THE ERRORS INVOLVED IN EVALUATING CORRELATION DETERMINANTS

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1. **Introduction.** Many statistical problems require for their solution the evaluation of correlation determinants. The method usually employed for such evaluation is that of Chio,[1] in which the order of the determinant is reduced by successive operations with selected pivotal elements. The repeated multiplications and subtractions involved in the method necessitate rounding off the elements in the successively reduced determinants. The calculated value of the original determinant is therefore in error; and so the question naturally arises as to the magnitude of this error.

Previous attempts to answer this question seem to be satisfied with finding an upper bound for the magnitude of the difference between the value of the original determinant and its value after its elements have been rounded off. Moreover, this bound is expressed in terms of the errors in the elements and the minors of the original determinant, whose values are assumed to be known exactly from calculation. However, several reductions are often needed before the value of the determinant can be obtained; and furthermore the minors are subject to the same type of errors as the determinant itself. The problem, therefore, is to find an upper bound for the magnitude of the difference between the final calculated value of the determinant and the determinant itself which involves only calculated quantities.

This paper treats the problem from two different points of view. In the first part an upper bound is obtained for the magnitude of the error. In the second part the first order error terms are given more detailed consideration, with the result that an upper probability bound is obtained for the error.

2. **Absolute Bounds.** Consider the correlation determinant $\Delta = |r_{ij}|$. To evaluate Δ by the method of Chio, it is convenient to select diagonal elements as pivots. It will be assumed without loss of generality that the upper left diagonal element is always chosen as the pivotal element in each reduction. After each reduction, elements are rounded off to a fixed decimal accuracy. Let a_{ij}^k represent the element i,j after the k-th reduction, x_{ij}^k the difference between the rounded value of element a_{ij}^k and a_{ij}^k itself. After k reductions, we arrive at the determinant

$$F^k = \begin{vmatrix} a_{k+1\,k+1}^k + x_{k+1\,k+1}^k & & \\ & \ddots & \\ & & a_{nn}^k + x_{nn}^k \end{vmatrix}$$

[1] See for example, Whittaker and Robinson *Calculus of Observations*, p. 71.

By treating F^k as a function of the x^k, it may be expanded by Taylor's formula as follows:

$$F^k = A^k + \sum_{i,j=k+1}^{n} x_{ij}^k A_{ij}^k + \frac{1}{2!} \sum_{k+1}^{n}\sum x_{ij}^k x_{pq}^k A_{ijpq}^k + \cdots, \tag{1}$$

where A^k is the value of F^k for all x^k zero, A_{ij}^k is the cofactor of a_{ij}^k in A^k, etc.

For a determinant of order n, the value of the determinant obtained after a single reduction is the value of the original determinant multiplied by the $n - 2$ power of the pivotal element used. Applying this to F^k, it follows that

$$\begin{aligned} A^k &= (a_{kk}^{k-1} + x_{kk}^{k-1})^{n-k-1} F^{k-1} = H_k^{n-k-1} F^{k-1} \\ A_{ij}^k &= H_k^{n-k-2} F_{ij}^{k-1} \\ A_{ijpq}^k &= H_k^{n-k-3} F_{ijpq}^{k-1}, \end{aligned}$$

etc., where the exponents of H_k are ordinary exponents rather than notation. Substituting in (1),

$$F^k = H_k^{n-k-1} F^{k-1} + H_k^{n-k-2} \sum_{k+1}^{n} x_{ij}^k F_{ij}^{k-1} + \frac{1}{2!} H_k^{n-k-3} \sum_{k+1}^{n}\sum x_{ij}^k x_{pq}^k F_{ijpq}^{k-1} + \cdots$$

In order to express F^k in terms of the original determinant, this expansion will be condensed by means of the following operational notation.

$$F^k = (1 + D + D^2 + \cdots + D^{n-k}) H_k^{n-k-1} F^{k-1}, \tag{2}$$

where D^i operates on $H_k^{n-k-1} F^{k-1}$ by reducing the exponent of H_k^{n-k-1} by i units, by summing from $k + 1$ to n the product of i terms in x^k with the corresponding cofactors of F^{k-1}, and dividing the result by factorial i. Using this as a recursion formula,

$$F^k = (1 + D + \cdots + D^{n-k}) H_k^{n-k-1} (1 + \cdots + D^{n-k+1}) H_{k-1}^{n-k} \cdots (1 + \cdots + D^{n-1}) H_1^{n-2} F^0.$$

However.

