

THE UNIVERSITY OF CHICAGO

Computational and Applied Mathematics & Statistics Student Seminar

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Prior-Free Characterization of Multimodal X-ray Reflectivity Landscapes through Smooth Forward Modeling

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ABSTRACT

Structural parameters of interfaces are obtained from specular reflectivity by fitting a forward model to the data, and the resulting fitting landscapes are often multimodal. Many analyses will explore these landscapes starting from a fitted point and subsequently enforce priors and constraints during a search, under-examining structures from other basins in the landscape and conflating analysis choices with the data. We argue that smoothness of the forward model with respect to its parameters should be a key design consideration, because it determines which optimization, sampling and diagnostic methods can be used effectively, and furthermore enables a prior-free search which disentangles exploration from basin weighting. As a case study, we reimplement the XModFit model for X-ray reflectivity from lipid monolayers, liquid-liquid interfaces and protein-lipid films as a continuously differentiable model with automatic differentiation (XPR). XPR reproduces the reflectivity of the original implementation to within 1.6% and evaluates 2-11 times faster. Smoothness makes a simple multistart protocol effective: for 76 datasets it yields a catalog of 3,720 certified local minima, from 3-7 per dataset for two-box lipid models to 42--104 for protein-lipid models. The catalogs reveal a near-degenerate pair of lipid structures in every two-box dataset, pairs of liquid-liquid minima related by reversal of the profile, two classes of protein-lipid solutions, and protein orientations that the data do not determine. The number of minima grows with the range of momentum transfer included in the fit. Applied to the original, nonsmooth implementation, the same protocol finds only 2-6 minima per protein dataset, because most of its local optimizations stop at discontinuities.