Poster Presentation

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Explicit and Implicit data merging in Crystallographic Least Squares

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For single crystals and twins the assumption that the background can be subtracted from an integrated intensity and the result regarded as a complete observation introduces a systematic error that is worst for the weakest reflections. Refinement and difference maps will be improved if the background is included in a model of peak-plus-background and the background and its associated error is known. A recent review [1] showed how an intensity associated with a sampling point in reciprocal space may be described in terms of partial observations that describe uncorrelated components of the intensity, one of which is the background. Thus Yo(h), the square root of the observed intensity, may be described as the vector sum of orthogonal components and the direction of Yo(h) is defined by an initial model that evolves with refinement. For any least squares refinement cycle the direction and magnitude of Yo(h) is assumed to be fixed by an initial model but Yo(h) does have a variance and the orthogonal components define partial observations. The variance of a residual |Yo(h)| - |Yc(h)| can also be subdivided into contributions that include the background. We can then can assess the fraction of a residual that is being refined and how much of that fraction is associated with individual parameters or combination of parameters. If we assume a variance for an unrefined parameter or combination of parameters we can evaluate what fraction of the total number of observations this is associated with. These ideas allow error distribution and the number of partial observations to be assessed for any feature of the model of the diffraction pattern. The refinement of partial observations of the integrated intensities can be separated from the refinement of the background and peak shapes. Information about the various integrated intensities is duplicated in different parts of the diffraction data. Proper notice should be taken of this duplication to obtain an integrated intensity and its associated partial observation.

[1] *Rae. A.D., (2013) "The use of partial observations, partial models, and partial residuals to improve the least squares refinement of crystal structures ", Crystallography Reviews, Vol. 20, 155-229, Taylor & Francis.*

Keywords: Least squares refinement, partial observations, data merging