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Weighted simultaneous iterative reconstruction technique for single-axis tomography

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ABSTRACT

Tomographic techniques play a crucial role in imaging methods such as transmission electron microscopy (TEM) due to their unique capabilities to reconstruct three-dimensional object information. However, the accuracy of the two standard tomographic reconstruction techniques, the weighted back-projection (W-BP) and the simultaneous iterative reconstruction technique (SIRT) is reduced under common experimental restrictions, such as limited tilt range or noise. We demonstrate that the combination of W-BP and SIRT leads to an improved tomographic reconstruction technique: the weighted SIRT. Convergence, resolution and reconstruction error of the W-SIRT are analyzed by a detailed analytical, numerical, and experimental comparison with established methods. Our reconstruction technique is not restricted to TEM tomography but can be applied to all problems sharing single axis imaging geometry.

1. Introduction

Electron tomography (ET) provides an unique access to the three-dimensional (3D) structural, chemical or electrical properties of organic and inorganic materials with nanometer resolution [1–3]. For example, ET significantly contributes to the understanding of the prokaryotic ultrastructure [4,5] as well as complex catalysts [6], polymers [7], and semiconductor nanostructures [8].

ET basically includes three steps: First, the acquisition of a tilt series in the transmission electron microscope (TEM), i.e., a series of 2D electron micrographs (projections) while tilting the specimen under the electron beam typically within ca. $\pm 70^{\circ}$ at increments of 1–3°. Second, the alignment of the tilt series for corrections of residual displacements between the projections with respect to a common tilt axis; and third, the computerized 3D reconstruction of the tilt series by specific reconstruction techniques yielding finally the electron tomogram.

The most notable experimental limitation of the technique is an incomplete tilt range (for example $\pm 70^{\circ}$ instead of $\pm 90^{\circ}$), which leads to a loss of information, visible as "missing wedge" in the Fourier transform (FT) of the tomogram. In real space, this corresponds to a reduced resolution in the tomogram in the direction of the missing wedge. Therefore, considerable effort is put into the development of adapted specimen geometries (e.g. needles [9]), holder designs (e.g. On-Axis Rotation Tomography Holder), and novel goniometers (e.g. TEAMstage [10]) facilitating at 180° tilt series acquisition. Accurate and stable rotation holders also reduce spurious drift of the sample which eases the requirements to the alignment procedure following the acquisition. Nonetheless, small alignment variations as well as detection noise and specimen damages cannot be completely avoided and impose a second important limitation, in particular when aiming for high-resolution tomograms. It is one important task of the reconstruction procedures to suppress the influence of these "non-projective" artifacts. This can be achieved by exploring additional information on the sample structure such as symmetries and by regularizing the reconstruction.

Nowadays, the tomographic reconstruction is usually performed either with the help of weighted back-projection (W-BP) methods [11–14] or iterative techniques, in particular the simultaneous iterative reconstruction technique (SIRT) [15,16]. Iterative methods are also often referred to as algebraic reconstruction techniques (ART) [17]. Numerous variations of these techniques have been developed in order to consider the above mentioned limitations: For example, the so-called Discrete ART (DART) [18] discretizes the range of the allowed reconstructions and can therefore robustly reconstruct samples that consist of only a few different materials (grey levels). More recently, another ART has been introduced which assumes a certain smoothness of the 3D data using compressive sensing [19].

In general, the mathematical structure of the projection–reconstruction corresponds to a matrix inversion, which usually only exists as a pseudoinverse [20]. This pseudoinverse is typically (mildly) ill conditioned (e.g. due to the missing wedge) and has to

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be regularized in order to be robust against the “non-projective” errors such as noise [20]. Such a regularization can be achieved by adding auxillary conditions weighted by a regularization parameter. Examples of such conditions are euclidean norm minimization (Tikhonov regularization, e.g. [21]), total variation minimization (TVM) [19] or basis function number minimization (compressive sensing) [22]. The iterative reconstruction techniques considered in the following utilize some sort of Tikhonov regularization where the regularization parameter is the number of iterations.

Here, we present a reconstruction algorithm that we refer to as Weighted SIRT (W-SIRT) because it is a combination of W-BP and SIRT. The combination of these two established methods (introduced in Section 2) and the advantage of a specific weighting filter (explained in Section 3.1) yield tomograms with higher signal fidelity and lateral resolution than those obtained from W-BP or SIRT. This is supported by comparing the results and the convergence behavior of W-SIRT or SIRT obtained from theoretical case studies (Section 4) and experimental examples (Section 5).

2. Two-dimensional weighted back-projection and SIRT

2.1. Radon transformation

If the tilt series is recorded at single axis geometry (one alternative is conical tilt geometry [23]), the description of the projection–reconstruction problem of a 3D (scalar) function $f(x,y,z)$ can be reduced to 2D by a separate treatment of slices $f(x,y=\text{const.},z)$ perpendicular to the tilt axis y (see Fig. 1). The process of projecting $f(x,z)$ along lines L determined by a tilt angle α and the distance to the origin l, i.e.

$$\hat{f}(l,\alpha)=\int_L f(x,z)\,\mathrm{d}\mathbf{s}, \tag{1}$$

is referred to as Radon transformation $\mathcal{R}$ [24], whose discrete result is also called *sinogram*. Thus, the tomographic reconstruction of a sinogram (y-slice through the tilt series) can be described mathematically as the inverse 2D Radon transformation ($\mathcal{R}^{-1}$). Therefore, algorithms for tomographic reconstruction optimally should be numerical realizations of $\mathcal{R}^{-1}$.

