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Denoising Atomic Resolution Hyperspectral Data with Tensor Singular Value Decomposition

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Hyperspectral data collected from electron energy loss spectroscopy (EELS), energy dispersive X-ray spectroscopy (EDS), and 4D scanning transmission electron microscopy (4D STEM)[1] are often corrupted by significant noise, giving rise to the need to denoise the data in order to extract useful information regarding the sample. Here we propose a new approach to denoising hyperspectral data by treating it as a noisy tensor and denoising the tensor by searching for a low-rank tensor approximation using tensor singular value decomposition (SVD)[2]. We assume that the ground truth can be represented by a low rank tensor due to periodic lattice structure and the repetition in real space. Compared with widely-used matrix SVD methods, tensor SVD has the potential to exploit additional structure in the data, for example by preserving spatial relationships between scattering from adjacent atomic columns. Compared to more sophisticated non-local hyperspectral denoising methods, tensor SVD achieves similar or better performance but is much more memory efficient, so it can be directly applied to multiple GB datasets with modest computing resources.

Tensor SVD denosing was tested on 4D STEM data with the two dimensions in diffraction space unfold into one single dimension to create a 3D tensor. Figure 1 shows tensor SVD's performance on data simulated from Si [110] edge dislocation structure. The image quality is significantly improved for both a reconstructed annular dark field (ADF) image and a single convergent beam electron diffraction (CBED) pattern. Tensor SVD consistently improves the peak signal-to-noise ratio (PSNR) of the denoised image versus the noisy image by about 20 dB. The same simulated 4D STEM data with reciprocal space truncated to 10-by-10 pixels was denoised with non-local principal component analysis (NLPCA)[3] and block-matching and 4D-filtering (BM4D)[4]. Tensor SVD either performs the best or close to the best under varying noise levels, and it runs at least 100 times faster than the other two methods.

4D STEM experimental data used to test the tensor SVD method was collected on a Thermo Fisher Titan with CBED patterns collected using a DE-16 direct electron camera. Both $SrTiO_3$ [100] single crystal sample and LiZnSb [] film on Al_2O_3 [] substrate were as test samples. Figure 2 shows a comparison between noisy data and denoised data in terms of reconstructed ADF images and single CBED patterns. Denoised ADF images show good SNR with clear atom sites in both structures, while denoised CBED patterns show much fewer noise points with clear arc features from the first-order Bragg diffraction disks as marked by the yellow arrow in figure 2f. The whole denoise process on these 3 GB experiment datasets took 2 minutes with single-threaded Matlab implementation on a personal computer with 2 GB peak memory consumption. Applications using the tensor SVD components for spectral unmixing will also be discussed.[5]

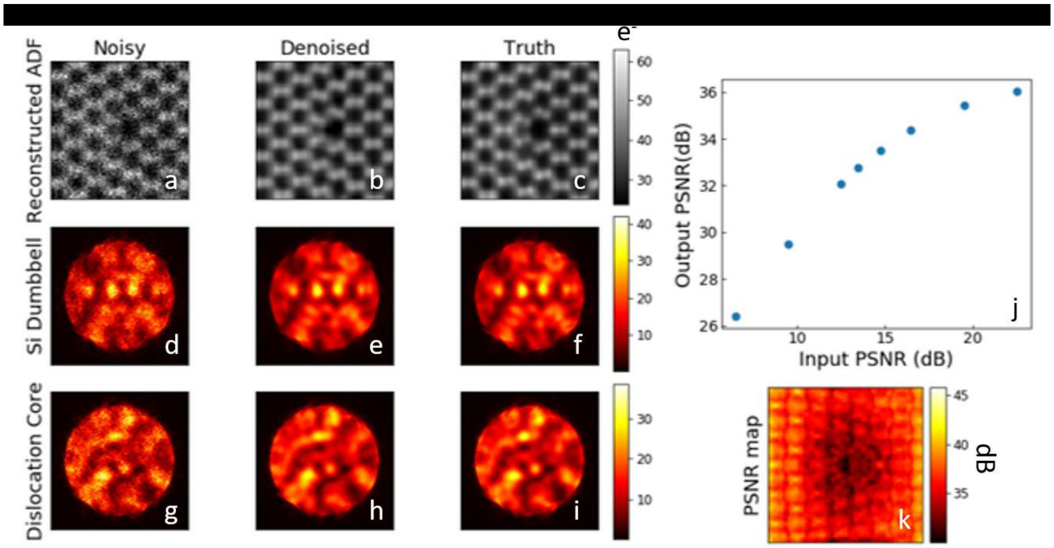

Figure 1. a-c: Comparison between noisy ADF, denoised ADF, and truth ADF image. d-i: Comparison between noisy CBED pattern, denoised CBED pattern, and truth CBED pattern from two different beam positions. j: Output PSNR vs. input PSNR under different noise levels. k: denoised performance measured by PSNR from different spatial locations.

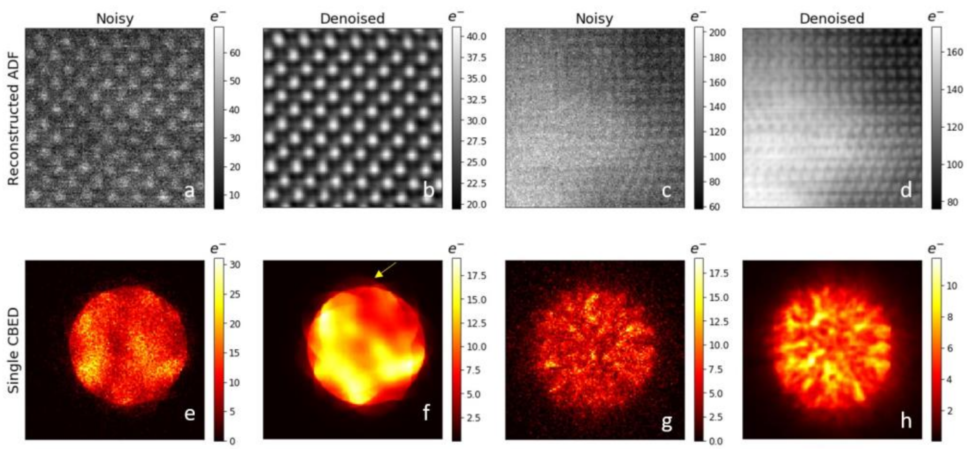

Figure 2. a-d: two pairs of comparison between noisy ADF images and reconstructed ADF images from experimental 4D STEM data collected from SrTiO3 [110] and LiZnSb/Al2O3 [11-20]. e-h: same comparison on the two datasets between noisy CBED patterns and denoised CBED patterns.

References

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