$$F^0 = \begin{vmatrix} a_{11} + x_{11} & & \\ & \ddots & \\ & & a_{nn} + x_{nn} \end{vmatrix} = \Delta,$$

since we assume that $x_{ij} = 0$ for our original determinant. Consequently,

$$F^k = (1 + \cdots + D^{n-k}) H_k^{n-k-1} (1 + \cdots + D^{n-k+1}) H_{k-1}^{n-k} \cdots (1 + \cdots + D^{n-1}) H_1^{n-2} \Delta. \tag{3}$$

Since D^i operates on F^{k-1} in (2) to extract the proper cofactor of i less rows than in F^{k-1}, which in turn reduces the exponent of all factors H_{k-1} in the expansion of F^{k-1} by i units, D^i reduces the exponent of all H's following it in the expansion of F^k in (3) by i units.

Following these rules of operation, and expanding so as to collect terms of the same degree in the x's, we may write

$$(4) \qquad \begin{aligned} F^k = H_k^{n-k-1} \cdots H_1^{n-2}\Delta + H_k^{n-k-2} \cdots H_1^{n-3} \text{ (terms in } x_{ij}) + \\ H_k^{n-k-3} \cdots H_1^{n-4} \text{ (terms in } x_{ij}x_{pq}) + \cdots . \end{aligned}$$

Letting $H = H_k H_{k-1} \cdots H_1$ and $C = H_k^{n-k-1} \cdots H_1^{n-2}$, we may write

$$I = F^k - C\Delta = C\left[\frac{1}{H}\text{ (terms in } x_{ij}) + \frac{1}{H^2}\text{ (terms in } x_{ij}x_{pq}) + \cdots\right];$$

and hence

$$(5) \qquad J = \frac{F^k}{C} - \Delta = \frac{1}{H}\text{ (terms in } x_{ij}) + \frac{1}{H^2}\text{ (terms in } x_{ij}x_{pq}) + \cdots .$$

Now J is the difference between the calculated value of Δ, using Chio's reduction method and rounding off after each reduction, and the true value of Δ. We are interested in finding an upper bound for the magnitude of J. To accomplish this we shall first overestimate the number of terms in the various sums of (5), then find an upper bound for the magnitude of the terms in these sums, and finally combine the two results.

In counting terms by means of (3), we may ignore the H's since they merely serve as coefficients of the x's. Therefore consider the nature of the terms in

$$(1 + \cdots + D^{n-k})(1 + \cdots + D^{n-k+1}) \cdots (1 + \cdots + D^{n-1})\Delta.$$

Now $(1 + \cdots + D^s)\Delta$ contains the sums $\sum_{n-s+1}^{n} x_{ij}\Delta_{ij}$, $\frac{1}{2!}\sum\sum_{n-s+1}^{n} x_{ij}x_{pq}\,\Delta_{ijpq}$, etc.; hence it contains s^2 terms in x_{ij}, $\frac{s^2(s-1)^2}{2}$ terms in $x_{ij}x_{pq}$, etc. Each of these is not greater than s^2, ${}_{s^2}C_2$, etc.; consequently, the number of terms of each type is not greater than the coefficient of the corresponding power of D in the expansion of $(1 + D)^{s^2}$. Therefore,

$$(6) \qquad (1 + D)^{(n-k)^2}(1 + D)^{(n-k+1)^2} \cdots (1 + D)^{(n-1)^2} = (1 + D)^m,$$

where $m = (n - k)^2 + \cdots + (n - 1)^2$, contains at least as many terms of each type as are found in the expansion of F^k. This gives us the desired overestimate of the number of terms in the various sums of (5).

In finding upper bounds for the magnitudes of terms, it is to be noted that (4) is written with all common factors extracted from each set of terms of the same degree in the x's. In the parenthesis containing terms consisting of the product of r x's, the first sum will have unity for its coefficient while the last sum will have $H_k^r H_{k-1}^r \cdots H_2^r$ as coefficient, with all sums between having as coefficients products of H's with exponents $\leq r$. Hence an upper bound for all coefficients in this parenthesis may be written as $\bar{H}^r$, where $\bar{H}$ is the magnitude of the product of those H's whose magnitude is greater than unity, but unity if none exceeds unity. Now terms in x_{ij} are multiplied by Δ_{ij}, those in $x_{ij}x_{pq}$ by Δ_{ijpq}, etc.; therefore let $\bar{\Delta}_{ij}$, $\bar{\Delta}_{ijpq}$, etc., be the absolute values of the largest in magnitude of such cofactors. With this notation for upper bounds for magnitudes of terms, and (6) giving an upper bound for the number of terms, we may write an upper bound for the magnitude of J as follows:

