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Scaling a set of intersecting reciprocal-lattice planes. By J. Kraut,*, *Department of Biochemistry, University of Washington, Seattle, U.S.A.*

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In the course of a current investigation of crystalline proteins very low-order three-dimensional intensity data were collected using the Buerger precession camera. This was done by taking nine different zero-level reciprocal-lattice planes which did not all intersect in a common row of reflections. For this reason, and since the number of moderately strong reflections in the most populous intersection did not exceed five, it seemed desirable to place all of the intensities on the same scale by a somewhat more systematic procedure than those which may come immediately to mind. At least such a method would have the advantage of producing the same results in the hands of different crystallographers. The procedure finally adopted may be of some interest to crystallographers in general and is therefore described here separately.

Begin by considering the ith and jth out of the total of n reciprocal-lattice planes, the intensities of the reflections in each being on an arbitrary scale which varies from plane to plane. Assume that one has computed the ratio of intensities for each pair of reflections common to the two planes, and has then averaged these ratios. Define r_{ij} as the average ratio so obtained over all the reflections in the intersection, that is

$$r_{ij} = \left\langle \frac{I_j(hkl)}{I_i(hkl)} \right\rangle_{\text{av.}} . \qquad (1)$$

In general r_{ij} is not equal to r_{ji}^{-1}.

Now denote the scaling constants being sought by k_i. In the absence of errors of measurement one would have simply $k_i/k_j = r_{ij}$. But in practice the best that can be achieved is to obtain a set of k_i which minimizes the deviations of the k_i/k_j from the experimentally estimated r_{ij}. The rest of this communication is devoted to demonstrating that such a set of k_i can be found by taking

$$k_i = \left[\prod_{j=1}^{n} \left(\frac{r_{ij} r_{jn}}{r_{ji} r_{nj}} \right) \right]^{\frac{1}{2n}} \qquad (2)$$

for which, of course, $k_n = 1$, i.e. all the other planes are being put on the same scale as the nth.

Instead of dealing directly with the quantities r_{ij} and k_i we choose rather to consider their logarithms, greatly simplifying the problem at hand. The function to be minimized, then, is

$$F(k_i, r_{ij}) = \sum_{i,j=1}^{n} \left(\log \frac{k_i}{k_j} - \log r_{ij} \right)^2 . \qquad (3)$$

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Note that if, as is usual, r_{ij} and hence k_i/k_j do not differ much from unity this is practically the customary sum of the squares of deviations.

For brevity, we introduce the two new symbols $l_i = \log k_i$ and $a_{ij} = \log r_{ij}$ and rewrite (3) as

$$F(l_i, a_{ij}) = \sum_{i,j=1}^{n} (l_i - l_j - a_{ij})^2 . \qquad (4)$$

Taking partial derivatives with respect to the l_i and equating to zero, one obtains

$$\sum_{j=1}^{n} [l_i - l_j - b_{ij}] = 0 , \quad i = 1, 2, \ldots, n \qquad (5)$$

where $b_{ij} = (a_{ij} - a_{ji})/2$ has been introduced. By summing both sides of all n such equations it is seen that they are linearly dependent. It is permissible therefore to assign the value of zero to l_n (i.e. to take $k_n = 1$) and to solve the first $n-1$ equations for the $n-1$ remaining l_i. This set of equations may be written in matrix notation

$$\begin{bmatrix} (n-1) & -1 & \ldots & -1 \\ -1 & (n-1) & \ldots & -1 \\ \vdots & \vdots & & \vdots \\ -1 & -1 & \ldots & (n-1) \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ \vdots \\ l_{n-1} \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \\ \vdots \\ B_{n-1} \end{bmatrix} \qquad (6)$$

or more briefly as

$$\mathbf{Ml} = \mathbf{B} . \qquad (6')$$

Here B_i has been written for $\sum_{j=1}^{n} b_{ij}$. By inspection one finds that the inverse of matrix $\mathbf{M}$ is

$$\mathbf{M}^{-1} = \frac{1}{n} \begin{bmatrix} 2 & 1 & \ldots & 1 \\ 1 & 2 & \ldots & 1 \\ \vdots & \vdots & & \vdots \\ 1 & 1 & \ldots & 2 \end{bmatrix} \qquad (7)$$

that is, the $n-1$ by $n-1$ matrix with $2/n$ on the diagonal and $1/n$ elsewhere. The solution of (6′) is therefore

$$\mathbf{l} = \mathbf{M}^{-1}\mathbf{B} . \qquad (8)$$

Upon writing out in full the expression for any l_i and using the fact that $\sum_{j=1}^{n} B_j = 0$, it is found that

$$l_i = \frac{1}{n} \sum_{j=1}^{n} (b_{ij} - b_{nj}) , \qquad (9)$$

which may be converted, upon taking antilogarithms, into equation (2) as desired.