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A Criterion to Evaluate Three Dimensional Reconstructions from Projections of Unknown Structures

MARCELLO BARBIERI

Max-Planck-Institut für Molekulare Genetik
1 Berlin 33 (Dahlem), Ihnestrasse 63–73, Germany

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A criterion is proposed to evaluate visually and quantitatively the three-dimensional reconstructions performed by non-linear algorithms from the projections of unknown structures.

Utilizing the informational content of this criterion the structure of an existing algorithm is modified and its performance is improved.

1. Introduction

The recent discoveries of algorithms for three dimensional reconstructions from projections (Cormack, 1963; De Rosier & Klug, 1968; Crowther, De Rosier & Klug, 1970; Vainshtein, 1970; Gordon, Bender & Herman, 1970; Berry & Gibbs, 1970; Ramachandran & Lakshminarayanan, 1971; Goitein, 1971; Matulka & Collins, 1971; Gilbert, 1972; Cormack, 1973; Sweeney & Vest, 1973; Smith, Peters & Bates, 1973) are of great interest to biologists because of the possibility of applying them to reconstruct three-dimensional structures from electron micrographs and radiographs. However, it has been shown that when the number of projections is limited the reconstruction problem is intrinsically indetermined (Frieder & Herman, 1971). In addition it has been realized that the actual processing of real data introduces anisotropy, erroneous contrast and noise amplification, which produces further elements of uncertainty (Goodman, 1968; De Rosier, 1970; Bellman, Bender, Gordon & Rowe, 1971; Herman, Lent & Rowland, 1973). Given this situation it is extremely important to have a quantitative criterion to evaluate *a posteriori* the reconstruction itself.

Gordon *et al.* (1970) propose as a criterion the δ-measure and, regarding the statement of Crowther & Klug (1971) that "δ is not a good measure because it reaches a low value once the large scale features are correct and it is relatively insensitive to errors in fine details", Frieder & Herman (1971) reply showing the contrary, i.e. that "δ is very sensible to fine details", Moreover, Frieder & Herman (1971) have shown that the choice of the δ-measure, being equivalent to the mean square error criterion so widely used in engineering, not only is a logical one, but it has also been recognized as effective by other authors in the same field of image processing. Unfortunately, however good δ is, the fact remains that we cannot calculate it for unknown objects, because δ requires the knowledge of the original structure. It should be possible to suggest that if an algorithm works well in terms of δ with test pictures we may be confident that it will perform satisfactory reconstructions even with unknown objects. We cannot rely on this extrapolation because it has been shown that the performances of all the algorithms are picture-dependent (Herman & Rowland, 1973).

In this paper a criterion will be presented which gives an approximate estimation of the reconstruction errors and may permit a visual and a quantitative evaluation of reconstructions performed from the projections of unknown objects. This criterion is based on a new way of extracting information from the projection data, and it will be shown that this information, once available, permits not only checking but even improving the reconstructions performed by non-linear algorithms.

2. Definitions

We will follow the terminology of Gordon *et al.* (1970) and of Herman *et al.* (1973), as well as their procedure of reducing the reconstruction problem from three dimensions to two by considering an object which is rotated around an axis perpendicular to the beam of rays which cross it.

The digitized version of a picture is a $n \times m$ matrix $[\mathbf{f}_{ij}]$ whose ray sums are given by

$$g_{\theta k} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij}^{\theta k} f_{ij} \tag{1}$$

where $\alpha_{ij}^{\theta k}$ is the area of the matrix cell (i, j) which falls within the ray (θ, k). A digital picture represented by a $n \times m$ matrix $[\mathbf{f}_{ij}]$ is said to be equivalent, within an error ε, to another digital picture represented by a $n \times m$ matrix $[\mathbf{f}_{ij}^*]$ if

$$\frac{1}{n \times m} \sum_{i=1}^{n} \sum_{j=1}^{m} |f_{ij} - f_{ij}^*| \leqslant \varepsilon \tag{2}$$

where ε is a real positive number. When $[\mathbf{f}_{ij}]$ is a reconstructed picture and $[\mathbf{f}_{ij}^*]$ is the original picture, ε is called the linear reconstruction error.

The expression (2) represents a definition of "overall equivalence" which is satisfactory only if the reconstruction performances are uniform all over the reconstructed matrix. If we suspect that this does not happen we may use a more restrictive definition of picture equivalence substituting (2) with the expression

$$\frac{1}{(k-h)}\cdot\frac{1}{(q-p)}\sum_{i=h}^{k}\sum_{j=p}^{q}|f_{ij}-f_{ij}^{*}| \leqslant \varepsilon \tag{3}$$

for any (h, k) and (p, q) such that

$$1 \leqslant h < k \leqslant n$$
$$1 \leqslant p < q \leqslant m.$$

The concept of equivalence depends therefore on the choice of ε, and ε, in its turn, has to be selected according to the specific purposes of the reconstruction. For example, if we want two pictures which are optically equivalent ε will be a quantity for which the differences between the two pictures are beyond the sensitivity of the human eye.

