correlation coefficient, ϱ, of 0·999, indicating an almost normal distribution of the weighted residuals. The corresponding values before the last least-squares refinement were 0·904 and

Table 2. *Analysis of* $\langle w|\varDelta F|^2\rangle$ *as a function of* (sin θ)/λ

Interval	Number of reflexions	$\langle|\varDelta F|^2\rangle$	$\langle w|\varDelta F|^2\rangle$
0·3084	110	3·093	1·106
0·3861	110	0·667	1·131
0·4418	110	0·520	0·878
0·4885	110	0·488	0·807
0·5302	110	0·706	1·103
0·5665	110	0·580	0·823
0·6049	110	0·932	1·116
0·6491	112	1·015	1·036
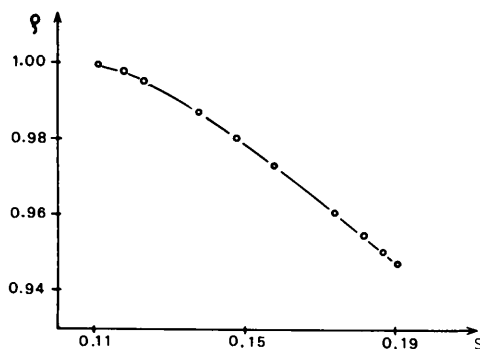
Fig. 1. Plot of the correlation coefficient, ϱ, *versus* weight index, S.

0·999 respectively. The averages of $w|\varDelta F|^2$ analysed with respect to F and (sin θ)/λ are shown in Tables 1 and 2 respectively. The values in the tables are scaled such that the total average is unity and refer to the second determination of the weight function.

Fig. 1 shows the correlation coefficient as a function of the weight index S for a fixed set $\varDelta F$. The different values of S and ϱ are obtained by varying the parameters in the weight function. The correlation coefficient, ϱ, tends to 1 with decreasing value of S, in which case the $w^{1/2}\varDelta F$ are drawn from a normal distribution, and the least-squares method and the maximum-likelihood method become equivalent (Kendall, 1946). Although, as a general feature, this remains to be proved, the present method, as demonstrated by the example, is nevertheless, together with a normal probability plot, a useful tool in the evaluation of crystal structure data.

References

ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A27, 157–165.

BRILLOUIN, L. (1962). *Science and Information Theory*, 2nd ed. New York: Academic Press.

CRUICKSHANK, D. W. J. (1970). In *Crystallographic Computing*, edited by F. R. AHMED, p. 195. Copenhagen: Munksgaard.

KENDALL, M. G. (1946). *The Advanced Theory of Statistics*, Vol. II, p. 59. London: Charles Griffin.

NELDER, J. A. & MEAD, R. (1964–65). *Comput. J.* 7, 308–313.

SØTOFTE, I. & NIELSEN, K. (1977). In preparation.

Further notes on the generalized inverse.

By D. N. J. WHITE, *Chemistry Department, The University, Glasgow* G12 8QQ, *Scotland*

Fast algorithms for 'inverting' singular matrices by modified Cholesky procedures produce a non-unique A^{r2} generalized reciprocal matrix rather than the generalized inverse A^+.

Some crystallographic applications of generalized inverse matrices have been described (Mackay, 1977) and further food for thought may be gleaned from standard texts (Pringle & Rayner, 1971; Boullion & Odell, 1971). In addition to these applications the use of generalized inverse matrices is currently undergoing something of a renaissance in a related area of physical science, namely empirical valence-force-field or molecular-mechanics calculations of crystal (Warshel & Lifson, 1970) and molecular structure (White, 1977). Unfortunately, the search for efficient algorithms to generate generalized inverses has precipitated several difficulties which have been discussed by Ermer (1975) although no explanation was offered. These problems have an almost exact parallel in the refinement of structure factors by the methods described in Mackay's paper and we offer the following clarification.

Some definitions are required because the nomenclature of generalized inverses is something of a semantic minefield. For any matrix P, square or rectangular, there exists a *unique* matrix Q satisfying the conditions

$$PQP = P \qquad (1)$$

$$QPQ = Q \qquad (2)$$

$$(PQ)^* = PQ \qquad (3)$$

$$(QP)^* = QP . \qquad (4)$$

Furthermore, (a) a one-condition, generalized reciprocal matrix of P is a matrix $Q = P^{r1}$ satisfying (1); (b) a two-condition, generalized reciprocal matrix of P is a matrix $Q = P^{r2}$ satisfying (1) and (2); (c) a left-weak, generalized reciprocal matrix of P is a matrix $Q = P^{r3}$ satisfying (1), (2) and (3); (d) a right-weak, generalized reciprocal matrix of P is a matrix $Q = P^{r3'}$ satisfying (1), (2) and (4); (e) the generalized inverse matrix of P is a matrix $Q = P^+$ satisfying (1)–(4).