2.2. Weighted back-projection

The W-BP is based on the *simple* or *direct* back-projection (S-BP) algorithm [4,16]. As the name back-projection suggests, each pixel of the sinogram is projected back into 2D space along the ray path, which contributed to the pixel during the projection process. The superposition of all back-projected paths yields the *layergram* (Fig. 1c), which reads in the continuous case [25]

$$f_b(x,z)=(2\pi)^{-1}\int \hat{f}(\mathbf{n}(\alpha)\cdot(x,z)^T,\alpha)\,\mathrm{d}\alpha \tag{2}$$

with $\mathbf{n}(\alpha)=(\cos\,\alpha,\,\sin\,\alpha)^T$.

The layergram is only a blurred version of the desired object function f. It can be abbreviated by

$$f_b(x,z)=\mathcal{R}^T\{\hat{f}(l,\alpha)\} \tag{3}$$

with the transpose or adjoint Radon transformation $\mathcal{R}^T$. However, the object function (tomogram) is computed by inverse Radon transformation by

$$f(x,z)=\mathcal{R}^{-1}\{\hat{f}(l,\alpha)\}. \tag{4}$$

The reason for the difference between f_b and f, i.e. the blurring, can be understood from the projection-slice (or central slice) theorem, which states (for 2D) that the 1D projection of a 2D object corresponds in Fourier space to a 1D slice (line) through the origin (center) of the Fourier transform ($\mathcal{F}$) of the 2D object. Thus, the S-BP corresponds to a summation (integration) of central slices in Fourier space. This in turn means an inhomogeneous sampling decreasing from lower to higher spatial frequencies, which can be described by a transfer function (TF) for S-BP [14]. Consequently, the modulation of spatial frequencies $\mathbf{g}=(g_x,g_z)$ in the Fourier transform of the layergram $F_b(g_x,g_z)=\mathcal{F}\{f_b(x,z)\}$ can be corrected by multiplication with a weighting function $W(\mathbf{g})$, the inverse of the TF. This is the concept of the Weighted BP (W-BP) which finally retrieves the object function by

$$f(x,z)=\mathcal{F}^{-1}\{\mathcal{F}\{f_b(x,z)\}\cdot W(g_x,g_z)\}. \tag{5}$$

In the continuous (analytical) case, i.e. infinitesimally small tilt increments and a tilt range of $\pm 90^\circ$, the transfer function of the S-BP is the reciprocal modulus of the spatial frequency. Thus, the weighting function or the so-called *analytical* weighting filter (WF) is

$$W_a(g_x,g_z)=|\mathbf{g}|. \tag{6}$$

Indeed the analytical WF is the 2D Jacobian for the Cartesian to polar coordinate transformation which is, however, missing if considering the S-BP (Eq. (2)) in Fourier space. However, in realistic cases, including possibly non-uniform tilt increments of about 2° and tilt ranges of about $\pm 70^\circ$, the transfer function is neither axially symmetric nor its slope in radial direction is unity. To consider the limited and discrete number of projections better than the analytical WF, Harauz and van Heel introduced a so-called *exact*

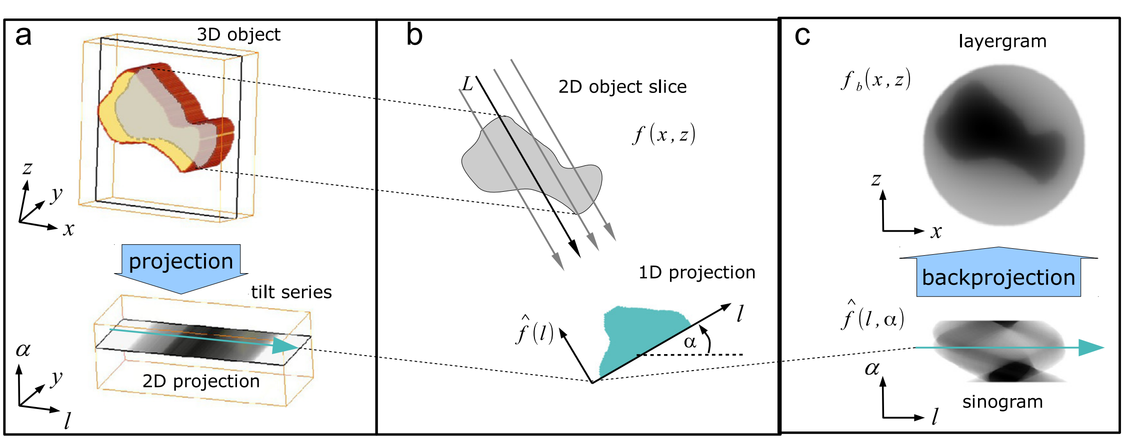

Fig. 1. Tomography in single-axis tilt geometry. (a) Schematic of the tilt series acquisition (projection) process. The tilt axis points in y-direction. The green arrow in the 2D projection corresponds to the 1D projection of the 2D object slice at a certain tilt angle α as shown in (b). (c) The sinogram is composed of all available 1D projections through the 2D object slice under different tilt angles. Its back-projection leads to the layergram, a blurred version of the original 2D object slice. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)