Together with the linear reconstruction error ε, a quadratic error δ is also used through the definition

$$\delta = \left[\frac{1}{n\times m}\sum_{i=1}^{n}\sum_{j=1}^{m}(f_{ij}-f_{ij}^{*})^2\right]^{\frac{1}{2}}. \tag{4}$$

The expressions (2) and (4) are also called the ε-measure and the δ-measure of the reconstruction.

3. The Ω-Matrix

Given a picture represented by a $n\times m$ matrix **P** let us define as a complementary picture an $n\times m$ matrix $\mathbf{P}^c$ such that

$$\mathbf{P}+\mathbf{P}^c = \mathbf{\Omega}_0 \tag{5}$$

where $\mathbf{\Omega}_0$ represents a uniform gray matrix with density values $\omega_{ij} = \omega_0$.

It is obvious that the addition of a constant to each element of $\mathbf{P}^c$ produces another complementary matrix, because

$$\mathbf{P}+(\mathbf{P}^c+\mathbf{K}) = (\mathbf{P}+\mathbf{P}^c)+\mathbf{K} = \mathbf{\Omega}_0+\mathbf{K} = \mathbf{\Omega}_0' \tag{6}$$

(where **K** is a constant $n\times m$ matrix) so that, given a picture, an infinite number of complementary pictures exist.

From an experimental point of view the projections of a complementary picture are obtained by taking photographic negatives of the plates which represent the projections of a given picture, but the process can also be simulated mathematically.

Indeed, an Ω_0 matrix which represents a uniform gray picture with density values ω_0 has ray sums given by

$$\sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij}^{\theta k} \omega_0 \tag{7}$$

From the expressions

$$\omega_{ij} = f_{ij} + f_{ij}^c \tag{8}$$

$$g_{\theta k} = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij}^{\theta k} f_{ij} \tag{9}$$

$$g_{\theta k}^c = \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij}^{\theta k} f_{ij}^c \tag{10}$$

it follows

$$g_{\theta k}^c = \left[\sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij}^{\theta k} \omega_0 \right] - g_{\theta k}. \tag{11}$$

Since $\alpha_{ij}^{\theta k}$ can be calculated and $g_{\theta k}$ are given values, it follows that in order to obtain $g_{\theta k}^c$ we have only to derive ω_0.

The exact evaluation of ω_0, however, is not essential because complementary matrices which differ only for a constant are, in many respects, equivalent. The only desirable property of ω_0 is that

$$\omega_0 \geqslant \max (f_{ij}) \tag{12}$$

because if this condition is not realized, from

$$f_{ij}^c = \omega_0 - f_{ij}$$

it follows that some values of the complementary matrix would be negative, and this should be avoided.

Condition (12), on the other hand, can be easily satisfied by choosing

$$\omega_0 = \max (g_{\theta k})$$

or, in many practical cases, by

$$\omega_0 = 2 \max \left(\frac{g_{\theta k}}{N_{\theta k}} \right)$$

($N_{\theta k}$ is the number of centre points which lie within the ray θ, k) or even by other convenient expressions which can be chosen at will.

We therefore conclude that, given the projection values of a picture, we can always obtain the projection values of a complementary picture, and the sum of these two matrices will be referred to as the **Ω**-matrix of the given picture.

At this point it might be pointed out that the reconstruction of a complementary matrix adds nothing to the knowledge we would get from the reconstruction of a matrix because, in terms of information, data and complementary data are equivalent. This, however, is true only if all the reconstruction operations are linear. The introduction of non-linear constraints—for example the density positivity constraint—would produce results which affect the two matrices differently and their **Ω**-matrix will not be a uniform gray one, i.e.

$$f_{ij}+f_{ij}^{c} = \omega_{ij} \neq \omega_0.$$

On the other hand, from the definition itself of complementary matrix it follows that the reconstructed **Ω**-matrix should always be constant, and we may regard its uniformity as a new kind of reconstruction constraint.

The information of the **Ω**-matrix is therefore directly related to the effects of the non-linear operations which are at the very heart of the **Ω**-matrix discontinuities.

