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The Estimation of an Orientation Relationship

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A numerical method is given for the determination of an orientation relationship with high accuracy. It is essentially a least-squares method.

Conventional methods for the determination of an orientation relationship are usually carried out by means of manipulations on a stereographic net. However, the accuracy of these manipulations is essentially limited, and if high accuracy is required resort must be made, at least in the final stages, to purely numerical methods. In recent years the accuracy of orientation determinations has improved considerably, and in at least one investigation, concerned with a change of phase in the solid state (Bowles, Barrett & Guttman, 1950), the accuracy approached 10 min. of arc. Thus, the need for purely numerical methods is apparent.

An orientation relationship is established when the rotation required to carry a standard orientation of a crystal into its actual orientation is known. If, on an actual crystal, exact measurements are made of the directions of at least two distinct normals with known specific indices this rotation can be determined. However, if the measurements are subject to error the angles between pairs of observed normals will not be exactly equal to their known true values and some adjustment procedure is necessary in order to estimate the rotation as precisely as possible. The method of adjustment proposed below was developed to solve a problem which arose in another connexion. It is numerical and analogous to the classical method of least squares for the solution of linear simultaneous equations. The method can be used whatever the precision of the observations but its main use lies in the final estimation of an orientation relationship of high accuracy.

The components of a vector relative to a fixed orthonormal basis can be written as the elements of a 3×1 column matrix. Therefore, let y_r be the column matrix representing the measured unit normal to the rth plane in the actual crystal and x_r that representing the known unit normal to the corresponding plane in the standard orientation. Then, if R is the 3×3 rotation matrix ($\mathsf{R}\mathsf{R}' = \mathsf{I}$) which is to be determined and $\theta_r (0 \le \theta_r \le \frac{1}{2}\pi)$ is the angular deviation of y_r from its true position $\mathsf{R}\mathsf{x}_r$,

$$\cos\theta_r = \mathsf{y}_r'\mathsf{R}\mathsf{x}_r, \quad (r = 1, \ldots, n)\,. \tag{1}$$

Now in the method of least squares R would be determined so that a sum of the type $\Sigma w_r\theta_r^2$ was a minimum. However, for θ_r small, $\cos\theta_r \simeq 1-\frac{1}{2}\theta_r^2$ so that an almost equivalent procedure is to maximize the sum

$$S = \sum_{r=1}^{n} w_r \cos\theta_r = \sum_{r=1}^{n} w_r \mathsf{y}_r'\mathsf{R}\mathsf{x}_r\,, \tag{2}$$

where each w_r is a known (positive) weight which should ideally be chosen inversely proportional to the variance of θ_r.

If X, Y are $3\times n$ matrices with x_r, y_r in their rth columns respectively and W is the $n\times n$ diagonal matrix with diagonal elements w_r, then

$$S = \mathrm{Tr}(\mathsf{W}\mathsf{Y}'\mathsf{R}\mathsf{X}) = \mathrm{Tr}(\mathsf{R}\mathsf{A})\,, \tag{3}$$

where

$$\mathsf{A} = \mathsf{X}\mathsf{W}\mathsf{Y}', \tag{4}$$

and Tr denotes the sum of the diagonal elements of a matrix; the last step follows from the result that $\mathrm{Tr}(\mathsf{B}\mathsf{C}) = \mathrm{Tr}(\mathsf{C}\mathsf{B})$ for all matrices B, C which can be multiplied together. Now, for any matrix A, rotation matrices R_1, R_2 can be found such that

$$\mathsf{A} = \mathsf{R}_2\Lambda\mathsf{R}_1'\,, \tag{5}$$

where Λ is a diagonal matrix with non-negative elements and the product $\mathsf{R}_2\mathsf{R}_1'$ is unique provided $\mathsf{A}'\mathsf{A}$ has not more than one characteristic root equal to zero. Murnaghan (1938) effectively proves this result when A is non-singular, but the general result, essentially proved below, is required since $\mathsf{A}'\mathsf{A}$ will have just one zero characteristic root if measurements are made on only two normals. Thus,

$$S = \mathrm{Tr}(\mathsf{R}_1'\mathsf{R}\mathsf{R}_2\Lambda) = \mathrm{Tr}(\mathsf{R}_0\Lambda)\,, \quad \text{say}\,. \tag{6}$$

Since the moduli of the elements of a rotation matrix are less than or equal to unity, S is maximum when $\mathsf{R}_0 = \mathsf{I}$ so that

$$\mathsf{R} = \mathsf{R}_1\mathsf{R}_2' = (\mathsf{R}_2\mathsf{R}_1')', \tag{7}$$

and

$$S_{\text{max.}} = \mathrm{Tr}(\Lambda)\,. \tag{8}$$

The procedure for determining R

The procedure is as follows: First the experimental data are used to compute A from (4), then R_1, R_2 are constructed as below and finally R is given by (7). The final result is unique, apart from symmetry rotations.

