Note added in proof: Dr T. Matsumoto (personal communication) has pointed out to us that some of the cases presented in Tables 2 and 3 do not hold as enhancement cases for pairs of geometrically and chemically identical substructures. It is still possible to obtain enhancement in some of those cases by combining more than two geometrically and chemically identical substructures, but, in any case, all the cases tabulated in this paper hold as enhancement cases in the more general instance of chemically different ('proportional') substructures.

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Some Information-Theory Aspects of Structure Determination

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The iterative procedure of phase determination in direct methods is considered as a filtering process. The use of different filter transforms for more effective filtering is proposed. The eigenvector transform for optimal extraction of reliable structure information from approximate densities is introduced.

1. Introduction

Since the first papers on direct methods for structure determination (Karle & Hauptman, 1950; Sayre, 1952) it was apparent that these methods were related to the *a priori* information present in the atomic arrangement and the electron density of the structure in question. The principles of positivity and atomicity together with the observed structure-factor amplitudes enabled the solution of structures of considerable complexity. Until then, the normal method of structure determination, the heavy-atom method or the more general partial-structure method, also used the atomicity principle but in a different way. The positioning of the heavy atom or partial structure and the consequent phasing of structure factors is of quite specific character and only pertains to the structure in question. However, the determination of the missing structure part by weighting the structure-factor amplitudes also relies on quite general principles and involves statistical considerations.

In contrast, the *a priori* information of direct methods is in most cases of an entirely general, statistical character. The natural way to estimate and measure the amount of information present in these principles is by information theory. In the following some information-theory aspects are used to derive results for both heavy-atom and direct methods to indicate their similarity. Furthermore the treatment is given of a special problem in structure determination as seen from information theory.

2. Structure determination as image filtering

X-ray structure determination can be considered as an imaging of an object (structure) where the Fourier transformation in the nonexistent X-ray lens is replaced by a calculated Fourier transformation to which the principles of optical image formation can be applied. Of special concern in this context is the separation of object and noise in an image.

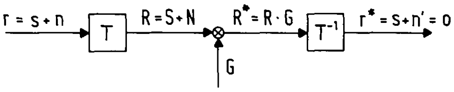

Fig. 1. Generalized Wiener filtering.

(*a*) *Spectral filtering*

The typical filtering process of noisy images is shown in Fig. 1. The object s and the noise n compose the total input $r(x)=s(x)+n(x)$ which is subjected to the transformation $\mathbf{T}$, then corrected by the filter $\mathbf{G}$ and transformed back by the transformation $\mathbf{T}^{-1}$ to give a filtered output $o(x)=s(x)+n'(x)$ with a reduced noise component $n'(x)$. Applying the quadratic measure of Wiener filtering one obtains (see, for example, Gallagher & Liu, 1975) an optimal filter as:

$$\langle|o-s|^2\rangle=\int|o-s|^2\mathrm{d}V=\text{minimum} \qquad (1)$$

$$\mathbf{G}(\boldsymbol{\omega})=\frac{\Phi_{rs}(\boldsymbol{\omega})}{\Phi_{rr}(\boldsymbol{\omega})}\,; \qquad (2)$$

where Φ_{rs} is the cross-spectral density between input r and objects s, whereas Φ_{rr} is the spectral density of the input r. The expressions Φ_{rs} and Φ_{rr} are calculated by the Fourier transformations

$$\Phi_{rs}(\boldsymbol{\omega})=\mathscr{F}\left\{\int r(\mathbf{x})*s(\mathbf{x})\mathrm{d}V\right\} \qquad (3a)$$

$$\Phi_{rr}(\boldsymbol{\omega})=\mathscr{F}\left\{\int r(\mathbf{x})*r(\mathbf{x})\mathrm{d}V\right\} \qquad (3b)$$

where the sign $*$ indicates a convolution and $\boldsymbol{\omega}$ is the spectral frequency.

