A Hamiltonian Monte Carlo-based method for boosting Bayesian parameter inference of stochastic differential equation models

Simone Ulzega, Carlo Albert

Eawag, Swiss Federal Institute of Aquatic Science and Technology
Überlandstrasse 133, 8600 Dübendorf (ZH), Switzerland

Bayesian parameter inference is a fundamental problem in data-driven modeling. Given observed data, which is believed to be a realization of some parameterized model the aim is to find a distribution of likely parameter values that are able to explain the observed data. This so-called posterior distribution expresses the probability of a given parameter to be the "true" one, and can be used for making probabilistic predictions. For truly stochastic models this posterior distribution is typically extremely expensive to evaluate. We propose a novel, exact and very efficient Hamiltonian Monte Carlo approach for generating posterior parameter distributions, for stochastic differential equation models calibrated to measured time-series. The algorithm is inspired by re-interpreting the posterior distribution as a statistical mechanics partition function of an object akin to a polymer, whose dynamics is confined by both the model and the measurements. We thus reduce the Bayesian inference problem to simulating the dynamics of a linear polymer represented by a chain of coupled harmonic oscillators in an external non-harmonic potential. Our approach is applicable to a wide range of inference problems and is highly parallelizable.