Title: Optimizing Markov State Models for enzymes (Robert Arbon)

Understanding the dynamics and stationary properties of enzymes is a key problem chemistry and biology. Being able to predict their properties could lead to new medical treatments and therapies as well as improving our fundamental understanding of nature. The transfer operator contains all the necessary information, through it's eigenvalues and eigenvectors, to understand such systems [1]. Using high-throughput molecular simulation it is now possible to estimate this operator's eigenspectrum by constructing a Markov state model. However, constructing such a model leaves open a wide variety of choices for the researcher which could lead to biased or misleading results. My work is focused on optimising an MSM's hyper-parameters using cross validation [2] and Bayesian optimisation with Gaussian process priors [3] and understanding their relationships to the properties of the model.

[1] Nu, F. et al., 2014. Variational Approach to Molecular Kinetics. J. Chem. Theory Comput. 2014, 10, 1739−1752
[2] McGibbon, R.T. & Pande, V.S., 2015. Variational cross-validation of slow dynamical modes in molecular kinetics. Journal of Chemical Physics, 142(12).
[3] Snoek, J., Larochelle, H. & Adams, R.P., Practical Bayesian Optimization of Machine Learning Algorithms.