Rewriting the procedure of Fig. 1 in crystallographic terms one obtains the following (Fig. 2). The input consists of the partial structure information $\varrho_p(\mathbf{x})$ considered as the total density $\varrho(\mathbf{x})$ with additional noise density $\varrho_n(\mathbf{x})$. After Fourier transformation one obtains the complex structure factor $\mathbf{F}^p_h=\mathscr{F}\{\varrho_p\}$ which is filtered with a function $\mathbf{G}_h$ after (2) to obtain an improved density $\varrho^*(\mathbf{x})$:

$$\varrho^*=\mathscr{F}^{-1}\{\mathbf{G}_h\,.\,\mathbf{F}^p_h\}\,.$$

The filter $\mathbf{G}_h$ is given by

$$\mathbf{G}_h=\frac{\Phi_{\varrho_p\varrho}(\mathbf{h})}{\Phi_{\varrho_p\varrho_p}(\mathbf{h})}\,. \qquad (2a)$$

The denominator $\Phi_{\varrho_p\varrho_p}$ is just the Patterson coefficient for the reciprocal vector $\mathbf{h}$:

$$\Phi_{\varrho_p\varrho_p}(\mathbf{h})=\mathscr{F}\left\{\int\varrho_p*\varrho_p\mathrm{d}V\right\}=|F^p_h|^2\,. \qquad (3b')$$

The numerator $\Phi_{\varrho_p\varrho}$ of (2*a*) is calculated as:

$$\begin{aligned}\Phi_{\varrho_p\varrho}(\mathbf{h})&=\mathscr{F}\left\{\int\varrho_p*\varrho\mathrm{d}V\right\}\\&=\mathbf{F}^p_h\,.\,\mathbf{F}_{-h}=F^p_hF_h\exp i(\alpha^p_h-\alpha_h)\,. \qquad (3a')\end{aligned}$$

The amplitudes F_h and F^p_h are given by observed and calculated values respectively. Only the phase factor has to be determined. Assuming a Gaussian distribution of $\mathbf{F}_h$ around $\mathbf{F}^p_h$ (Fig. 3) and taking the expectation value one obtains (Cochran, 1955):

$$\begin{aligned}\langle\exp i(\alpha^p_h-\alpha_h)\rangle&=\langle\cos(\alpha_h-\alpha^p_h)\rangle\\&=\langle\cos\Delta\alpha_h\rangle=\frac{I_1(X_h)}{I_0(X_h)}\,;\end{aligned}$$

$$X_h=\frac{2F_hF^p_h}{|F^n_h|^2}\,.$$

The total weighting factor is then given by:

$$G_h=\frac{F^p_hF_h}{|F^p_h|^2}\,\frac{I_1(X_h)}{I_0(X_h)}\,. \qquad (2b)$$

The filtered Fourier coefficient $\mathbf{R}^*_h$ becomes

$$\mathbf{R}^*_h=\frac{F_h}{F^p_h}\,\frac{I_1(X_h)}{I_0(X_h)}\,\mathbf{F}^p_h=\frac{I_1(X_h)}{I_0(X_h)}\,F_h\exp(i\alpha^p_h)\,. \qquad (4)$$

This is the optimal weighting of a partial-structure Fourier synthesis and is well known in crystallography (Sim, 1960; Woolfson, 1956). It is based on a purely statistical relation between the partial and the final structure and under the above assumptions reaches the best signal-to-noise ratio of all weighting schemes (Gassmann, 1966; Nixon & North, 1976).

(*b*) *Spatial filtering*

An optimal filtering of the above type in direct space is not directly possible, since, for a certain location $\mathbf{x}$, no specific or statistical property of $\varrho(\mathbf{x})$ is known. Only the general properties of ϱ at all locations $\mathbf{x}$ (positivity, atomicity, *etc.*) can be assumed to be known.

The filtering to be applied must therefore rely on these properties, so it would be more appropriate to call this a statistical or *a priori* filter. Starting from the optimal filter condition

$$\langle(\varrho-\varrho^*)^2\rangle=\int(\varrho-\varrho^*)^2\mathrm{d}V=\text{minimum}$$

and the positivity condition

$$1\geq\varrho,\varrho^*\geq0$$

where ϱ^* is the filtered density, one can formulate general conditions which have to be met by the filtering process (Gassmann, 1976*a*).

In many structure determinations the only available indication for the behaviour of the final density ϱ is the given initial density ϱ_p. The filtering factor g in these cases must therefore depend on this initial density: $g=g(\varrho_p)$. The filtering process as indicated in Fig. 4 is equivalent to the iterative procedure of direct methods in structure determination (Gassmann, 1976*b*).

Comparison with the normal filtering of Figs. 1 and 2 shows, however, that there are essential differences. First, knowledge of the structure factor amplitudes F^{obs}_h allows iterative filtering. The Fourier coefficients $\mathbf{F}^*_h$ of the filtered density ϱ^* combined with these values

$F_h^{\rm obs}$ result in new initial structure factors $\mathbf{F}_h^p$, which can be used as new input to the filtering process.

