

and, of course at the point 0, where the Fourier coefficient is the average density ρ_0 .

The space group $p8gm$ has

$$\Phi_m(2\zeta^j + \zeta^{j\pm 1}) \equiv \frac{1}{2}, \quad \Phi_r(2\zeta^j + \zeta^{j\pm 1}) \equiv 0. \quad (5.8)$$

If we take the Fourier coefficients at the lattice vectors (5.7) to be given by

$$\rho(2\zeta^j + \zeta^{j\pm 1}) = \pm \rho_1, \quad j = 0, \dots, 7, \quad (5.9)$$

where ρ_1 is a constant overall amplitude, then it is evident from Fig. 2 and the defining relation (2.4) that mirrorings and rotations of (5.9) are indeed characterized by the phase functions (5.8).

The symmetry of the resulting real-space density is shown in Fig. 3, by coloring the plane black or white depending on the sign of $\rho - \rho_0$. To aid the reader in deciding to what extent 'quasi-glide lines' are present in this pattern, we display in Fig. 4 the corresponding symmorphic pattern with $p8mm$ symmetry given by taking all 16 Fourier coefficients in (5.9) to have the same sign.

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A Note on the Rotational Superposition Problem

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Abstract

A rotation axis vector with magnitude $\tan(\theta/2)$ for a rotation angle θ and a closely related unit vector of dimension 4 are used to show that: (i) the quadratic residual (weighted sum of squares of coordinate differences) that results when one vector set is rotated relative to another is a quadratic form of order 4, (ii) the stationary values of the residual are given by the eigenvalues of a matrix of order 4, (iii) the minimum residual is given by the largest eigenvalue, (iv) the rotations required to obtain such residuals are uniquely defined by the corresponding eigenvectors, and (v) the stationary values are related by the operations of 222 symmetry. No precautions against the generation of improper rotations are required. In addition, an equivalent solution based on a scalar iteration is presented, together with some relationships of general interest.

Introduction

The problem of the optimal superposition of one vector set on another by pure rotation arises notably in the comparison of parts of related protein molecules, and its solution has attracted the attention of a number of writers, notably McLachlan (1972, 1979, 1982), Kabsch (1976, 1978), Diamond (1976) and Lesk (1986).

McLachlan's earlier method is iterative and analogous to rotating one vector set about the axis of the prevailing couple to reduce that couple to zero, when the couple is supposed to be the sum of the moments arising from forces along the lines separating equivalent points in the two vector sets having magnitudes proportional to those separations. His later method is an eigenvalue/vector method using a symmetric matrix of order 6. Kabsch's method is an eigenvalue/vector method based on matrices of order

3 but requires the use of Lagrange multipliers to constrain the resulting matrix to be orthogonal. Diamond's method does not impose orthogonality on the transformation relating the vector sets, but allows it to be a general transformation which is then interpreted rigorously as the combination of rotation and homogeneous or inhomogeneous strain. Lesk's approach, leading to the solution of a polynomial of order 4, is possibly the one most closely related to the present work.

In this paper we show that the analysis of the problem is simplified and enriched by casting the algebra in terms of half the required angle of rotation, $\theta/2$, rather than θ itself, leading to an unconstrained eigenvalue/vector problem of order 4, or to a scalar iteration involving inversion of a matrix of order 3.

What follows is valid for the rotation of one vector set onto another using any prevailing origins for these vector sets. It is well known that the optimal rotational superposition is achieved if the data sets are referred to their respective centroids as origins, and it is assumed that if this is required, then this step has been performed as a preliminary, and no further attention is given to translational components.

The representation of rotation

We define three 3-vectors, \mathbf{l} , \mathbf{r} and $\boldsymbol{\lambda}$ and a 4-vector $\boldsymbol{\rho}$ such that

$\mathbf{l}^T = (l, m, n)$ is a unit vector of direction cosines of the axis of rotation,

$$\mathbf{r}^T = (r_1, r_2, r_3) = (u, v, w) = t\mathbf{l}^T \quad \text{with } t = \tan(\theta/2), |\mathbf{r}| = r = t, \quad (1)$$

$$\boldsymbol{\lambda}^T = (\lambda_1, \lambda_2, \lambda_3) = (\lambda, \mu, \nu) = s\mathbf{l}^T \quad \text{with } s = \sin(\theta/2),$$

$$\boldsymbol{\rho}^T = (\lambda, \mu, \nu, \sigma) = (\boldsymbol{\lambda}^T, \sigma) \quad \text{with } \sigma = \cos(\theta/2).$$

By definition $\mathbf{l}^T \mathbf{l} = \boldsymbol{\rho}^T \boldsymbol{\rho} = 1$, but the elements of \mathbf{r} are independent, equivalent and unbounded.

