 | .136 | 1.022 | 1.010 | .968 | 4 |
| .40 | -.35 | -.65 | -.200 | -.226 | .864 | .963 | 1.173 | 5 |
| .35 | .25 | -.70 | -.033 | -.038 | .974 | 1.011 | 1.015 | 5 |
| .35 | -.10 | -.95 | -.233 | -.304 | .646 | 1.093 | 1.261 | 6 |
| .35 | -.75 | -.85 | -.417 | -.487 | .535 | .788 | 1.677 | 6 |
| .30 | -.00 | -.45 | -.050 | -.053 | .978 | 1.003 | 1.019 | 5 |
| .30 | -.45 | -.65 | -.267 | -.297 | .831 | .933 | 1.237 | 5 |
| .25 | .05 | -.20 | .033 | .034 | 1.008 | .999 | .993 | 4 |
| .25 | -.10 | -.85 | -.233 | -.277 | .738 | 1.070 | 1.191 | 6 |
| .20 | .20 | .10 | .167 | .167 | 1.010 | .995 | .995 | 4 |
| .20 | -.10 | -.85 | -.250 | -.295 | .718 | 1.085 | 1.197 | 5 |
| .15 | -.45 | -.65 | -.317 | -.342 | .812 | .943 | 1.246 | 5 |
| .10 | -.15 | -.20 | -.083 | -.084 | .989 | .994 | 1.017 | 4 |
| .05 | .05 | -.75 | -.217 | -.242 | .816 | 1.092 | 1.092 | 5 |
| .05 | -.40 | -.50 | -.283 | -.294 | .905 | .953 | 1.142 | 5 |
| -.00 | -.60 | -.65 | -.417 | -.440 | .797 | .857 | 1.345 | 5 |
| -.05 | -.20 | -.60 | -.283 | -.295 | .854 | 1.042 | 1.104 | 5 |
| -.05 | -.50 | -.65 | -.400 | -.418 | .790 | .941 | 1.269 | 5 |
| -.10 | -.25 | -.40 | -.250 | -.252 | .947 | 1.001 | 1.052 | 4 |
| -.15 | -.15 | -.20 | -.167 | -.167 | .993 | 1.003 | 1.003 | 4 |
| -.15 | -.40 | -.50 | -.350 | -.355 | .906 | .974 | 1.118 | 4 |
| -.25 | -.40 | -.40 | -.350 | -.351 | .971 | .971 | 1.059 | 4 |
| -.35 | -.35 | -.65 | -.450 | -.458 | .776 | 1.112 | 1.112 | 5 |

Figure 3.4.4. Selected values of $\hat{\rho}$ and $\hat{\lambda}_i^2$ from 7035 sample correlation matrices, with best theoretical bounds from Figure 3.4.3.




| $\hat{\rho}$ | $\hat{\lambda}_i^2$ | $\hat{\rho}$ | $\hat{\lambda}_i^2$ |
|---|---|---|---|
| -.492 | 1.920 | -.044 | 1.045 |
| -.475 | 1.861 | .096 | 1.059 |
| -.452 | 1.765 | .200 | 1.105 |
| -.399 | 1.662 | .301 | 1.134 |
| -.352 | 1.544 | .401 | 1.154 |
| -.300 | 1.402 | .498 | 1.150 |
| -.248 | 1.342 | .595 | 1.135 |
| -.205 | 1.244 | .691 | 1.130 |
| -.151 | 1.157 | .802 | 1.079 |
| -.102 | 1.093 | .884 | 1.049 |

| $\hat{\rho}$ | $\hat{\lambda}_i^2$ | $\hat{\rho}$ | $\hat{\lambda}_i^2$ |
|---|---|---|---|
| -.499 | .008 | -.044 | .971 |
| -.475 | .247 | .102 | .918 |
| -.451 | .351 | .205 | .882 |
| -.399 | .484 | .297 | .832 |
| -.351 | .569 | .393 | .819 |
| -.300 | .650 | .503 | .822 |
| -.251 | .745 | .596 | .839 |
| -.201 | .817 | .690 | .868 |
| -.147 | .869 | .802 | .917 |
| -.101 | .918 | .884 | .960 |

Now $s^2 - 2 = -1 + 2x(n+d) + 2nd \leq 2x(n+d) - x^2$, since $2nd \leq n^2 + d^2 = 1 - x^2$. Thus (3.4.47) holds provided $s[2(n+d) - x] \leq 9nd$, $x \neq 0$. That is $2(n+d)^2 + x(n+d) - x^2 \leq 9nd$ or $2(d-n)^2 + x(n+d) - x^2 \leq nd$. If

$$(3.4.48) \qquad \epsilon = x - d \quad ; \quad \delta = d - n,$$

we need $\epsilon^2 + \epsilon\delta - 2\delta^2 \geq 0$, which is so whenever $\epsilon \geq \delta$. To prove (3.4.47) when $\epsilon < \delta$ we write $s^2 - 2 = -1 + 2n(d+x) + 2dx \leq 2n(d+x) - n^2$, since $2dx \leq x^2 + d^2 = 1 - n^2$. Thus we need $s[2(d+x) - n] \leq 9dx$, $n \neq 0$. [When $n = 0$ we need $s^2 - 2 \leq 0$ which follows from $(d+x)^2 - 2 = x^2 + d^2 + 2xd - 2 \leq 2(x^2+d^2-1) = 0$.] Substituting (3.4.48) we obtain $2\epsilon^2 + n(d+x) - n^2 \leq dx$ or $\delta^2 + \epsilon\delta - 2\epsilon^2 \geq 0$, which is so provided $\delta \geq \epsilon$, thus completing the proof. (qed)

COROLLARY 3.4.1. _Let_ $u_i$, $i = 1, 2, 3$, _be three nonnegative quantities with_ $\sum_{i=1}^{3} u_i^2 = 3$. _Then_

$$(3.4.49) \qquad 2\left(\sum_{i=1}^{3} u_i^3 - \sum_{i=1}^{3} u_i\right) \geq \sum_{i=1}^{3} u_i - 3\prod_{i=1}^{3} u_i,$$

_with equality if and only if all the_ $u_i$ _are equal._

The inequality (3.4.49) follows from (3.4.44) by substituting $u_i = \sqrt{3}\, x_i$. An interpretation of the differences compared in (3.4.49) may be made as follows. From the Cauchy-Schwarz inequality $\Sigma u_i^3 \cdot \Sigma u_i \geq (\Sigma u_i^2)^2 = 9$ and $\Sigma u_i \leq 3$ [cf. (3.3.3)]. Thus

$$(3.4.50) \qquad \sum_{i=1}^{3} u_i^3 \geq 3 \geq \sum_{i=1}^{3} u_i,$$

while by the arithmetic mean/geometric mean inequality, (3.4.51) $$\sum_{i=1}^{3} u_i \geq 3\prod_{i=1}^{3} u_i^{1/3} \geq 3 \prod_{i=1}^{3} u_i .$$

Thus (3.4.49) asserts that twice a Cauchy-Schwarz inequality-type-difference is at least as large as an arithmetic mean/geometric mean inequality-type-difference.

We use Corollary 3.4.1 to establish part of:

RESULT 3.4.2. <u>When</u> $p = 3$, <u>either</u>

(3.4.52) $$-\tfrac{1}{2} < \hat{\rho} \leq r \leq 0,$$

<u>or</u>

(3.4.53) $$0 \leq r \leq \hat{\rho} < 1,$$

<u>where</u> $r = (r_{12} + r_{13} + r_{23})/3$ <u>is the average sample correlation coefficient and</u> $\hat{\rho}$ <u>is the maximum likelihood estimate of</u> $\rho$ <u>as given by the unique solution of (3.4.27) and</u> $\sum_{i=1}^{3} \hat{\lambda}_i^2 = 3$.

Using (3.4.31) we have when $\hat{\rho} \neq 0$,

(3.4.54) $$r = \frac{(1+\hat{\rho}+\hat{\rho}^2)\sum_{i=1}^{3} \hat{\lambda}_i - (1+\hat{\rho})\sum_{i=1}^{3} \hat{\lambda}_i^3}{3\hat{\rho}\prod_{i=1}^{3} \hat{\lambda}_i},$$

so that $r \leq \hat{\rho}$ $(\hat{\rho} > 0)$ or $r \geq \hat{\rho}$ $(\hat{\rho} < 0)$ provided

(3.4.55) $$\hat{\rho}^2\left(\sum_{i=1}^{3} \hat{\lambda}_i - 3\prod_{i=1}^{3} \hat{\lambda}_i\right) - (\hat{\rho}+1)\left(\sum_{i=1}^{3} \hat{\lambda}_i^3 - \sum_{i=1}^{3} \hat{\lambda}_i\right) \leq 0.$$

Applying Lemma 3.4.1 we find that the negative root from (3.4.55) is at most $-\frac{1}{2}$ and the positive root at least one provided

(3.4.56) $$2\left(\sum_{i=1}^{3} \hat{\lambda}_i^3 - \sum_{i=1}^{3} \hat{\lambda}_i\right) \geq \sum_{i=1}^{3} \hat{\lambda}_i - 3\prod_{i=1}^{3} \hat{\lambda}_i,$$

which holds by (3.4.49). Equality holds if and only if $\hat{\rho} = r$ ; $\hat{\lambda}_i^2 = 1; i = 1, 2, 3$, as observed in §3.1. When $\hat{\rho} \neq 0$, all $r_{ij} = r$ in addition. It follows from Result 3.4.1 that $\hat{\rho} = 0$ if and only if $r = 0$, and so $\hat{\rho} = r$ if and only if $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$ for all $\hat{\rho}$ in $(-\frac{1}{q}, 1)$.

It remains to be shown that $\hat{\rho}$ and $r$ have the same sign. This is so provided

$$(3.4.57) \qquad (1+\hat{\rho}+\hat{\rho}^2)\sum_{i=1}^{3}\hat{\lambda}_i > (1+\hat{\rho})\sum_{i=1}^{3}\hat{\lambda}_i^3,$$

making the numerator in (3.4.54) positive ($\hat{\rho}$ positive or negative).

