The Annals of Statistics
1975, Vol. 3, No. 3, 780–786

THE CHARACTERISTIC POLYNOMIAL OF THE INFORMATION MATRIX FOR SECOND-ORDER MODELS

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The characteristic polynomial is derived for the information matrix M for those main-effect and second-order models based on fractions of the 3^n factorial which render the model symmetric under permutation of the factors. Explicit formulas for the determinant of M and the trace of M^{-1} result.

1. The patterned information matrix for a permutation-invariant second-order model. Let X be the design matrix for a second-order linear model based on some regular or irregular fraction Z of the 3^n factorial. The model is

$$E(y) = \mu + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} x_i x_j . \tag{1.1}$$

Then the matrix $M = X'X$ arising in the normal equations may be partitioned into ten submatrices corresponding to the general mean, linear and quadratic components of main effects, and the first-order two-factor interactions. In (1.2), $i \neq j$,

$$M = \begin{array}{c} \begin{matrix} \mu & \{\beta_i\} & \{\beta_{ii}\} & \{\beta_{ij}\} \end{matrix} \\ \begin{bmatrix} M_{00} & M_{01} & M_{02} & M_{03} \\ & M_{11} & M_{12} & M_{13} \\ \text{Sym.} & & M_{22} & M_{23} \\ & & & M_{33} \end{bmatrix} \begin{matrix} \mu \\ \{\beta_i\} \\ \{\beta_{ii}\} \\ \{\beta_{ij}\} \end{matrix} \end{array} . \tag{1.2}$$

The dimensions of M are $N_2(n) \times N_2(n)$ where $N_2(n) = (n+1)(n+2)/2$. Each row and each column of M correspond to exactly one pairing of parameters from $\boldsymbol{\beta}$ where $\boldsymbol{\beta}$ is the arrangement in lexicographic order of all parameters up through two factor interactions. Thus, the element in the (i, j) position of M, call it $p(i, j)$, corresponds to the element in the ith and jth positions of $\boldsymbol{\beta}$.

We assume throughout that Z renders M positive definite and that Z is a partially balanced array of strength at least four (see [3]). This guarantees that M is invariant under permutation of the factors and contains at most fourteen distinct elements. For any $1 \leqq i, j, k, l \leqq n$ where $i \neq j \neq k \neq l$, these elements are

$$\begin{aligned} &p_1 = p(\mu, \mu), && p_2 = p(\mu, \beta_i) = p(\beta_i, \beta_{ii}), \\ &p_3 = p(\beta_i, \beta_i), && p_4 = p(\beta_i, \beta_j) = p(\mu, \beta_{ij}) = p(\beta_{ii}, \beta_{ij}), \\ &p_5 = p(\mu, \beta_{ii}), && p_6 = p(\beta_i, \beta_{jj}), \qquad p_7 = p(\beta_{ii}, \beta_{ii}), \\ &p_8 = p(\beta_{ii}, \beta_{jj}), && p_9 = p(\beta_i, \beta_{ij}), \qquad p_{10} = p(\beta_i, \beta_{jk}), \end{aligned}$$

Received November 1973.

AMS 1970 *subject classification*. 60.

Key words and phrases. Patterned information matrices, second-order models, characteristic polynomial, determinant, trace.

$$p_{11} = p(\beta_{ii}, \beta_{jk})\,, \qquad p_{12} = p(\beta_{ij}, \beta_{ij})\,, \qquad p_{13} = p(\beta_{ij}, \beta_{ik})\,,$$
$$p_{14} = p(\beta_{ij}, \beta_{kl})\,.$$

For a particular design it is possible to use the frequency operator of [1] as well as the three symbols which define the parameter set for a partially balanced array to get explicit expressions for all the p_i.