If the vector \mathbf{d} (Fig. 1) is rotated through an angle θ about \mathbf{l} to \mathbf{d}' then

$$\mathbf{d}' = \mathbf{d} + (\mathbf{l} \times \mathbf{d}) \sin \theta + [\mathbf{l} \times (\mathbf{l} \times \mathbf{d})](1 - \cos \theta) \quad (2)$$

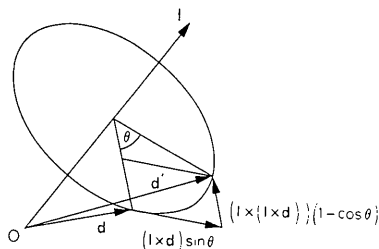


Fig. 1. The manner in which the rotated vector \mathbf{d}' is made up from the unrotated vector \mathbf{d} and two additional vectors. \mathbf{l} is a unit vector in the direction of the axis of rotation.

because $|\mathbf{l} \times \mathbf{d}|$ is the radius of the arc along which \mathbf{d} moves. The identities

$$\sin \theta = \frac{2t}{1+t^2}, \quad \cos \theta = \frac{1-t^2}{1+t^2} \quad (3)$$

then give

$$\mathbf{d}' = \mathbf{d} + \frac{2}{1+t^2} \{(\mathbf{r} \times \mathbf{d}) + [\mathbf{r} \times (\mathbf{r} \times \mathbf{d})]\} \quad (4)$$

$$= \mathbf{d} + 2\{\sigma(\boldsymbol{\lambda} \times \mathbf{d}) + [\boldsymbol{\lambda} \times (\boldsymbol{\lambda} \times \mathbf{d})]\}. \quad (5)$$

These expressions are linear on \mathbf{d} , and may be expanded to give the orthogonal matrix satisfying $\mathbf{d}' = \mathbf{R}\mathbf{d}$ as

$$\mathbf{R} = \frac{1}{(1+t^2)} \begin{pmatrix} (1+u^2-v^2-w^2) & 2(uv-w) & 2(uw+v) \\ 2(uv+w) & (1-u^2+v^2-w^2) & 2(vw-u) \\ 2(uw-v) & 2(vw+u) & (1-u^2-v^2+w^2) \end{pmatrix}. \quad (6)$$

Equation (6) may alternatively be obtained from the standard form of \mathbf{R} based on \mathbf{l} and θ using the identities (3). Similarly (5) gives

$$\mathbf{R} = \begin{pmatrix} (\lambda^2 - \mu^2 - \nu^2 + \sigma^2) & 2(\lambda\mu - \nu\sigma) & 2(\lambda\nu + \mu\sigma) \\ 2(\lambda\mu + \nu\sigma) & (-\lambda^2 + \mu^2 - \nu^2 + \sigma^2) & 2(\mu\nu - \lambda\sigma) \\ 2(\lambda\nu - \mu\sigma) & 2(\mu\nu + \lambda\sigma) & (-\lambda^2 - \mu^2 + \nu^2 + \sigma^2) \end{pmatrix}. \quad (7)$$

Note that improper rotations are excluded by this definition, and that negation of l, m, n and θ (which leaves the rotation unchanged) leaves \mathbf{r} and $\boldsymbol{\rho}$ unchanged, and negation of $\boldsymbol{\rho}$ (which leaves $\boldsymbol{\rho}^T \boldsymbol{\rho}$ unchanged, see below) adds 2π to θ .

