equivalent to unconstrained refinement followed by judicious averaging – and we reject this as being of no advantage. Thus the efficacy of the C & D procedure rests on the difficulty of going from the constrained to the unconstrained result in one cycle; the more difficult this is the nearer the C & D procedure is to strict constraints. A rough guess for a value of $S$ would be in excess of 70%: the one cycle mentioned finds more than 70% of the total shift. With a value as high as this the usefulness of the C & D procedure is in grave doubt.

Table 1. *$R_w$ for pyrazole*

| | | $R_w$ |
|---|---|---|
| Constraint (*a*)* | best value | 254 |
| Constraint (*b*)* | after 1 cycle | 243 |
| | after 2 cycles | 241 |
| Unconstrained | after 1 cycle | 229 |
| | after 2 cycles | 228 |

* See Pawley (1972).

In all the cases in my experience this figure has been in excess of 70%. An example, the first to hand in my files, is given by pyrazole. The residual $R_w=\sum_{\mathbf{h}} w_{\mathbf{h}}(\Delta F_{\mathbf{h}})^2$ varied as in Table 1 where $R_w$ improved by $S=90\%$ in the first cycle after removing the constraints.

If their procedure is to be established as worthwhile, Chesick & Davidon should perform detailed calculations to compare the results of their method with the strictly constrained and the unconstrained results.

## References

CHESICK, J. P. & DAVIDON, W. C. (1975). *Acta Cryst.* A**31**, 586–591.

PAWLEY, G. S. (1972). *Advances in Structure Research by Diffraction Methods*, edited by W. HOPPE & R. MASON. Oxford: Pergamon Press.

*Acta Cryst.* (1976). A**32**, 922

## A solution for the best rotation to relate two sets of vectors.

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A simple procedure is derived which determines a best rotation of a given vector set into a second vector set by minimizing the weighted sum of squared deviations. The method is generalized for any given metric constraint on the transformation.

In various crystallographic situations the problem arises of finding a best rotation to fit a given atomic arrangement to approximately measured coordinates. Examples have been given by McLachlan (1972) and Diamond (1976). Diamond determines the best unconstrained transformation between the two sets of coordinates and factorizes it into a symmetric and an orthogonal matrix. McLachlan finds a best rotation between the two sets of coordinates by an iterative process. The analysis below shows that a direct solution is also possible, despite the non-linear character of the problem.

Let $\mathbf{x}_n$ and $\mathbf{y}_n$ $(n=1,2,\ldots,N)$ be two given vector sets and $w_n$ the weight corresponding to each pair $\mathbf{x}_n,\mathbf{y}_n$. The problem is then to find an orthogonal matrix $\mathsf{U}=(u_{ij})$ which minimizes the function

$$E=\tfrac{1}{2}\sum_n w_n(\mathsf{U}\mathbf{x}_n-\mathbf{y}_n)^2 \qquad (1)$$

subject to the constraints

$$\sum_k u_{ki}u_{kj}-\delta_{ij}=0 \qquad (2)$$

where the $\delta_{ij}$ are the elements of the unit matrix. A translation, if admitted, can always be removed from the problem by shifting the centroids of the vector sets to the origin.

Introducing a symmetric matrix $\mathsf{L}=(l_{ij})$ of Lagrange multipliers an auxiliary function (see, for example, Brand, 1958)

$$F=\tfrac{1}{2}\sum_{i,j} l_{ij}\Big(\sum_k u_{ki}u_{kj}-\delta_{ij}\Big) \qquad (3)$$

is constructed and added to $E$ to form the Lagrangian function

$$G=E+F. \qquad (4)$$

Since for each different condition (2) an independent number $l_{ij}$ is available, the constrained minimum of $E$ is now included among the free minima of $G$. A free minimum of $G$ can only occur where

$$\frac{\partial G}{\partial u_{ij}}=\sum_k u_{ik}\Big(\sum_n w_n x_{nk}x_{nj}+l_{kj}\Big)-\sum_n w_n y_{ni}x_{nj}=0 \qquad (5)$$

and

$$\frac{\partial^2 G}{\partial u_{mk}\partial u_{ij}}=\delta_{mi}\Big(\sum_n w_n x_{nk}x_{nj}+l_{kj}\Big) \qquad (6)$$

are the elements of a positive definite matrix. $x_{nk}$ and $y_{nk}$ are the $k$th components of the vectors $\mathbf{x}_n$ and $\mathbf{y}_n$.

Let

$$r_{ij}=\sum_n w_n y_{ni}x_{nj} \qquad (7)$$

and

$$s_{ij}=\sum_n w_n x_{ni}x_{nj} \qquad (8)$$

be the elements of a matrix $\mathsf{R}=(r_{ij})$ and a symmetric matrix $\mathsf{S}=(s_{ij})$, respectively. For $i=m=1$ from equation (6), a minimum of the Lagrangian function $G$ requires that $\mathsf{S}+\mathsf{L}$ is positive definite, and – by rewriting equation (5) – that

$$\mathsf{U}\,.\,(\mathsf{S}+\mathsf{L})=\mathsf{R}. \qquad (9)$$

The problem is now to find a symmetric matrix L of Lagrange multipliers such that U is orthogonal. If both sides of (9) are multiplied by their transposed matrices, the unknown orthogonal matrix U can be eliminated:

$$\mathsf{U}(\widetilde{\mathsf{S}+\mathsf{L}})\mathsf{U}(\mathsf{S}+\mathsf{L})=(\widetilde{\mathsf{S}+\mathsf{L}})\tilde{\mathsf{U}}\mathsf{U}(\mathsf{S}+\mathsf{L}) =(\mathsf{S}+\mathsf{L})(\mathsf{S}+\mathsf{L})=\tilde{\mathsf{R}}\mathsf{R}\,. \quad (10)$$