We verified by computer that subject to $\Sigma\hat{\lambda}_i^2 = 3$ and $\hat{\lambda}_m < \hat{\lambda}_i < \hat{\lambda}_M$,

$$(3.4.58) \qquad \max \frac{\Sigma\,\hat{\lambda}_i^3}{\Sigma\,\hat{\lambda}_i} = \frac{\hat{\lambda}_M^3 + \hat{\lambda}_d^3 + \hat{\lambda}_m^3}{\hat{\lambda}_M + \hat{\lambda}_d + \hat{\lambda}_m},$$

where $\hat{\lambda}_d^2 = 3 - \hat{\lambda}_M^2 - \hat{\lambda}_m^2$. We evaluated (3.4.58) numerically using (3.4.18) through (3.4.20) for $\hat{\lambda}_m$ and $\hat{\lambda}_M$ and $\hat{\rho} = -.4995(.0005)-.495(.005)-.245, -.2(.1).9$, and found (3.4.58) exceeding $1 + \hat{\rho}^2/(1+\hat{\rho})$ with $\hat{\rho} \geq -.4965$. For $-.4995 \leq \hat{\rho} \leq -.4970$, (3.4.58) made $|\underset{\sim}{R}| < 0$; the largest value of the left-hand side of (3.4.58) with $|\underset{\sim}{R}| > 0$ was found always to be larger than $1 + \hat{\rho}^2/(1+\hat{\rho})$ in this range. Thus (3.4.57) and our result are established.

### 3.4.4 Case of all Sample Correlation Coefficients with Same Sign.

Further bounds on $\hat{\lambda}_i^2$ apply when all sample correlation coefficients have the same sign. Suppose first that all $r_{ij} > 0$. If $\hat{\rho} < 0$ then from (3.3.1)

$$(3.4.59) \qquad [1 + \hat{\rho}(q-1)]\hat{\lambda}_i^2 < \hat{\alpha}.$$

Summing from $i = 1, \ldots, p$ we obtain $0 < -\hat{\rho}^2 q$ which is not possible. Hence $\hat{\rho} > 0$. This proves:

THEOREM 3.4.2. *When $\hat{\rho} > 0$ at least one sample correlation coefficient is positive, and when $\hat{\rho} < 0$ at least one is negative. When all sample correlation coefficients have the same sign, $\hat{\rho}$ also has that sign.*

We thus have the reverse inequality to (3.4.59) regardless of sign. Similarly from (3.3.31),

$$[1 + (q-1)\hat{\rho}]\hat{\lambda}_i^2 - \hat{\alpha} < \tfrac{1}{2}pq\hat{\rho}^2. \tag{3.4.60}$$

Combining these results we have the following:

THEOREM 3.4.3. *When the sample correlation coefficients are either all positive or all negative and* $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$,

$$1 - \frac{q\hat{\rho}^2}{1+(q-1)\hat{\rho}} < \hat{\lambda}_i^2 < 1 + \frac{qt\hat{\rho}^2}{1+(q-1)\hat{\rho}} \; ; \; i = 1, \ldots, p. \tag{3.4.61}$$

As $\hat{\rho}$ tends to 0 both bounds converge to 1, while as $\hat{\rho}$ tends to $-1/q$ or to 1, they converge to 0 and $\frac{1}{2}p$. Both bounds are weaker than previous bounds for most positive $\hat{\rho}$ and even quite small p, but are uniformly tighter for all negative $\hat{\rho}$ and all p. We remark that the bounds (3.4.61) are symmetric about $\hat{\rho} = 0$ with the positive side inflated to q times the negative side.

Using the strongest of the bounds (3.4.61), (3.3.11), and (3.3.38) in Corollary 3.2.1, we found by numerical evaluation that (3.4.5) was always positive, $\hat{\rho} > 0$, $p \geq 4$. Thus $|\underset{\sim}{H}_1|$ is positive, $\hat{\rho} > 0$, when all sample correlation coefficients are positive.

When $p = 3$, (3.4.61) becomes

$$(3.4.62) \qquad 1 - \frac{2\hat{\rho}^2}{1+\hat{\rho}} < \hat{\lambda}_i^2 < 1 + \frac{\hat{\rho}^2}{1+\hat{\rho}} \; ; \; i = 1, 2, 3,$$

which we sketch in Figure 3.4.3. Applying (3.4.62) to Corollary 3.2.1 yields for $\hat{\rho} < 0$,

$$(3.4.63) \qquad m = \frac{1 + \frac{1}{2}\hat{\rho}}{1 - \hat{\rho}^3} \; ; \; M = \frac{1}{\hat{\alpha}} \; ,$$

which substituted in (3.4.5) gives

$$(3.4.64) \qquad d = \frac{\hat{\rho}^2}{\hat{\alpha}(1-\hat{\rho}^3)} \, [2\hat{\rho}^3 - \hat{\rho}^2 + 2\hat{\rho} + \tfrac{3}{2}].$$

The cubic in (3.4.64) has one real root of $\hat{\rho} = -\frac{1}{2}$ and is monotonically increasing. Hence (3.4.64) is positive for $\hat{\rho} > -\frac{1}{2}$ and so $|\underset{\sim}{H}_1| > 0$ for $-\frac{1}{2} < \hat{\rho} < 0$ and all sample correlation coefficients negative.

## 3.5 Iterative Solution of the Maximum Likelihood Equations.

The maximum likelihood equations in Theorem 3.1.1 may be solved iteratively by the procedures given in §2.4. We use the Newton-Raphson process based on the initial trial solution of $\hat{\underset{\sim}{\lambda}} = \underset{\sim}{e}$ and $\hat{\rho} = r$, the average sample correlation coefficient. By substitution in (3.1.31) through (3.1.33), (3.1.4), and (3.1.11), we find the first iterate to be, using (2.4.5),

$$(3.5.1) \quad \begin{pmatrix} \underset{\sim}{\lambda}_1 \\ \rho_1 \end{pmatrix} = \begin{pmatrix} \underset{\sim}{e} \\ r \end{pmatrix} - \begin{bmatrix} 2(\overline{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} + \underset{\sim}{I}), & 2[(1+rq)^2\underset{\sim}{I} - (1+r^2q)\underset{\sim}{R}] \, \underset{\sim}{e}/a^2 \\ 2\underset{\sim}{e}'[(1+rq)^2\underset{\sim}{I} - (1+r^2q)\underset{\sim}{R}]/a^2, & pq(1+r^2q)/a^2 \end{bmatrix}^{-1} \begin{pmatrix} 2(\overline{\underset{\sim}{R}}^{-1} * \underset{\sim}{R} - \underset{\sim}{I})\underset{\sim}{e} \\ 0 \end{pmatrix},$$

where $\overline{\underset{\sim}{R}}$ and $a$ are $\underset{\sim}{R}$ and $\alpha$, respectively, with $r$ replacing $\rho$. As in §2.9 we substitute $\overline{\underset{\sim}{R}}$ for $\underset{\sim}{R}$ in the matrix of second derivatives and obtain

$$(3.5.2)\quad \begin{pmatrix} \lambda_1^* \\ \rho_1^* \end{pmatrix} = \begin{pmatrix} e \\ r \end{pmatrix} + \begin{pmatrix} \frac{1}{2}I, & 0 \\ 0', & 1 \end{pmatrix} \begin{bmatrix} \frac{1}{2}(\bar{R}^{-1}*\bar{R}+I), & -rqe/a \\ -rqe'/a, & pq(1+r^2q)/a^2 \end{bmatrix}^{-1} \begin{pmatrix} (I-\bar{R}^{-1}*R)e \\ 0 \end{pmatrix}.$$

The matrix to be inverted is (3.1.35) with $r$ replacing $\rho$. Using (3.1.39) we have

$$(3.5.3)\quad \begin{pmatrix} \lambda_1^* \\ \rho_1^* \end{pmatrix} = \begin{pmatrix} e \\ r \end{pmatrix} + \begin{bmatrix} \frac{2a}{2a+pr^2} I + r^2 ee'\left(\frac{1}{2a+pr^2} + \frac{q}{p}\right), & are/p \\ are'/p, & a^2/pq \end{bmatrix} \begin{bmatrix} (I-\bar{R}^{-1}*R)e \\ 0 \end{bmatrix}.$$

Since $\bar{R}^{-1}*R = \frac{1}{1-r} I - \frac{r}{a} R$, we obtain $(\bar{R}^{-1}*R)e = [1+r(q-1)]e/a - r\underline{r}/a$, where $\underline{r} = (R-I)e$, the vector of row sums of sample correlations. Thus $(I-\bar{R}^{-1}*R)e = r\underline{r}/a - qr^2e/a$ and $e'(I-\bar{R}^{-1}*R)e = 0$. Hence $\rho_1^* = r$ and

$$(3.5.4)\quad \lambda_1^* = \frac{r}{2a+pr^2}\underline{r} + \left(1 - \frac{qr^2}{2a+pr^2}\right)e,$$

which is (2.9.11) with $r$ replacing $\rho$. Han (1967) obtained (3.5.4) and proved that $\sqrt{N}\,(\sigma_*^{(\ell)} - \sigma^{(\ell)})$, where $\sigma_*^{(\ell)} = (D^{-1}\lambda_1^*)^{(-\ell)}$, has a limiting multivariate normal distribution with mean $0$ and covariance matrix proportional to the upper left-hand corner of (3.1.24). It follows that $\sqrt{N}\,(\gamma_1^* - \gamma)$ has the same limiting distribution as given in Theorem 3.1.4, where $\gamma = (\sigma^{(2)'}, \rho)'$. Han (1967, 1968) obtained large sample tests of homogeneity of variances based on (3.5.4) similar to those given in §2.9.4 and compared them with other tests. Anderson (1963), Lawley (1963), and Gleser (1968) have given related large sample tests for testing homogeneity of correlation coefficients.

