

Quantifying the Advantages of Compressive Sensing and Sparse Reconstruction for Scanning Transmission Electron Microscopy

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From the perspective of information theory, it's easy to suspect that current methods for extracting information using STEM can't possibly be optimal. After all, when we try to make sense of the multi-GB data sets produced by spectrum imaging, STEM diffraction, and other similar techniques, usually the first thing we do is apply aggressive data reduction techniques. Each EELS spectrum might be represented as a combination of a small number of component spectra (using any of a variety of techniques including principal component analysis, independent component analysis, and Bayesian dictionary learning), and the residual is normally thrown away as noise. In STEM diffraction, often an entire diffraction pattern with a MB or more of data is reduced to just three parameters giving the 3D orientation of the crystal at that point. In both cases, the analyzed data might be 100 times smaller than the raw data and yet may still contain virtually all of the information the user cared about.

Even after data reduction, such data sets can still be highly compressible. Atomic-resolution images typically have most of their information crammed into the vicinity of a handful of spatial frequency vectors. In nanometer-resolution images the spectrum or diffraction pattern from one pixel almost always looks nearly identical to that of one or more nearby pixels, and when it does not, then most likely something went wrong with the measurement and that pixel needs to be discarded anyway. Standard data-compression algorithms can eliminate this redundant information, reducing the byte count by perhaps another factor of 10 without losing a significant amount of real, useful information.

Compressive sensing (CS) is a fast-growing field that has been proposed as a solution to this problem [1-3]. CS raises the question: Why acquire all of this redundant information in the first place? Every byte that's thrown away represents wasted electron dose and data-acquisition capacity. What if we could avoid this? What if we could operate the instrument in a clever way that, in effect, applies data-compression algorithms before the signal even hits the analog-to-digital convertors? Would that enable dramatic improvements in data throughput, time resolution, and/or the ability to study radiation-sensitive materials?

We embarked on an extensive series of simulations to answer this question, using existing CS algorithms and new ones invented for the purpose, and determined that the answer to this yes-or-no question is a very decisive "maybe." The answer is surprisingly sensitive to the details of how you're going to implement CS in a STEM and, more importantly, on why you're doing CS in the first place. If you're using it to reduce the number of acquisitions needed, perhaps because of the limited bandwidth of your detection and/or data storage system or the speed of *in situ* processes you're interested in studying, then there are certainly advantages to be had. The answer still depends on the hardware-implementation details, but there are undoubtedly regimes where CS has a substantial advantage.

But if your intent is to reduce radiation dose to the sample, the results are not so encouraging. In fact, over a very broad class of problems and acquisition parameters, we found that non-adaptive CS-STEM has essentially no practical advantage over conventional STEM in terms of radiation dose, and results

appearing to show otherwise are due to the inherent denoising properties of CS reconstruction algorithms and not to the change in acquisition mode. Reducing electron dose in CS-STEM runs into serious problems with Poisson noise, which has highly detrimental effects on the compression/distortion scaling laws that allow CS to work in the first place [4]. This cloud has two silver linings: First, many of the apparent advantages of CS can be had without having to do anything difficult or clever with the acquisition hardware; advanced data analysis methods applied to conventionally acquired data produce equivalent or better results. Second, the result only applies to non-adaptive CS. Adaptive CS techniques are another question entirely, and in some cases they may prove highly effective at reducing radiation dose. But this will not come about by accident; a great many devils lurk in the details. We will close with some proposed solutions to these problems.

Figure 1. Example simulation, showing reconstruction of a 10,000-pixel STEM-diffraction virtual dark field image using 2000 measurements, each of which uses a thresholded power-law spatial mask, and reconstructed using the Poisson-noise-aware "SPIRAL-TV" algorithm [4]. The lower-left image shows the reconstruction, while the lower-right shows the (much worse) reconstruction using conventional l_2 -norm-based techniques.

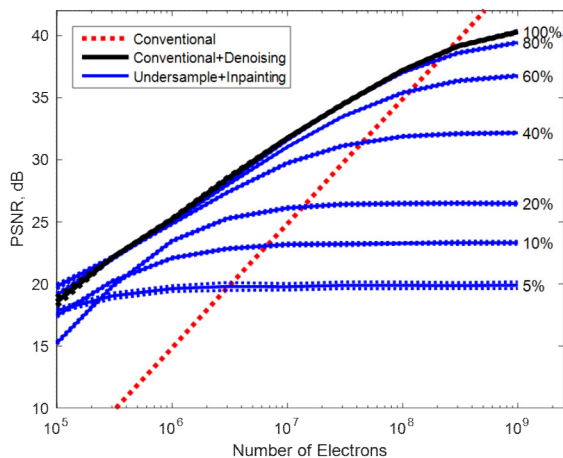
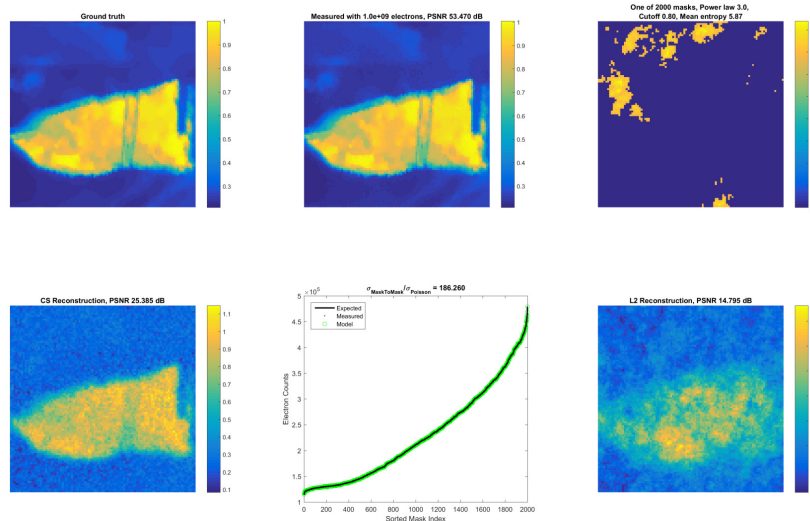


Figure 2. Results from an ensemble of undersampling-and-inpainting simulations, showing the peak-signal-to-noise ratio (PSNR) of the reconstruction as a function of the number of electrons. PSNR values of ~25 dB or more are of acceptable quality, while those much above ~35 dB are approaching overexposure. Throughout the useful range, undersampling and inpainting (blue, with varying sampling fractions) appears to outperform conventional measurements (red) but only if we ignore the availability of sparsity-based denoising algorithms (black).

[1] P. Binev *et al.*, "Compressed Sensing and Electron Microscopy," pp. 73-126 in *Modeling Nanoscale Imaging in Electron Microscopy*, Springer (2012).
 [2] A. Stevens *et al.*, *Microscopy* **63**, 41 (2014).
 [3] A. Béché *et al.*, arXiv:1509.06656v1 (2015).
 [4] Z. Harmany, R. F. Marcia, and R. M. Willett, *IEEE Trans. Image Proc.* **21**, 1084 (2012).
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