$$|J| \leq \left(\frac{\bar{H}}{H}\epsilon\right) {}_mC_1\bar{\Delta}_{ij} + \left(\frac{\bar{H}}{H}\epsilon\right)^2 {}_mC_2\bar{\Delta}_{ijpq} + \cdots, \tag{7}$$

where $\epsilon \geq |x|$ is the maximum error of rounding. This result is valid for any determinant with real elements. All quantities on the right are available from calculations except the $\bar{\Delta}$; consequently this upper bound will be useful only if satisfactory bounds exist for the minors of the determinant. It can be shown that (7) holds for any minor of Δ, say Δ_{uv}, if the $\bar{\Delta}$ have uv added as subscripts; and therefore it may be applied to the question of the accuracy of least square solutions.

For the correlation determinant Δ it can be shown that the magnitude of a minor of order $n - k$ is bounded by $k!/2^{\frac{1}{2}k}$ for k even and $k!/2^{\frac{1}{2}(k-1)}$ for k odd. Setting $a = \frac{\bar{H}}{H}\epsilon$ and substituting these bounds in (7),

$$\begin{aligned} |J| &\leq am + a^2{}_mC_2\frac{2!}{2} + a^3{}_mC_3\frac{3!}{2} + a^4{}_mC_4\frac{4!}{2^2} + \cdots \\ &\leq am + \frac{a^2m^2}{2} + \frac{a^3m^3}{2} + \frac{a^4m^4}{2^2} + \cdots \\ &\leq am + \frac{a^2m^2}{2} + \frac{a^3m^3}{2(1-am)}, \end{aligned} \tag{8}$$

for $am < 1$. Since am is obtainable from the calculations for Δ, this is the desired upper bound for the error in question.

3. Probability Bounds. In order to find probability bounds for this error, it will be necessary to expand the H's since they involve the variables x. Consider $H_k = a_{kk}^{k-1} + x_{kk}^{k-1}$. Since a_{kk}^{k-1} came from repeated reductions of Δ, it is expressible in terms of the x's and the minors of Δ. To obtain this expansion of H_k consider

$$G^s = \begin{vmatrix} a_{k-s+1\,k-s+1}^{k-s} + x_{k-s+1\,k-s+1}^{k-s} & & \\ & \ddots & \\ & & a_{kk}^{k-s} + x_{kk}^{k-s} \end{vmatrix}$$

Using the same methods as for F^k, this may be written as

$$G^s = B^s + \sum_{k-s+1}^{k} x_{ij}^{k-s}B_{ij}^s + \frac{1}{2!}\sum\sum_{k-s+1}^{k} x_{ij}^{k-s}x_{pq}^{k-s}B_{ijpq}^s + \cdots,$$

where B^s is the value of G^s for all x^{k-s} zero, etc., and where $B^s = H_{k-s}^{s-1}G^{s+1}$, $B_{ij}^s = H_{k-s}^{s-2}G_{ij}^{s+1}$, etc. Substituting,

$$G^s = H_{k-s}^{s-1}G^{s+1} + H_{k-s}^{s-2} \sum x_{ij}^{k-s} G_{ij}^{s+1} + \frac{1}{2!} H_{k-s}^{s-3} \sum\sum x_{ij}^{k-s} x_{pq}^{k-s} G_{ijpq}^{s+1} + \cdots$$

Using operational notation here also, this may be written as

$$G^s = (1 + E + E^2 + \cdots + E^s)H_{k-s}^{s-1}G^{s+1},$$

where the E's operate the same as the D's, except that sums are taken from $k - s + 1$ to k rather than from $n - s + 1$ to n. Treating this as a recursion formula,

$$H_k = G^1 = (1 + E)H_{k-1}^0(1 + E + E^2)H_{k-2}^1 \cdots (1 + \cdots + E^{k-1})H_1^{k-2}G^k.$$

However,

$$G^k = \begin{vmatrix} a_{11} + x_{11} & & \\ & \ddots & \\ & & a_{kk} + x_{kk} \end{vmatrix} = \begin{vmatrix} a_{11} & & \\ & \ddots & \\ & & a_{kk} \end{vmatrix} = \Delta_k.$$

Consequently,

$$H_k = (1 + E)H_{k-1}^0(1 + E + E^2)H_{k-2}^1 \cdots (1 + \cdots + E^{k-1})H_1^{k-2}\,\Delta_k. \tag{9}$$

