

Comparing an algebraic least squares 3D reconstruction algorithm with back projection and SIRT

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In 1970, Crowther et al. [1] proposed an algebraic reconstruction method based on a least squares solution of the set of projection equations. The application of this method requires large computing power, which has become available only in recent years. While methods such as the weighted back projection [2] or SIRT (simultaneous iterative reconstruction technique) [3] are widely used, the "least squares reconstruction" method is not commonly applied. So far it has not been explored systematically. Here we present a first thorough analysis of the least squares reconstruction algorithm using a Siemens star as a test object.

Solving the set of projection equations $H \cdot \mathbf{x} = \mathbf{b} + \boldsymbol{\varepsilon}$ (with H the projector matrix, \mathbf{x} vector of all unknown density points of the object and $(\mathbf{b} + \boldsymbol{\varepsilon})$ vector of the known projections with errors) is equivalent to an inversion of the normal matrix, because the classical solution that minimizes the sum of the squares of errors $\boldsymbol{\varepsilon}^T \boldsymbol{\varepsilon}$ is $H^T H \cdot \mathbf{x} = H^T \cdot \mathbf{b}$. $H^T H$ cannot be inverted directly. Therefore, determining density \mathbf{x} involves numerically calculating the normal matrix Eigenvalue spectrum and the corresponding Eigenfunctions in order to solve the equations in the subspace of significant Eigenfunctions. Their number can be determined beforehand by considering the Crowther criterion [1], which then leads to a well defined reconstruction superposition of the relevant Eigenfunctions.

In the case of ideal data (high signal to noise ratio, SNR) all geometrically meaningful Eigenfunctions can be included into the reconstruction, resulting in an exceptional reconstruction quality. Figure 1 illustrates this for the test object, which can be reconstructed with a Fourier ring correlation of almost 0.9 at Nyquist frequency. This very high achievable resolution compares favourably with the more conventional reconstructions (see reconstruction of an ideal edge as illustrated in Fig. 2).

The reconstruction of more realistic, noisy data (Fig. 3) reveals the intrinsic properties of the three methods compared here: The SNR of a reconstructed test object is best when using SIRT, while - at moderate noise level - the "least squares reconstruction" will always produce highest reconstruction quality (e.g. reproduced radial density profiles) and resolution, as shown by the Fourier ring correlation (Fig. 3d).

The "least squares reconstruction" method has already been applied to an object with helical symmetry (myosin-decorated actin filaments [4]), which illustrates the applicability of the method to 3D data reconstruction. With increasing computing power, in principle every reconstruction of axial tomographic projection geometry can be easily calculated. Preliminary results on tomographic data are comparable to the results shown here for 2D.

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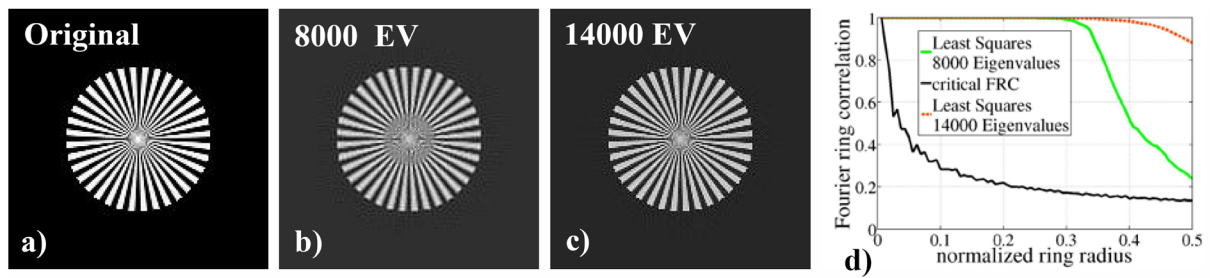


Figure 1. Effect of Eigenfunction selection on the quality of the reconstruction (no noise added). **a)** - Siemens star as test object for all 2D reconstruction simulations. **b)** - Algebraic least squares reconstruction using the 8000 highest Eigenvalues. **c)** - Algebraic least squares reconstruction using the 14000 highest Eigenvalues. **d)** - Fourier ring correlation between original Siemens star and reconstructions (b, c).

