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Bayesian Optimization for Multi-dimensional Alignment: Tuning Aberration Correctors and Ptychographic Reconstructions

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Bayesian optimization (BO) is an automatic sequential strategy searching for global optimization of a target function inside a high-dimensional parameter space. We have applied BO both to tune aberration corrector in a scanning transmission electron microscope (STEM) and refine the parameters used for ptychographic reconstructions [1] from 4D-STEM data. Both are problems where the resulting image quality depends on a large number of coupled parameters and imperfect measurements. We implemented BO with the open-source package BoTorch [2]. Our results show that BO can optimize the target function effectively even when the measurements are noisy.

The mechanism of BO is sketched in figures 1(a) and (b) using a one-dimensional parameter space as an example. With a set of sample points, BO predicts the unknown function with uncertainty at each point in the parameter space. Then it selects the next observation point by maximizing the acquisition function, which would be a point with the best chance to optimize the unknown function. By repeating this process, BO can quickly get a good understanding of the unknown function and meanwhile optimize the value of the function.

We have applied BO to tune an octupole aberration corrector on a Nion UltraSTEM by minimizing the emittance growth of the beam. The emittance is a metric that characterizes the volume occupied by the beam in phase space [3] and is minimized for an optimal alignment. We trained a convolutional neural network (CNN) to determine the normalized beam emittance from a single Ronchigram. The output of the CNN is minimized to reduce the aberrations, as shown in figure 1(c). The comparison between initial Ronchigram, Ronchigram after automatic tuning, and Ronchigram after tuning with the microscope's software are shown in figure 1(d) – (f). The phase errors are reduced and at least comparable to the level of standard tuning software after 120 iterations of optimization with BO. The process took about two minutes to finish, which is generally faster with less human bias compared to the standard tuning software. The speed of the latter also depends much on the operator.

We have also applied BO to automatically select the reconstruction parameters for the mixed state ptychography. We selected the reconstruction error as the target function to be minimized; and convergence angle, defocus, and scan rotation as the parameters to be explored. The progress of minimizing the reconstruction error over the two stages is shown in figure 2(a). The final refined parameters are then used to run a complete reconstruction of 1,000 iterations. Figure 2(b) - (e) show the reconstructed phase object of a $MoSe_2$/WS_2/BN multilayer structure and the probe for both the nominal parameters estimated for the instrument (figure 2(b), (c)) and the optimized parameters determined by the BO (figure 2(d), (e)). The results from the optimized parameters show both better resolution in the phase of the object and a more physical probe shape.

Overall, we have shown that BO is a useful tool for hyperparameter tuning both in aberration corrector alignment and ptychography reconstruction. It is capable of exploring high-dimensional complex parameter space with many local minimums under high noise and can significantly reduce the amount of human interaction [4].