EXAMPLE. Suppose we code the three levels of a factor as 0, 1, 2 and have n factors. Let $[j_1; j_2; n - j_1 - j_2]$ denote the set of all $\binom{n}{j_1, j_2, n-j_1-j_2}$ assemblies obtained by permuting one assembly having $j_1$0's, $j_2$1's, and $n - j_1 - j_2$2's. For $n \geqq 4$, consider the design composed of the $N_2(n) + n$ assemblies $[n; 0; 0]$, $[1; 0, n - 1]$, $[1; n - 1; 0]$, $[n - 2; 0; 2]$, and $[0; 1; n - 1]$.
For this design it is the case $p_9(n) \equiv p_6(n) \equiv p_2(n)$, so there are really only twelve distinct $p_i(n)$. They are:

$$\begin{aligned}
p_1(n) &= 0.5n^2 + 2.5n + 1\,, & p_2(n) &= -0.5n^2 + 4.5n - 7\,,\\
p_3(n) &= 0.5n^2 + 1.5n + 1\,, & p_4(n) &= 0.5n^2 - 2.5n + 3\,,\\
p_5(n) &= 0.5n^2 - 0.5n + 1\,, & p_7(n) &= 0.5n^2 + 5.5n + 1\,,\\
p_8(n) &= 0.5n^2 + 5.5n - 17\,, & p_{10}(n) &= -0.5n^2 + 8.5n - 28\,,\\
p_{11}(n) &= 0.5n^2 - 2.5n\,, & p_{12}(n) &= 0.5n^2 + 1.5n - 1\,,\\
p_{13}(n) &= 0.5n^2 - 2.5n + 2\,, & p_{14}(n) &= 0.5n^2 - 6.5n + 21\,.
\end{aligned}$$

The optimality properties of this design are presented in [5] and [6]. It serves as a good example here because it is highly nonorthogonal. Thus, without our Theorem 2, the derivation of $|M - \lambda I|$, $|M|$, trace (M^{-1}), etc., would be possible only by computer analysis for fixed n and λ.

2. The characteristic polynomial and associated quantities. Now, let M be the information matrix for a complete main-effects plan involving the first $N_1(n) = 2n + 1$ terms of (1.1). Then

$$M = \begin{bmatrix} M_{00} & M_{01} & M_{02} \\ & M_{11} & M_{12} \\ \text{Sym.} & & M_{22} \end{bmatrix} \tag{2.1}$$

where only the first eight p_i are involved. Some expressions in the p_i needed later are:

$$\begin{aligned}
\alpha_{11} &= p_3 + (n-1)p_4\,, & \delta_{11} &= p_3 - p_4\,,\\
\alpha_{12} &= p_2 + (n-1)p_6\,, & \delta_{12} &= p_2 - p_6\,,\\
\alpha_{22} &= p_7 + (n-1)p_8\,, & \delta_{22} &= p_7 - p_8\,.
\end{aligned} \tag{2.2}$$ and

Then we have proved

THEOREM 1. *The characteristic polynomial of M may be written*

$$|M - \lambda I| = (-\lambda^3 + c_1\lambda^2 - c_2\lambda + c_3)(\lambda^2 - c_4\lambda + c_5)^{n-1} \tag{2.3}$$

where

$$c_1 = p_1 + \alpha_{11} + \alpha_{22}\,,$$
$$c_2 = p_1(\alpha_{11} + \alpha_{22}) + \alpha_{11}\alpha_{22} - \alpha_{12}^2 - n(p_2^2 + p_5^2)\,,$$
$$c_3 = p_1(\alpha_{11}\alpha_{22} - \alpha_{12}^2) + 2\alpha_{12}np_2p_5 - \alpha_{11}np_5^2 - \alpha_{22}np_2^2\,, \tag{2.4}$$
$$c_4 = \delta_{11} + \delta_{22}\,,$$
and
$$c_5 = \delta_{11}\delta_{22} - \delta_{12}^2\,.$$

