MS20-O2

Nonisomorphism - diagnostics and metrics

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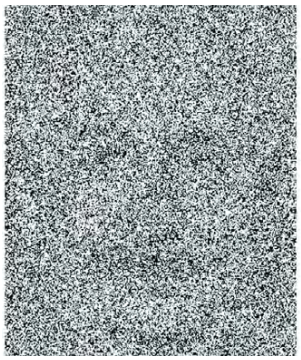
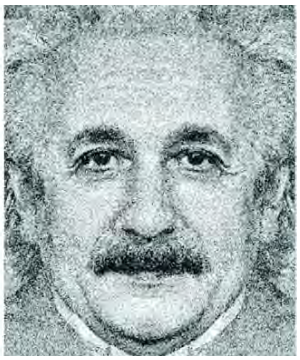
Datasets measured from different crystals are affected by both random and systematic errors. Systematic errors may arise from different properties of the crystals (e.g. composition and conformation of molecules, or their hydration state) or from experimental conditions (e.g. beam fluctuations or detector non-linearities). Datasets differing systematically are called non-isomorphous, and current crystallographic procedures are far from being able to capture and analyse the various sources of systematic error.

Often, a correlation coefficient is used for inter-dataset comparison [1], but the relations between datasets are not obvious from the matrix of pairwise correlations since the numerical value of the correlation coefficient is lowered by both random and systematic differences. It is therefore desirable to develop methods that can separate random and systematic effects on data.

The talk presents a novel type of analysis [1] of the pairwise correlation coefficients which positions datasets within a low-dimensional space whose axes are associated with the types of systematic differences between the datasets. This dimensionality reduction can not only be used for classification purposes (e.g. to find out which datasets are so similar in their properties that they can be merged), but can also derive dataset relations on a continuous scale, and directly relates to previous work [3] which introduced CC1/2 for describing the precision of crystallographic data.

This novel analysis has numerous applications in Structural Biology, but also in other fields.





References:

[1]. Diederichs, K. (2017) Dissecting random and systematic differences between noisy composite data sets. Acta Cryst. D73, 286-293.Keywords: nonisomorphism, data quality, heterogeneity

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MS20-O3

Combining a nine-crystal multianalyser stage with a Pilatus3 X CdTe detector for high-resolution X-ray powder diffraction at ESRF-ID22

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The high-resolution powder diffraction beamline at ESRF (ID22), built with a dual-undulator source on the 6 GeV storage ring, combines a wide continuous range of incident energy (6-80 keV) with high brightness, offering the possibility to carry out high-flux, high-resolution powder diffraction measurements above 30 keV. In routine operation, a bank of nine scintillation detectors is scanned vertically to measure the diffracted intensity as a function of 2θ, each detector being preceded by a Si 111 analyzer crystal. The current detector system has operated successfully for the past 20 years. Nevertheless developments in detector technology can be exploited to improve the overall performance. In particular, at low diffraction angle, the axial acceptance of the detectors results in broadened and asymmetric peaks owing to the curvature of the Debye-Scherrer cones. At high diffraction angles, detection efficiency could be improved by up to an order of magnitude by increasing the axial acceptance of the detectors as the scattering power of the sample falls off naturally. In order to improve the detection efficiency behind the 9 analyzer crystals, a Pilatus3 X CdTe 300K-W was mounted on the arm of the diffractometer, and used for standard continuous-scanning acquisition on several test samples (Si, LaB6, ceria, ZSM-5 zeolite). By using a small area detector, the axial aperture can be varied with 2θ, narrow at low angles where the curvature is most marked, and wider at higher angles, where the curvature is less. In this way, as well as increasing overall counting efficiency, resolution and peak shapes at low angle are improved as compared to the current fixed, 4-mm-wide receiving aperture. In addition, by carefully selecting the diffraction region on the 2D images, parasitic signals can be avoided. Combining the high efficiency of a hybrid photon-counting area detector with the high resolution given by analyzer crystals is an effective approach to improving the overall performance of high resolution powder diffraction.

Keywords: high-resolution X-ray powder diffraction, Pilatus detector