

Lecture "Machine Learning for Electron Microscopy: from Imaging to Atomic Fabrication"

Tuesday, 14 September 2021 16:45 (1 hour)

I will discuss recent progress in automated experiment in electron microscopy, ranging from feature to physics discovery via active learning. The applications of classical deep learning methods in streaming image analysis are strongly affected by the out of distribution drift effects, and the approaches to minimize though are discussed. We further present invariant variational autoencoders as a method to disentangle affine distortions and rotational degrees of freedom from other latent variables in imaging and spectral data and decode physical mechanisms. Extension of encoder approach towards establishing structure-property relationships will be illustrated on the example of plasmonic structures. Finally, I illustrate transition from post-experiment data analysis to active learning process. Here, the strategies based on simple Gaussian Processes often tend to produce sub-optimal results due to the lack of prior knowledge and very simplified (via learned kernel function) representation of the system. Comparatively, deep kernel learning (DKL) methods allow to realize both the exploration of complex systems towards the discovery of structure-property relationship, and enable automated experiment workflows targeting physics (rather than simple spatial feature) discovery. The latter is illustrated via experimental discovery of the edge plasmons in STEM/EELS in MnPS₃, a lesser-known 2D material.

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