4. The Ω-Matrix Functions

The parallel reconstructions of a picture and its complementary picture with algorithms which make use of non-linear operations produce an **Ω**-matrix (8) about which we may calculate expressions similar to the ε-measure (2) and the δ-measure (4).

$$\varepsilon_\omega = \frac{1}{n\times m}\sum_{i=1}^{n}\sum_{j=1}^{m}|\omega_{ij}-\omega_0| \tag{13}$$

$$\delta_\omega = \left[\frac{1}{n\times m}\sum_{i=1}^{n}\sum_{j=1}^{m}(\omega_{ij}-\omega_0)^2\right]^{\frac{1}{2}} \tag{14}$$

Expressions (13) and (14) are referred to as the ε_ω-measure and the δ_ω-measure, or, respectively, the linear and the quadratic **Ω**-matrix errors.

From the expressions (8), (2), (4), (13) and (14) it follows

$$\varepsilon_\omega \leqslant \varepsilon+\varepsilon^c$$

and

$$(\delta_\omega)^2 = (\delta)^2+(\delta^c)^2+2\left[\frac{1}{n\times m}\sum_i\sum_j (f_{ij}-f_{ij}^*)(f_{ij}^c-f_{ij}^{c*})\right],$$

i.e. the **Ω**-matrix errors are functions of the same terms which define the reconstruction errors but are not identical with them. We have already seen, in the previous section, that the **Ω**-matrix discontinuities are a direct consequence of non-linear operations and therefore the **Ω**-matrix errors represent measures of the algorithm non-linearities. The **Ω**-matrix errors appear therefore substantially different from the reconstruction errors, but nevertheless they may be of some value in estimating the performances of a non-linear reconstruction algorithm.

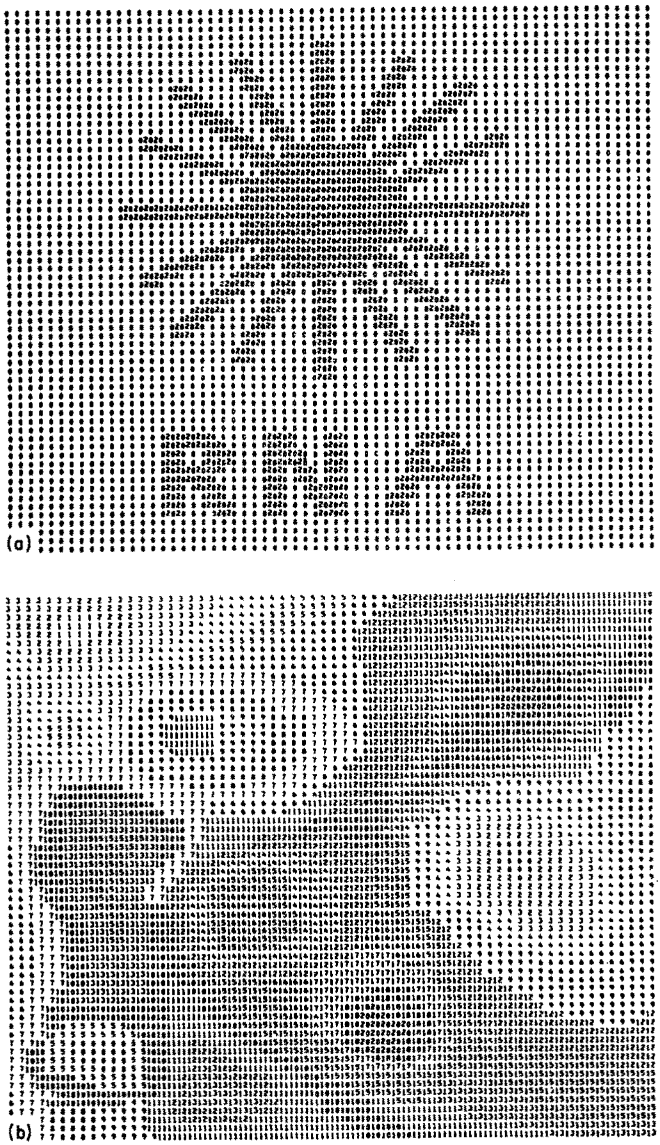

FIG. 1. Original test patterns of the "sun" picture (a) and the "gradient" picture (b).

5. Two Examples

In order to evaluate the information displayed by an **Ω**-matrix and to compare the **Ω**-matrix errors with the reconstruction errors let us examine the results obtained with two test pictures which have been reconstructed with additive ART (Gordon *et al.*, 1970) for 20 iterations, with 12 projections taken at equally spaced angles in a 180° range.

The two pictures have been chosen because they represent two opposite categories: one is relatively smooth and does not contain familiar features; the second represents a recognizable pattern and contains sharp density discontinuities. They have been called the "gradient" and the "sun" pictures, and are represented in Fig. 1.