The following inclusion relations are true

$$P^+ \subseteq P^{r3} \subseteq P^{r2} \subseteq P^{r1}$$

$$P^+ \subseteq P^{r3'} \subseteq P^{r2}$$

with equality holding throughout if and only if P is non-singular. It is also possible to express P^{r2}, P^{r3}, $P^{r3'}$ and P^+ in terms of one-condition generalized reciprocals (P^r_{11}, $P^r_{21} \ldots P^r_{n1}$):

$$P^{r2} = P^r_{11}PP^r_{21} \tag{5}$$

$$P^{r3} = (P*P)^{r_1}P* \tag{6}$$

$$P^{r3'} = P*(PP*)^{r_1} \tag{7}$$

$$P^+ = P*(PP*)^{r_1}P(P*P)^{r_1}P* \tag{8}$$

or

$$P^+ = P^{r3'}PP^{r3} . \tag{9}$$

Consider now the solution of a system of linear equations

$$Ax = b \tag{10}$$

where A is a symmetric matrix. For molecular-mechanics calculations

$$A = \frac{\partial^2 V}{\partial p_i \partial p_j} \quad \text{and} \quad b = \frac{\partial V}{\partial p_j}$$

where V is the potential energy and p_i are the atomic co-ordinates *etc*. The corresponding formulation for crystallographic least squares would be

$$A = \sum_{hkl} \omega \frac{\partial |F_c|}{\partial p_i} \frac{\partial |F_c|}{\partial p_j} \quad \text{and} \quad b = \sum_{hkl} \omega \Delta \frac{\partial |F_c|}{\partial p_j} .$$

The general solutions of (10) for the vector, x, of corrections to the p_j is

$$x = A^+ b$$

and two procedures have been described for 'inverting' A (which is singular in the general case). (i) Construction of A^+ from the eigenvalues (λ) and eigenvectors (E) of A so that

$$A^+ = E \, \text{diag}(1/\lambda)E*$$

which is analogous to Mackay's use of *F01BHF* for rectangular matrices.

(ii) Rao's (1955) method which is a modification of the Cholesky inversion procedure for symmetric, positive de-finite matrices. The procedures described by Ermer (1975) and Altona & Faber (1974) and the practice of, for instance, fixing the arbitrary y parameter during crystallographic least-squares refinement in the space group $P2_1$ are simply inelegant implementations of Rao's method.

Ermer has found that method (ii) is eight times faster than method (i) (see also the timings for *F01BHF* and *F01ADF* in the Nottingham Algorithms Group NAG library manual) resulting in an overall reduction of run time by a factor of three for a complete energy-minimization calculation. Although Rao's method does not give A^+, its speed of execution provides a powerful incentive to its use. The fact that Rao's method gives a *non-unique* A^{r2} generalized reciprocal does not appear to be widely known. This explains Ermer's residual difficulties, namely that the results of his energy-minimization calculations varied slightly depending on how the molecule was placed in the coordinate frame (in general, Ermer was able to circumvent the convergence difficulties mentioned by Mackay). Although these variations are real they are small and, as far as energy-minimization calculations go, can be ignored in practice. Whether this is true for crystallographic least-squares calculations remains to be seen (Mackay, 1977).

References

ALTONA, C. & FABER, D. H. (1974). *Top. Curr. Chem.* **45**, 1–38.

BOULLION, T. L. & ODELL, P. L. (1971). *Generalized Inverse Matrices*. New York: Interscience.

ERMER, O. (1975). *Tetrahedron*, **31**, 1849–1854.

MACKAY, A. L. (1977). *Acta Cryst.* A**33**, 212–215.

PRINGLE, R. M. & RAYNER, A. A. (1971). *Generalized Inverse Matrices*, Griffin's Statistical Monographs & Courses No. 28, edited by A. STUART. London: Griffin.

RAO, C. R. (1955). *Sankhyā*, **15**, 253–280.

WARSHEL, A. & LIFSON, S. (1970). *J. Chem. Phys.* **53**, 582–594.

WHITE, D. N. J. (1977). *Comput. Chem.* **2**. In the press.