PROOF. (Sketch only). Upon suitable rearrangement of the rows and columns in M, we have

$$M^* = \begin{bmatrix} M_{11} & M_{10} & M_{12} \\ M_{01} & M_{00} & M_{02} \\ M_{21} & M_{20} & M_{22} \end{bmatrix}. \tag{2.5}$$

Let

$$M_{22}^* = \begin{bmatrix} M_{00} & M_{02} \\ M_{20} & M_{22} \end{bmatrix}.$$

Then the characteristic polynomial for M equals the characteristic polynomial for M^* and the latter is

$$|M^* - \lambda I| = |M_{11} - \lambda I_n| \cdot |M_{22}^* - \lambda I_{n+1} - p(\lambda)| \tag{2.6}$$

where $p(\lambda)$ is the $(n + 1) \times (n + 1)$ product of matrices

$$\begin{bmatrix} M_{01} \\ M_{21} \end{bmatrix} [M_{11} - \lambda I_n]^{-1}[M_{10}, M_{12}]\,.$$

Each of the factors of (2.6) can be shown to be the determinant of a well-known patterned matrix (see [4], page 185) and the coefficients $\{c_i, i = 1, \cdots, 5\}$ follow by some tedious algebra.

COROLLARY 1. *For the same M as in* (2.1)

$$|M| = c_3 c_5^{n-1} \tag{2.7}$$

and

$$\text{trace}\,(M^{-1}) = \frac{c_2}{c_3} + (n - 1)\frac{c_4}{c_5}\,. \tag{2.8}$$

PROOF. Having assumed M to be positive definite, none of its characteristic roots can be zero. Thus, letting $\lambda = 0$ in (2.3) we get (2.7). In order to get the characteristic polynomial of M^{-1}, change λ to $1/\lambda$ in (2.3), divide both sides by $|M|$, and acquire

$$|M^{-1} - \lambda I| = \left\{-\lambda^3 + \frac{c_2}{c_3}\lambda^2 - \frac{c_1}{c_3}\lambda + \frac{1}{c_3}\right\}\left\{\lambda^2 - \frac{c_4}{c_5}\lambda + \frac{1}{c_5}\right\}^{n-1}. \tag{2.9}$$

The trace of a matrix equals the sum of its characteristic roots. From (2.9) we see that three of the five roots, λ_1^{-1}, λ_2^{-1} and λ_3^{-1}, are of multiplicity one each; while the remaining two, λ_4^{-1} and λ_5^{-1}, are of multiplicity $n - 1$ each. Therefore,

$$\text{trace}\,(M^{-1}) = (\lambda_1^{-1} + \lambda_2^{-1} + \lambda_3^{-1}) + (n - 1)(\lambda_4^{-1} + \lambda_5^{-1})\,. \tag{2.10}$$

However, in a monic polynomial $x^n + b_{n-1}x^{n-1} + \cdots + b_1 x + b_0$, the term $-b_{n-1}$ is the sum of its roots. Thus, we get

$$\lambda_1^{-1} + \lambda_2^{-1} + \lambda_3^{-1} = \frac{c_2}{c_3} \quad \text{and} \quad \lambda_4^{-1} + \lambda_5^{-1} = \frac{c_4}{c_5}$$

which, with (2.10), proves (2.8).

Now, in the rest of this section, let M be the information matrix (1.2) for a second-order model involving all $N_2(n)$ terms of (1.1) and all $\{p_i, i = 1, \cdots, 14\}$. In addition to the expressions at (2.2), some other needed expressions in the p_i are

$$\gamma_{13} = (n-1)p_9 + \binom{n-1}{2}p_{10}, \qquad \gamma_{23} = (n-1)p_4 + \binom{n-1}{2}p_{11},$$
$$\pi_1 = p_{12} + 2(n-2)p_{13} + \binom{n-2}{2}p_{14},$$
$$\pi_2 = p_{12} + (n-4)p_{13} - (n-3)p_{14}, \qquad \text{and}$$
$$\pi_3 = p_{12} - 2p_{13} + p_{14}.$$

