Acta Cryst. (1989). A**45**, 657

A comparison of three recently published methods for superimposing vector sets by pure rotation.

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(*Received* 8 *March* 1989; *accepted* 30 *May* 1989)

Abstract

Solutions to the rotational superposition problem published recently by Diamond [*Acta Cryst.* (1988), A**44**, 211-216] Kearsley [*Acta Cryst.* (1989), A**45**, 208-210] and MacKay [*Acta Cryst.* (1984), A**40**, 165-166] are compared. It is shown that the first two of these are identical and that MacKay's solution underestimates the rotation unless the initial orientation is optimal or perfect fitting is possible, or the residual vectors after optimal fitting are all parallel to the corresponding rotation axis.

We refer to the papers by Diamond (1988), Kearsley (1989) and MacKay (1984) as (I), (II) and (III) respectively.

The last equation in (II) is identical to equation (23) of (I) since Kearsley's matrix is $E_0\mathbf{I}-2\mathbf{P}$ in the notation of (I). Combination of two terms into one in this way makes the associated eigenvalue spectrum independent of the original orientation, whereas in (I) it is floating, but there is no other difference apart from the ordering of the elements and the manner of the derivation.

In (III) MacKay shows that if a vector $\mathbf{x}$ is rotated to become the vector $\mathbf{X}$ then

$$\mathbf{X}-\mathbf{x}=\mathbf{r}\times(\mathbf{X}+\mathbf{x}), \quad (1)$$

where $\mathbf{r}$ has the direction of the axis of rotation and magnitude $\tan(\theta/2)$ for a rotation angle θ. This relationship, linear in $\mathbf{r}$, may form the basis of a least-squares solution for $\mathbf{r}$ when many vector pairs exist for which $\mathbf{X}$ is not necessarily an exact rotation of $\mathbf{x}$. We define the square matrix $(\boldsymbol{\varepsilon}\mathbf{v})$ by

$$(\varepsilon v)_{IJ}=\varepsilon_{IJk}v_k, \quad \varepsilon_{IJK}=(I-J)(J-K)(K-I)/2 \quad (2)$$

and treat all vectors as columns. The individual residual vectors in MacKay's method are then

$$\mathbf{e}_M=(\boldsymbol{\varepsilon}(\mathbf{X}+\mathbf{x}))\mathbf{r}-(\mathbf{X}-\mathbf{x}) \quad (3)$$

and the residual

$$E_M(\mathbf{r})=\sum W\mathbf{e}_M^T\mathbf{e}_M \quad (4)$$

where the summation is over the point pairs of the vector sets with weights W. $E_M(\mathbf{r})$ is quadratic in $\mathbf{r}$ and therefore has one minimum and no maximum, and the minimum is reached in one cycle of least squares. In contrast, the more usual residual, $E_N(\mathbf{r})$, the weighted sum of squares of coordinate differences between the points $\mathbf{X}$ and the rotated $\mathbf{x}$, has one minimum, one maximum and two saddle points. MacKay is thus minimizing a different residual and the question arises as to whether or not its minimum coincides with the minimum of $E_N(\mathbf{r})$.

So long as the vectors $\mathbf{x}$ remain unrotated we may write MacKay's solution, $\mathbf{r}_M$, as

$$\mathbf{r}_M=\mathbf{r}-[\nabla^2E_M(\mathbf{r})]^{-1}\nabla E_M(\mathbf{r}) \quad (5)$$

for any vector $\mathbf{r}$, and in particular

$$\nabla E_M(\mathbf{r}_N)=2\sum W(\boldsymbol{\varepsilon}(\mathbf{X}+\mathbf{x}))^T\{(\boldsymbol{\varepsilon}(\mathbf{X}+\mathbf{x}))\mathbf{r}_N-(\mathbf{X}-\mathbf{x})\} \quad (6)$$

$$\nabla^2E_M(\mathbf{r}_N)=2\sum W(\boldsymbol{\varepsilon}(\mathbf{X}+\mathbf{x}))^T(\boldsymbol{\varepsilon}(\mathbf{X}+\mathbf{x}))\equiv 2\mathbf{A} \quad (7)$$

where $\mathbf{r}_N$ minimizes $E_N(\mathbf{r})$.

