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Multi-objective Bayesian Optimization for High-resolution Electron Ptychography

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Electron ptychography enables deep sub-angstrom spatial resolution of atomic structures by solving the inverse problem of electron scattering through the sample, provided the complete distribution of transmitted electrons enabled by a new generation of detectors for scanning transmission electron microscopy (STEM). However, in practice, ptychographic reconstructions are computationally intensive and require a delicate selection of both experimental and algorithmic parameters, heavily relying on the trials and errors of user experiences. Here we propose an automatic parameter selection scheme based on multi-objective Bayesian optimization. We show that introducing Fourier ring correlation (FRC) as an additional objective in addition to the Fourier reconstruction error captures the subtle differences in resolution and circumvents unphysical local minima. Instead of a single optimum produced by a black box optimization, the multi-objective framework produces a Pareto front of equally feasible solutions that lead to the best reconstruction result.

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