Formation of the antisymmetric part of the product $\mathbf{R} = \mathbf{R}_2 \mathbf{R}_1$ using (6) shows that the combination of two rotations is given by

$$\mathbf{r} = \frac{\mathbf{r}_2 + \mathbf{r}_1 + \mathbf{r}_2 \times \mathbf{r}_1}{1 - \mathbf{r}_2 \cdot \mathbf{r}_1} \quad (8)$$

or, equivalently,

$$\begin{aligned} \boldsymbol{\lambda} &= \boldsymbol{\lambda}_2 \sigma_1 + \boldsymbol{\lambda}_1 \sigma_2 + \boldsymbol{\lambda}_2 \times \boldsymbol{\lambda}_1 \\ \sigma &= \sigma_1 \sigma_2 - \boldsymbol{\lambda}_2 \cdot \boldsymbol{\lambda}_1 \end{aligned} \quad (9)$$

as given by Aharonov, Farach & Poole (1977). It follows that any two rotations for which $\mathbf{r}_1 \cdot \mathbf{r}_2 = 1$ result in a combined rotation of 180° .

The superposition problem

In this section we use a subscript notation in which lower- or upper-case subscripts denote summation or no summation respectively. The subscript a relates to points (atoms) in the vector sets, other subscripts relate to coordinates.

The weighted sum of squares of errors, E , between the vector set \mathbf{X} and the rotated vector set $\mathbf{R}\mathbf{x}$, is

$$E = W_a(X_{ia} - R_{ij}x_{ja})(X_{ia} - R_{ik}x_{ka}) \quad (10)$$

$$= W_a(X_{ia}X_{ia} - R_{ij}x_{ja}X_{ia} - X_{ia}R_{ik}x_{ka} + x_{ja}x_{ja}) \quad (11)$$

$$R_{ij}x_{ja} = x_{IA} + \frac{2}{1+r^2}(\varepsilon_{ijk}r_jx_{ka} + \varepsilon_{ijk}r_j\varepsilon_{klm}r_lx_{mA}) \quad (12)$$

$$E = W_a \left(X_{ia}X_{ia} - 2 \left\{ x_{ia} + \frac{2}{1+r^2} [\varepsilon_{ijk}r_jx_{ka} + (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl})r_jr_lx_{ma}] \right\} X_{ia} + x_{ja}x_{ja} \right) \quad (13)$$

$$= W_a \left[(X_{ia} - x_{ia})(X_{ia} - x_{ia}) - \frac{4X_{ia}}{1+r^2} \times (\varepsilon_{ijk}r_jx_{ka} + r_jr_lx_{ja} - r_jr_lx_{ia}) \right]. \quad (14)$$

Hence E is minimized by the (unconstrained) vector \mathbf{r} which maximizes

$$\varphi = \frac{4W_aX_{ia}}{1+r^2}(\varepsilon_{ijk}r_jx_{ka} + r_lr_lx_{ja} - r_jr_lx_{ia}). \quad (15)$$

Defining the matrices \mathbf{M} and \mathbf{Q} and the vector \mathbf{V} by

$$M_{IJ} = W_ax_{Ia}X_{Ja} \quad (16)$$

$$\mathbf{Q} = \mathbf{M} + \mathbf{M}^T - 2\mathbf{I} \operatorname{tr} \mathbf{M} \quad (17)$$

$$V_I = \varepsilon_{Ijk}W_ax_{ja}X_{ka} = \varepsilon_{Ijk}M_{jk} \quad (18)$$

gives

$$\varphi = \frac{2}{1+r^2}(2\mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r}) \quad (19)$$

$$= 2(2\sigma\lambda \cdot \mathbf{V} + \lambda^T \mathbf{Q} \lambda) \quad (20)$$

$$= 2\boldsymbol{\rho}^T \mathbf{P} \boldsymbol{\rho} \quad (21)$$

in which

$$\mathbf{P} = \begin{pmatrix} \mathbf{Q} & \mathbf{V} \\ \mathbf{V}^T & 0 \end{pmatrix}. \quad (22)$$