Second, the spatially filtered structure factors $\mathbf{F}_h^*$, or rather their phases φ_h^*, are not taken directly to calculate the new input density in combination with the observed structure factor amplitudes. According to the above derivations it would be optimal to filter structure factors $\mathbf{F}_h^*$ according to (4). However, the spectral noise density $|F_h^n|^2$ of a modified density is not known in general. This is in contrast to the partial-structure method where this spectral noise density can be taken as $|F_h^n|^2 = \sum\limits_{j=1}^{L} f_j^2(h)$ (L=number of unknown atoms, f_j=atomic form factor). Therefore, one approximates the spectral noise density by the average total spectral density $|F_h^n|^2 = \sum\limits_{j=1}^{N} f_j^2(h)$ (N=total number of atoms), which certainly for the initial iteration cycles is a very good approximation, and obtains:

$$X_h = \frac{2F_h^* F_h^{\rm obs}}{\sum\limits_{j=1}^{N} f_j^2} = 2E_h^* E_h^{\rm obs}$$

(E=normalized structure factor) and a filtered coefficient $\mathbf{R}_h^*$ as:

$$\mathbf{R}_h^* = \frac{I_1(X_h)}{I_0(X_h)} F_h^{\rm obs} \exp{(i\varphi_h^*)}\,. \tag{4a}$$

The values $\mathbf{R}_h^*$ are used as new input $\mathbf{F}_h^p$ to calculate a new density.

The values of $\mathbf{F}_h^*$ (or $\mathbf{E}_h^*$) must be scaled appropriately to form a vector triangle with $\mathbf{F}_h$ and $\mathbf{F}_h^n$ according to Fig. 3. Consequently, if $\mathbf{E}_h^*$ is expressed as convolution products of $\mathbf{E}_h$ this introduces powers of $\sqrt{N}$ into the expression for the value X_h (Gassmann, 1975).

Usually, (4a) is not applied strictly. Only those phases ϱ_h^* whose structure factors $\mathbf{E}_h^*$ form the largest products $X_h = 2E_h^* E_h^{\rm obs} >$ limit are accepted as iterative input.

Third, the iterative procedure of Fig. 4 is impossible with the spectral filtering of Fig. 2 where the statistical information leads only to a scalar weighting or filtering. In that case each spectral component $\mathbf{F}_h^p$ is weighted only individually in amplitude and not in phase [see (4)]. Therefore, spatial filtering of density, *i.e.* direct methods of structure determination by vector filtering of the input, alone permit the use of iterative procedures which incorporate the measured amplitudes $F_h^{\rm obs}$.

Furthermore, the known amplitudes $F_h^{\rm obs}$ contain information about the total density ϱ. This is important for the convergence of the iterative process. Rewriting the density ϱ as a sum of atomic densities

$$\varrho(\mathbf{x}) = \sum_{j=1}^{N} \varrho_j(\mathbf{x})$$

where

$$\int \varrho_j \varrho_k \mathrm{d}V \sim \delta_{jk}$$

one can show from very general mathematical principles (Zurmühl, 1964) that, starting with any initial density ϱ_p which contains information (possibly incomplete) about all ϱ_j, the correct density ϱ can be obtained by iterations with an appropriately chosen filter factor g. This ensures that the total density can in principle be recovered from the initial density.

Lastly, the filter factor g at a certain space point $\mathbf{x}$ must not only depend on the density at this space point $\varrho(\mathbf{x})$, but can also take into account the density in the whole unit cell and the specific properties and constraints known about the structure. Typical examples of such constraints are atomic distances, molecular compounds, empty or solvent regions and non-crystallographic symmetries.

(*c*) *Matched filtering*

To obtain the initial phases for spectral filtering in reciprocal space from heavy-atom or partial-structure

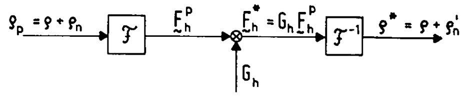

Fig. 2. Optimal filtering in reciprocal space for structure determination. Each spectral component is multiplied by a scalar filtering factor G_h.

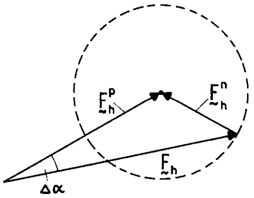

Fig. 3. Decomposition of the input structure factor $\mathbf{F}_h^p$ into the 'signal' structure factor $\mathbf{F}_h$ and the 'noise' structure factor $\mathbf{F}_h^n$. For calculation of the spectral filtering factor a Gaussian distribution of $\mathbf{F}_h$ around $\mathbf{F}_h^p$ is assumed.

