

Acta Cryst. (1961). **14**, 83

On the treatment of ill-conditioning. By JERRY DONOHUE and EDGAR HEILBRONNER, *Swiss Federal Institute of Technology, (E.T.H.), Zürich, Switzerland*

(Received 25 January 1960 and in revised form 13 June 1960)

Schomaker, Waser, Marsh & Bergman (1959) have recently pointed out that in fitting, by least squares, a plane to a set of points, x^i , the normal equations

$$ax = \xi \quad (1)$$

may be badly ill-conditioned under certain conditions. They propose instead that the equations

$$Am = \lambda gm \quad (2)$$

be used, the roots $\lambda^{(i)}$ yielding not only a *best* plane, but also a 'worst' plane and an intermediate plane. Since there is in general little use for knowledge on the planes of the latter two types, their solution leads to unwanted results, even though the procedure recommended by Schomaker *et al.* is, as was pointed out by them, 'quite simple', since only about 500 digits (decimal) were required to be recorded when the work was done on a desk calculator, as shown by their example (model of calculator not stated). They further remark that the normal equations (1) may possibly remain ill-conditioned, though not badly, if, when 'trouble threatens', the origin is moved, although they appear to have incomplete understanding on this point (not a member of the set x^i). This doubt concerning the ill-conditioning is of course rather vexing.

We have accordingly carried out a direct test of the first method, using as our example the x^i of Schomaker *et al.*, as given in the rows j_i , $i = 1, 2, 3, 4, 5, 6$, and columns i_j , $j = 2, 3, 4$, of their Table 1, transforming, however, the x^i into

$$x^j = Ax^i \quad (3)$$

the elements a_{ij} of A being defined as

$$(1 - [x^i]/nx^i + m^i da/x^i)\delta_{ij}, \quad (4)$$

where the m^i are obtained from a preliminary solution of equations (1), δ_{ij} is as defined by Kronecker, and a is an arbitrary constant. We shall not concern ourselves explicitly with the trivial case when $d = a_{ij}$, $i \neq j$, since it is easily dealt with by an obvious method. Because an appropriate desk calculator was unavailable to us at the time, the numerical experiment on the dependence of the ill-conditioning upon a was carried out with punched cards on an IBM 650.

Our results, presented in Table 1, give the distances $\Delta_i(a)(A)$ obtained by the above method. In our opinion, the use of (3) removes all doubt (within the limits of error of the numbers used) concerning the residual ill-conditioning.*

In conclusion we remark that neither method will lead to an acceptable result if the set x^i is empty.

We wish to thank Prof. J. D. Dunitz for his persistent criticism on points of detail, Mr A. Reber, Chef der Lochkarten-Sektion der Eidg. Post, Telephon, u. Telegraphen-Verwaltung (Zürich) for permission to use the IBM 650, Mr W. Dürig for assistance with the computations, the National Science Foundation (U.S.A.) for a fellowship granted to one of us, and the Schweizerische Nationalfonds for additional financial support.

References

- MARCUS, M. (1960). *Nat. Bur. Stand., Appl. Math. Ser.* **57**, 21.
SCHOMAKER, V., WASER, J., MARSH, R. E. & BERGMAN, G. (1959). *Acta Cryst.* **12**, 600.

* Various references on ill-conditioning, but not its treatment, have been collected by Marcus (1960).

Table 1. *Numerical data for least-squares plane*

Atom	$D(A)^*$	$D(A)^\dagger$	$\Delta(d)(A)$	$\Delta(5)(A)$	$\Delta(10)(A)$	$\Delta(20)(A)$
1	0.0030	0.0051	0.0051	0.00307	0.00306	0.00307
2	0.0034	0.0048	0.0048	0.00344	0.00344	0.00345
3	-0.0049	-0.0054	-0.0054	-0.00485	-0.00485	-0.00485
4	0.0000	-0.0017	-0.0017	0.00001	0.00001	0.00001
5	0.0062	0.0049†	0.0052	0.00622	0.00622	0.00621
6	-0.0079	-0.0070	-0.0070	-0.00786	-0.00786	-0.00787
[]	-0.0002	0.0007	0.0010	0.00003	0.00002	0.00002

* Obtained by Schomaker *et al.* by their 'correct' method.

† Obtained by Schomaker *et al.* by their 'incorrect' method.

‡ Incorrect value obtained by 'incorrect' method (discrepancy may arise from rounding-off errors).