Hence φ is maximized by the normalized eigenvector $\boldsymbol{\rho}$ of largest eigenvalue of the matrix

$$\begin{pmatrix} \mathbf{Q} & \mathbf{V} \\ \mathbf{V}^T & 0 \end{pmatrix}.$$

$\boldsymbol{\rho}$ then, by definition, determines the axis of rotation and the angle, including its quadrant. The residual E is then given by

$$E = E_0 - 2\boldsymbol{\rho}^T \mathbf{P} \boldsymbol{\rho} \quad (23)$$

in which

$$E_0 = W_a(X_{ia} - x_{ia})(X_{ia} - x_{ia}) \quad (24)$$

is the initial value of E and the corresponding rotation matrix is given by (7) above. Rotations determined in this way are accurate and reliable, and there are no special cases. An angle of 179.999° for which $\tan(\theta/2) = 10^5$ has been correctly measured using single-length working (24-bit mantissa) without requiring any special care. Note that \mathbf{M} and \mathbf{P} each have nine independent elements and thus the same information content.

Equation (23) is valid for all unit vectors $\boldsymbol{\rho}$ in 4-space and their associated matrices (7) and there are four stationary values of E corresponding to the four eigenvalues, p , of \mathbf{P} .

If \mathbf{x}' represents the vector set \mathbf{x} in an alternative initial orientation, for which may be calculated the corresponding E'_0 and \mathbf{P}' , then, since the same stationary values of E are accessible by rotation from the alternative initial orientation, it follows that the eigenvalue spectra of \mathbf{P} and of \mathbf{P}' are the same except for an offset given by $\frac{1}{2}(E_0 - E'_0)$, and that the interval (p_{\min}, p_{\max}) contains the origin. $p_{\max} = 0$ occurs if the initial orientation of \mathbf{x} is, in fact, the best superposition on \mathbf{X} , and $p_{\min} = 0$ occurs if the initial orientation is the worst fit.

If the initial (arbitrary) orientation of the vector set \mathbf{x} is designated by a subscript zero, and the orientations corresponding to the stationary values of E are designated by subscripts 1 to 4, then the rotation vector \mathbf{r}_{01} rotates \mathbf{x} from the initial orientation to orientation 1, \mathbf{r}_{02} is from the initial orientation to orientation 2 and \mathbf{r}_{12} rotates from orientation 1 to orientation 2, then we may rotate from 1 to 2 either by applying \mathbf{r}_{12} or by applying $-\mathbf{r}_{01}$ followed by \mathbf{r}_{02} ; therefore (8) gives

$$\mathbf{r}_{12} = \frac{\mathbf{r}_{02} - \mathbf{r}_{01} - \mathbf{r}_{02} \times \mathbf{r}_{01}}{1 + \mathbf{r}_{01} \cdot \mathbf{r}_{02}}. \quad (25)$$

Now the eigenvectors of \mathbf{P} correspond to $\boldsymbol{\rho}_{01}$, $\boldsymbol{\rho}_{02}$ etc. and, being eigenvectors of a real symmetric matrix, are orthogonal, *i.e.*

$$\boldsymbol{\rho}_{01}^T \boldsymbol{\rho}_{02} = 0 = \lambda_{01}^T \lambda_{02} + \sigma_{01} \sigma_{02} \quad (26)$$

$$\therefore \mathbf{r}_{01} \cdot \mathbf{r}_{02} + 1 = 0.$$

Therefore $|\mathbf{r}_{12}| = \infty$ and the corresponding rotation $\theta_{12} = \pi$.

Thus the orthogonality of the eigenvectors demonstrates that the four orientations with stationary values of E are related by the operations of 222 symmetry.

If \mathbf{X} and \mathbf{x} are interchanged, \mathbf{Q} is unchanged but \mathbf{V} is negated. Thus new eigenvectors are obtained by negating σ , consistent with the requirement that if θ optimally rotates \mathbf{x} onto \mathbf{X} , then a rotation $-\theta$ about the same axis optimally rotates \mathbf{X} onto \mathbf{x} .

\mathbf{X} and \mathbf{x} may also be superposed by rotating each through an angle $\pm\theta/2$ using

$$\mathbf{R}^{1/2} = \begin{pmatrix} \left(\frac{\lambda^2}{1+\sigma} + \sigma \right) & \left(\frac{\lambda\mu}{1+\sigma} - \nu \right) & \left(\frac{\lambda\nu}{1+\sigma} + \mu \right) \\ \left(\frac{\lambda\mu}{1+\sigma} + \nu \right) & \left(\frac{\mu^2}{1+\sigma} + \sigma \right) & \left(\frac{\mu\nu}{1+\sigma} - \lambda \right) \\ \left(\frac{\lambda\nu}{1+\sigma} - \mu \right) & \left(\frac{\mu\nu}{1+\sigma} + \lambda \right) & \left(\frac{\nu^2}{1+\sigma} + \sigma \right) \end{pmatrix} \quad (27)$$

and its transpose.