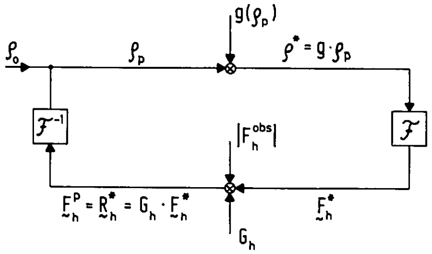

Fig. 4. Iterative procedure of direct methods. The input density ϱ_p is spatially filtered to represent better the final density. The resulting Fourier coefficients F_h^* are spectrally filtered to optimize the contributions $\mathbf{R}_h^* = G_h \mathbf{F}_h^* = [I_1(X_h)/I_0(X_h)] F_h^{\rm obs} \exp{(i\varphi_h^*)}$ to form a new input density.

positions one normally has to use Patterson search techniques. There exists a strong correspondence between the rotation and translation search procedures in structure determination (for chronological references see Karle, 1972) and matched filtering (see for example, Turin, 1960; van der Lugt, 1964). These search techniques are a generalization of matched filtering for an arbitrarily oriented and situated signal. The information comparison or matching is done between the convolution product of the total signal (Patterson function) $\sigma^{\rm Patt}=\varrho*\varrho$ and the convolution product of the known signal form (convolution molecule) $\sigma^{\rm conv}=\varrho_p*\varrho_p$, or their respective Fourier coefficients. If one requires that the information content of the given $\sigma^{\rm Patt}$ about the correct position of $\sigma^{\rm conv}$ is not to be decreased by a filter operation, the correlation function

$$\int \sigma^{\rm Patt}\sigma^{\rm conv}(\boldsymbol{\theta},\mathbf{t}){\rm d}V=K(\boldsymbol{\theta},\mathbf{t}) \tag{5}$$

must be a maximum (see, for example, Woodward, 1953) with respect to the rotation parameters $\boldsymbol{\theta}$ and the translation parameters $\mathbf{t}$. Rewriting (5) one obtains the representation in reciprocal space:

$$\sum_h |F_h|^2|F_h^{\varrho}(\boldsymbol{\theta},\mathbf{t})|^2=K(\boldsymbol{\theta},\mathbf{t}) \rightarrow K_1(\boldsymbol{\theta})K_2(\mathbf{t})\,. \tag{5a}$$

The separation of the rotation and translation dependency of this cross-correlation allows the successive rotation and translation operations to be determined.

3. Information content of crystal structures

As a crystal structure may be regarded as being defined by the atomic locations one can ask what amount of information is present in such a representation, and what is the best coding of this information. This coding will be shown to be of importance for evaluating the minimum number of free parameters necessary to determine a structure.

Subdividing an elementary cell into M small units which may contain an atom or be empty, one obtains a bit representation of this structure. The N units (N=atoms per unit cell) containing an atom are labelled '1'; the rest are labelled '0', so a sequence of the M bits codes the structure information. Thus, for an orthogonal unit cell, say, of volume V Å^3 and a subunit length of $1/m$ Å the number of bits would be very large, namely of the order $M=Vm^3$ bits.

As a result of the sparse distribution of atoms in the subunits, it is obvious that the normal coding with atomic coordinates is much more compact. One atom needs for location determination with the above assumed subdivision $A_1+A_2+A_3$ bits, where A_i is at least the next power of two larger than ma_i (a_i=unit-cell dimension). The total structure is then given by $(A_1+A_2+A_3)N$ bits. To find the optimal coding one must calculate the information entropy of the structure. This is given by (Shannon, 1949):

$$H=-\varepsilon\log_2\varepsilon-(1-\varepsilon)\log_2(1-\varepsilon) \tag{7}$$

where ε is the probability of finding an atom indication in one of the subdivision units. For small ε this is rewritten as:

$$H\simeq\varepsilon(1-\log_2\varepsilon);\quad \varepsilon=\frac{N}{M}=\frac{N}{Vm^3}\ll 1\,. \tag{7a}$$