$\mathbf{A}$ is positive definite unless all vectors $(\mathbf{X}+\mathbf{x})$ are parallel, as can happen if the requisite rotation is 180°. Using equations (16), (17), (18), (23), (31) and (36) of (I) we obtain from (6)

$$\nabla E_M(\mathbf{r}_N)=2[E_N(\mathbf{r}_N)\mathbf{I}-\sum W(\mathbf{X}-\mathbf{x})(\mathbf{X}-\mathbf{x})^T]\mathbf{r}_N \equiv 2\mathbf{B}\mathbf{r}_N. \quad (8)$$

Since $\mathbf{R}_N\mathbf{r}_N=\mathbf{R}_N^T\mathbf{r}_N=\mathbf{r}_N$

$$\begin{aligned}\mathbf{r}_N^T\nabla E_M(\mathbf{r}_N)&=2\mathbf{r}_N^T[E_N(\mathbf{r}_N)\mathbf{I}\\&\quad-\sum W(\mathbf{X}-\mathbf{R}_N\mathbf{x})(\mathbf{X}^T-\mathbf{x}^T\mathbf{R}_N^T)]\mathbf{r}_N\\&=2\mathbf{r}_N^T[\sum W\mathbf{e}_N^T\mathbf{e}_N\mathbf{I}-\sum W\mathbf{e}_N\mathbf{e}_N^T]\mathbf{r}_N\\&=2\mathbf{r}_N^T[\sum W(\boldsymbol{\varepsilon}\mathbf{e}_N)^T(\boldsymbol{\varepsilon}\mathbf{e}_N)]\mathbf{r}_N\\&=2\sum W|\mathbf{r}_N\times\mathbf{e}_N|^2,\end{aligned} \quad (9)$$

in which $\mathbf{R}_N$ is the rotation matrix constructed from $\mathbf{r}_N$ and the $\mathbf{e}_N$ vectors are the residual vectors $\mathbf{X}-\mathbf{R}_N\mathbf{x}$. This vanishes if perfect fitting is possible, or if the initial orientation is optimal, or if every residual vector $\mathbf{e}_N$ is parallel to $\mathbf{r}_N$. Otherwise this quantity is positive which shows that E_M increases with increasing $|\mathbf{r}|$ in the vicinity of $\mathbf{r}_N$ and that therefore $\mathbf{r}_M$ underestimates the rotation angle with respect to the criterion E_N.

By similarly interposing $\mathbf{R}_N^T$ in the last factor in $\mathbf{B}$ and replacing $(\mathbf{X}-\mathbf{x})$ by $[\mathbf{X}-\mathbf{R}_N\mathbf{x}+(\mathbf{R}_N-\mathbf{I})\mathbf{x}]$ we find from (5), (7) and (8)

$$\mathbf{r}_M=\mathbf{r}_N-\mathbf{A}^{-1}\{\sum W[(\boldsymbol{\varepsilon}\mathbf{e}_N)^T(\boldsymbol{\varepsilon}\mathbf{e}_N)-(\mathbf{R}_N\mathbf{x}-\mathbf{x})\mathbf{e}_N^T]\}\mathbf{r}_N \quad (10)$$

which permits the calculation of $\mathbf{r}_M$ from $\mathbf{r}_N$ but not the reverse. The first term in the square bracket is positive semi-definite and the second contributes a vector in the plane $\perp\mathbf{r}_N$.

The vectors $\mathbf{r}_M$ and $\mathbf{r}_N$ specify the rotations to reach either superposition from the initial orientation of $\mathbf{x}$. If a corrective rotation $\mathbf{R}_C$ is required such that $\mathbf{R}_N=\mathbf{R}_C\mathbf{R}_M$ then the associated correction rotation vector is given by

$$\mathbf{r}_C=\frac{\mathbf{r}_N-\mathbf{r}_M-\mathbf{r}_N\times\mathbf{r}_M}{1+\mathbf{r}_N\cdot\mathbf{r}_M}. \quad (11)$$

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0108-7673/89/090657-01$03.00