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Subsampling and inpainting approaches for electron tomography

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ABSTRACT

With the aim of addressing the issue of sample damage during electron tomography data acquisition, we propose a number of new reconstruction strategies based on subsampling (which uses only a subset of a full image) and inpainting (recovery of a full image from subsampled one). We point out that the total-variation (TV) inpainting model commonly used to inpaint subsampled images may be inappropriate for 2D projection images of typical TEM specimens. Thus, we propose higher-order TV (HOTV) inpainting, which accommodates the fact that projection images may be inherently smooth, as a more suitable image inpainting scheme. We also describe how the HOTV method can be extended to 3D, a scheme which makes use of both image data and sinogram data. Additionally, we propose gradient subsampling as a more efficient scheme than random subsampling. We make a rigorous comparison of our proposed new reconstruction schemes with existing ones. The new schemes are demonstrated to perform better than or as well as existing schemes, and we show that they outperform existing schemes at low subsampling rates.

1. Introduction

One of the greatest challenges associated with electron tomography (and electron microscopy in general) is avoiding significant sample damage due to prolonged exposure to the electron beam. Hence for tomographic data acquisition the microscopist must somehow minimize the electron dose, all the while knowing that most attempts to do so will result in a loss of accuracy in the 3D reconstruction. Typically the electron beam intensity is set, based on experience, to a level that maintains a suitably high signal-to-noise ratio while not producing obvious sample damage. In addition, the number of tilt-series orientations must be limited to a suitable number, which is again typically gauged by experience.

A recent and more cunning approach for limiting the dose in electron microscopy is *subsampling*, i.e., sampling only a fraction (e.g., 20%) of the total number of pixels in the image domain. Possibilities for implementing subsampling experimentally in a scanning transmission electron microscope (STEM) are discussed briefly later in this article. A general prevailing strategy to interpret the subsampled images is to *inpaint* the missing pixels. Inpainting generally refers to any mathematical model that can be solved numerically to interpolate (recover) missing parts of an image. Many popular inpainting models, including those used in the present work, are characterized as ℓ_1 regularization or compressed sensing models.[1] For instance, the works of Anderson et al. [1] and Oxvig et al. [2] used a discrete cosine transform (DCT) for the ℓ_1 regularization model to inpaint subsampled microscopy images. An alternative approach for inpainting of atomic-resolution images using Bayesian dictionary learning was studied by Stevens et al. [3]. More generally within the mathematical community, a wide variety of inpainting strategies have been studied [4–7], many of which also fall under the umbrella of ℓ_1 regularization with combinations of frames and other transforms.

Recently, Saghi et al. [8] demonstrated the potential effectiveness of inpainting for 3D electron tomography. In that work, a total variation (TV) model was used to inpaint the 2D projection images of a tilt series data set that was subsampled post mortem (the original data set was not acquired in a subsampled manner). As with other attempts to reduce the electron dose, subsampling will result in some loss of accuracy in the final 3D reconstruction. Part of the goal of the present study is to determine how we can limit this loss.

As explained further below, the ℓ_1 regularization models work by minimizing an appropriate ℓ_1 norm, which is chosen based on prior knowledge of the behavior, or *smoothness*, of the image or

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[1] Uncoincidentally, these models are popular for tomographic reconstruction in a wide range of scientific fields.

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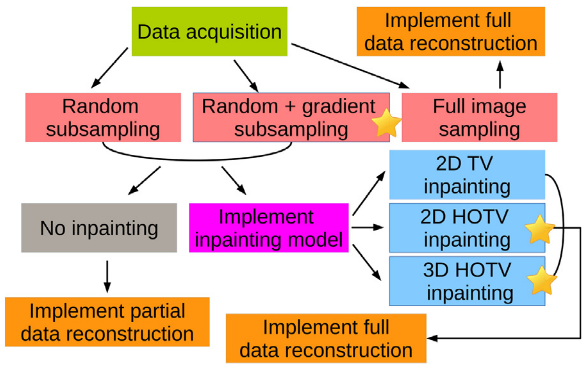

Fig. 1. Work flow for the various tomographic reconstruction strategies studied in the present work. Blocks highlighted by yellow stars indicate new strategies proposed here. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

function which we are trying to recover. The TV ℓ_1 regularization model is a popular choice, which assumes that the imaging scene consists essentially of constant values with a small number of jumps or boundary points. For example, in the relatively simple case of homogeneous nanoparticles resting on a weakly-scattering support, the imaging scene can be approximated as a binary image in 3D (or more generally a piecewise constant function), and so the TV assumption is approximately satisfied. More recently, higher-order TV (HOTV) models have also been proposed for electron tomographic reconstruction [9]. The latter models are more general and have the benefit of allowing for smooth changes in the imaging scene, characterized by low-order polynomial behavior. Related to the work in this paper, others have proposed using similar higher-order regularization methods known as TGV [10]. In Ref. [11], the latter method was applied to inpaint missing wedges in 2D sinograms . An approach to inpaint sinograms with limited angular sampling using dictionary learning was also proposed in Ref. [12]. In Refs. [11,12] images at the known projection angles were fully sampled (as opposed to subsampled), and additional 1D projections were recovered by the algorithm. This problem differs significantly from the present work where we work with subsampled projection images. Moreover, here we extend the inpainting problem to the full 3D domain of the reconstruction.

