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To fit a plane to a set of points by least squares.

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A correct solution is offered to the least-squares plane problem by Schomaker, Waser, Marsh & Bergman (1959) (SWMB), in which the whole calculation is carried through in crystal lattice coordinates. This may cause a more simple and direct method of solution, attained by working in Cartesian coordinates, to be overlooked. In Cartesian coordinates, as SWMB mention, g is the unit matrix. The secular equation $|A-\lambda g|=0$ is then readily solved without calculation of an adjoint matrix. It may be expanded

$$-\lambda^3+\alpha\lambda^2+\beta\lambda+\gamma=0\,, \qquad (1)$$

where

$$\alpha=\sum_i A^{ii}$$

$$\beta=-\sum_i A^{ii}A^{jj}+\sum_i (A^{ij})^2$$

$$\gamma=\prod_i A^{ii}+2\prod_i A^{ij}-\sum_i A^{ii}(A^{jk})^2.$$

Here $A^{ij}=\Sigma w x_i x_j-\bar{x}_i\bar{x}_j\Sigma w$ as in SWMB, but in Cartesian coordinates*; $i=1, 2, 3$; j and k are obtained by cyclic permutation of i. The cubic equation (1) is accurate, but tedious to solve directly. Since for atoms near a plane the desired solution for λ is small, an approximation to λ may be found and refined, for example, by the Newtonian method. For puckered rings the approximate solution,

$$\lambda_{(1)}=[-\beta-(\beta^2-4\alpha\gamma)^{\frac{1}{2}}]/2\alpha \qquad (2)$$

is usually accurate to about 1%, while for 'good' planes it normally suffices to calculate

$$\lambda_{(0)}=-\gamma/\beta\,. \qquad (3)$$

In either case it is important to check the effect of neglected terms of (1) and to refine the solution if necessary.

When λ is known, values of μm_i, where μ is an undetermined multiplier, can be calculated from any two of SWMB's equations (7), the third being used as a check. One choice would be

$$\mu m_1=\begin{vmatrix} A^{22}-\lambda & A^{23} \\ A^{12} & A^{13}\end{vmatrix};\quad \mu m_2=\begin{vmatrix} A^{11}-\lambda & A^{13} \\ A^{12} & A^{23}\end{vmatrix};$$

$$\mu m_3=\begin{vmatrix} A^{12} & A^{11}-\lambda \\ A^{22}-\lambda & A^{12}\end{vmatrix}.$$

Since $\Sigma m_i^2=1$, the m_i can now be calculated.

No matrix manipulation is needed; the calculation is simplified; and the solution refines rapidly to the correct solution for λ without a special rule being needed.†

In Cartesian coordinates the m_i are direction cosines of the plane normal, so that angular relationships are immediately accessible. These advantages are attained at the cost of transforming to Cartesian coordinates.

Table 1. *Numerical example of least-square plane*

Unit weights. Data in italics, results in bold-face. All lengths in Å.

Atom	x_1	x_2	x_3	D
1	*0.1860*	*4.9741*	*4.4804*	**0·0030**
2	*0.0697*	*6.1712*	*3.8151*	**0·0034**
3	*0.0994*	*7.3637*	*4.5212*	**−0·0048**
4	*0.2618*	*7.3200*	*5.9058*	**0·0000**
5	*0.3883*	*6.1238*	*6.6023*	**0·0062**
6	*0,3302*	*4.9323*	*5.8446*	**−0·0079**
Sum	1·3354	36·8851	31·1694	0·0001
Mean	0·22257	6·14752	5·19490	

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0·080467	−0·199234	0·651103
−0·199234	5·708601	−0·003002
0·651103	−0·003002	5·776348

α	β	γ
	0·463638	2·653456
≈11	−33·899871	+0·000779
	−33·436233	−0·299293
		−0·000001
		−2·420076
		0·004865

$\lambda_{(0)}=1{\cdot}46\times10^{-4}$: corrections negligible.

μm_i	3·7162	0·1295	−0·4188
m_i	**0·9931**	**0·0346**	**−0·1119**
d	**−0·1476**		

In Table 1 are reproduced all the steps in the calculation of the mean plane of the benzene ring of phenyl *cyclo*butenedione. The data are taken from SWMB and transformed to Cartesian coordinates so that the x_1 and x_2 axes coincide with the crystal axes x^1, x^2.

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Reference

Schomaker, V., Waser, J., Marsh, R. E. & Bergman, G. (1959). *Acta Cryst.* **12**, 600.

* Schomaker, Waser & Marsh, in a personal communication, have remarked that the equation $|A-\lambda g|=0$ may be written $|g^{-1}A-\mathbf{1}\lambda|=0$ where **1** represents the unit matrix. In this way an expansion in the form (1) may be made in any coordinate system. The matrix $g^{-1}A$ is, in general, only symmetric in the case of an orthogonal coordinate system, so that further terms would be required in the coefficients α, β, γ. Thus, Cartesian coordinates usually offer the most convenient method for the practical solution of the secular equation.

† This is obvious in the practical case of a reasonably planar distribution. It is, moreover, true in general. Since λ is a sum of squares, all solutions of (1) must be positive, and since A is a symmetric matrix all three solutions are real. The required solution is, of course, the least of these. If we think of the cubic function (1) plotted as a function of λ, it is clear that (2) represents a solution provided by a parabola which approximates to the cubic at small λ. The form of (2) gives the smaller of the two (necessarily positive) solutions. γ must always be negative (since (3) is a solution obtained from the straight line tangent to the cubic at $\lambda=0$), so that $(\beta^2-4\alpha\gamma)$ is always positive and a real solution to (2) exists. Since, at the solution of (2), the (negative) slope of the cubic must always be steeper than that of the quadratic, refinement by the Newtonian method will always lead to the smallest solution.