Figures 2 and 3 represent the behaviour of the δ and δ_ω measures for the two pictures. It is evident that for the gradient matrix δ_ω converges as δ does, but for the sun matrix δ_ω reaches a minimum at the second iteration whereas δ continuously decreases for all 20 iterations.

Figure 4 shows the reconstructions of the gradient matrix, together with the corresponding **Ω**-matrix. In this case the performance of ART is without doubt excellent as can be verified mathematically from the δ and δ_ω values, or visually from an examination of the **Ω**-matrix.

Figure 5 shows the reconstruction displays of the sun matrices at the second iteration, when δ_ω reaches its minimum value, and Fig. 6 the corresponding displays at the 20th iteration.

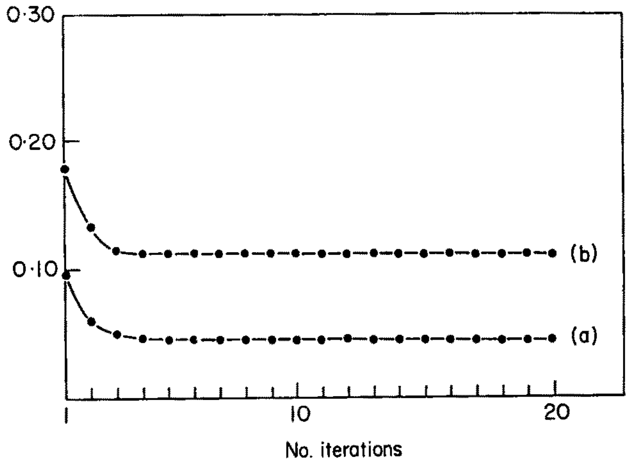

FIG. 2. The δ (a) and the δ_ω (b) measures versus number of iterations for the reconstruction of the "gradient" picture by ART from 12 projections.

The Ω-matrix of iteration 20 contains a higher contrast than iteration 2 because its maximum and minimum values are 38 and 7 compared with the values of 33 and 14 in the Ω-matrix of iteration 2. This fact is reflected in the sun reconstruction displays. The central region of the sun should have had a homogeneous density, but whereas at the iteration 2 the minimum and maximum values inside this region are 10 and 33, at the iteration 20 they are 7 and 38. It is obvious that in this case from iteration 2 to iteration 20 ART has increased the contrast in a region where the contrast should have

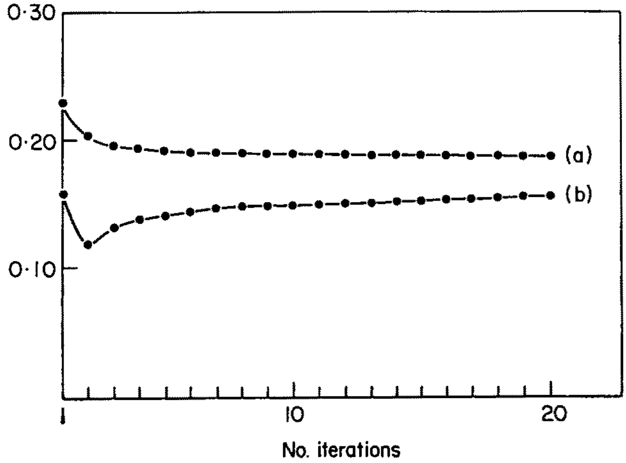

FIG. 3. The δ (a) and the δ_ω (b) measures versus number of iterations for the reconstruction of the "sun" picture by ART from 12 projections.

been decreased. This behaviour is detected by δ_ω but not by δ and this reveals that δ_ω is a very sensible measure of the reconstruction algorithm performance. We may say therefore that when δ_ω converges uniformly as in Fig. 2 we may be confident that at each iteration the reconstruction is getting progressively and uniformly better.

When, instead, the δ_ω behaviour is like Fig. 3 we should be careful in taking for granted the progressive improvement of the reconstruction. This improvement, in fact, can take place only in certain regions of the reconstruction matrix, whereas in other regions negative effects may appear.

We conclude, therefore, that the behaviour of δ_ω gives us precious information about the convergence of a reconstruction performed by an iterative non-linear algorithm and that, in any case, a monotonic convergence of δ_ω is a much more reliable guarantee than a monotonic convergence of δ.

