Data-driven Phasing Algorithms for Bragg Coherent Diffractive Imaging

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Immediately following the announcement of Shannon' Information Theorem, David Sayre proposed a solution to the crystallographic "phase problem": if diffraction can be sampled more than twice as finely as the Bragg peak spacing, the problem is overdetermined and can be solved [1]. Sayre did not explicitly mention the need for X-ray coherence, which has been happily solved with the development of the latest synchrotron sources. This produces speckle in the diffraction patterns which can be oversampled to overdetermine the phase problem. Sayre also did not specifically propose a closed form solution of the phase problem either, and that is lacking to this day. Many methods have been proposed to invert the diffraction to real space images over the 68 years since, all of them iterative algorithms that converge on the solution. But despite "proofs" to the contrary, these methods are usually prone to local minima giving multiple solutions with real experimental data containing noise. In this presentation we will introduce the possibility that the speckle inversion "phase problem" may be amenable to data-driven Machine Learning approaches in the future. Our first demonstration is published [2] and a more general 3D result is submitted [3].

[1] Some implications of a theorem due to Shannon, D. Sayre, Acta Cryst. 5, 843 (1952).

[2] Complex Imaging of Phase Domains by Deep Neural Network Longlong Wu, Pavol Juhas, Shinjae Yoo and Ian Robinson, IUCrJ 8 12-21 (2021)

[3] 3D Coherent X-ray Imaging via Deep Convolutional Neural Networks, Longlong Wu, Shinjae Yoo, Ana F. Suzana, Tadesse A. Assefa, Jiecheng Diao, Ross J. Harder, Wonsuk Cha and Ian K. Robinson, to be published
https://arxiv.org/ftp/arxiv/papers/2103/2103.00001.pdf