The following construction of R_1 and R_2 is based on the facts that, if A is given by (5), $\mathsf{R}_1'\mathsf{A}'\mathsf{A}\mathsf{R}_1 = \mathsf{R}_2'\mathsf{A}\mathsf{A}'\mathsf{R}_2 = \Lambda^2$ and that $\mathsf{A}'\mathsf{A}$ is symmetrical and has no negative characteristic roots, i.e. a positive semi-definite matrix (Albert, 1941). It follows (Ferrar, 1941, 1951) that a set of mutually orthogonal unit vectors u_1, u_2, u_3 can be determined such that

$$\mathsf{A}'\mathsf{A}\mathsf{u}_r = \lambda_r^2\mathsf{u}_r, \quad \lambda_r \geq 0\,, \tag{9}$$

where the λ_r^2 are the roots of the determinantal equation

$$\det\,[\mathsf{A}'\mathsf{A}-\lambda^2\,\mathsf{I}] = 0\,. \tag{10}$$

Thus, a possible choice for R_1 is

$$\mathsf{R}_1 = (\mathsf{u}_1, \mathsf{u}_2, \mathsf{u}_3)\,, \tag{11}$$

and the diagonal elements of Λ are λ_r. Multiplying (9) on the left by A shows that, provided $\lambda_r \neq 0$,

$$\mathsf{v}_r = \mathsf{A}\mathsf{u}_r \tag{12}$$

is a characteristic vector of $\mathsf{A}\mathsf{A}'$ belonging to the characteristic root λ_r^2. Further, it is easily shown that the v_r so found are mutually orthogonal and of magnitude λ_r. Thus, when all the λ_r are positive, a possible choice for R_2 is

$$\mathsf{R}_2 = (\mathsf{v}_1/\lambda_1, \mathsf{v}_2/\lambda_2, \mathsf{v}_3/\lambda_3)\,, \tag{13}$$

and this is the only choice consistent with (5) and (11).

If $\lambda_3 = 0$ is the only zero characteristic root, the first two columns of R_2 are found as above while the last column is the unique unit vector v satisfying the equation

$$\mathsf{A}'\mathsf{v} = 0\,. \tag{14}$$

It can now be verified readily that $\mathsf{R}_1'\mathsf{A}'\mathsf{R}_2 = \Lambda$ so that A is given by (5). Further, if all the characteristic roots λ_r are different the u_r and v_r are unique so that R_1, R_2 are each unique, while if the λ_r are not all different it can be shown that the product $\mathsf{R}_1\mathsf{R}_2'$ is unique although R_1 and R_2 separately are not.

The above estimate of R can be made reasonable from the statistical point of view. For, if, following Fisher (1953), it is assumed that the observations are independent and that the probability density of each $\cos\theta_r$ is proportional to

$$\exp\,(\kappa w_r \cos\theta_r)\,, \tag{15}$$

where κw_r is approximately equal to the reciprocal of the variance of θ_r, then the above estimate of R which maximizes S is just the maximum likelihood estimate. Using this density function, the problems of determining the probability distributions of R and of $S_{\text{max.}}$ do not appear to be simple and no estimate of confidence limits can be made at present. However, the weighted mean of the expectation values of the $\cos\theta_r$ is approximately $1-1/\kappa\,\mathrm{Tr}(\mathsf{W})$. Calling this quantity $\cos\theta_0$ and using the maximum likelihood estimate for κ gives

$$\cos\theta_0 = 1-[\mathrm{Tr}(\mathsf{W})-S_{\text{max.}}]/n\,\mathrm{Tr}(\mathsf{W})\,, \tag{16}$$

and θ_0 may be taken as a rough estimate of the 'reasonably likely' variations in the angle of rotation determined by R; θ_0 will be related in some way to the standard error of this angle of rotation.

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