Since the E's operate on the following H's to reduce their exponents, the number of terms of various types, that is, of various degrees in the x's, will not be decreased if the order of H's is disregarded and their exponents held fixed. Therefore consider

$$H_k' = (1 + E)(1 + E + E^2) \cdots (1 + \cdots + E^{k-1})\Delta_k H_{k-1}^0 \cdots H_1^{k-2} \tag{10}$$

as an ordinary recursion formula in the H's for overestimating the number of terms of various types. If (10) is substituted for successive H's within itself in a systematic manner until no H's remain, it will be found that

$$\begin{aligned} H_k' &= (1 + E) \cdots (1 + \cdots + E^{k-1})\Delta_k \\ &\quad [(1 + E) \cdots (1 + \cdots + E^{k-3})\Delta_{k-2}]^{2^0} \cdots [(1 + E)\Delta_2]^{2^{k-4}}[\Delta_1]^{2^{k-3}}. \end{aligned} \tag{11}$$

To merely count terms it is permissible to combine like terms to give

$$\begin{aligned} H_k' &= (1 + E)^{2+2+2^2+\cdots+2^{k-4}}(1 + E + E^2)^{2+2+2^2+\cdots+2^{k-5}} \cdots (1 + \cdots + E^{k-1})K \\ &= (1 + E)^{2^{k-3}}(1 + E + E^2)^{2^{k-4}} \cdots (1 + \cdots + E^{k-1})K, \end{aligned}$$

where K is the product of the Δ's. Since the E's operate like the D's, the same arguments as those used to arrive at (6) may be used to replace $(1 + E + \cdots + E^s)$ by $(1 + E)^{s^2}$ for overestimating the number of terms. Hence, the number of terms of various types in H_k is not greater than those in

$$(1 + E)^{2^{k-3}}(1 + E)^{2^2 \cdot 2^{k-4}} \cdots (1 + E)^{(k-2)^2 \cdot 2^0}(1 + E)^{(k-1)^2} = (1 + E)^{w_k},$$

where $w_k = 2^{k-3} + 2^2 \cdot 2^{k-4} + \cdots + (k-2)^2 \cdot 2^0 + (k-1)^2$. Therefore the number of terms of various types in $H_k^{n-k-1} \cdots H_1^{n-2}$ is not greater than in

$$(12) \qquad (1+E)^{(n-k-1)w_k + (n-k)w_{k-1} + \cdots + (n-2)w_1} = (1+E)^t.$$

It is easily shown that t can be condensed into the form

$$(13)\ t = [2^{k-2}(n-k)-1] + 2^2[2^{k-3}(n-k)-1] + \cdots + (k-1)^2[2^0(n-k)-1].$$

From (3) it is evident that the number of terms of various types in F^k will not be greater than those in the expansion of F^k when the exponents of the H's are held fixed. But from (6) we have an upper bound for the number of terms arising from the D's, and from (12) those arising from the H's; hence the number of terms in question will certainly be bounded by those in

$$(14) \qquad (1+D)^{m+t} = (1+D)^{\mu}.$$

Now consider the magnitude of terms. The terms arising from the operation of D's contain minors of Δ as factors, while those arising from the operation of E's contain minors of Δ_i, where i ranges from 1 to k. Let Δ'_{ij}, etc., denote an upper bound for the magnitudes of all such minors of the same number of subscripts. It is easily shown that Δ' with $2r$ subscripts is not less than the magnitude of the product of several minors whose subscripts total $2r$ in number. The terms of various types also contain as factors products of the constant terms in the H's. The constant term in H_k, which will be denoted by h_k, can be obtained from (11) by operating with all ones since it will be unaffected by disregarding the order of operation. Hence,

$$h_k = \Delta_k \Delta_{k-2} \Delta_{k-3}^2 \cdots \Delta_2^{2^{k-4}} \Delta_1^{2^{k-3}}.$$

Since the Δ_i are principal minors of a positive definite determinant with no element greater than unity, h_k has unity for an upper bound. Thus, an upper bound for the magnitude of any term in the product of i x's will be ϵ^i times Δ' with $2i$ subscripts.