Then we have proved

THEOREM 2. *Let $n' = n(n-3)/2$. The characteristic polynomial of M may be written*

$$|M - \lambda I| = (\lambda^4 - c_1\lambda^3 + c_2\lambda^2 - c_3\lambda + c_4) \times (-\lambda^3 + c_5\lambda^2 - c_6\lambda + c_7)^{n-1}(\pi_3 - \lambda)^{n'} \tag{2.11}$$

where x denotes continuation of a product between lines and

$$c_1 = \pi_1 + p_1 + \alpha_{11} + \alpha_{22},$$
$$c_2 = \pi_1 p_1 - \binom{n}{2}p_4^2 + (\pi_1 + p_1)(\alpha_{11} + \alpha_{22}) + \alpha_{11}\alpha_{22} - \alpha_{12}^2 - n(p_2^2 + p_5^2) - \frac{2}{n-1}\gamma_{13}^2 - \frac{2}{n-1}\gamma_{23}^2,$$
$$c_3 = \left(\pi_1 p_1 - \binom{n}{2} \cdot p_4^2\right)(\alpha_{11} + \alpha_{22}) + (\pi_1 + p_1)(\alpha_{11}\alpha_{22} - \alpha_{12}^2) - n\pi_1(p_2^2 + p_5^2) + n(2\alpha_{12}p_2p_5 - \alpha_{11}p_5^2 - \alpha_{22}p_2^2) + 2np_2p_4\gamma_{13} + 2np_5p_4\gamma_{23} + 4\alpha_{12}\frac{\gamma_{13}\gamma_{23}}{n-1} - 2(p_1 + \alpha_{22})\frac{\gamma_{13}^2}{n-1} - 2(p_1 + \alpha_{11})\frac{\gamma_{23}^2}{n-1},$$
$$c_4 = \left(\pi_1 p_1 - \binom{n}{2}p_4^2\right)(\alpha_{11}\alpha_{22} - \alpha_{12}^2) + n\pi_1(2\alpha_{12}p_2p_5 - \alpha_{11}p_5^2 - \alpha_{22}p_2^2) + 2np_4(p_2\alpha_{22} - p_5\alpha_{12})\gamma_{13} + 2np_4(p_5\alpha_{11} - p_2\alpha_{12})\gamma_{23} + \frac{2}{n-1}(np_5^2 - p_1\alpha_{22})\gamma_{13}^2 + \frac{2}{n-1}(np_2^2 - p_1\alpha_{11})\gamma_{23}^2 - \frac{4}{n-1}(np_2p_5 - p_1\alpha_{12})\gamma_{13}\gamma_{23},$$
$$c_5 = \pi_2 + \delta_{11} + \delta_{22},$$
$$c_6 = \pi_2(\delta_{11} + \delta_{22}) + \delta_{11}\delta_{22} - \delta_{12}^2 - (n-2)(p_9 - p_{10})^2 - (n-2)(p_4 - p_{11})^2,$$
$$c_7 = \pi_2(\delta_{11}\delta_{22} - \delta_{12}^2) - (n-2)(p_9 - p_{10})^2\delta_{22} - (n-2)(p_4 - p_{11})^2\delta_{11} + 2(n-2)\delta_{12}(p_9 - p_{10})(p_4 - p_{11}).$$

PROOF. Let $M_c' = [M_{30}, M_{31}, M_{32}]$ of dimensions $\binom{n}{2} \times (1 + 2n)$. Then the characteristic polynomial is

$$|M - \lambda I| = |M_{33} - \lambda I| \cdot p(\lambda) \tag{2.12}$$

where the factor

$$p(\lambda) = |M^* - \lambda I_{2n+1} - M_c\{M_{33} - \lambda I\}^{-1} M_c'| . \tag{2.13}$$

Here

$$M^* = \begin{bmatrix} M_{00} & M_{01} & M_{02} \\ & M_{11} & M_{12} \\ \text{Sym.} & & M_{22} \end{bmatrix} \tag{2.14}$$

is the information matrix for that portion of the model involving main effects only. Algebraic analysis will reveal to us that $M^* - M_c\{M_{33} - \lambda I\}^{-1}M_c'$ has a form exactly the same in its general structure as that for M^*.