Here we propose a number new strategies for both image subsampling and appropriate inpainting models in the context of electron tomography. First, we argue that HOTV models are more appropriate for inpainting subsampled 2D images (e.g., subsampled STEM images).[2] Second, we extend the HOTV model to a 3D inpainting model, which makes use of the data points in the images taken at nearby orientations. In other words, the 3D inpainting model also makes use of the data visualized as both 2D images *and* as a set of sinograms. Finally, we propose a "smarter" subsampling strategy, whereby a greater number of samples are taken at the important image regions, which in this work we regard as those regions where we estimate the magnitude of the gradient to be large. A diagram summary of this work in the electron tomography data processing work flow is provided in Fig. 1, where we have omitted the important alignment procedure that is a multifaceted problem and somewhat disjoint from this work. In the diagram we highlight three blocks with yellow stars to indicate the new investigations in this paper.

[2] We note here that a number of higher order methods have been proposed [10,13,14] and would likely be a suitable alternative to our approach, pending the available software.

2. Problem description

Electron tomography works by first acquiring a *tilt series*, where a transmission electron microscope is used to acquire images of the specimen from a number of viewing angles. These images are then carefully processed by image registration and reconstruction methods to yield a 3D approximation of the imaging scene, where each pixel in the 2D images is mathematically viewed as a data point used to reconstructed the 3D structure. These 3D images allow us a more accurate and detailed understanding of materials applications in technology, medicine, and science [15–19].

Let the imaging scene that we want to reconstruct be denoted by f, a function defined in 3D space over some finite rectangular domain given by $\Omega = [\Omega_x \times \Omega_y \times \Omega_z]$. The data acquired in electron tomography are traditionally 2D projection images of the form

$$P_\theta(f)(x,y) = \int_{\Omega_z} f(x, (y,z)Q_\theta)\, dz,$$

$$\text{where} \quad Q_\theta = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}. \tag{1}$$

This projection data is acquired with an electron microscope by orienting the sample at a finite number of angles $\{\theta_j\}_{j=1}^m$. For each orientation, the specimen is sampled over a discretization of the domain $[\Omega_x \times \Omega_y]$, denoted by $\{(x_a, y_b)\}_{a,b=1}^N$, where a typical value for N is 1024 and the number of angles m is on the order of 50 to 100. This makes for a total of mN^2 data points.

A simple strategy for subsampling is to reduce the number of grid points (and hence, in an experiment, reduce the electron dose) by *randomly* sampling the specimen at some subset of the full $N \times N$ mesh. For each angle θ_j, we denote some subset of the full mesh by $S_j = \{(x_{i(j,1)}, y_{i(j,2)})\}_{i=1}^M$, where $M < N^2$. Here, $i(j, 1)$ and $i(j, 2)$ are some the index mappings for jth subsampled image and the x and y coordinates respectively, and the subsampling rate is defined by M/N^2.

With the subsampled data, one can of course attempt to use the data given and implement a traditional reconstruction algorithm, such as a Fourier-based algorithm. However, Fourier-based methods will not work because transforming the data into Fourier space via the Fourier slice theorem requires the full projection data.

To introduce the concept of inpainting let us describe the TV inpainting method for the 2D projection images. First, let $I_{S_j} \in \mathbb{R}^{M \times N^2}$ denote the identity matrix containing only the rows from the subset S_j, and let $\vec{p}_{\theta_j}(f) \in \mathbb{R}^M$ denote the vectorized version of the subsampled projection data. Then recovery of the full 2D projection image by the TV inpainting model is given by[3]

$$\vec{q}_{\theta_j}(f) = \underset{q \in \mathbb{R}^{N^2}}{\operatorname{argmin}}\, TV(q) \quad \text{s.t.} \quad I_{S_j} q = \vec{p}_{\theta_j}(f). \tag{2}$$

which, in words, means that the full 2D projection image $\vec{q}_{\theta_j}(f)$ is that set of N^2 values that possesses minimum total variation, subject to being entirely consistent with the subsampled projection data $\vec{p}_{\theta_j}(f)$. Here the anisotropic TV norm of an image $g \in \mathbb{R}^{N \times N}$ is given by

$$TV(g) = \sum_{i=1}^{N} \sum_{j=1}^{N-1} |g_{i,j+1} - g_{i,j}| + \sum_{j=1}^{N} \sum_{i=1}^{N-1} |g_{i+1,j} - g_{i,j}|, \tag{3}$$

and this definition is naturally altered if the image is in vectorized form as in (2). The isotropic variant of the TV norm is given by

$$TV_I(g) = \sum_{i=1}^{N-1} \sum_{j=1}^{N-1} \sqrt{(g_{i+1,j} - g_{i,j})^2 + (g_{i,j+1} - g_{i,j})^2} \tag{4}$$

[3] The minimum in (2) cannot be guaranteed to be unique, in which case the solution will depend on the solver.