## 3.6 Efficiencies of the Sample Quantities.

In this section we evaluate the limiting relative efficiencies of $D^2e$ and $r$ and compare our results with those of §2.9.3. From (3.1.24) the limiting covariance matrix of the maximum likelihood estimate is

$$(3.6.1) \qquad 2\begin{bmatrix} \underset{\sim}{\Delta}^2(\frac{2\alpha}{2\alpha+p\rho^2}\underset{\sim}{I} + \rho^2\underset{\sim}{ee}'[\frac{1}{2\alpha+p\rho^2} + \frac{q}{p}])\underset{\sim}{\Delta}^2, & (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)} \\ (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)\prime}, & \alpha^2/pq \end{bmatrix}$$

while that of the sample quantities is

$$(3.6.2) \qquad 2\begin{bmatrix} \underset{\sim}{\Delta}^2[(1-\rho^2)\underset{\sim}{I} + \rho^2\underset{\sim}{ee}']\underset{\sim}{\Delta}^2, & (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)} \\ (\alpha\rho/p)\underset{\sim}{\sigma}^{(2)\prime}, & \alpha^2/pq \end{bmatrix}$$

from (2.9.42), (2.9.40), and (2.9.36). We thus see immediately that the average sample correlation coefficient is an asymptotically efficient estimate of $\rho$. Using (2.6.3) we obtain:

THEOREM 3.6.1. <u>The asymptotic relative efficiency of the sample variances in a multivariate normal distribution with equal but unknown correlations is given by</u>

$$(3.6.3) \qquad \frac{1}{[(1-\rho^2)(1 + \frac{p\rho^2}{2\alpha})]^{p-1}}.$$

<u>Proof</u>. The efficiency is the ratio of the determinants of the upper left-hand corners of (3.6.1) and (3.6.2). In (3.6.1), the $p \times p$ matrix has a multiple root of $2\alpha/(2\alpha+p\rho^2)$ and a simple root of $1 + q\rho^2$, while that in (3.6.2) has a multiple root of $1 - \rho^2$ and the same simple root, establishing (3.6.3). (qed)

We note that (3.6.3) is the same as (2.9.55), the asymptotic efficiency of the modified estimator $\bar{\underset{\sim}{\sigma}}^{(2)} = (1 + [\rho(\rho-r)q]/2\alpha)^2\underset{\sim}{D}^2\underset{\sim}{e}$, when $\rho$ is known. Thus Table 2.9.2 and Figures 2.9.1 and 2.9.2 also apply to (3.6.3). The joint asymptotic efficiency of $\underset{\sim}{D}^2\underset{\sim}{e}$ and $r$ is also given by (3.6.3). To see this we must prove(3.6.3) the ratio of the determinants of (3.6.1) and (3.6.2). Using the Frobenius-Schur method the desired efficiency reduces to

$$(3.6.4)\qquad \frac{\left|\frac{2\alpha}{2\alpha+p\rho^2}\left(\underset{\sim}{I}+\frac{\rho^2}{2\alpha}\underset{\sim}{ee}'\right)\right|}{\left|(1-\rho^2)\underset{\sim}{I}+\rho^2\underset{\sim}{ee}'(1-q/p)\right|}\ ;$$

the matrix in the numerator has multiple root $2\alpha/(2\alpha+p\rho^2)$ and simple root 1, while that in the denominator has multiple root $1-\rho^2$ and simple root also 1. Thus (3.6.4) equals (3.6.3) as claimed.

Corollary 2.9.4 also applies to the asymptotic efficiency in Theorem 3.6.1. That is (3.6.3) tends to 1 as $\rho$ tends to 1, and has a minimum value over positive $\rho$ at

$$(3.6.5)\qquad \rho = \frac{p-4+\sqrt{p(p+8)}}{4(p-1)}\ ,$$

as in (2.9.58). Values of (3.6.3) at (3.6.5) are tabulated in Table 2.9.3 and illustrated in Figure 2.9.3.

## 3.7 Case of Variances Equal but Unknown.

When all the variances are equal but still unknown, the maximum likelihood equations can be solved explicitly. We write the covariance matrix

$$(3.7.1)\qquad \underset{\sim}{\Sigma} = \sigma^2\underset{\sim}{R} = \sigma^2[(1-\rho)\underset{\sim}{I}+\rho\underset{\sim}{ee}']$$

and study the problem in terms of $\rho$ and $\lambda$ where following (3.1.2),

$$(3.7.2)\qquad \lambda\underset{\sim}{De} = \underset{\sim}{De}/\sigma = \lambda\underset{\sim}{d} = \underset{\sim}{\lambda}.$$

Maximizing the likelihood is equivalent to minimizing

(3.7.3) $\ell = \lambda^2 \underset{\sim}{d}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R})\underset{\sim}{d} - 2p \log \lambda + \log |\underset{\sim}{R}|,$

using (3.1.3). Differentiating with respect to $\lambda$ yields

(3.7.4) $\frac{\partial \ell}{\partial \lambda} = 2\lambda \underset{\sim}{d}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R})\underset{\sim}{d} - 2p/\lambda,$

and with respect to $\rho$ gives, as in (3.1.11),

(3.7.5) $\frac{\partial \ell}{\partial \rho} = \frac{\lambda^2 \underset{\sim}{d}'\underset{\sim}{d}}{(1-\rho)^2} - \frac{(1+\rho^2 q)\lambda^2}{\alpha^2} \underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d} - \frac{\rho p q}{\alpha} .$

Setting (3.7.4) and (3.7.5) equal to zero, and substituting (3.1.8) in (3.7.4) yields

(3.7.6) $\hat{\lambda}^2 = \frac{p\hat{\alpha}}{(1+\hat{\rho}q)\underset{\sim}{d}'\underset{\sim}{d} - \hat{\rho}\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}} = \frac{pq\hat{\rho}\hat{\alpha}}{(1+\hat{\rho}q)^2\underset{\sim}{d}'\underset{\sim}{d} - (1+\rho^2 q)\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}} ,$

from which follows immediately that

(3.7.7) $1 + \hat{\rho}q = \underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}/\underset{\sim}{d}'\underset{\sim}{d},$

in parallel to (3.1.14), and

(3.7.8) $\hat{\rho} = \underset{\sim}{d}'(\underset{\sim}{R}-\underset{\sim}{I})\underset{\sim}{d}/q\underset{\sim}{d}'\underset{\sim}{d},$

which equals r, the average sample correlation coefficient when all the sample variances are equal. Substituting in (3.7.6) yields

(3.7.9) $\hat{\lambda}^2 = p/\underset{\sim}{d}'\underset{\sim}{d} = 1/\hat{\sigma}^2.$

As in Theorem 3.1.3 we deduce from (3.7.7) that

(3.7.10) $-\frac{1}{q} < \frac{1}{q}\, ch_p(\underset{\sim}{R}-\underset{\sim}{I}) \leq \hat{\rho} \leq \frac{1}{q}\, ch_1(\underset{\sim}{R}-\underset{\sim}{I}) < 1.$

We obtain the covariance matrix of the limiting distribution of

$\sqrt{N}\,(\hat{\sigma}^2 - \sigma^2,\ \hat{\rho} - \rho)$ from the second derivatives of $\ell$. From (3.7.4) we have

$$(3.7.11)\qquad \frac{\partial^2 \ell}{\partial \lambda^2} = 2\underset{\sim}{d}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R})\underset{\sim}{d} + 2p/\lambda^2,$$

while from (3.7.5) we obtain

$$(3.7.12)\qquad \frac{\partial^2 \ell}{\partial \lambda \partial \rho} = \frac{2\lambda \underset{\sim}{d}'\underset{\sim}{d}}{(1-\rho)^2} - \frac{2\lambda(1+\rho^2 q)}{\alpha^2}\,\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}.$$

Using (3.1.33) the second derivative with respect to $\rho$ is

$$(3.7.13)\qquad \frac{\partial^2 \ell}{\partial \rho^2} = \frac{2\lambda^2 \underset{\sim}{d}'\underset{\sim}{d}}{(1-\rho)^3} + \frac{2(q-1-3\rho q-\rho^3 q^2)}{\alpha^3}\,\lambda^2 \underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d} - \frac{pq(1+\rho^2 q)}{\alpha^2}\,.$$

Following the proof of Theorem 3.1.4 the desired covariance matrix is the limit of

$$(3.7.14)\qquad \tfrac{1}{2}\begin{bmatrix} -1/2\sigma^3, & 0 \\ 0, & 1 \end{bmatrix} E \begin{bmatrix} \dfrac{\partial^2 \ell}{\partial \lambda^2}, & \dfrac{\partial^2 \ell}{\partial \lambda \partial \rho} \\ \dfrac{\partial^2 \ell}{\partial \rho \partial \lambda}, & \dfrac{\partial^2 \ell}{\partial \rho^2} \end{bmatrix} \begin{pmatrix} -1/2\sigma^3, & 0 \\ 0, & 1 \end{pmatrix},$$

since $d(1/\sigma)/d\sigma^2 = -1/2\sigma^3$. Substituting, (3.7.14) becomes

$$(3.7.15)\qquad \tfrac{1}{2}p \begin{bmatrix} 1/\sigma^2, & 0 \\ 0, & 1 \end{bmatrix} \begin{bmatrix} 1, & -\rho q/\alpha \\ -\rho q/\alpha, & q(1+\rho^2 q)/\alpha^2 \end{bmatrix} \begin{bmatrix} 1/\sigma^2, & 0 \\ 0, & 1 \end{bmatrix},$$

in parallel to (3.1.34); inverting yields

$$(3.7.16)\qquad \frac{2}{p} \begin{pmatrix} (1+\rho^2 q)\sigma^4, & \alpha\rho\sigma^2 \\ \alpha\rho\sigma^2, & \alpha^2/q \end{pmatrix},$$

which also follows directly from (3.1.39) by pre- and postmultiplication by

$$(3.7.17)\qquad \begin{pmatrix} \underset{\sim}{e}'/p, & 0 \\ \underset{\sim}{0}', & 1 \end{pmatrix}.$$

The first term in (3.7.16) can also be obtained immediately from Corollary 2.4.2.

