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A Bayesian Data Modelling Framework for Chemical Processes using Adaptive Sequential Design with Gaussian Process Regression

Chemical Processes are traditionally simulated using physical computer models to capture the highly non-linear behaviours exhibited by features such as reaction kinetics and recycle loops. Traditional statistical models have been, historically, poor predictors of process performance. Here, an alternative, Bayesian treatment of a process modelling problem is presented, modelled on an existing process simulator as a proof-of-concept. We present a poster examining how Gaussian Process Regression (GPR) may be used to overcome the inflexibility of typical statistical modelling techniques and introduce an inherently probabilistic treatment of our modelling problem. In tandem, we also explain the advantages of a Bayesian adaptive design of experiments for chemical processes and explore the implementation details of such an approach as applied to our process simulator.

An iterative procedure combining sequential design and GPR is outlined, with some thoughts given on model selection for GPR and a kernel principal component analysis (kPCA) based method of dimensionality reduction. We present our results from a GPR model fitted to 104 data points over a noiseless process simulator which show good predictive performance (maximum error under 5%, typical error under 1%) over an unseen test set of 20 points, with little evidence to suggest overfitting. We finish by looking at the limitations of our framework with respect to noise and data resolution and forward some developments for the framework.

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