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Sampling limits for electron tomography with sparsity-exploiting reconstructions

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ABSTRACT

Electron tomography (ET) has become a standard technique for 3D characterization of materials at the nano-scale. Traditional reconstruction algorithms such as weighted back projection suffer from disruptive artifacts with insufficient projections. Popularized by compressed sensing, sparsity-exploiting algorithms have been applied to experimental ET data and show promise for improving reconstruction quality or reducing the total beam dose applied to a specimen. Nevertheless, theoretical bounds for these methods have been less explored in the context of ET applications. Here, we perform numerical simulations to investigate performance of ℓ_1-norm and total-variation (TV) minimization under various imaging conditions. From 36,100 different simulated structures, our results show specimens with more complex structures generally require more projections for exact reconstruction. However, once sufficient data is acquired, dividing the beam dose over more projections provides no improvements—analogous to the traditional dose-fraction theorem. Moreover, a limited tilt range of ±75° or less can result in distorting artifacts in sparsity-exploiting reconstructions. The influence of optimization parameters on reconstructions is also discussed.

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1. Introduction

Electron tomography (ET) attempts to reconstruct the 3D structure of physical and biological materials from an angular range of 2D images collected by a (scanning) transmission electron microscope ((S)TEM) [1–8]. The set of images is often referred to as a tilt series and modeled as projections of the original object. Unfortunately, in typical ET experiments, radiation damage, contamination, and acquisition time limit the signal-to-noise ratio (SNR) and the number of projections (ca. ∼70–140). Furthermore, specimen and stage geometry usually restrict the tilt range (ca. ±70°), leaving a large missing wedge of information in Fourier space. Consequently, conventional reconstruction algorithms, such as weighted back projection, that only make use of measured data suffer from elongation and blurring artifacts that are disruptive to accurate characterizations.

Recently, there is a growing interest in developing reconstruction techniques that incorporate additional prior knowledge about the specimen [9–11]. Inspired by the field of compressed sensing, a majority of these methods [11–15] exploit the notion of image sparsity and obtain reconstructions via minimizing the ℓ_1-norm of the object vector in some domain. Unlike back projection, sparsity-exploiting methods have considerable flexibility in designing reconstructions based on users' assumptions about the specimen as well as the desired utility of the reconstruction [16]. A typical form of the optimization problem can be written as

$$\overbrace{\min \|\underbrace{D(x)}_{\text{Reconstruction}}\|_1}^{\text{Objective Function}} \ \text{s.t.}\ \overbrace{\|\underbrace{A}_{\text{Measurement Matrix}}x-\underbrace{b}_{\text{Data}}\|_2 \le \underbrace{\varepsilon}_{\text{Data-Tolerance Parameter}}}^{\text{Data Constraint}},$$

where x and b represent the reconstructed image and measured data. A is referred to as the "*measurement matrix*", which *models* the experimental imaging process and depends on sampling schemes such as pixel/voxel size, the number of projections and tilt range. A scalar "*data-tolerance parameter*" ε is introduced to accommodate inconsistencies between data (b) and imaging model (Ax). Higher SNR data generally allows a smaller ε to be used because there are fewer discrepancies between the measured data

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and the reconstruction model. The function $D(x)$ transforms the reconstruction to a domain in which the object is assumed to be sparse. Two most popular transformations are identity ($D(x) = x$) and gradient magnitude ($D(x) = \nabla x_2$). The ℓ_1-norm of the gradient-magnitude image is also known as the TV-norm (x_{TV}) [17] and has been used in image processing and reconstruction algorithms for over two decades [18,19]. Furthermore, for STEM tomography, it is also beneficial to enforce additional constraint that restricts pixels/voxels to be non-negative.

To date, several experimental works have demonstrated that sparsity-exploring methods can reduce artifacts and improve overall reconstruction quality [11,12,14] for under-sampled data. Nevertheless, theoretical limitations of such algorithms are seldom discussed in the context of ET, especially when and how they fail. In essence, the reconstruction (a solution of the optimization problem) can be interpreted as a multivariable function that depends on *A, b*, and ε. Different experimental conditions, such as sampling scheme or data quality, and the data-tolerance parameter can lead to significantly different reconstructions. It is generally onerous, if not impossible, to explore the entire parameter space when characterizing optimization-based reconstructions. Thus, in this work, we carry out extensive simulation studies of both x_1 and x_{TV} minimization techniques and investigate four key parameters that are of practical interests: number of projections, data-tolerance parameter, data noise, and tilt range. Our results demonstrate some fundamental behaviors of sparsity-exploiting methods:

1. The number of projections required for exact reconstruction increases with specimen complexity.
2. In the presence of Poisson noise, the quality of sparsity-exploiting reconstructions degrades quickly. With a sufficient number of projections, the root-mean-square error (RMSE) of the reconstruction depends only on the total electron counts (i.e. dose). Using more projections with lower SNR has insignificant influence on the reconstruction. This resembles the traditional dose-fraction theorem for weighted back projection [20,21].
3. Sparsity-exploiting reconstructions suffer from distorting artifacts when the tilt range is less than ±75°.
4. The data-tolerance parameter also has significant impact on reconstructions. For TV minimization, small ε can produce noisy artifacts, while large ε results in over-smoothed reconstructions.