First, it is shown in [2], page 162 that M_{33} can be written

$$M_{33} = p_{12}B_{33}^{(0)} + p_{13}B_{33}^{(1)} + p_{14}B_{33}^{(2)} \tag{2.15}$$

where $B_{33}^{(j)}$ $(j = 0, 1, 2)$ is the association matrix for jth associates in a PBIBD with two associate classes and a triangular association scheme. It follows from previous work on such PBIBD's that

$$|M_{33} - \lambda I| = (\pi_1 - \lambda)(\pi_2 - \lambda)^{n-1}(\pi_3 - \lambda)^{n'} . \tag{2.16}$$

Next, it is proved in [7] that

$$Q_{33} = \{M_{33} - \lambda I\}^{-1} = q_{12}(\lambda)B_{33}^{(0)} + q_{13}(\lambda)B_{33}^{(1)} + q_{14}(\lambda)B_{33}^{(2)}$$

where $q_{12}(\lambda)$, $q_{13}(\lambda)$, $q_{14}(\lambda)$ are expressions in the reciprocals $(\pi_i - \lambda)^{-1}$ $(i = 1, 2, 3)$. By means of certain identities among these $q_i(\lambda)$, those block submatrices $M_{i3} \cdot Q_{33} \cdot M_{3j}$ $(i, j = 0, 1, 2)$ that comprise $M_c Q_{33} M_c'$ can have their entries written out in manageable form. Finally, after considerable algebraic simplification the difference matrices

$$DM_{ij} = M_{ij} - M_{i3}Q_{33}M_{3j} \quad (i, j = 0, 1, 2)$$

that comprise $M^* - M_c Q_{33} M_c'$ can be written out in full. These are

$DM_{00} = \text{scalar} = (\pi_1 - \lambda)^{-1}[p_1(\pi_1 - \lambda) - \binom{n}{2}p_4^2]$.

$DM_{01} = (p_2 - \alpha_{01})1_n'$ where $p_2 - \alpha_{01} = (\pi_1 - \lambda)^{-1}[p_2(\pi_1 - \lambda) - p_4\gamma_{13}]$.

$DM_{11} = \xi_{11}I_n + \zeta_{11}(J_n - I_n)$ where $J_n = 1_n 1_n'$ and

$$\xi_{11} = (\pi_1 - \lambda)^{-1}\left[\alpha_{11}(\pi_1 - \lambda) - \frac{2}{n-1}\gamma_{13}^2\right],$$

$$\zeta_{11} = (\pi_2 - \lambda)^{-1}[\delta_{11}(\pi_2 - \lambda) - (n - 2)(p_9 - p_{10})^2] .$$

$DM_{02} = (p_5 - \alpha_{02})1_n'$ where $p_5 - \alpha_{02} = (\pi_1 - \lambda)^{-1}[p_5(\pi_1 - \lambda) - p_4\gamma_{23}]$.

$DM_{12} = \xi_{12}I_n + \zeta_{12}(J_n - I_n)$ where

$$\xi_{12} = (\pi_1 - \lambda)^{-1}\left[\alpha_{12}(\pi_1 - \lambda) - \frac{2}{n-1}\gamma_{13}\gamma_{23}\right],$$

$$\zeta_{12} = (\pi_2 - \lambda)^{-1}[\delta_{12}(\pi_2 - \lambda) - (n - 2)(p_9 - p_{10})(p_4 - p_{11})] .$$