We verify that (3.7.8) and (3.7.9) maximize the likelihood by showing that the matrix formed from (3.7.11) through (3.7.13) is positive definite when (3.7.8) and (3.7.9) are satisfied. Substituting (3.7.8) in (3.7.11) yields $4p/\hat{\lambda}^2$, and in (3.7.12) gives $2\hat{\rho}pq/2\hat{\lambda}$ using (3.7.5). Substitution in (3.7.13) completes the matrix to be

$$(3.7.18) \qquad \begin{pmatrix} 4p/\hat{\lambda}^2, & 2\hat{\rho}pq/\hat{\alpha}\hat{\lambda} \\ 2\hat{\rho}pq/\hat{\alpha}\hat{\lambda}, & pq(1+\hat{\rho}^2q)/\hat{\alpha}^2 \end{pmatrix}$$

It suffices for positive definiteness to prove the determinant positive since the diagonal elements are clearly so. Expansion gives $4p^2q/\hat{\alpha}^2\hat{\lambda}^2$ for the determinant and so (3.7.18) is positive definite. We assemble these results in the following:

THEOREM 3.7.1. _In a p-variate normal population with covariance matrix_

$$(3.7.19) \qquad \underset{\sim}{\Sigma} = \sigma^2[(1-\rho)\underset{\sim}{I} + \rho\underset{\sim}{e}\underset{\sim}{e}'],$$

_the maximum likelihood estimates are_

$$(3.7.20) \qquad \hat{\sigma}^2 = \underset{\sim}{d}'\underset{\sim}{d}/p \ ; \ \hat{\rho} = \underset{\sim}{d}'(\underset{\sim}{R}-\underset{\sim}{I})\underset{\sim}{d}/q\underset{\sim}{d}'\underset{\sim}{d},$$

_where_ $\underset{\sim}{d}$ _is the vector of sample standard deviations,_ $\underset{\sim}{R}$ _is the sample correlation matrix, and_ $q = p - 1$. _The limiting distribution of_ $\sqrt{N}\,(\hat{\sigma}^2 - \sigma^2, \hat{\rho} - \rho)$, _where_ N _is the sample size, is bivariate normal with mean vector_ $\underset{\sim}{0}'$ _and covariance matrix_

$$(3.7.21) \qquad \frac{2}{p}\begin{pmatrix} (1+\rho^2q)\sigma^4, & \alpha\rho\sigma^2 \\ \alpha\rho\sigma^2, & \alpha^2/q \end{pmatrix},$$

_where_ $\alpha = (1-\rho)(1+\rho q)$.

The maximum likelihood estimate $\hat{\sigma}^2$ is the average sample variance, while $\hat{\rho}$ is the ratio of the average sample covariance to the average sample variance. Using (3.6.2), we find that $\sqrt{N}(\hat{\sigma}^2 - \sigma^2, r - \rho)$, where $r$ is the average sample correlation coefficient, and $\sqrt{N}(\hat{\sigma}^2 - \sigma^2, \hat{\rho} - \rho)$ have the same limiting distribution.

The exact marginal distributions of $\hat{\sigma}^2$ and $\hat{\rho}$ may be found as follows. If $\underset{\sim}{x}_\beta$, $\beta = 1,\ldots, N$, is a random sample from $N(\underset{\sim}{\mu}, \underset{\sim}{\Sigma} = \sigma^2[(1-\rho)\underset{\sim}{I} + \rho \underset{\sim}{e}\underset{\sim}{e}'])$, then $\underset{\sim}{P}'\underset{\sim}{x}_\beta$, $\beta = 1,\ldots, N$, is a random sample from $N(\underset{\sim}{P}'\underset{\sim}{\mu}, \underset{\sim}{P}'\underset{\sim}{\Sigma}\underset{\sim}{P})$, where $\underset{\sim}{P}$ is an orthogonal matrix with first column $\underset{\sim}{e}/\sqrt{p}$ and

$$(3.7.22) \quad \underset{\sim}{P}'\underset{\sim}{\Sigma}\underset{\sim}{P} = \sigma^2 \begin{bmatrix} (1+\rho q) & \underset{\sim}{0}' \\ \underset{\sim}{0} & (1-\rho)\underset{\sim}{I} \end{bmatrix} .$$

Thus $\hat{\sigma}^2(1+\hat{\rho}q)$ follows the same distribution as $\sigma^2(1+\rho q)\chi^2_{N-1}/N$ independently of $q\hat{\sigma}^2(1-\hat{\rho})$ which is distributed as $\sigma^2(1-\rho)\chi^2_{q(N-1)}/N$. Hence $\hat{\sigma}^2$ is distributed as

$$(3.7.23) \quad \sigma^2[(1+\rho q)\chi^2_{N-1} + (1-\rho)\chi^2_{q(N-1)}]/Np,$$

where the chi-squares are independent, and $\hat{\rho}$ follows the same distribution as

$$(3.7.24) \quad 1 - \frac{p}{q + \frac{1+\rho q}{1-\rho} F_{N-1,q(N-1)}} ,$$

which we note is independent of $\sigma^2$.

This model with equal variances and covariances is often referred to as that of intraclass correlation (cf. Olkin & Pratt (1958), Selliah (1964), for example). The maximum likelihood estimates $\hat{\sigma}^2$

and $\hat{\rho}$ and their distribution are given by Selliah (1964), who observes that $\hat{\sigma}^2$ is the unique minimum variance unbiased estimator of $\sigma^2$, since it is unbiased and $[\underset{\sim}{d}'\underset{\sim}{d},\ \underset{\sim}{d}'(\underset{\sim}{R}-\underset{\sim}{I})\underset{\sim}{d}]$ is a complete sufficient statistic. The estimator $\hat{\rho}$ is not unbiased; Olkin & Pratt (1958), however, have shown that $\hat{\rho}\ F(\frac{1}{2},\ 1;\ \frac{1}{2}N;\ 1 - \hat{\rho}^2)$ is the unique minimum variance unbiased estimate of $\rho$, where

$$(3.7.25)\qquad F(\eta,\ \nu;\ \gamma;\ x) = \sum_{k=0}^{\infty} \frac{\Gamma(\eta+k)\Gamma(\nu+k)\Gamma(\gamma)}{\Gamma(\eta)\Gamma(\nu)\Gamma(\gamma+k)}\ \frac{x^k}{k!}$$

is the hypergeometric function.

## 3.8 Case of Variances Known.

When the variances are known the maximum likelihood equation for the common correlation coefficient $\rho$ is a cubic. We write the covariance matrix

$$(3.8.1)\qquad \underset{\sim}{\Sigma} = \underset{\sim}{R} = (1-\rho)\underset{\sim}{I} + \rho\underset{\sim}{e}\underset{\sim}{e}',$$

setting the variances equal to unity, which loses no generality. Then from (3.7.5), with $\lambda = 1$,

$$(3.8.2)\qquad \frac{\partial \ell}{\partial \rho} = \frac{\underset{\sim}{d}'\underset{\sim}{d}}{(1-\rho)^2} - \frac{(1+\rho^2 q)}{\alpha^2}\,\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d} - \frac{\rho p q}{\alpha}\ ,$$

which put equal to 0 gives the cubic equation

$$(3.8.3)\qquad pq^2\hat{\rho}^3 + q\hat{\rho}^2[q(\underset{\sim}{d}'\underset{\sim}{d}-p) - (\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}-p)] + \hat{\rho}q(2\underset{\sim}{d}'\underset{\sim}{d}-p) + (\underset{\sim}{d}'\underset{\sim}{d}-\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}) = 0.$$

When $\hat{\rho} = 1$ the left-hand side of (3.8.3) equals $p(p\underset{\sim}{d}'\underset{\sim}{d}-\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d})$, which by Lemma 3.1.1 is always positive; when $\hat{\rho} = -1/q$, we obtain $-(p/q)\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}$ which is always negative. Hence (3.8.3) always admits one real root between $-1/q$ and 1; in general, (3.8.3) must have one or three real roots, and in the latter case two roots may fall between $-1/q$ and 1 and both give relative maxima of the likelihood. We would in such a case choose the root which gives the larger value of the likelihood, or the smaller value of

(3.8.4) $$\ell = \underset{\sim}{d}'(\underset{\sim}{R}^{-1} * \underset{\sim}{R})\underset{\sim}{d} + \log |\underset{\sim}{R}|.$$

A root of (3.8.3) will give a relative maximum of the likelihood when the corresponding value of the second derivative of $\ell$ is positive. Using (3.7.13) we have

(3.8.5) $$\frac{\partial^2 \ell}{\partial \rho^2} = \frac{2\underset{\sim}{d}'\underset{\sim}{d}}{(1-\rho)^3} + \frac{2(q-1-3\rho q-\rho^3 q^2)\underset{\sim}{d}'\underset{\sim}{Rd}}{\alpha^3} - \frac{pq(1+\rho^2 q)}{\alpha^2}.$$

Substituting $\underset{\sim}{d}'\underset{\sim}{d}$ satisfying (3.8.3) gives

(3.8.6) $$q(1-\hat{\rho})[p(1+\hat{\rho}q)(\hat{\rho}^2 q+2\hat{\rho}-1) + 2(1-\hat{\rho})\underset{\sim}{d}'\underset{\sim}{Rd}]/\hat{\alpha}^3.$$

A necessary and sufficient condition for (3.8.6) to be positive is that

(3.8.7) $$2(1-\hat{\rho})\underset{\sim}{d}'\underset{\sim}{Rd} > p(1+\hat{\rho}q)(1-2\hat{\rho}-\hat{\rho}^2 q),$$

or equivalently

(3.8.8) $$2\hat{\alpha}\underset{\sim}{d}'\underset{\sim}{d} > p(1+2\hat{\rho}(q-1) - 4\hat{\rho}^2 q - \hat{\rho}^4 q^2),$$

found by substituting (3.8.3) in (3.8.7).