These results provide basic insights on data acquisition and reconstructions for ET. Because the number of projections required for sparsity-exploiting reconstruction is specimen-dependent, one should be cautious when reducing the number of projections or tilt range in practical experiments. With proper choice of the optimization parameter, however, sparsity-exploiting reconstructions are robust to a small missing wedge (~30°, i.e. tilt range of greater than ±75°) and follow the traditional dose-fraction theorem. Increasing data SNR generally improves reconstruction quality.

2. Background

2.1. Image model for ET

Most optimization-based reconstruction methods are built upon the *discrete-to-discrete model* [22] in which both image (x) and data (b) are represented as vectors and related via the measurement matrix as $Ax = b$ (Eq. (1). In this model, tomographic reconstruction is an inverse problem of solving x for a given system of linear equations.

In ET, each measurement is often interpreted as line integrals (i.e. a projection) across the specimen [23]. If data is *ideal*, that is, $b = Ax$, one can define a *sufficient projection number* as the smallest number of projections that gives a full rank measurement matrix [24], which guarantees that Eq. (1) has a unique solution. Due to experimental limitations, the sufficient projection number is rarely achieved in practice. For instance, in order to reconstruct a 512×512 image from data with 1024 measurements in each projection, one needs to record at least 256 projections (the exact number depends on how A is constructed). To overcome data insufficiency, additional knowledge beyond Eq. (1) needs to be incorporated into the imaging model so that the reconstruction is closer to the actual specimen.

2.2. Sparse model and compressed sensing

The notion of sparsity has become widely used in optimization-based reconstruction techniques. Mathematically, sparsity refers to the number non-zero elements in a vector (also known as the ℓ_0-norm). A sparse model assumes only a small fraction of the elements in the image vector (x), or some transform of it, are non-zero. Because direct ℓ_0-norm minimization is NP-hard [25], alternative approaches have been developed to approximate sparse solutions. In 2002, Li et al. [26] used an ℓ_1-norm minimization method to reconstruct sparse blood vessels from 15 X-ray computed tomography (CT) projections. The idea of ℓ_1-norm minimization is further reinforced by the work of Candes et al. [27], which proved that if the measurement matrix satisfies a restricted isometry property (RIP), it is highly probable the sparsest solution and minimal ℓ_1-norm solution are equivalent, given there are enough non-zero measurements. This result led to the field of compressed sensing [27,28] and re-invigorated developments in optimization-based methods.

Despite the popularity of compressed sensing, its theoretical conclusions are of limited use in practice. It is well known that compressed sensing typically favors dense and random measurement matrices [29]. In ET or X-ray CT, on the other hand, measurement matrices are much more sparse and structured (See Fig. 1 in ref. [38]. Studies using radon transforms have shown not only the existence of sparse vectors that cannot be reconstructed by ℓ_1-norm minimization [30], but RIP-based guarantee only holds for extremely sparse vectors [31]. Moreover, it is computationally intractable (NP-hard) to examine whether a measurement matrix satisfies the properties required by compressed sensing [32]. Without theoretical guarantees, it is imperative to carry out simulation studies using an ensemble of objects with well-defined features to understand the recoverability of any algorithm.

3. "Phase diagram" analysis for ℓ_1-norm minimization

In this section, we perform a "phase diagram" analysis to study the recoverability of ℓ_1-norm minimization method at various imaging conditions. Adapting the work by Jørgensen et al. [33,34], we establish an average-case relation between image sparsity and the number of projections needed for exact reconstruction. In Fig. 1, the simulation results are summarized as a function of the percentage of non-zero pixels (k) of the object intensity and relative sampling (μ), which is defined as the ratio of the number of projections to the sufficient projection number. For each pair of (k, μ) in this phase space, we generate 100 semi-realistic test objects with similar complexity. Details of object generation are summarized in supporting information and the source code is included in the tomography software *tomviz* (www.tomviz.org) [49]. For ideal data, a reconstruction is obtained by solving the basis pursuit optimization problem: $\min ||x||_1 \; s.t. \; Ax = b$ [36]. A total of 36,100 different structures are used in the phase diagram and we report the percentage of "accurate" reconstructions whose RMSE are less than 0.05 in Fig. 1a.

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