Since $\tilde{\mathsf{R}}\mathsf{R}$ is a symmetric positive definite matrix the positive eigenvalues $\mu_k$ and the corresponding eigenvectors $\mathbf{a}_k$ can be found by well established procedures. Since S+L is symmetric and positive definite also, it is evident from (10) that it must have the same normalized eigenvectors $\mathbf{a}_k$ and the positive eigenvalues $\sqrt{\mu_k}$.

It can be easily verified that the Lagrange multipliers are then

$$l_{ij}=\sum_k \sqrt{\mu_k}\quad a_{ki}a_{kj}-s_{ij} \quad (11)$$

where $a_{ki}$ denotes the $i$th component of $\mathbf{a}_k$. The effect of the orthogonal matrix U on these eigenvectors $\mathbf{a}_k$ is determined from (9) and defines unit vectors $\mathbf{b}_k$ as

$$\mathbf{b}_k=\mathsf{U}\,.\,\mathbf{a}_k=\frac{1}{\sqrt{\mu_k}}\,\mathsf{U}(\mathsf{S}+\mathsf{L})\mathbf{a}_k=\frac{1}{\sqrt{\mu_k}}\,\mathsf{R}\mathbf{a}_k\,. \quad (12)$$

The orthogonal matrix U is finally constructed as

$$u_{ij}=\sum_k b_{ki}a_{kj} \quad (13)$$

and the problem to find the constraint minimum of the function $E$ is solved.

Sometimes it may happen that all of the vectors $\mathbf{x}_n$ or $\mathbf{y}_n$ lie in a plane. Then one of the eigenvalues of $\tilde{\mathsf{R}}\mathsf{R}$, *e.g.* $\mu_3$, will be zero. In this case a complete set of vectors $\mathbf{a}_k, \mathbf{b}_k$ is constructed by setting

$$\mathbf{a}_3=\mathbf{a}_1\times\mathbf{a}_2 \qquad \mathbf{b}_3=\mathbf{b}_1\times\mathbf{b}_2\,. \quad (14)$$

Note that the procedure described in this article can be easily extended to vector spaces of higher dimensions.

It is possible also to replace the constraints of equation (2) by the more general constraints

$$\tilde{\mathsf{U}}\mathsf{U}=\mathsf{M}\,, \quad (15)$$

where M is a symmetric and positive definite matrix. If B is any specific solution of (15), it is easy to prove that all possible other solutions U of that equation can be written as

$$\mathsf{U}=\mathsf{V}\,.\,\mathsf{B} \quad (16)$$

with an orthogonal matrix V. If the initial vector set $\mathbf{x}_n$ is transformed into $\mathbf{x}'_n=\mathsf{B}\mathbf{x}_n$ then this problem is reduced to minimizing $E'=\frac{1}{2}\sum_n w_n(\mathsf{V}\mathbf{x}'_n-\mathbf{y}_n)^2$ with the constraint $\tilde{\mathsf{V}}\mathsf{V}=1$.

I would like to thank Dr K. C. Holmes for reading the manuscript.

### References

DIAMOND, R. (1976). *Acta Cryst.* A**32**, 1–10.
MCLACHLAN, A. D. (1972). *Acta Cryst.* A**28**, 656–657.
BRAND, L. (1958). *Advanced Calculus*, pp. 194–198. New York: John Wiley.

*Acta Cryst.* (1976). A**32**, 923

## A comment on the close-packing of hyperspheres.

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The packing of hyperspheres in more than three dimensions is discussed.

Lifchitz (1976) has drawn attention to a type of lattice packing for hyperspheres in which there is one hypersphere per unit cell (at the origin) and where the unit cell has a metric matrix in which the diagonal elements are 1 and all other elements are $\frac{1}{2}$. This matrix can be factorized into an upper triangular matrix and its transpose to obtain the orthonormal coordinates as required.

This packing is, however, except for dimensions 1, 2 and 3, by no means the closest packing of hyperspheres. The general solution remains unknown but the packing fraction for four-dimensional close-packing is $\pi^2/16=0{\cdot}61685$ and corresponds to a hypercubic cell centred at $(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})$ with 24 contacts per sphere. This is denser than the type of packing described by Lifchitz, which for four dimensions gives the value $\pi^2/(8\times 5^{1/2})=0{\cdot}55173$ for the packing fraction and 20 contacts per sphere. Leech (1964) has given a table of what, up to that date, were believed to be the closest packings in up to 12 dimensions. The packing fraction for 12 dimensions exceeded by a factor of more than 8 that for the Lifchitz type of packing, and there are 756 contacts per hypersphere as compared with 156.

The French words 'assemblage compact' might thus be better translated as 'close-ish packing' rather than as 'close-packing'.

### References

LEECH, J. (1964). *Canad. J. Math.* **16**, 657–682.
LIFCHITZ, A. (1976). *Acta Cryst.* A**32**, 50–53.