Bayesian Inference with Optimal Maps

Predictive modeling of complex physical systems: new tools for statistical inference, uncertainty quantification, and experimental design

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Abstract

Bayesian inference provides a natural framework for quantifying uncertainty in parameter estimates and model predictions, for fusing heterogeneous sources of information, and for conditioning sequential predictions on data. Posterior simulation in Bayesian inference often proceeds via Markov chain Monte Carlo (MCMC), but the associated computational expense and convergence issues can present significant bottlenecks in large-scale problems.

We present a new approach to Bayesian inference that entirely avoids Markov chain simulation, by constructing a map that *pushes forward* the prior measure to the posterior. Existence and uniqueness of a suitable measure-preserving map is established by formulating the problem in the context of optimal transport theory. We discuss various means of explicitly parameterizing the map and computing it efficiently through solution of an optimization problem, exploiting gradient information from the forward model when possible. The resulting scheme overcomes many of the computational bottlenecks associated with MCMC. Advantages of the map-based representation of the posterior distribution include analytical expressions for posterior moments and the ability to generate arbitrary numbers of independent posterior samples without additional likelihood evaluations or forward solves. The approach also provides clear convergence criteria for posterior approximation, and facilitates model selection through automatic evaluation of the marginal likelihood.

We demonstrate the accuracy and efficiency of the method on nonlinear inverse problems of varying dimension, involving point and distributed parameters appearing in ordinary and partial differential equations.