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Hierarchical Bayesian approach for adaptive integration of Bragg peaks in time-of-flight neutron scattering data

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The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) operates in the event mode. Time-of-flight (TOF) information about each detected neutron is collected separately and saved as a descriptive entry in a database enabling unprecedented accuracy of the collected experimental data. Nevertheless, the common data processing pipeline still involves the binning of data to perform analysis and feature extraction. For weak reflections, improper binning leads to sparse histograms with low signal-to-noise ratios, rendering them uninformative. In this study, we propose the Bayesian ML approach for the identification of Bragg peaks in TOF diffraction data. The method is capable of adaptively handling the varying sampling rates found in different regions of the reciprocal space. Unlike histogram fitting methods, our approach focuses on estimating the true neutron flux function. We accomplish this by employing a profile fitting algorithm based on the event-level likelihood, along with a multiresolution histogram-level prior. By using this approach, we ensure that there is no loss of information due to data reduction in strong reflections and that the search space is appropriately restricted for weak reflections. To demonstrate the effectiveness of our proposed model, we apply it to real experimental data collected at the TOPAZ single crystal diffractometer at SNS.

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