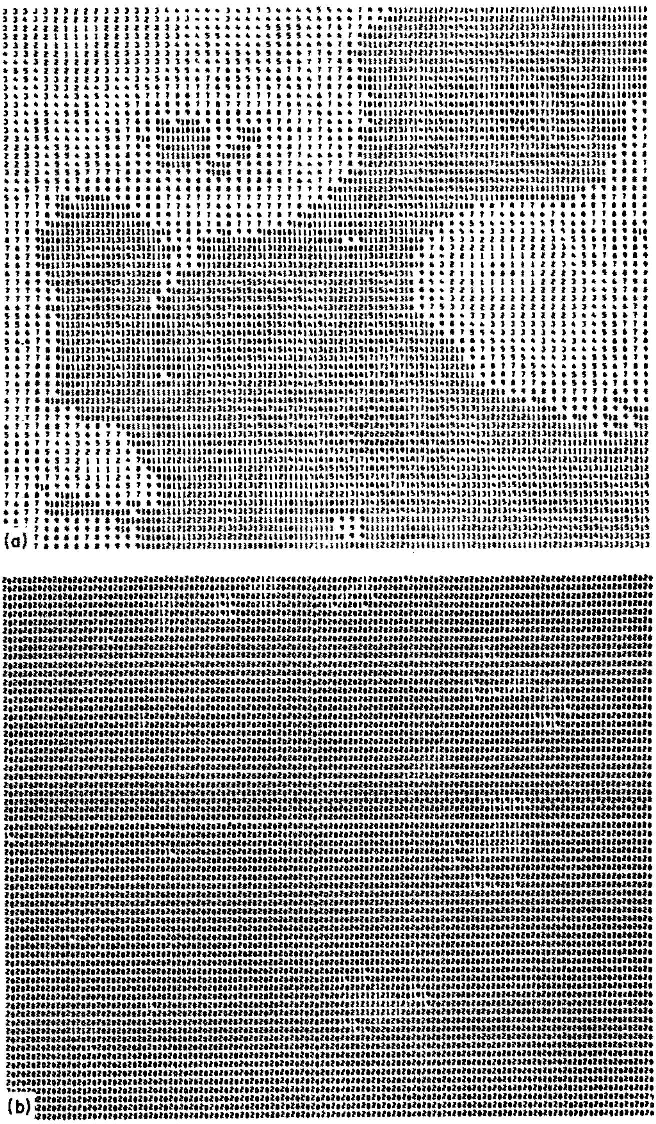

FIG. 4. Reconstruction by ART of the "gradient" picture (a) and its corresponding Ω-matrix (b) from 12 projections in the 180° angular range with 20 iterations.

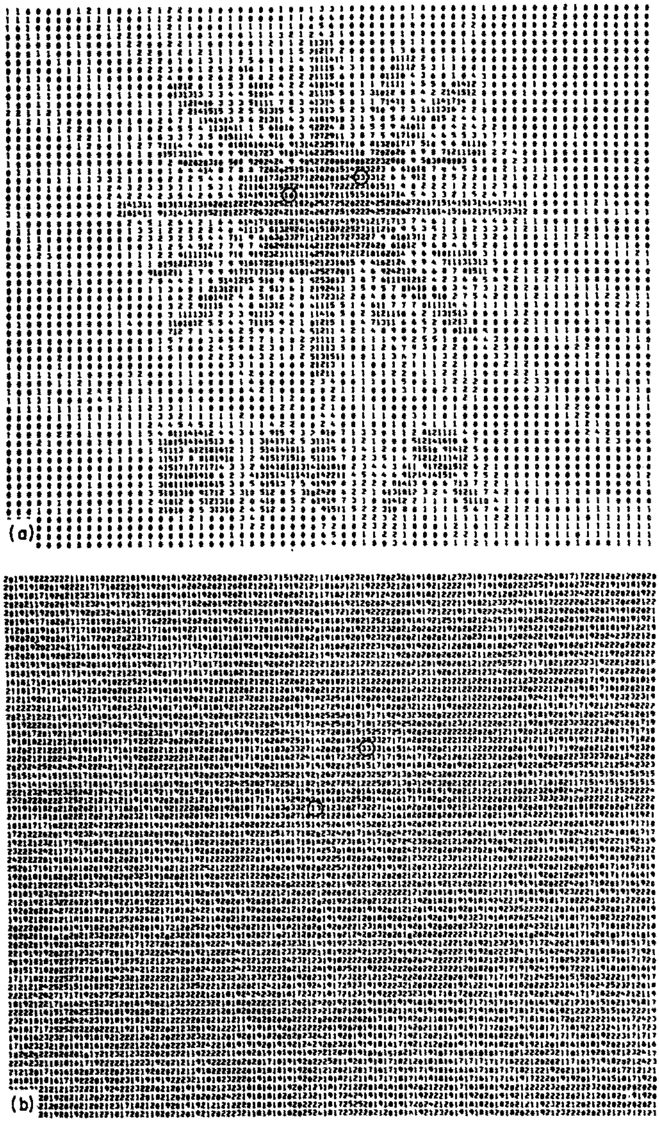

FIG. 5. Reconstruction after two iterations of ART of the "sun" picture (a) and its corresponding Ω-matrix (b) from 12 projections in the 180° angular range.

