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Model comparison in X-ray crystallography DAVID SIVAK, NATHAN BABCOCK, Dept. of Physics, Simon Fraser University, DANIEL KEEDY, JAMES FRASER, Dept. of Bioengineering and Therapeutic Sciences, University of California, San Francisco — X-ray crystallographers conventionally infer a single best-fit structure from experimental data. Recently, attention has turned to inference of multiple structures and more generally to more complex model types that improve quality of fit—yet potentially increase overfitting to experimental noise. Significant research effort has been focused on inferring the best-fit parameters within a given model type, yet comparatively little attention has been given to selection between model types. Using metrics from the statistics community, we develop a model comparison framework for statistically-rigorous inference of protein conformational heterogeneity. We compare these information criteria to conventional model comparison criteria, and we assess their utility for judging different model types on their balance between quality of fit and model parsimony.

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