If the vectors in either \mathbf{X} or \mathbf{x} or both are collinear \mathbf{P} is degenerate, the eigenvalues are equal in pairs and a \mathbf{p} vector which is any linear combination (subject to unit norm) of the two relevant eigenvectors produces a stationary residual. Equation (25) then establishes that such degenerate solutions are related by arbitrary rotation about the line of collinearity.

As an alternative to solving a 4×4 eigenproblem

$$\varphi = \frac{2}{1+r^2} (2\mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r}) \quad (28)$$

$$\nabla \varphi = \frac{-4\mathbf{r}}{(1+r^2)^2} (2\mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r}) + \frac{2}{1+r^2} (2\mathbf{V} + 2\mathbf{Q} \mathbf{r}) \quad (29)$$

giving stationary values when

$$\mathbf{r} [2\mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r}] = (1+r^2)(\mathbf{V} + \mathbf{Q} \mathbf{r}). \quad (30)$$

One may define

$$\begin{aligned} \alpha &= \frac{2\mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r}}{1+r^2} \\ &= (\mathbf{r}^T \mathbf{1}) \begin{pmatrix} \mathbf{Q} & \mathbf{V} \\ \mathbf{V}^T & 0 \end{pmatrix} \begin{pmatrix} \mathbf{r} \\ 1 \end{pmatrix} / (\mathbf{r}^T \mathbf{1}) \begin{pmatrix} \mathbf{r} \\ 1 \end{pmatrix} \\ &= \mathbf{p}^T \mathbf{P} \mathbf{p}, \end{aligned} \quad (31)$$

form the scalar product of (30) with \mathbf{r} and substitute α to give

$$\alpha r^2 = \mathbf{r} \cdot \mathbf{V} + \mathbf{r}^T \mathbf{Q} \mathbf{r} \quad (32)$$

as the equation to be solved. Substitution of $\mathbf{r}^T \mathbf{Q} \mathbf{r}$ from here into the definition of α gives

$$\alpha = \frac{2\mathbf{r} \cdot \mathbf{V} + (\alpha r^2 - \mathbf{r} \cdot \mathbf{V})}{1+r^2}. \quad (33)$$

Therefore

$$\alpha = \mathbf{r} \cdot \mathbf{V} \quad (34)$$

and the equation to be solved for \mathbf{r} is [from (30) and (31)]

$$\mathbf{r}(\mathbf{V} \cdot \mathbf{r}) = \mathbf{V} + \mathbf{Q} \mathbf{r}, \quad (35)$$

i.e.

$$(\alpha \mathbf{I} - \mathbf{Q}) \mathbf{r} = \mathbf{V} \quad (36)$$

$$\mathbf{r} = (\alpha \mathbf{I} - \mathbf{Q})^{-1} \mathbf{V} \quad (37)$$

$$\mathbf{V}^T \mathbf{r} = \alpha = \mathbf{V}^T (\alpha \mathbf{I} - \mathbf{Q})^{-1} \mathbf{V}. \quad (38)$$

This may be solved for α iteratively with reference to Fig. 2, in which the straight line represents the left-hand side of (38) and the other four branches represent the right-hand side, with singularities where α is an eigenvalue of \mathbf{Q} . The solution may be obtained by iterating

$$\mathbf{r}_n = (\alpha_n \mathbf{I} - \mathbf{Q})^{-1} \mathbf{V} \quad (39)$$

$$\alpha_{n+1} = \frac{\mathbf{V} \cdot \mathbf{r}_n + \alpha_n r_n^2}{1+r_n^2}, \quad (40)$$

and to obtain the smallest E the largest α must be found since $E = E_0 - 2\alpha$ by (23) and (31). Hence a good initial iterate is

$$\alpha_0 = E_0/2 \quad (41)$$

and the corresponding transformation is given by using the elements of \mathbf{r} from (39) in (6).

