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Breaking the barriers in understanding your data: Unbiased model selection for muon spin relaxation spectroscopy

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The analysis of muon spin relaxation experiments typically relies on model fitting under conditions that are ill-posed. Typically models are selected to fit the data based on the inductive bias (physical intuition) of the experimentalist. Although recent studies have demonstrated the application of unsupervised machine learning to automatically detect model changes [https://doi.org/10.1088/1361-648x/abe39e], the use of physical models remains essential for gaining insights into the physics and chemistry of the systems under study. This invites the question - can we use a principled approach, in concert with the inductive bias of experienced researchers to select the best models for fitting a given data set? In this contribution we demonstrate how Bayesian model selection can be applied to select the optimal model from a finite set, for fitting data from a given experiment, avoiding both over- and under-fitting. We use a series of simulated experimental data sets, with different underlying models and levels of noise. We show how comparison of Bayes factors, obtained by integration of Markov Chain Monte Carlo (MCMC) sampling of the parameter space, provides robust and principled comparison of possible models for fitting the data, and also provides parameter estimation with associated uncertainties. The latter can be used to determine the point at which sufficient experimental data have been collected to satisfactorily assign parameters to the underlying model. Finally, we also explore the application of nested sampling [https://doi.org/10.1063/1.1835238], a method of efficiently sampling posterior distributions, which could allow the extension of this scheme of model selection to higher-dimensional models (D>5) while remaining computationally tractable.

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