The value ε is proportional to $N/V=k$ which is approximately constant ($1/k\simeq 20$ Å^3 atom^{-1}). For example, a subdivision length of $1/m=(\frac{1}{4}$ Å) along each unit-cell dimension would result in

$$\varepsilon=\frac{N}{V}\tfrac{1}{64}\simeq 10^{-3}\,.$$

Insertion of the value for ε in (7a) leads to:

$$H=\frac{N}{V}\frac{1}{m^3}\left(1-\log_2\frac{N}{Vm^3}\right)$$
$$=\frac{k}{m^3}(1+3\log_2 m-\log_2 k) \tag{7b}$$

which only depends on the subunit division m. The optimal coding, *i.e.* the minimal number of bits required for this information is given by:

$$B=HM=N(1+3\log_2 m-\log_2 k)\,. \tag{8}$$

The minimal number of coding bits per atom is

$$b=\frac{B}{N}=\left(1-\log_2\frac{N}{M}\right)=(1+3\log_2 m-\log_2 k) \tag{8a}$$

independent of the structure size, whereas coordinate coding, for example, increases with the unit-cell size.

A typical example with assumed unit-cell dimensions $a_i=16$ Å ($i=1,2,3$) and a subdivision of $1/m=\frac{1}{4}$ Å indicates the different orders of magnitude for the coding of an atom:

subunit coding:

$$b=\frac{M}{N}=\frac{Vm^3}{N}=\frac{m^3}{k}\simeq 10^3 \text{ bits};$$

coordinate coding:

$$b=A_1+A_2+A_3=18 \text{ bits};$$

minimal coding:

$$b=(1+3\log_2 m-\log_2 k)\simeq 11 \text{ bits}\,.$$

It should be pointed out that this minimal coding does not take into account further, Markov-type knowledge such as interatomic distances, which would lower the entropy still further.

How is structural information coded by Fourier coefficients in reciprocal space? As in coordinate coding $A_1+A_2+A_3-3$ bits are needed to give the re-

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† Heavy atoms could be coded as multiple normal atoms at the same location. The number N must then be changed appropriately.

flexion index $\mathbf{h}$. In addition the complex structure factor must be coded, and if a sufficient accuracy is to be achieved, a normalized structure factor can be coded by four bits for the amplitude and eight bits for the phase information in the acentric case. In the centric case, however, only 1 bit for sign information is needed.

From our own experience and that of others (see, for example, Lessinger, 1976) one knows that the order of $5N$ to $10N$ reflexions is necessary to represent atomic positions in a crystal structure unambiguously. Coding by Fourier coefficients in reciprocal space is, therefore, less compact than coding for atomic coordinates in real space.

This influences the relative effectiveness of different filtering procedures. A better, more concise coding contains less redundant information and has more effect on a filtering operation. Consequently real-space filtering should be more effective than reciprocal-space spectral filtering. On the other hand, one must prevent noise enhancement in the more effective filtering procedure. In spatial filtering of crystal structures quite arbitrary filters are possible. One form of filtering often used is clipping of density (Kartha, 1969; Hoppe, Gassmann & Zechmeister, 1970; Barrett & Zwick, 1971; Collins, 1975; Nixon & North, 1976) which, unfortunately, may lead to considerable aliasing and wrong phase and structure indications, which are not always correctable by the inclusion of the known structure-factor amplitudes.

4. Image filtering by unitary transformations

As indicated by the general principle of filtering (Fig. 1) this process can be implemented by any unitary transform $\mathbf{T}$. The use of the Fourier transform $\mathbf{T}=\mathcal{F}$ in structure determination (Figs. 2 and 4) has great advantages, since the experimentally determined structure-factor amplitudes $|F_h|$ immediately give the spectral power density. Nevertheless, the relatively inefficient coding of structure information by Fourier components raises the question of effecting a more compact coding by other transforms. So, for example, the Walsh or Haar transforms seem to be candidates because of the form of their eigenfunctions which approaches better atomic densities and the coding of the atomic coordinates discussed above.

However, the difficult sequency problem (see, for example, Beauchamp, 1975) must be taken into account. An intermediate solution of this could be the combination of Fourier components approaching the eigenfunctions of these transforms.

Another filter transform which enables quite general information filtering and compression is the eigenvector transformation (sometimes called principal component, Hotelling, or Karhunen–Loève transform).