We can solve (3.8.3) explicitly (cf. Birkhoff & Maclane (1953), pp. 96, 112-113) as follows. Let

(3.8.9) $$a = pq^2;\ 3b = q^2(\underset{\sim}{d}'\underset{\sim}{d}-p) - q(\underset{\sim}{d}'\underset{\sim}{Rd}-p)$$

(3.8.10) $\quad 3c = q(2\underset{\sim}{d}'\underset{\sim}{d}-p); \; d = \underset{\sim}{d}'\underset{\sim}{d}-\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}.$

Then we transform (3.8.3) by the substitution $y = a\hat{\rho} + b$ into

(3.8.11) $\quad y^3 + 3hy + g = 0,$

where

(3.8.12) $\quad g = a^2d - 3abc + 2b^3 \; ; \; h = ac - b^2.$

Making the so-called Vieta substitution

(3.8.13) $\quad y = x - h/x$

we obtain the quadratic $x^3 - h^3/x^3 + g = 0$ so that

(3.8.14) $\quad x^3 = \frac{1}{2}(-g \pm \sqrt{g^2 + 4h^3})$

which gives six solutions for $x$ in the form of cube roots. Substituting these in (3.8.13), we get three pairs of solutions for $y$, and hence $\hat{\rho}$, paired solutions being equal. One root will always be real, while the other two are complex conjugates of each other provided the discriminant in (3.8.14),

(3.8.15) $\quad g^2 + 4h^3 > 0 \; ;$

otherwise there are three real roots.

Following the discussion by Kendall & Stuart (1967), pp. 38-39, for the special case $p = 2$ (which we study in §3.8.1), we find

THEOREM 3.8.1. The maximum likelihood equation for the common correlation coefficient in a multivariate normal population with known variances admits a unique solution between $-1/(p-1)$ and

1 <u>with probability tending to</u> 1 <u>as the sample size</u> $N \to \infty$.

<u>Proof</u>. It suffices to prove that the limit in probability of the left-hand side of (3.8.15) is positive. Let the limits in probability of b, c, d, g, and h be the corresponding quantity with an asterisk. Then from (3.8.9) and (3.8.10), since $\underset{\sim}{d}'\underset{\sim}{d}$ tends in probability to p and $\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}$ to $p(1+\rho q)$, we have

$$(3.8.16) \qquad 3b^* = -pq^2\rho; \; 3c^* = pq; \; d^* = -pq\rho.$$

Hence, using (3.8.12), we obtain

$$(3.8.17) \qquad g^* = \frac{-2p^3q^5\rho}{3}\left(1 + \frac{q\rho^2}{9}\right); \; h^* = \frac{p^2q^3}{3}\left(1 - \frac{q\rho^2}{3}\right),$$

so that the left-hand side of (3.8.15) tends in probability to

$$(3.8.18) \qquad 4p^6q^9(1 + q\rho^2)^2/27,$$

which is always positive. (qed)

Writing $\alpha = (1-\rho)(1+\rho q)$ as before, we find that the expectation of (3.8.5) tends to

$$(3.8.19) \qquad pq(1+\rho^2 q)/\alpha^2.$$

Thus $\sqrt{N}(\hat{\rho} - \rho)$ has a limiting normal distribution with mean 0 and variance $2\alpha^2/pq(1+\rho^2 q)$, where N is the sample size and $\hat{\rho}$ the real solution of (3.8.3) between $-1/q$ and 1 which makes (3.8.4) the smallest. From Theorem 3.7.1 we recall that $\sqrt{N}(r - \rho)$, where r is the average sample correlation coefficient, has a limiting normal distribution with mean 0 and variance $2\alpha^2/pq$. Thus the asymptotic efficiency of r is

(3.8.20) $1/(1 + \rho^2 q); \quad - 1/q < \rho < 1.$

As $\rho$ tends to $- 1/q$, (3.8.20) tends to $q/p$, which for $p$ not too small is near 1. For $\rho \neq 0$, (3.8.20) decreases as the dimension $p$ becomes large.

Another estimator of $\rho$ is the average sample covariance (we are taking all variances equal to unity):

$$r^* = \sum_{i \neq j} c_{ij}/pq. \tag{3.8.21}$$

From Lemma 2.9.3 we find that $\sqrt{N}(r^* - \rho)$ has a limiting normal distribution with mean 0 and variance $4/p^2q^2$ times the sum of the elements in the lower right-hand corner of (2.9.34),

$$2[\{1 + \rho(q-1)\}^2 + \rho^2 q]/pq. \tag{3.8.22}$$

Thus the asymptotic efficiency of $r^*$ is

$$\alpha^2/(1+\rho^2 q)[\{1 + \rho(q-1)\}^2 + \rho^2 q] \tag{3.8.23}$$

which is always less than or equal to the efficiency of $r$ since $\alpha^2 < \{1 + \rho(q-1)\}^2 + \rho^2 q$. We see this by expanding $\alpha^2$ and cancelling common terms, obtaining $\rho^2 q - 2\rho(q-1) - 3 < 0$ as an equivalent condition. The result then follows by Lemma 3.4.1 with $u = 1$ and $v = - 1/q$.

### 3.8.1 Case of $p = 2$.

When $p = 2$ the maximum likelihood equation (3.8.3) simplifies but remains a cubic. Substituting $\underset{\sim}{d}'\underset{\sim}{d} = c_{11} + c_{22}$ and $\underset{\sim}{d}'R\underset{\sim}{d} = c_{11} + c_{22} + 2c_{12}$ in (3.8.3), we obtain (cf. Kendall & Stuart

(1967), pp. 38-39)

$$(3.8.24)\qquad \hat\rho^3 - c_{12}\hat\rho^2 + (c_{11} + c_{22} - 1)\hat\rho - c_{12} = 0.$$

The condition (3.8.8) that a solution $\hat\rho$ maximizes the likelihood reduces to

$$(3.8.25)\qquad (1-\hat\rho^2)(c_{11} + c_{22}) > 1 - 4\hat\rho^2 - \hat\rho^4.$$

In an unpublished paper, Madansky (1958) obtained the complete solution of (3.8.24) for the maximum likelihood estimate $\hat\rho$. Let

$$(3.8.26)\qquad v = c_{12}^2 - 3(c_{11} + c_{22} - 1),$$

$$(3.8.27)\qquad w = c_{12}[9(4 - c_{11} - c_{22}) + 2c_{12}^2]/2|v|^{3/2}.$$

Then the solution of (3.8.24) which maximizes the likelihood is:

$$\begin{aligned}(3.8.28)\qquad \hat\rho &= \tfrac{2}{3}|v|^{\frac12}\sinh\left(\tfrac{1}{3}\sinh^{-1}w\right) + \frac{c_{12}}{3}\ ;\ v < 0,\\ &= \tfrac{2}{3}\,v^{\frac12}\cosh\left(\tfrac{1}{3}\cosh^{-1}w\right) + \frac{c_{12}}{3}\ ;\ v > 0,\ |w| \geq 1,\\ &= \tfrac{2}{3}\,v^{\frac12}\cos\left(\tfrac{1}{3}\cos^{-1}w + \tfrac{4\pi}{3}\right) + \frac{c_{12}}{3}\ ;\ v > 0,\ |w| < 1,\\ &= \frac{c_{12}}{3} + \left(c_{12} + \frac{c_{12}^3}{27}\right)^{\frac13};\ v = 0.\end{aligned}$$

The last solution occurs with probability zero. Asymptotically the first solution applies since $v$ tends in probability to $\rho^2 - 3 < 0$. Madansky's method apparently does not generalize directly to the case of arbitrary $p > 2$. Differentiating the left-hand side of (3.8.3) gives the quadratic

$$(3.8.29)\qquad 3pq^2\hat\rho^2 + 2q\hat\rho[q(\underset{\sim}{d}'\underset{\sim}{d}-p) - (\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}-p)] + q(2\underset{\sim}{d}'\underset{\sim}{d}-p)$$

with discriminant

$$(3.8.30) \quad q^2[q(\underset{\sim}{d}'\underset{\sim}{d}-p) - (\underset{\sim}{d}'\underset{\sim}{R}\underset{\sim}{d}-p)]^2 - 3pq^3(2\underset{\sim}{d}'\underset{\sim}{d}-p).$$

This tends in probability to $p^2q^3(q\rho^2-3)$ which is negative for all $\rho$ between $-1/q$ and $1$ only for $q \leq 3$ or $p \leq 4$. When $p = 2$, $q = 1$ and (3.8.30) reduces to $4v$.

The asymptotic efficiency of $\underline{r}$, now the only sample correlation coefficient is

$$(3.8.31) \quad 1/(1+\rho^2),$$

from (3.8.20), while that of $r^*$, now the only sample covariance is

$$(3.8.32) \quad (1-\rho^2)^2/(1+\rho^2)^2,$$

from (3.8.23), as given by Madansky (1958). We sketch (3.8.31) and (3.8.32) in Figure 3.8.1 below for $-1 < \rho < 1$.