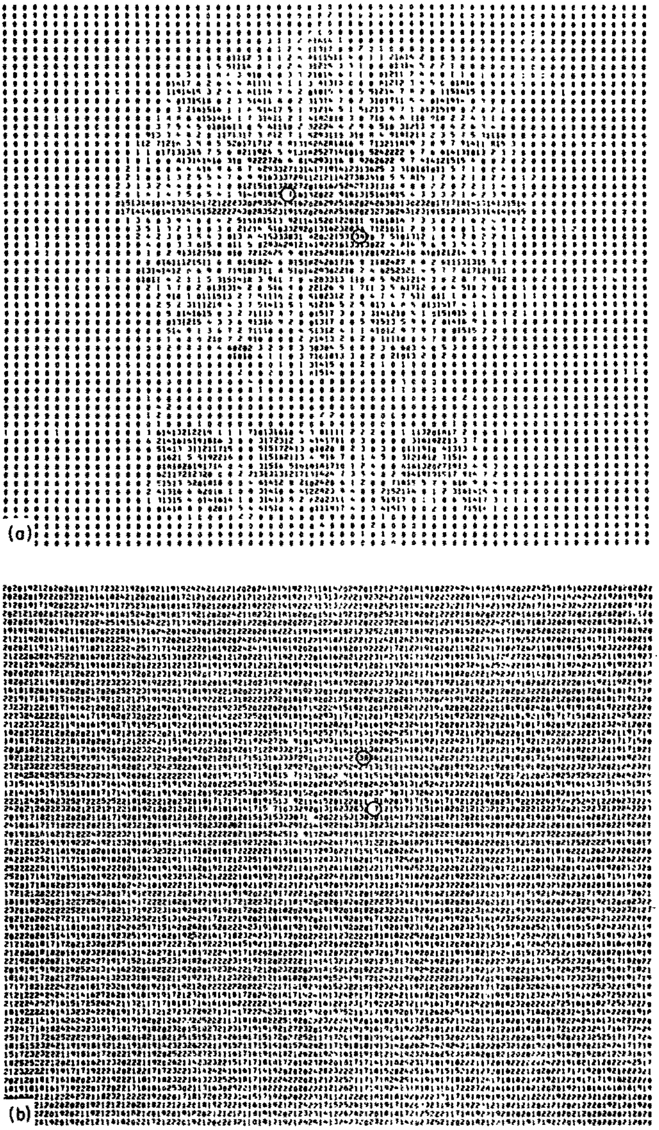

FIG. 6. Reconstruction after 20 iterations of ART of the "sun" picture (a) and its corresponding Ω-matrix (b) from 12 projections in the 180° angular range.

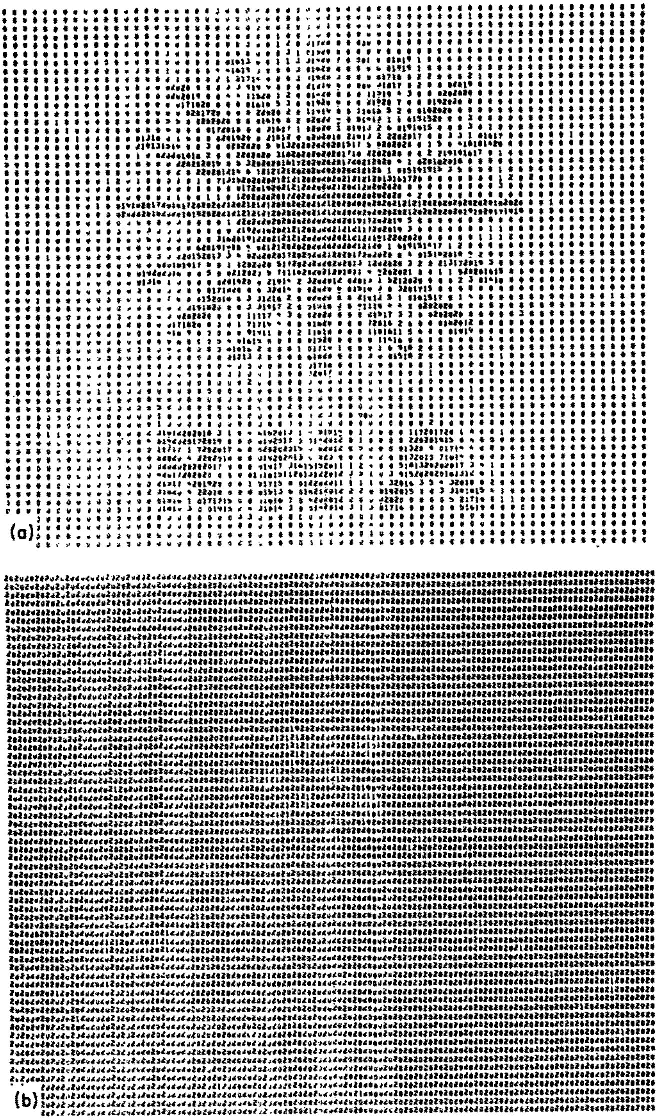

FIG. 7. Reconstruction after 20 iterations of MART of the "sun" picture (a) and its corresponding Ω-matrix (b) from 12 projections in the 180° angular range.