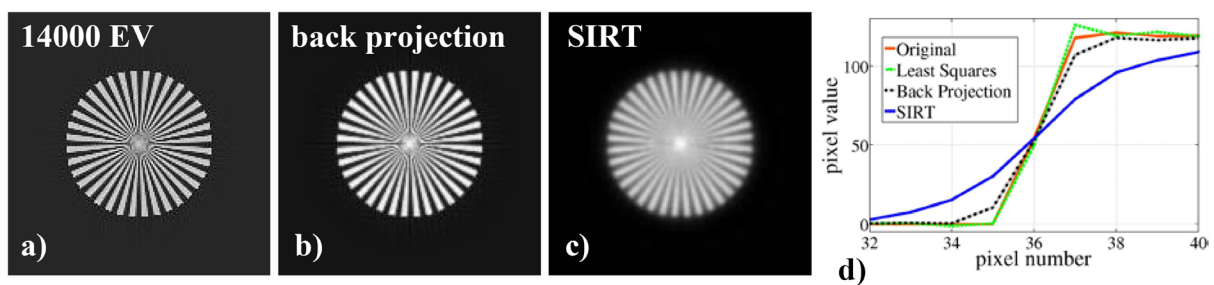


Figure 2. Comparing algebraic reconstruction, back projection and SIRT reconstruction of a Siemens star (no noise added). **a)** - Algebraic least squares reconstruction using 14000 Eigenvalues. **b)** - Weighted back projection reconstruction using SPIDER operation BPW2 [2]. **c)** - SIRT reconstruction using XMIPP programme reconstruct_art with 100 iterations [3]. **d)** - Reconstructed edge of the Siemens star for the three reconstruction algorithms (a,b,c). Reconstructions were rotationally averaged and the central lines plotted as profile.

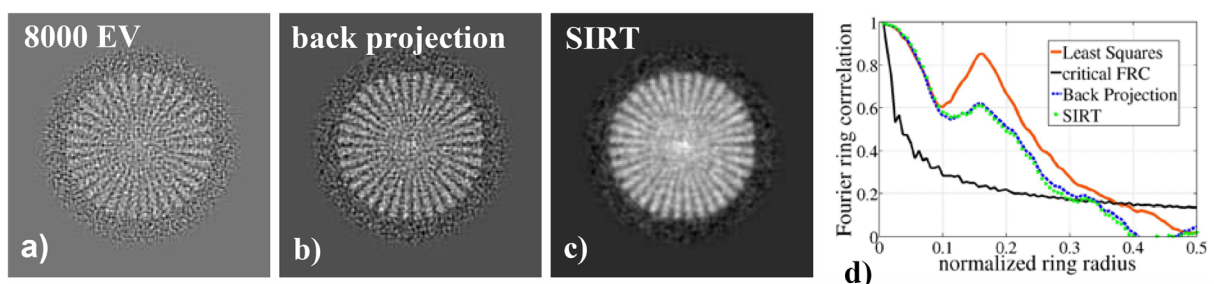


Figure 3. Reconstructions and Fourier ring correlation of a Siemens star with added noise (noise with SNR=2 was added to the projected profiles before reconstruction). **a)** - Algebraic least squares reconstruction using 8000 Eigenvalues. **b)** - Weighted back projection reconstruction using SPIDER operation BPW2 [2] followed by a low frequency Fermi filter. **c)** - SIRT reconstruction using XMIPP programme reconstruct_art with 100 iterations [3] followed by a low frequency Fermi filter. **d)** - Fourier ring correlation of the reconstructions (a,b,c) with the original Siemens star.