Poster

A Robust Beamstop Shadow Outlier Rejection: Combining Crystallographic Statistics with Modern Clustering Method

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In crystallographic diffraction experiments, outlier reflection intensities occur as a result of unaccounted-for or partially masked beamstop shadows and are a known issue in both manual and automatic data reduction [1, 2]. Traditional statistical diagnostics have only limited effectiveness in identifying these outliers, termed Not-Excluded-unMasked-Outliers (NEMOs). The diagnostic tool AUSPEX [3] now allows visual inspection of NEMOs, revealing that they typically exhibit a pattern of clusters at the low-resolution end of the AUSPEX plots of intensity or amplitudes versus *d*-spacing.

By combining statistical inference with machine learning concepts such as clustering and hyperparameter tuning, we have developed a method to identify and exclude NEMOs with better reliability than previously possible. Our approach suggests that by accurately pinpointing the source and recognizing the pattern of the corresponding error (which is only possible with sufficient amount of raw data deposition [4]), it becomes feasible to exclude such errors during automatic data processing.

Re-refinement results indicate that excluding the identified NEMOs can effectively enhance the quality of subsequent structure determination steps.

In this talk, we will reason the resilience of NEMOs, explain the new automatic detection method (**Fig. 1**) and demonstrate how it can be used in AUSPEX (e.g. determine the inner-shell resolution without unnecessary loss of information.)

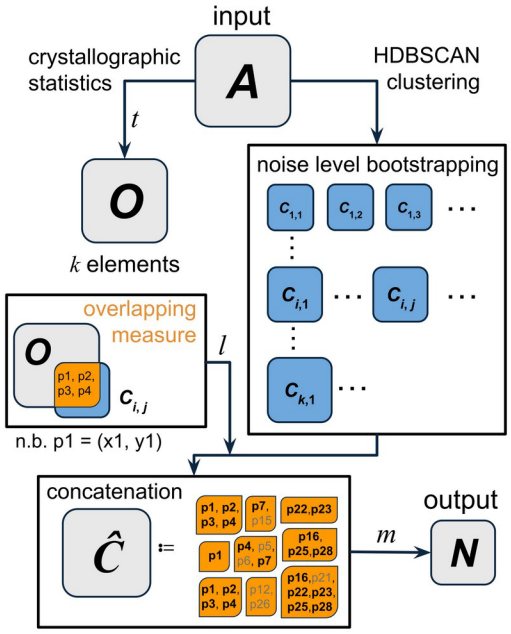

Figure 1. Schematic workflow of the automatic NEMO detection algorithm.

[1] Read, R. J. (1999). *Acta Crystallogr. D Biol. Crystallogr.* **55**, 1759–1764.

[2] Read, R. J. & McCoy, A. J. (2016). *Acta Crystallogr. D Struct. Biol.* **72**, 375–387.

[3] Thorn, A., Parkhurst, J., Emsley, P., Nicholls, R. A., Vollmar, M., Evans, G. & Murshudov, G. N. (2017). *Acta Crystallogr. D Struct. Biol.* **73**, 729–737.

[4] Gao, Y., Thorn, V. & Thorn, A. (2023). *Acta Crystallogr. D Struct. Biol.* **79**, 206–211.