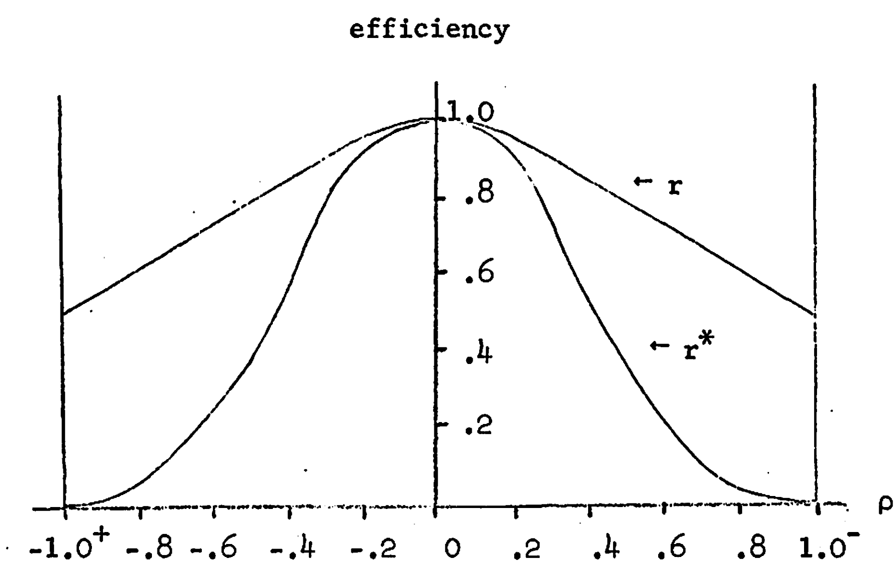



Figure 3.8.1. Efficiency of sample correlation coefficient $r$ and sample covariance $r^*$ when variances are known and $p = 2$.

## IV. OTHER CORRELATION STRUCTURES

We can extend the procedures used in Sections II and III to more general assumptions about the correlation matrix. Motivated by Anderson (1966) and (1968) we study the situation where the covariance matrix

$$(4.1) \qquad \underset{\sim}{\Sigma} = \underset{\sim}{\Delta}(\underset{\sim}{I} + \sum_{g=1}^{m} \rho_g \underset{\sim}{K}_g)\underset{\sim}{\Delta} = \underset{\sim}{\Delta}\underset{\sim}{R}\underset{\sim}{\Delta},$$

or the correlation matrix has linear structure. We assume that the diagonal matrix $\underset{\sim}{\Delta}$ of standard deviations is unknown, and that $\underset{\sim}{K}_1, \underset{\sim}{K}_2, \ldots, \underset{\sim}{K}_m$ are $m$ given symmetric linearly independent zero-axial matrices with unknown coefficients $\rho_1, \rho_2, \ldots, \rho_m$ so chosen that $\underset{\sim}{R}$ is positive definite. The component matrices may be zero-axial, i.e., have diagonal elements all zero, since $\underset{\sim}{R}$ has diagonal elements all unity.

In Section III we studied the special case of (4.1) with $m = 1$ and $\underset{\sim}{K}_1 = \underset{\sim}{e}\underset{\sim}{e}' - \underset{\sim}{I}$. Other special cases of (4.1) are considered by Jöreskog (1963) and Aitkin, Nelson, & Reinfurt (1968).

We will estimate the unknown variances and coefficients $\rho_1, \ldots, \rho_m$ by the method of maximum likelihood. As in Section III we study the problem in terms of

$$(4.2) \qquad \underset{\sim}{\lambda} = \underset{\sim}{D}\underset{\sim}{\sigma}^{(-1)},$$

where, as in (3.1.2), the elements of $\underset{\sim}{\lambda}$ are ratios of sample to population standard deviations. Maximizing the likelihood is equivalent to minimizing

$$(4.3)\qquad \ell = \underset{\sim}{\lambda}'(\underset{\sim}{R}^{-1}*\underset{\sim}{R})\underset{\sim}{\lambda} - 2\underset{\sim}{e}'\underset{\sim}{\lambda}^{(\ell)} + \log|\underset{\sim}{R}| + 2\log|\underset{\sim}{D}|,$$

as in (3.1.3). We differentiate (4.3) with respect to $\underset{\sim}{\lambda}$ and $\rho_1,\ldots,\rho_m$. From (3.1.4) we recall that

$$(4.4)\qquad \frac{\partial\ell}{\partial\underset{\sim}{\lambda}} = 2[(\underset{\sim}{R}^{-1}*\underset{\sim}{R})\underset{\sim}{\lambda} - \underset{\sim}{\lambda}^{(-1)}].$$

Let us write

$$(4.5)\qquad \underset{\sim}{\rho} = (\rho_1,\ldots,\rho_m)'.$$

Then writing $\{\partial\underset{\sim}{R}^{-1}/\partial\underset{\sim}{\rho}\}$ for $\partial\underset{\sim}{R}^{-1}/\partial\rho_g$; $g = 1,\ldots, m$, etc., we find

$$(4.6)\qquad \{\frac{\partial\underset{\sim}{R}^{-1}}{\partial\underset{\sim}{\rho}}\} = -\underset{\sim}{R}^{-1}\{\frac{\partial\underset{\sim}{R}}{\partial\underset{\sim}{\rho}}\}\underset{\sim}{R}^{-1} = \{-\underset{\sim}{R}^{-1}\underset{\sim}{K}_g\underset{\sim}{R}^{-1};\ g = 1,\ldots, m\}$$

and (cf. Anderson (1958), p. 347)

$$(4.7)\qquad \frac{\partial\log|\underset{\sim}{R}|}{\partial\underset{\sim}{\rho}} = \operatorname{tr}\underset{\sim}{R}^{-1}\{\frac{\partial\underset{\sim}{R}}{\partial\underset{\sim}{\rho}}\}$$

$$= \{\operatorname{tr}\underset{\sim}{R}^{-1}\underset{\sim}{K}_g;\ g = 1,\ldots, m\}$$

so that

$$(4.8)\qquad \frac{\partial\ell}{\partial\underset{\sim}{\rho}} = \{\operatorname{tr}\underset{\sim}{R}^{-1}\underset{\sim}{K}_g - \underset{\sim}{\lambda}'(\underset{\sim}{R}^{-1}\underset{\sim}{K}_g\underset{\sim}{R}^{-1}*\underset{\sim}{R})\underset{\sim}{\lambda};\ g = 1,\ldots, m\}$$

$$= \{\operatorname{tr}\underset{\sim}{R}^{-1}\underset{\sim}{K}_g(\underset{\sim}{I} - \underset{\sim}{R}^{-1}\underset{\sim}{\Lambda}\underset{\sim}{R}\underset{\sim}{\Lambda});\ g = 1,\ldots, m\}.$$

We equate (4.4) and (4.8) to zero to obtain

THEOREM 4.1. The maximum likelihood equations for the unknown quantities in the covariance matrix $\underset{\sim}{\Sigma} = \underset{\sim}{\Delta}(\underset{\sim}{I} + \Sigma\rho_g\underset{\sim}{K}_g)\underset{\sim}{\Delta}$ in a p-dimensional normal population are

(4.9) $(\hat{R}^{-1} * R)\hat{\lambda} = \hat{\lambda}^{(-1)}$

and

(4.10) $\mathrm{tr}\ \hat{R}^{-1}K_g = \mathrm{tr}\ \hat{R}^{-1}K_g\hat{R}^{-1}\hat{\Lambda}R\hat{\Lambda};\ g = 1,\ldots, m,$

where $\hat{R}$ and $R$ are the maximum likelihood estimate and sample correlation matrices, and $\hat{\lambda}^{(-1)} = \hat{\Lambda}^{-1}e$ is the Hadamard inverse of $\hat{\lambda} = \hat{\Lambda}e$ which contains ratios of sample to maximum likelihood estimate standard deviations.

Premultiplying (4.9) by $\hat{\lambda}'$ yields

(4.11) $\hat{\lambda}'(\hat{R}^{-1} * R)\hat{\lambda} = p = \mathrm{tr}\ \hat{R}^{-1}\hat{\Lambda}R\hat{\Lambda},$

while multiplying (4.10) by $\hat{\rho}_g$ and summing over $g = 1,\ldots, m$ gives

(4.12) $\mathrm{tr}\ \hat{R}^{-1} = \mathrm{tr}\ \hat{R}^{-1}\hat{\Lambda}R\hat{\Lambda}\hat{R}^{-1} = \hat{\lambda}'(\hat{R}^{-2} * R)\hat{\lambda},$

using (4.11).

As shown by Anderson (1958), p. 47 and Anderson (1966) the equations in Theorem 4.1 admit at least one real solution. When there is more than one we choose that which minimizes (4.3). From Chanda (1954) and Anderson (1966) we find that (4.11) and (4.12) admit a consistent solution and the usual asymptotic theory applies.

We proceed by finding the second derivatives of $\ell$. From (4.4) we find

(4.13) $\frac{\partial^2 \ell}{\partial \lambda \partial \lambda^T} = 2(R^{-1} * R + \Lambda^{-2})$

as in (3.1.31), and

(4.14) $\frac{\partial^2 \ell}{\partial \lambda \partial \rho^T} = \{-\ 2(R^{-1}K_g R^{-1} * R)\lambda;\ g = 1,\ldots, m\}.$

From (4.8) we obtain

$$(4.15) \qquad \frac{\partial^2 \ell}{\partial \lambda \partial \rho'} = \{\mathrm{tr}\, R^{-1} K_g (2R^{-1}\Lambda R \Lambda - I) R^{-1} K_h;\ g,\ h = 1, \ldots, m\}.$$

Following the proof of Theorem 3.1.4 we have:

THEOREM 4.2. The limiting distribution of $\sqrt{N}\,(\hat{\sigma}^{(2)'} - \sigma^{(2)'},\ \hat{\rho}' - \rho')$ is multivariate normal with mean $0'$ and covariance matrix

$$(4.16) \qquad 2\begin{pmatrix} \Delta^2 & 0 \\ 0 & I \end{pmatrix} \begin{bmatrix} \frac{1}{2}(R^{-1} * R + I), & \{(R^{-1} * K_h) e\} \\ \{e'(R^{-1} * K_g)\}, & \{\mathrm{tr}\, R^{-1} K_g R^{-1} K_h\} \end{bmatrix}^{-1} \begin{pmatrix} \Delta^2 , & 0 \\ 0 , & I \end{pmatrix},$$

where $g,\ h = 1, \ldots, m$.