6. A Modified Algebraic Algorithm

In this section it is shown that the elimination of the **Ω**-matrix discontinuities brings about a sensible improvement in the performances of a non-linear algorithm. In other words, we say that the **Ω**-matrix contains truthful information because utilizing, at least in part, this information we get a better reconstruction. Unfortunately a complete use of the informational content of the **Ω**-matrix is not possible now because it is not known if a general relationship exists between the density distributions of the reconstructed picture, the reconstructed complementary picture and their corresponding **Ω**-matrix.

At present, however, we may reasonably assume the simpler alternative that the reconstructed matrix and the reconstructed complementary matrix are equally responsible, point by point, for the density deviations of the **Ω**-matrix from a uniform gray matrix. In this case we may correct the reconstructed density values in the following way. Given the three reconstructed matrices $[\mathbf{f}_{ij}]$, $[\mathbf{f}^c_{ij}]$ and $[\boldsymbol{\omega}_{ij}]$ with

$$f_{ij}+f^c_{ij} = \omega_{ij} \neq \omega_0$$

set

$$\bar{f}_{ij} = f_{ij}+\tfrac{1}{2}(\omega_0-\omega_{ij}) \tag{15}$$

and

$$\bar{f}^c_{ij} = f^c_{ij}+\tfrac{1}{2}(\omega_0-\omega_{ij}) \tag{16}$$

so that

$$\bar{f}_{ij}+\bar{f}^c_{ij} = \bar{\omega}_{ij} = \omega_0.$$

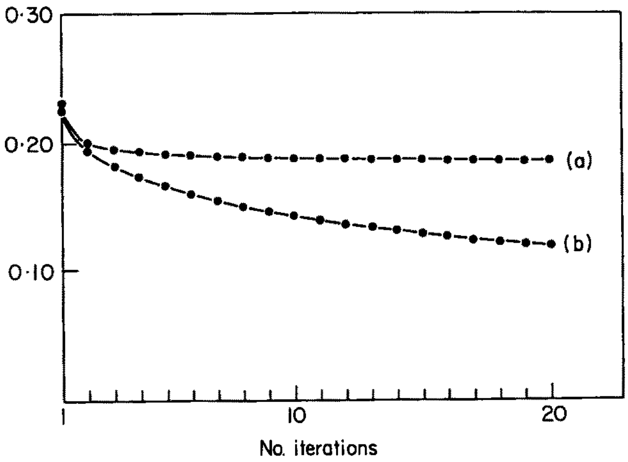

FIG. 8. The δ-measure versus number of iterations for the reconstruction of the "sun" picture by ART (a) and by MART (b) from 12 projections.

This simple way of utilizing the **Ω**-matrix information has been found particularly effective with the Algebraic Reconstruction Technique of Gordon *et al.* (1970) applying the expressions (15) and (16) after each iteration, which produces a new version of ART called MART (Modified Algebraic Reconstruction Technique).

Figure 7 represents the reconstruction of the "sun" picture with MART together with the corresponding **Ω**-matrix.

Figure 8 represents the δ functions of the reconstructions performed with MART and ART.

It must be pointed out that other ways of extracting information from the **Ω**-matrix exist and the expressions (15) and (16) represent only a first attempt. In addition, the **Ω**-matrix uniformity constraint may be equally well implemented not only with the ART method but also with other non-linear reconstruction algorithms. Work in this direction is still in progress but in the Appendix the scheme of a Generalized Iterative Method is presented which permits the implementation of any desired reconstruction constraint with any desired reconstruction algorithm.

7. Conclusion

A comparative examination of a reconstructed matrix and its correspondent **Ω**-matrix (see Figs 4, 5, 6 and 7) reveals that even if the deviations of the **Ω**-matrix from a uniform gray matrix are not identical with the differences between the reconstructed picture and the original, nevertheless they are sufficiently close to those differences in every region of the matrix to support the conclusion that the **Ω**-matrix errors may be convenient approximations of the reconstruction errors. The visual and the quantitative evaluation of the **Ω**-matrix become therefore a candidate-criterion for evaluating reconstructions of unknown structures.

