

Variational Inference for Scaling Unconventional Diffraction Data

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In order to obtain electron density, integrated reflection intensities must be averaged and converted to structure factors. Intensities cannot be merged directly because they are contaminated with systematic errors which vary throughout the data set. These errors originate from a variety of sources including the volume of crystal in the X-ray beam, the mosaic properties of the crystal, and fluctuations in beam intensity. In the conventional setting, it is straightforward to correct these errors through an optimization algorithm known as scaling. In the case of serial and time-resolved crystallography, scaling is complicated by the experimental design. Unlike conventional, rotation-method crystallography, reflections originating from short, monochromatic X-ray pulses are partial; they do not reflect the full intensity of the corresponding Bragg peak. Partiality may either be corrected using a model of the Bragg peaks' shape or by averaging over a large number of images. I will present a third alternative which is agnostic to the lineshape of Bragg peaks and works with a small number of images. This method uses a statistical technique known as variational inference combined with deep learning to jointly learn structure factors along with a scaling model. In this way, the model chooses the optimal corrections for each particular experiment. Though it is applicable to conventional data as well, I anticipate this technique will be most valuable for time-resolved and serial experiments with both mono and polychromatic X-rays.