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Position-Blind Ptychography for Single Particle Imaging: Viability of image reconstruction via data-driven variational inference

Recent innovations in X-ray optics can achieve a beam focus with a spot size of below 3 nanometers, which is well within the size range of single biological macromolecules. Here, we are interested in using such highly focused X-ray Free Electron Laser (XFEL) beams for single-particle imaging (SPI) to maximize the photon flux through the sample and hence increase the measurement SNR. When the illuminating beam (probe) is concentrated in a region that is roughly as large as - or smaller than - the object under investigation, the involved measurements become ptychographic: only a part of the illuminated object meaningfully contributes to each measurement. A key difficulty of this imaging modality lies in the fact that, due to the uncontrolled flight of the particles through the region of the beam, the scan positions are fully unknown and must be recovered jointly with the image. We hence call this kind of imaging “position-blind ptychography”.

In this work, we computationally investigate the viability of a simplified type of position-blind ptychography with 2-dimensional objects based on synthetic complex-valued images and simulated measurements. We develop and compare methods based on optimization and on variational inference, and investigate the use of modern data-driven image priors in the form of diffusion models for this task. We provide insights into the optimal structure and size of the probe for position recovery and image quality, and show that we can achieve successful reconstructions with a mean PSNR of about 25 dB and >90% of positions recovered correctly in our simplified problem setting. We will also discuss missing pieces and challenges towards full 3-D ptychographic SPI.

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