We verify that substitution of $m = 1$, $K_1 = ee' - I = K$, say, confirms (3.1.35). We have $R^{-1} = \frac{1}{1-\rho} I - \frac{\rho}{\alpha} ee'$, where $\alpha = (1-\rho)(1+\rho q)$, $q = p - 1$. Hence $R^{-1} * K = \rho(I - ee')/\alpha$ and so $(R^{-1} * K)e = -\rho q\, e/\alpha$. Furthermore $\mathrm{tr}\, R^{-1} K R^{-1} K = e'(R^{-1}K)^{(2)} e$ and $(R^{-1}K)^{(2)} = [(\rho^2 q^2 - 1) I + ee']/\alpha^2$ so that $\mathrm{tr}\, R^{-1} K R^{-1} K = pq(1 + \rho^2 q)/\alpha^2$.

The solution $\hat{\lambda}$, $\hat{\rho}$ maximizes the likelihood provided the matrix of second derivatives formed by (4.13) through (4.15) is positive definite there. We obtain

$$(4.17) \qquad \begin{bmatrix} 2(\hat{R}^{-1} * R + \hat{\Lambda}^{-2}), & \{-2(\hat{R}^{-1} K_h \hat{R}^{-1} * R)\hat{\lambda}\} \\ \{-2\hat{\lambda}'(\hat{R}^{-1} K_g \hat{R}^{-1} * R)\}, & \{\mathrm{tr}\, \hat{R}^{-1} K_g (2\hat{R}^{-1}\hat{\Lambda} R \hat{\Lambda} - I) \hat{R}^{-1} K_h\} \end{bmatrix},$$

where $g,\ h = 1, \ldots, m$. Whenever $\hat{R}$ is positive definite the top $p \times p$ submatrix in (4.17) is also positive definite. Thus for any set of solutions $\hat{\rho}_1, \ldots, \hat{\rho}_m$ the corresponding vector $\hat{\lambda}$, and hence $\hat{\sigma}^{(2)}$, is determined uniquely. The lower $m \times m$ submatrix is positive definite provided $2\hat{R}^{-1}\hat{\Lambda} R \hat{\Lambda} - I$ is positive definite, though this is not necessary.

From (4.9) we note that $2\hat{R}^{-1}\hat{\Lambda}R\hat{\Lambda} - I$ has all diagonal elements equal to unity.

In general the maximum likelihood equations in Theorem 4.1 cannot be solved analytically. We can solve them iteratively, however, by the Newton-Raphson process, for example (cf. §2.4). An initial consistent solution is $\lambda_o = e$ and

$$(4.18)\qquad \rho_o = \{e'(K_g * K_h)e\}^{-1}\{e'[(R-I)*K_h]e\}$$
$$= \{\mathrm{tr}\, K_g K_h\}^{-1}\{\mathrm{tr}(R-I)K_h\},$$

where $g, h = 1,\ldots, m$. We note that $R - I$ is a consistent estimate of $\sum_{g=1}^{m} \rho_g K_g$ and $\{\mathrm{tr}\, K_g K_h\}$ is positive definite since the $K_g$ are assumed linearly independent [cf. Anderson (1966)]. The first Newton-Raphson iterate, which leads to the same limiting distribution as that in Theorem 4.1 (cf. §2.4), is $(\sigma_1^{(2)'}, \rho_1')$ with $\sigma_1^{(2)} = (D^{-1}\lambda_1)^{(-2)}$, where $D$ is the diagonal matrix of sample standard deviations and

$$(4.19)\qquad \begin{pmatrix}\lambda_1\\ \rho_1\end{pmatrix} = \begin{pmatrix} e \\ \rho_o\end{pmatrix} - \begin{bmatrix} 2(R_o^{-1}*R + I), & \{-2(R_o^{-1}K_h R_o^{-1}*R)e\} \\ \{-2e'(R_o^{-1}K_h R_o^{-1}*R)\}, & \{\mathrm{tr}R_o^{-1}K_g(2R_o^{-1}R-I)R_o^{-1}K_h\}\end{bmatrix}^{-1} \begin{pmatrix} 2(R_o^{-1}*R-I)e \\ \{\mathrm{tr}R_o^{-1}K_g(I-R_o^{-1}R)\}\end{pmatrix},$$

$g, h = 1,\ldots, m$ and $R_o$ based on $\rho_o$.

Simplifications to the above expressions result if we assume all $K_g$ to commute or have unit rank. These will be the subject of further study.

Another structure motivated by Anderson's research is

$$(4.20)\qquad \Sigma^{-1} = \Delta^{-1}\left(\sum_{h=0}^{k} \tau_h L_h\right)\Delta^{-1} = \Delta^{-1}R^{-1}\Delta^{-1},$$

where the inverse of the correlation matrix has linear structure. Let us write

$$(4.21) \qquad \underset{\sim}{\tau} = (\tau_o, \tau_1, \ldots, \tau_k)'.$$

Then in parallel to (4.6),

$$(4.22) \qquad \{\frac{\partial \underset{\sim}{R}^{-1}}{\partial \underset{\sim}{\tau}}\} = \{\underset{\sim}{L}_h;\ h = 0, \ldots, k\}$$

and

$$(4.23) \qquad \frac{\partial \log|\underset{\sim}{R}^{-1}|}{\partial \underset{\sim}{\tau}} = \{\text{tr } \underset{\sim}{R}\underset{\sim}{L}_h;\ h = 0, \ldots, k\},$$

so that using (4.3),

$$(4.24) \qquad \frac{\partial \ell}{\partial \underset{\sim}{\tau}} = \{\underset{\sim}{\lambda}'(\underset{\sim}{L}_h * \underset{\sim}{R})\underset{\sim}{\lambda} - \text{tr } \underset{\sim}{R}\underset{\sim}{L}_h;\ h = 0, \ldots, k\}$$

$$= \{\underset{\sim}{\lambda}'(\underset{\sim}{L}_h * \underset{\sim}{R})\underset{\sim}{\lambda} - \underset{\sim}{e}'(\underset{\sim}{L}_h * \underset{\sim}{R})\underset{\sim}{e};\ h = 0, \ldots, k\}$$

$$= \{\text{tr } \underset{\sim}{L}_h(\underset{\sim}{\Lambda}\underset{\sim}{R}\underset{\sim}{\Lambda} - \underset{\sim}{R});\ h = 0, \ldots, k\}.$$

Equating (4.24) to zero and using (4.9) we obtain:

THEOREM 4.3. <u>The maximum likelihood equations for the unknown quantities in the covariance matrix $\underset{\sim}{\Sigma} = \underset{\sim}{\Delta}(\Sigma\ \tau_h \underset{\sim}{L}_h)^{-1}\underset{\sim}{\Delta}$ in a p-dimensional normal population are</u>

$$(4.25) \qquad (\hat{\underset{\sim}{R}}^{-1} * \underset{\sim}{R})\hat{\underset{\sim}{\lambda}} = \hat{\underset{\sim}{\lambda}}^{(-1)} = \sum_{h=0}^{k} \hat{\tau}_h(\underset{\sim}{L}_h * \underset{\sim}{R})\hat{\underset{\sim}{\lambda}}$$

<u>and</u>

$$(4.26) \qquad \underset{\sim}{e}'(\underset{\sim}{L}_h * \hat{\underset{\sim}{R}})\underset{\sim}{e} = \hat{\underset{\sim}{\lambda}}'(\underset{\sim}{L}_h * \underset{\sim}{R})\hat{\underset{\sim}{\lambda}}, \qquad h = 0, 1, \ldots, k,$$

<u>where $\hat{\underset{\sim}{R}}$ and $\underset{\sim}{R}$ are the maximum likelihood estimate and sample correlation matrices, and $\hat{\underset{\sim}{\lambda}}^{(-1)}$ is the Hadamard inverse of $\hat{\underset{\sim}{\lambda}}$ which</u>

contains ratios of sample to maximum likelihood estimate standard deviations.

Multiplying (4.26) by $\hat{\tau}_h$ and summing over $h = 0, \ldots, k$ yields (4.11) which follows from (4.25) by pre-multiplication by $\hat{\lambda}'$.

The second derivatives of $\ell$ are

$$(4.27) \qquad \frac{\partial^2 \ell}{\partial \lambda \partial \tau'} = \{2(L_h * R)\lambda;\ h = 0, \ldots, k\}$$

and

$$(4.28) \qquad \frac{\partial^2 \ell}{\partial \tau \partial \tau'} = \{e'(L_g * RL_h R)e;\ g, h = 0, \ldots, k\}.$$

In parallel to Theorem 4.2 we have

THEOREM 4.4. The limiting distribution of $\sqrt{N}(\hat{\sigma}^{(2)'} - \sigma^{(2)'}, \hat{\tau}' - \tau')$ is multivariate normal with mean $0'$ and covariance matrix

$$(4.29) \qquad 2\begin{pmatrix} \Delta^2, & 0 \\ 0, & I \end{pmatrix} \begin{bmatrix} \frac{1}{2}(R^{-1} * R + I), & -\{(L_h * R)e\} \\ -\{e'(L_g * R)\}, & \{\mathrm{tr}\ L_g R L_h R\} \end{bmatrix}^{-1} \begin{pmatrix} \Delta^2, & 0 \\ 0, & I \end{pmatrix},$$

where $g, h = 0, 1, \ldots, k$.

