XRAI: Simulation Informed Neural Networks for Guiding Crystallography Experiments

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Protein crystallographers value rapid feedback during beamtime for guiding experiments. Commonly, a human visually scans diffraction images for signs of crystal quality. Recently, we have developed a framework for replacing this human interpreter: we have built models whose inputs are diffraction images, and whose outputs are parameters of interest. Notably, these parameters include crystal resolution/B-factor, and the presence of multi-lattice scattering, determined on a per-shot basis. **Most importantly, we train the models using simulated diffraction images, providing us full control over the space of learnable parameters.** The simulations, however, are sufficiently realistic such that the trained models perform well when tested on real user data. These diffraction AI models, which we collectively call XRAI, can easily be incorporated at different user facilities, due to their simplicity, requiring a single image array as input.

During the talk, we will discuss the development of these models, from their underlying architectures to the simulation software used to create their training data. We will also explore how XRAI is incorporated in the Structural and Molecular Biology beamlines at the Stanford Synchrotron, and how other beamline groups might tune the models to their specific needs.