SHORT COMMUNICATIONS

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Full-matrix inversion procedure for minimum-variance Fourier coefficient (MVFC) refinement.

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Abstract

A fast matrix inversion procedure is suggested for matrices containing a large diagonal block as is the case in minimum-variance Fourier coefficient refinement.

Since the MVFC refinement procedure was introduced by Sygusch (1977, 1985), it has been widely accepted as a powerful phase refinement tool for the isomorphous replacement method. However, for most applications, the cross terms of the least-squares normal matrix relating phases and heavy-atom parameters are ignored to avoid the high computational cost of inverting a huge matrix, thus compromising the rate of convergence and the accuracy in phase error estimation. The fact is that a full-matrix inversion can be a cost-effective and viable approach, if one takes advantage of the special property of the normal matrix. Here, we propose an alternative algorithm for this matrix inversion problem, which is also applicable to other cases where similar types of matrices are encountered, such as scaling and absorption corrections for area detector data (He & Carter, 1988).

First let us give an anatomy for the problem at hand. The least-squares normal matrix for the MVFC procedure usually takes the form

$$\mathbf{A}=\begin{pmatrix}\mathbf{A}_{mm} & \mathbf{A}_{mn}\\ \mathbf{A}_{nm} & \mathbf{A}_{nn}\end{pmatrix},$$

where m is the number of reflections to be phased, n is the number of heavy-atom parameters (usually $m \gg n$), $\mathbf{A}_{mm}$ is a diagonal square matrix of order m, $\mathbf{A}_{nn}$ is a full or block-diagonal square matrix of order n, and $\mathbf{A}_{mn}$ ($=\mathbf{A}_{nm}^T$; superscript T represents transpose) is a rectangular matrix of order m by n, the elements of which are the cross terms relating phases and heavy-atom parameters and are usually ignored in the matrix inversion procedure. If we take a closer look at the fact that $\mathbf{A}_{mm}$ is diagonal, and hence its inverse is also a diagonal matrix with elements equal to the reciprocal of the corresponding elements in the original matrix, the problem becomes much easier to tackle.

Let us denote the inverse of $\mathbf{A}$ as $\mathbf{X}$ and partition it accordingly.

$$\mathbf{X}=\begin{pmatrix}\mathbf{X}_{mm} & \mathbf{X}_{mn}\\ \mathbf{X}_{nm} & \mathbf{X}_{nn}\end{pmatrix}.$$

Since $\mathbf{AX}=\mathbf{I}$, we have

$$\mathbf{A}_{mm}\mathbf{X}_{mn}+\mathbf{A}_{mn}\mathbf{X}_{nn}=\mathbf{0} \quad (1)$$

$$\mathbf{A}_{mm}\mathbf{X}_{mm}+\mathbf{A}_{mn}\mathbf{X}_{nm}=\mathbf{I} \quad (2)$$

$$\mathbf{A}_{nm}\mathbf{X}_{mn}+\mathbf{A}_{nn}\mathbf{X}_{nn}=\mathbf{I} \quad (3)$$

where $\mathbf{0}$ is a null matrix and $\mathbf{I}$ is the identity matrix. Solve (1) for $\mathbf{X}_{mn}$ by multiplying by $(\mathbf{A}_{mm})^{-1}$ (note: not to be confused with $\mathbf{X}_{mm}$!), leading to

$$\mathbf{X}_{mn}=-(\mathbf{A}_{mm})^{-1}\mathbf{A}_{mn}\mathbf{X}_{nn}. \quad (4)$$

Substituting (4) into (3) and solving for $\mathbf{X}_{nn}$, one gets

$$\mathbf{X}_{nn}=[\mathbf{A}_{nn}-\mathbf{A}_{nm}(\mathbf{A}_{mm})^{-1}\mathbf{A}_{mn}]^{-1}. \quad (5)$$

Solving (2) for $\mathbf{X}_{mm}$, one gets directly

$$\mathbf{X}_{mm}=(\mathbf{A}_{mm})^{-1}(\mathbf{I}-\mathbf{A}_{mn}\mathbf{X}_{nm}). \quad (6)$$

With these relationships we can invert the matrix $\mathbf{A}$ in three steps: (i) calculate $\mathbf{X}_{nn}$ using (5) through matrix inversion, which is trivial for a small matrix; (ii) calculate $\mathbf{X}_{mn}$ using (4); (iii) calculate $\mathbf{X}_{mm}$ using (6).

At this point, the full-matrix inversion of $\mathbf{A}$ is achieved.

References

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