A Gaussian Process Approach for Accelerating Parameter Inference over Nonlinear ODEs

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Abstract

Nonlinear dynamical models consisting of multiple interacting differential equations are frequently employed to describe the behaviour of a wide variety of biochemical systems. Such mechanistic approaches to modelling however are made difficult by an incomplete knowledge of the system structure and/or the specific parameter values defining the observed behaviour. Standard Bayesian and indeed non-Bayesian methods for model comparison and parameter estimation involve evaluating likelihood functions, which requires the explicit numerical solution of the differential equations describing the model. This computationally expensive task must often be repeated hundreds of thousands of times during the inference/optimisation procedure, resulting in extremely slow running times, particularly as the number of species and parameters employed in the model increases. This is exacerbated in models exhibiting sloppy characteristics. We present a novel alternative method employing nonparametric regression which avoids the need to explicitly solve the differential equations and allows greatly accelerated sampling of the required posterior distributions within the Bayesian framework. We demonstrate our method on a nonlinear ODE model describing the dynamics of spike potentials in neurons, and also on a DDE model describing transcription in a genetic regulatory network, for which our approach is around 400 times faster than standard methods.