Supervised and Unsupervised Machine Learning for Large, Noisy STEM Data*

Paul M. Voyles
Department of Materials Science and Engineering
University of Wisconsin-Madison

Abstract

Developments in instrumentation for high-resolution scanning transmission electron microscopy (STEM) in the past decade have been pushing consistently for faster and faster acquisition of more and more finely sampled data – more probe positions, more spectral channels, and more pixels in diffraction patterns. This trend creates opportunities to measure new signals and derive new information about both the structure of materials at the atomic scale and their functional properties, but it poses significant challenges as well. One challenge is increasingly noisy data as a fixed number of electrons are more finely divided. We have worked to mitigate noise by adapting non-rigid image registration from medical imaging [1] and by adapting non-local denoising [2, 3] and tensor dimensional reduction [4] approaches to Poisson-noise corrupted, highly structured, atomic-resolution STEM data sets. The other challenge is greater data volume. We have started to develop convolutional neural networks to support human microscopists in screening and analyzing this large volume of data [5]. Many other researchers on working on similar approaches, so we have also begun developing benchmark data sets for deep learning applications in STEM to aid performance comparisons for existing models and development of new models.

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