The solution $\hat{\lambda}, \hat{\tau}$ maximizes the likelihood provided the matrix of second derivatives formed from (4.13), (4.27), and (4.28) is positive definite. We obtain

$$(4.30) \qquad \begin{bmatrix} 2(\hat{R}^{-1} * R + \hat{\Lambda}^{-2}), & \{2(L_h * R)\hat{\lambda}\} \\ \{2\hat{\lambda}'(L_g * R)\}, & \{\mathrm{tr}\ L_g \hat{R} L_h \hat{R}\} \end{bmatrix},$$

where $g, h = 0, 1, \ldots, k$. Whenever $\hat{R}$ is positive definite the upper $p \times p$ and lower $(k+1) \times (k+1)$ submatrices of (4.30) are positive definite. Thus given a solution $\hat{\lambda}$ the corresponding vector $\hat{\tau}$ is uniquely defined and vice versa. To show complete uniqueness we would need in addition that

$$(4.31) \qquad \underset{\sim}{e}'(\underset{\sim}{L}_g\hat{\underset{\sim}{R}}*\hat{\underset{\sim}{R}}\underset{\sim}{L}_g)\underset{\sim}{e} \geq 2\hat{\underset{\sim}{\lambda}}'(\underset{\sim}{L}_g*\underset{\sim}{R})(\hat{\underset{\sim}{R}}^{-1}*\underset{\sim}{R} + \hat{\underset{\sim}{\Lambda}}^{-2})^{-1}(\underset{\sim}{L}_g*\underset{\sim}{R})\hat{\underset{\sim}{\lambda}}, \quad g = 0,\ldots, k,$$

which appears hard to establish in general.

Iterative solution of the equations in Theorem 4.3 can be effected similarly to that outlined for the equations in Theorem 4.1. Simplifications of the expressions result if all $\underset{\sim}{L}_h$ are assumed to commute or to have unit rank. We will study these later.

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## INDEX TO NOTATION

| | |
|---|---|
| $\underset{\sim}{A} = \{a_{ij}\}$ | matrix generated by $a_{ij}$ |
| $\underset{\sim}{C} = \underset{\sim}{X}'\underset{\sim}{C}_e\underset{\sim}{X}/N = \{c_{ij}\} = \underset{\sim}{DRD}$ | sample covariance matrix |
| $\underset{\sim}{C}_e = \underset{\sim}{I} - \underset{\sim}{ee}'/p$ | centering matrix of order $p$ |
| $\underset{\sim}{C}_\mu = \sum_{\alpha=1}^{N} (\underset{\sim}{x}_\alpha - \underset{\sim}{\mu})(\underset{\sim}{x}_\alpha - \underset{\sim}{\mu})'/N$ | covariance matrix about $\underset{\sim}{\mu}$ |
| $ch_j\underset{\sim}{A}$, $ch\,\underset{\sim}{A}$ | ($\underline{j}$-th largest) characteristic root of $\underset{\sim}{A}$ |
| $\underset{\sim}{d} = \underset{\sim}{De}$ | column vector of sample standard deviations |
| $\underset{\sim}{D} = \{\sqrt{c_{ii}}\}_{dg}$ | diagonal matrix of sample standard deviations |
| $(\quad)_{dg}$ | diagonal matrix |
| $\underset{\sim}{e}$ | column vector with each element 1 |
| $\underset{\sim}{e}_j$ | column vector with all elements 0 except j-th which is 1 |
| $\underset{\sim}{H} = \begin{bmatrix} \frac{\partial^2 \ell}{\partial\underset{\sim}{\lambda}\partial\underset{\sim}{\lambda}'}, & \frac{\partial^2 \ell}{\partial\underset{\sim}{\lambda}\partial\rho} \\ \frac{\partial^2 \ell}{\partial\rho\partial\underset{\sim}{\lambda}'}, & \frac{\partial^2 \ell}{\partial\rho^2} \end{bmatrix}_{\underset{\sim}{\lambda}=\hat{\underset{\sim}{\lambda}},\ \rho=\hat{\rho}}$ | matrix of second derivatives of $\ell$, where $\underset{\sim}{R} = (1-\rho)\underset{\sim}{I} + \rho\underset{\sim}{ee}'$, at solutions of the likelihood equations |
| $\underset{\sim}{H}_o$, $\underset{\sim}{H}_1$ | $\underset{\sim}{H}$ when $\hat{\rho} = 0$, $\hat{\rho} \neq 0$ |
| $\underset{\sim}{I} = \{\delta_{ij}\}$ | identity matrix, generated by Kronecker delta |
| $\ell = -\frac{2}{N}\log L - p\log 2\pi$ <br> $= tr\,\underset{\sim}{\Sigma}^{-1}\underset{\sim}{C} + \log\lvert\underset{\sim}{\Sigma}\rvert$ | reduced function of likelihood (after maximization with respect to $\underset{\sim}{\mu}$), the minimization of which is equivalent to maximizing the likelihood |

| | |
|---|---|
| $\ell_\mu = \frac{2}{N}\log L_\mu - p\log 2\pi$ <br> $= \operatorname{tr} \Sigma^{-1}C_\mu + \log\lvert\Sigma\rvert$ | reduced function of likelihood, the minimizing of which is equivalent to maximizing the likelihood |
| $L = \dfrac{\exp[-\frac{N}{2}\operatorname{tr}\Sigma^{-1}C]}{\lvert\Sigma\rvert^{N/2}(2\pi)^{Np/2}}$ | joint likelihood of N observations on $N(\mu, \Sigma)$ after maximization with respect to $\mu$ |
| $L_\mu = \dfrac{\exp[-\frac{N}{2}\operatorname{tr}\Sigma^{-1}C_\mu]}{\lvert\Sigma\rvert^{N/2}(2\pi)^{Np/2}}$ | joint likelihood of N observations on $N(\mu, \Sigma)$ |
| m, M | $\mathrm{ch}_p, \mathrm{ch}_1[\frac{1}{2}(\hat{R}^{-1} * R + \hat{\Lambda}^{-2})]$ |
| p | dimension of distribution studied |
| $q = p - 1$ | dimension less one |
| $r = \sum_{i \neq j} r_{ij}/p(p-1)$ | average sample correlation coefficient |
| $r = (R - I)e$ | column vector of row sums of sample correlations |
| $R = \{r_{ij}\} = D^{-1}CD^{-1}$ | sample correlation matrix |
| $R = \{\rho_{ij}\} = \Delta^{-1}\Sigma\Delta^{-1}$ | population correlation matrix |
| $t = \frac{1}{2}(q-1) = \frac{1}{2}p - 1$ | half the dimension, less one |
| $\operatorname{tr} A = \sum_{i=1}^{p} a_{ii}$ | trace of square matrix $A$ of order $p$ |
| $u = q - 2 = p - 3$ | dimension less three |
| $X = \{x_1, \ldots, x_N\}'$ | matrix of sample observations, order $N \times p$ |
| $\alpha = (1-\rho)(1+\rho q)$ <br> $= 1 + \rho(q-1) - \rho^2 q$ | product of the simple and multiple characteristic roots of $(1-\rho)I + \rho ee'$ |
| $\Delta = \{\sqrt{\sigma_{ii}}\}_{dg} = \{\sigma_i\}_{dg}$ | diagonal matrix of population standard deviations |

| | |
|---|---|
| $\underset{\sim}{\lambda} = \underset{\sim}{\Lambda e} = \underset{\sim}{D\sigma}^{(-1)}$ | column vector of ratios of sample to population standard deviations |
| $\underset{\sim}{\hat{\lambda}} = \underset{\sim}{\hat{\Lambda} e} = \underset{\sim}{D\hat{\sigma}}^{(-1)}$ | column vector of ratios of sample to maximum likelihood estimate standard deviations |
| $\underset{\sim}{\lambda}_1$ | first iterated estimate of $\underset{\sim}{\hat{\lambda}}$ |
| $\hat{\lambda}_m^2, \hat{\lambda}_M^2$ | $\min_{i=1,\ldots,p}$, $\max_{i=1,\ldots,p}$ $\hat{\lambda}_i^2$ |
| $\underset{\sim}{\Lambda} = \underset{\sim}{D\Delta}^{-1} = \{\sqrt{c_{ii}/\sigma_{ii}}\}_{dg}$ | diagonal matrix of ratios of sample to population standard deviations |
| $\underset{\sim}{\sigma} = \underset{\sim}{\Delta e} = \{\sqrt{\sigma_{ii}}\} = \{\sigma_i\}$ | column vector of population standard deviations |
| $\underset{\sim}{\hat{\sigma}} = \underset{\sim}{\hat{\Delta} e} = \{\sqrt{\hat{\sigma}_{ii}}\} = \{\hat{\sigma}_i\}$ | column vector of maximum likelihood estimate standard deviations |
| $\underset{\sim}{\Sigma} = \{\sigma_{ij}\} = \underset{\sim}{\Delta R \Delta}$ | population covariance matrix |

Special Symbols

| | |
|---|---|
| $\underset{\sim}{A} * \underset{\sim}{B} = \{a_{ij} b_{ij}\}$ | Hadamard product of $\underset{\sim}{A}$ and $\underset{\sim}{B}$, generated by elementwise products |
| $\underset{\sim}{A}^{(2)} = \underset{\sim}{A} * \underset{\sim}{A} = \{a_{ij}^2\}$ | Hadamard square of $\underset{\sim}{A}$ |
| $\underset{\sim}{A}^{(-1)} = \{1/a_{ij}\}$ | Hadamard inverse of $\underset{\sim}{A}$ |
| $\underset{\sim}{A}^{(\ell)} = \{\log_e a_{ij}\}$ | matrix of natural logarithms of elements in $\underset{\sim}{A}$ |
| $\{\frac{\partial \underset{\sim}{A}}{d \underset{\sim}{u}}\} = \{\frac{\partial \underset{\sim}{A}}{\partial u_i}, i = 1, \ldots, p\}$ | system of partial derivative matrices of the matrix $\underset{\sim}{A}$ with respect to the elements in the vector $\underset{\sim}{u}$ |
| $\lvert \underset{\sim}{A} \rvert$ | determinant of square matrix $\underset{\sim}{A}$ |
| $\underset{\sim}{\hat{\theta}}$ | maximum likelihood estimate of column vector $\underset{\sim}{\theta}$ |