

MS38 Computations with/for Pair Distribution Functions

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Unsupervised and supervised machine learning for total scattering and PDF analyses

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Abstract

I will describe recent efforts to apply machine learning to the analysis of total scattering and PDF data and modelling. This includes the use of deep neural nets for finding the unknown space-group of a measured PDF and automatically finding chemically reasonable components in large sets of powder diffraction and PDF measurements from, for example, an in situ synthesis experiment, using unsupervised machine learning methods. I will also present preliminary results of applying variational conditional autoencoders to do structure solution from PDF data, at least in a very limited way. Some of these tools are available as cloud-hosted web services at PDFitc.org and are free to use by the community.

References

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