It has to be said, however, that the results presented in this paper have been obtained only by reconstructing test pictures from pseudo and not from real projection data and in the absence of noise. In addition only the density positivity constraint has been used as a non-linear operation.

At present, therefore, the proposal of assuming the non-linearity measures as approximate estimates of the reconstruction errors remains necessarily a suggestion which needs further confirmation. In any case, whatever the exact relationship between **Ω**-matrix errors and reconstruction errors, and however limited the evidence derived from a few test pictures, it seems possible to conclude that some real advantages may actually be gained by making use of the **Ω**-matrix information.

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APPENDIX

A Generalized Iterative Method

The application of an algorithm A to a set of original projection values $g^{\circ}_{\theta k}$ produces an approximate reconstruction $\mathbf{f}^{q}_{ij}$ and we may describe this process by the notation:

$$A[g^{\circ}_{\theta k}] \rightarrow [\mathbf{f}^{q}_{ij}]. \tag{A1}$$

We may also say that the "true" matrix $[\mathbf{f}^t_{ij}]$ is related to the reconstructed matrix $[\mathbf{f}^q_{ij}]$ through an unknown "correction matrix" $[\mathbf{f}^\gamma_{ij}]$, i.e.:

$$f^q_{ij} = f^t_{ij} + f^\gamma_{ij}. \tag{A2}$$

It is obvious, therefore, that if we could estimate, in some way, the correction matrix $\mathbf{f}^\gamma_{ij}$ we could improve our reconstruction.

From equation (A2) we obtain

$$f^\gamma_{ij} = f^q_{ij} - f^t_{ij}$$

and taking the projections

$$g^\gamma_{\theta k} = g^q_{\theta k} - g^\circ_{\theta k}. \tag{A3}$$

We may therefore consider the correction matrix like any other matrix which has to be reconstructed from its projection values (A3). It is quite likely that a reconstruction algorithm applied to the projection data (A3) produces only an approximate evaluation of the correction matrix, but we can easily use these values to produce a first restoration of the reconstruction, then recalculate the projections of a second correction matrix and so on.

The expressions (A3) however do not represent the best choice for calculating the projections of the correction matrix. They correspond, in fact, to ray sums obtained through the expression

$$\sum_i \sum_j \alpha^{\theta k}_{ij} f^\gamma_{ij} = \sum_i \sum_j \alpha^{\theta k}_{ij}(f^q_{ij} - f^t_{ij}). \tag{A4}$$

It is obvious that the differences $(f^q_{ij} - f^t_{ij})$ have in general both positive and negative values and their sum largely cancels the contributions of opposite signs.

We may, however, avoid this result simply by adding a positive constant λ to all the values of the reconstruction matrix, where λ has to be chosen large enough to guarantee that all the differences $(f^q_{ij} - f^t_{ij})$ are positive.

We have, therefore,

$$f^{*q}_{ij} = f^q_{ij} + \lambda = f^t_{ij} + f^\gamma_{ij}$$

and

$$g^{\gamma q}_{\theta k} = \left[\sum_i \sum_j \alpha^{\theta k}_{ij} f^{*q}_{ij}\right] - g^\circ_{\theta k}.$$

The implementation of any desired reconstruction constraint can be expressed by the notation

$$f^{q+1}_{ij} = C[f^q_{ij}]$$

where $C[f^q_{ij}]$ means "apply to the value f^q_{ij} the operation C and consider the result as f^{q+1}_{ij}".

In this way our Generalized Iterative Method has the following scheme

$$\left.\begin{array}{ll}
\text{(a)} & A^{\circ}[g^{\circ}_{\theta k}] \to [\mathbf{f}^{\circ}_{ij}] \\
\text{(b)} & f^{*q}_{ij} = f^{q}_{ij} + \lambda^{q} \\
\text{(c)} & g^{\gamma q}_{\theta k} = g^{*q}_{\theta k} - g^{\circ}_{\theta k} = \left[\sum_i \sum_j \alpha^{\theta k}_{ij} f^{*q}_{ij}\right] - g^{\circ}_{\theta k} \\
\text{(d)} & A^{q}[g^{\gamma q}_{\theta k}] \to [\mathbf{f}^{\gamma q}_{ij}] \\
\text{(e)} & f^{q+1}_{ij} = C^{q}[f^{*q}_{ij} - f^{\gamma q}_{ij}].
\end{array}\right\} \quad \text{(A5)}$$

Where A^q is any desired reconstruction algorithm and C^q is any desired set of reconstruction constraints. The index q in the terms A^q and C^q means that during the iterative process even different Algorithms and Constraints can be alternated in any desired sequence to obtain any convenient combinations of their performances.