This iteration has the attractive property that if \mathbf{x} and \mathbf{X} are exactly superposable then the initial iterate, α_0 , is the analytic solution, the first cycle produces no change and the iteration terminates immediately. Only if \mathbf{x} is an inexact image of \mathbf{X} (as when either or both involve experimentally determined coordinates) is an iteration required at all.

If the required rotation is 180° then $(\alpha \mathbf{I} - \mathbf{Q})$ is singular at the end of the iteration. This is recognizable by its determinant being small (e.g. 10^{-6}) in relation to the product of its trace with the trace of its adjoint. Its adjoint is then of rank 1 and the product of the adjoint with \mathbf{V} gives the direction of \mathbf{r} . A 180° rotation about this vector is given by the limiting form of (6) as $t^2 \rightarrow \infty$, i.e.

$$\mathbf{R}_\pi = 2\mathbf{I} \mathbf{I}^T - \mathbf{I}. \quad (42)$$

If, in addition, \mathbf{V} is an eigenvector of \mathbf{Q} the product $[\text{adj}(\alpha \mathbf{I} - \mathbf{Q})] \mathbf{V}$ may also vanish, and in this case any

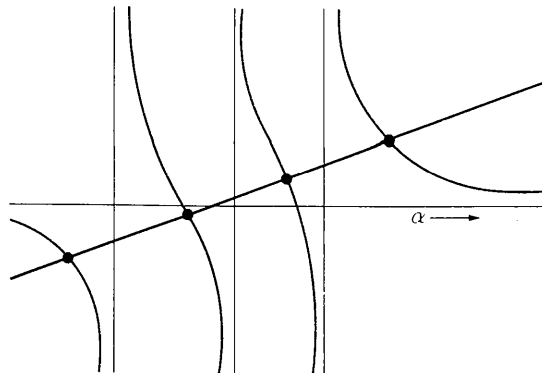


Fig. 2. Graphs of the left- and right-hand sides of equation (38) showing the four possible solutions of that equation. The required solution is the one with largest α . The vertical asymptotes occur where α is an eigenvalue of \mathbf{Q} .

non-vanishing row or column of the adjoint will do to establish I. However, if \mathbf{x} and \mathbf{X} are superposable, rotation angles measured are correct to 0.01° or better, provided the angle differs from 180° by 0.1° or more.

If the rotation required is close to π and \mathbf{x} and \mathbf{X} are not exactly superposable, then there is a possibility of α going below the largest eigenvalue of \mathbf{Q} , recognizable by the determinant of $(\alpha\mathbf{I} - \mathbf{Q})$ going negative. The iteration will then converge on the next best stationary value of E unless stopped immediately. Such cases are better handled by the previous approach using eigenvectors of \mathbf{P} . However, such cases have only occurred when the coordinate errors (*i.e.* departures of \mathbf{x} from an image of \mathbf{X}) are comparable with the coordinates themselves and with the more usual problems where \mathbf{x} and \mathbf{X} are closely similar, convergence has always been accurate in one cycle, and the speed of the iteration is thought to outweigh this limitation.

Some further relationships of interest

We define matrices Λ , \mathbf{S} and \mathbf{T} by

$$\Lambda_{IJ} = \varepsilon_{IJK}\lambda_k - \sigma\delta_{IJ} \quad (43)$$

and

$$\mathbf{S} = \begin{pmatrix} \Lambda & \boldsymbol{\lambda} \\ \boldsymbol{\lambda}^T & \sigma \end{pmatrix} = \begin{pmatrix} -\sigma & \nu & -\mu & \lambda \\ -\nu & -\sigma & \lambda & \mu \\ \mu & -\lambda & -\sigma & \nu \\ \lambda & \mu & \nu & \sigma \end{pmatrix}$$

$$\mathbf{T} = \begin{pmatrix} -\Lambda & \boldsymbol{\lambda} \\ -\boldsymbol{\lambda}^T & \sigma \end{pmatrix} = \begin{pmatrix} \sigma & -\nu & \mu & \lambda \\ \nu & \sigma & -\lambda & \mu \\ -\mu & \lambda & \sigma & \nu \\ -\lambda & -\mu & -\nu & \sigma \end{pmatrix}. \quad (44)$$