$DM_{22} = \xi_{22} I_n + \zeta_{22}(J_n - I_n)$ where

$$\xi_{22} = (\pi_1 - \lambda)^{-1}\left[\alpha_{22}(\pi_1 - \lambda) - \frac{2}{n-1}\gamma_{23}^2\right],$$

$$\zeta_{22} = (\pi_2 - \lambda)^{-1}[\delta_{22}(\pi_2 - \lambda) - (n-2)(p_4 - p_{11})^2] .$$

$[DM_{ij}]$ is now exactly in the form of the information matrix for Theorem 1 and by appeal to that theorem the factor $p(\lambda)$ of (2.12) may be evaluated. One problem here is that the resulting expression involves many powers of the reciprocals $(\pi_1 - \lambda)^{-1}$ and $(\pi_2 - \lambda)^{-1}$. By properly distributing the factors of $|M_{33} - \lambda I|$ throughout (2.12), however, we have proved that all those parts of polynomial coefficients from Theorem 1 which involve powers of reciprocals now sum to zero. Finally, after going through algebraic simplification involving the grouping of terms according to powers of λ, one gets the expression for $|M - \lambda I|$ as given at (2.11).

COROLLARY 2. *For the same M as in* (1.2),

$$|M| = c_4 c_7^{n-1} \pi_3^{n'} \tag{2.17}$$

and

$$\text{trace}\,(M^{-1}) = \frac{c_3}{c_4} + (n-1)\frac{c_6}{c_7} + \frac{n'}{\pi_3} . \tag{2.18}$$

The technique of proof is identical with that of Corollary 1.

In our example, the seven c_i of (2.11) become for any $n \geqq 4$

$$c_1(n) = 0.25n^4 - 2.5n^3 + 25.25n^2 - 64n + 71 ,$$

$$c_2(n) = 3n^6 - 47.75n^5 + 388.5n^4 - 1541.25n^3 + 3298.5n^2 - 3633n + 1798 ,$$

$$c_3(n) = 8n^8 - 170n^7 + 1605n^6 - 8176.5n^5 + 25392n^4 - 50668.5n^3 + 64564n^2 - 47506n + 15624 ,$$

$$c_4(n) = 81n^7 - 36n^6 - 3492n^5 + 18342n^4 - 44721n^3 + 61974n^2 - 46044n + 13896 ,$$

$$c_5(n) = 4n^2 - 23n + 70 ,$$

$$c_6(n) = 156n^2 - 930n + 1728 \quad \text{and}$$

$$c_7(n) = 1476n^2 - 9036n + 13896 .$$

These polynomials were computed in double precision arithmetic on a 32-bit word computer and are exact. Utilizing (2.17) and (2.18), explicit expressions for the determinant and trace result *for any* $n \geqq 4$.

REFERENCES

[1] BOSE, R. C. and SRIVASTAVA, J. N. (1964). Analysis of irregular factorial fractions. *Sankhyā Ser. A* **26** 117–144.

[2] BOSE, R. C. and SRIVASTAVA, J. N. (1964). Multidimensional partially balanced designs and their analysis with applications. *Sankhyā Ser. A* **26** 145–168.

[3] CHAKRAVARTI, I. M. (1956). Fractional replication in asymmetrical factorial designs and partially balanced arrays. *Sankhyā* **17** 143–164.

[4] GRAYBILL, F. (1969). *Introduction to Matrices with Applications in Statistics.* Wadsworth Publishing Company.

[5] HOKE, A. T. (1972). Economic second-order designs in sequences of partially balanced fractions of the 3^n factorial. Ph. D. dissertation, Columbia Univ.

[6] HOKE, A. T. (1974). Economical second-order designs based on irregular fractions of the 3^n factorial. *Technometrics* **16** 375–384.

[7] SRIVASTAVA, J. N. and CHOPRA, D. V. (1971). On the characteristic roots of the information matrix of 2^m balanced factorial designs of resolution V, with applications. *Ann. Math. Statist.* **42** 722–734.

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