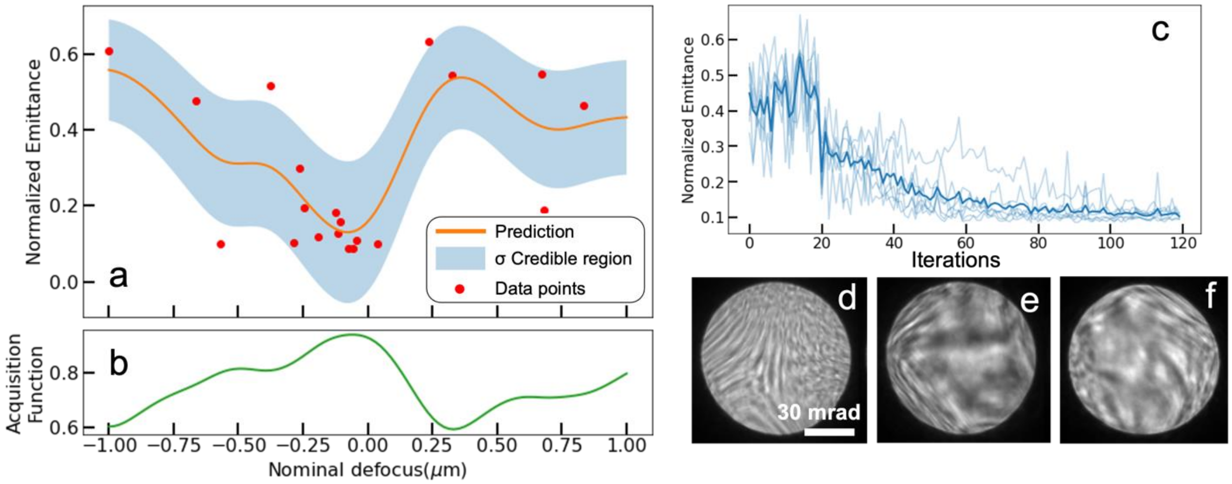

Figure 1. (a) BO predicted emittance as a function of the nominal defocus value based on the collected data points, (b) acquisition function used by BO to determine the next sample point, (c) progress of emittance minimization with BO under seven trials with different random starting points, the solid blue curve marks the average of the seven trials, (d) starting Ronchigram, (e) Ronchigram after auto-tuning from one of the trials, and (f) Ronchigram after manual tuning with microscope software.

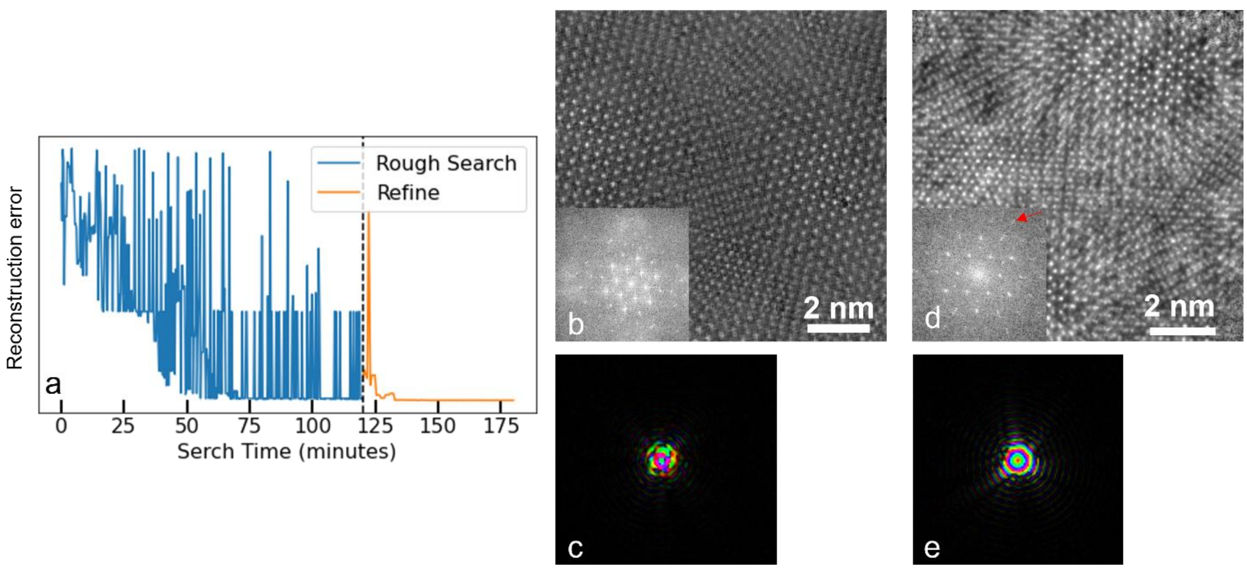

Figure 2. Application of BO to select the ptychography reconstruction parameter on 4D STEM data collected from $MoSe_2$/WS_2/BN multilayer structure. (a) the evolution of ptychography reconstruction error as BO searches for the optimized parameters. (b), (c) the reconstructed phase object and probe using default parameters read from the instrument, (d), (e) the reconstructed phase object and probe using parameters found by the BO. The phase object from parameters found by BO shows a higher information limit (pointed out by the red arrow in the Fourier transform) compare to the reconstruction using default parameters. It also reconstructs a more plausible probe shape, and the structure of phase object in the aligned region of the sample better matches the hexagonal lattice of the layers.

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