Then \mathbf{S} and \mathbf{T} are orthogonal, \mathbf{S} has the property that

$$\mathbf{S}^2 = \begin{pmatrix} \mathbf{R} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \quad (45)$$

according to (7), and \mathbf{T} has the property that the rotation vector $\boldsymbol{\rho}_n$ resulting from compounding n rotations is given by

$$\boldsymbol{\rho}_n = \mathbf{T}_n \mathbf{T}_{n-1} \dots \mathbf{T}_1 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad (46)$$

thus permitting the direct calculation of axes and rotation angles. Cayley's theorem (Courant & Hilbert, 1953, 1962) gives

$$\Lambda(\Lambda^T)^{-1} = \mathbf{R}. \quad (47)$$

Fig. 3 shows some relationships that arise when two rotations are compounded and represents a

stereogram in which the directions of rotation axes are plotted, labelled by their 4-dimensional counterparts. The points marked ρ_1 and ρ_2 are the axes of first and second rotations with angles θ_1 and θ_2 , and with an angle φ between them. Evidently rotation 1 moves A to B and rotation 2 moves B back to A . Therefore the combined rotation leaves the direction of A unchanged so that A must be the axis of the combined rotation. Similarly for B if rotation 2 is applied first. Since the first rotation leaves ρ_1 unchanged and the second moves it to ρ'_1 , the combined rotation angle θ about A is as indicated.

Solution of the spherical triangle $\rho_1\rho_2A$ generates the second equation (9). Solution of the spherical triangle $\rho_1\rho_2C$ shows that

$$\boldsymbol{\rho}_1^T \boldsymbol{\rho}_2 = \cos \psi. \quad (48)$$

If we construct a matrix \mathbf{S}_2 , which is an \mathbf{S} matrix formed from the elements of the rotation vector $\boldsymbol{\rho}_2$, then the product $\mathbf{S}_2\boldsymbol{\rho}_1$ plots at D since

$$\mathbf{S}_2\boldsymbol{\rho}_1 = \begin{pmatrix} \lambda_2\sigma_1 - \lambda_1\sigma_2 - \lambda_2 \times \lambda_1 \\ \sigma_1\sigma_2 + \lambda_2 \cdot \lambda_1 \end{pmatrix} = \begin{pmatrix} \lambda_3 \\ \sigma_3 \end{pmatrix} = \boldsymbol{\rho}_3, \quad (49)$$

which corresponds to the compound rotation given by (9) with λ_1 (but not σ_1) negated, *i.e.* to a rotation $-\theta_1$ about λ_1 followed by θ_2 about λ_2 . Of these two steps the first moves D to C and the second returns it to D . Since the same two operations move ρ_1 to ρ'_1 the rotation associated with $\boldsymbol{\rho}_3$ is 2ψ . Similarly, forming the product $\mathbf{S}_2\boldsymbol{\rho}_3$ corresponds to a rotation -2ψ about D followed by θ_2 about λ_2 , which operation