The principles of the eigenvector transform can be described as follows. A given set of n incomplete or noisy images $\boldsymbol{\varrho}=(\varrho_1,\varrho_2,\ldots\varrho_n)$ is to be combined in an optimal way to result in another set of images $\boldsymbol{\varrho}^*=(\varrho^*_1,\varrho^*_2,\ldots\varrho^*_n)$ where ϱ^*_1 contains the maximum of reliable information. In matrix form this transformation reads:

$$\boldsymbol{\varrho}^*=\mathbf{A}(\boldsymbol{\varrho}-\langle\boldsymbol{\varrho}\rangle)\,, \tag{9}$$

where $\langle\boldsymbol{\varrho}\rangle$ is the average value of the known structural content of the image set. The $n\times n$-matrix $\mathbf{A}$ is calculated from the covariance matrix $\mathbf{c}=||c_{ij}||$ where

$$c_{ij}=\langle(\varrho_i-\langle\varrho_i\rangle)\,(\varrho_j-\langle\varrho_j\rangle)\rangle\,. \tag{10}$$

The relative magnitudes of the eigenvalues λ_k as solutions of

$$||\mathbf{c}-\boldsymbol{\lambda}||=0\,; \tag{11}$$

indicate the information content of the successive component images ϱ^*_k. The normalized eigenvectors are the rows of the transformation matrix $\mathbf{A}$.

An immediate application of this transform in crystal structure determination is apparent. In direct methods of structure determination starting with different initial phase sets or different symbolic or numerical phase values a number of densities may be obtained which exhibit only incomplete pictures of the atomic positions. Often the orientation of a molecular partial structure is correct but the translation parameters have to be found from a translation search (Karle, 1972). The elements of the correlation matrix are calculated as:

$$c_{ij}=\langle\varrho_i\varrho_j\rangle=\sum_h \mathbf{F}^i_h\mathbf{F}^j_{-h} \tag{10a}$$

because the F_o term is not normally included. If a partial structure is known, $\langle\varrho_k\rangle\neq0$ and can be included in the calculation. Since the density in an equal-atom structure is limited to $0\leq\varrho\leq1$ it can also be of advantage to restrict the variance calculation of (10) to this range. Thereby one eliminates those images which show one or a few abnormally high peaks above the upper density limit $\varrho=1$, but little further structure details. Even more complicated and structure-dependent covariance definitions are possible.

The solution of the eigenvalue equation (11) leads

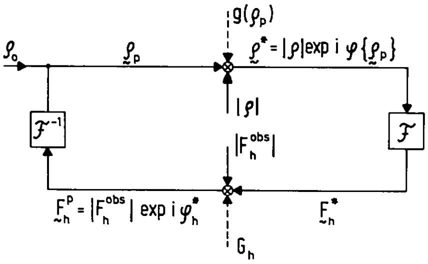

Fig. 5. Phase determination in electron microscopy. Instead of weighting the density ϱ_p and the Fourier coefficients $\mathbf{F}^*_h$, the known amplitudes of both the complex density and the Fourier coefficients are inserted as 'filter'. An additional weighting of the density and the Fourier coefficients corresponding to the *a priori* knowledge about the object would also be possible.

to the eigenvalues and the eigenvectors, from which the transformation matrix **A** is found.

The consequence of this procedure is, that by simple coherent addition of images one does not obtain optimal information extraction. This is only accomplished by superposition according to (9).

This superposition is of even greater importance for three-dimensional structure determination in electron microscopy (Hoppe, Schramm, Sturm, Hunsmann & Gassmann, 1976). Because of experimental limitations, radiation-damaged density projections of different quality have to be combined. Furthermore, individual structural objects reconstructed from different experimental data must be superposed to increase the incomplete information of a single three-dimensional image.

5. Conclusion

The ideas and procedures for image filtering in crystallographic structure determination have developed relatively independently from related fields. There exists however a large amount of work on optimal filtering, generalized filter transforms, pattern recognition and feature extraction.

For example, in electron microscopy a procedure quite similar to the iterative procedure of direct methods has been proposed (Gerchberg & Saxton, 1972). The only difference, compared with the process of Fig. 4, consists of the assumed knowledge of the amplitude of the complex density in real space (Fig. 5). Starting with arbitrary phases the convergence to the correct phases under these assumptions has been investigated (Schiske, 1974, 1975; Huiser, Drenth & Ferwerda, 1976). Generalized transforms have also been considered in electron microscopy (Hawkes, 1974) and in signal processing (see, for example, Pratt, 1972), whereas the eigenvector transformation has been used for optical pattern recognition and feature extraction (see, for example, Foley & Sammon, 1975; Therrien, 1975).

A careful analysis of these and similar ideas might show further relevance for structure determination.

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