With upper bounds now available for the number of terms and the magnitudes of terms, we are in a position to consider the complete expansion of I in which the coefficients of the x's will be constants rather than H's. Evidently the terms in x_{ij} will come from the terms in x_{ij} of (4) with the H's replaced by the constant terms in their expansions. If Z denotes these terms, then

$$(15) \qquad Z = h_k^{n-k-2} \cdots h_1^{n-3}\left[\sum_{k+1}^{n} x_{ij}^{k} \Delta_{ij} + h_k \sum_{k}^{n} x_{ij}^{k-1} \Delta_{ij} + \cdots + h_k \cdots h_2 \sum_{2}^{n} x_{ij}^{1} \Delta_{ij}\right].$$

Now consider an upper bound for $|I - Z|$. Since $I - Z$ involves only terms in the product of two or more x's, we need consider an upper bound for such terms only. From the results of the two preceding paragraphs, we obtain

$$|I - Z| \leq \epsilon^2 {}_{\mu}C_2 \Delta'_{ijpq} + \epsilon^3 {}_{\mu}C_3 \Delta'_{ijpquv} + \cdots.$$

But from the paragraph containing (8), bounds are available for the Δ'; hence

$$|I - Z| \leq \epsilon^2{}_\mu C_2 + \epsilon^3{}_\mu C_3 \frac{3!}{2} + \epsilon^4{}_\mu C_4 \frac{4!}{2^2} + \cdots$$

$$\leq \frac{\epsilon^2 \mu^2}{2} + \frac{\epsilon^3 \mu^3}{2(1 - \epsilon\mu)} = \Phi,$$

for $\epsilon\mu < 1$. Since Z is of order ϵ, Φ will ordinarily be small compared with Z; therefore consider the nature of the distribution of Z.

If we write $Z = a_1x_1 + \cdots + a_px_p$, then, since the x's are independently distributed with rectangular distributions, it is easily shown that $\mu_2 = \frac{\epsilon^2}{3} \sum a_i^2$, $\alpha_3 = 0$, $\alpha_4 = 3 - \frac{8}{5} \sum a_i^4/(\sum a_i^2)^2$. If the a_i are approximately equal in magnitude, then α_4 is approximately equal to $3 - 1/p$. But from (15) $p \geq \frac{1}{2}(n - k)^2 + \cdots + \frac{1}{2}(n - 1)^2$, which is sufficiently large for determinants employing Chio's method to justify the assumption that Z is approximately normally distributed. Setting $L = h_k^{n-k-2} \cdots h_1^{n-3}$,

$$\mu_2 = \frac{L^2\epsilon^2}{3}\left[\left(\sum_{k+1}^{n} \Delta_{ii}^2 + 4 \sum_{i<j} \Delta_{ij}^2\right) + \cdots + h_k^2 \cdots h_2^2\left(\sum_{2}^{n} \Delta_{ii}^2 + 4 \sum_{i<j} \Delta_{ij}^2\right)\right]$$

$$\leq \frac{2\epsilon^2}{3}[(n - k)^2 + \cdots + (n - 1)^2 - \tfrac{1}{2}\{(n - k) + \cdots + (n - 1)^2\}]$$

$$\leq \frac{2\epsilon^2}{3}\left[(n - k)^2 + \cdots + (n - 1)^2 - \frac{k}{4}(2n - k - 1)\right] = \Psi^2.$$

Hence, the probability is $>.95$ that $|Z| < 2\Psi$. Since $|I - Z| \leq \Phi$, the probability is $>.95$ that $|I| < 2\Psi + \Phi$; and therefore the probability is $>.95$ that

$$(16) \qquad |J| < \frac{2\Psi + \Phi}{C}.$$

This inequality will usually give a smaller bound for $|J|$ than (8). However, when Δ is small the H's may be small, with the result that C will be small and (16) may not give a satisfactory bound for $|J|$. In such cases the bound given by (8) may not prove satisfactory either.

4. **Example.** Consider a correlation determinant of order 7 in which the elements are accurate to 4 decimal places. If Chio's reduction method is applied until a 2 rowed determinant is obtained, then $n = 7$, $k = 5$, $\epsilon = .00005$, $m = 90$, $\mu = 176$, $\Psi = .00005\sqrt{160}/3$, and we obtain from (8) that

$$|J| < \left(\frac{\bar{H}}{H}\right).0045 + \left(\frac{\bar{H}}{H}\right)^2 .00001 + \left(\frac{\bar{H}}{H}\right)^3 \frac{.00000005}{1 - .0045\,\bar{H}/H}$$

where $\bar{H}/H$ is obtained from calculations involved in evaluating the determinant. From (16) we obtain that the probability is $>.95$ that

$$|J| < \frac{.0008}{C}.$$

The relative advantage of the second inequality over the first depends on the size of the pivotal elements, as does the usefulness of either inequality.

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