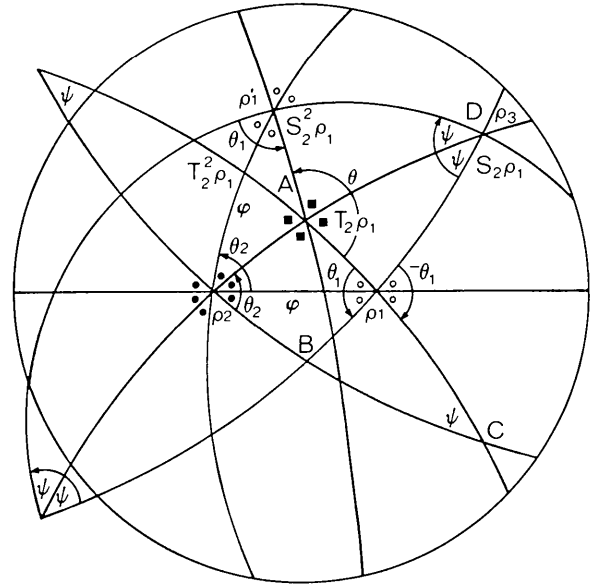


Fig. 3. Stereogram showing how rotation of θ_1 , about ρ_1 followed by θ_2 about ρ_2 is related to the matrix products $\mathbf{S}_2\boldsymbol{\rho}_1$, $\mathbf{S}_2^2\boldsymbol{\rho}_1$, $\mathbf{T}_2\boldsymbol{\rho}_1$ and $\mathbf{T}_2^2\boldsymbol{\rho}_1$. $\mathbf{T}_2^2\boldsymbol{\rho}_1$ defines the axis of the compound rotation θ_1 about ρ_1 , followed by $n\theta_2$ about ρ_2 , and $\mathbf{S}_2^2\boldsymbol{\rho}_1$ rotates the vector ρ_1 through θ_2 about ρ_2 . Similarly marked angles are equal.

leaves ρ'_1 unchanged, in agreement with the requirement

$$\begin{pmatrix} \lambda'_1 \\ \sigma_1 \end{pmatrix} = \mathbf{S}_2 \rho_3 = \mathbf{S}_2^2 \rho_1 = \begin{pmatrix} \mathbf{R}_2 \lambda_1 \\ \sigma_1 \end{pmatrix}. \quad (50)$$

Similarly, if the point marked ρ_1 in Fig. 3 now represents the direction of any position vector \mathbf{d} , then \mathbf{d} may be augmented to homogeneous coordinates

$$\xi = \begin{pmatrix} \mathbf{e} \\ f \end{pmatrix} = \begin{pmatrix} \mathbf{d} \\ 1 \end{pmatrix} (1 + d^2)^{-1/2} \quad (51)$$

and the normalized 4-vector ξ contains all the information in \mathbf{d} . Forming the product $\mathbf{R}_2 \mathbf{d}$ is seen to be analogous to forming $\mathbf{S}_2^2 \xi$. In this sense the transforming of a position vector \mathbf{d} and the compounding of two rotations are seen to be equivalent operations.

The vectors $\pm[1000]$, $\pm[0100]$ and $\pm[0010]$ represent 180° rotations about each of X, Y and Z, and $\pm[0001]$ gives the identity. It follows from (9) that the first three rows of \mathbf{S} , regarded as ρ vectors, correspond to the rotation ρ followed by 180° rotations about each of the reference axes, and the columns likewise correspond to ρ preceded by 180° rotations about them. Letting ρ_1 be the first row of \mathbf{S} and ρ_2 the second column allows the corresponding ψ to be identified as the angle between the unrotated X axis and the Y axis rotated by ρ , consistent with (45).

The top row of \mathbf{S} , as already stated, is the ρ vector which corresponds to the rotation ρ followed by a rotation of 180° about X. This compound rotation has

ρ vector $[-\sigma, \nu, -\mu, \lambda]$ and the corresponding \mathbf{S} matrix is therefore

$$\begin{pmatrix} -\lambda & -\mu & -\nu & -\sigma \\ \mu & -\lambda & -\sigma & \nu \\ \nu & \sigma & -\lambda & -\mu \\ -\sigma & \nu & -\mu & \lambda \end{pmatrix}.$$

In the original rotation σ is algebraically distinct from λ , μ and ν in the ways in which it enters into the equations that arise. However, this example shows that the four rotations (the original, and three produced from it by compounding with 180° about X, Y and Z) collectively form a set in which λ , μ , ν and σ all have equivalent status and none is unique.

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Phase Extension by Combined Entropy Maximization and Solvent Flattening

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Abstract

An efficient algorithm is described for finding the maximum entropy density distribution under the constraint that $\langle \sum |F| \cos(2\pi \mathbf{h} \cdot \mathbf{r} - \varphi) \rangle$, where the sum is over a subset of reflections whose phase has been determined, is constant. This algorithm is combined with solvent flattening in a procedure for extending phases to higher resolution. A test of the procedure on the structure of ribonuclease A and its application

to the determination of two previously unknown structures are discussed.

Introduction

In crystallography, as in other branches of physics such as spectroscopy and radio astronomy, the observable data depend on Fourier transforms of density distributions that the experimenter wishes to determine. Because only the amplitude, not the phase,