EXPLORING THE CONNECTION BETWEEN SAMPLING PROBLEMS IN BAYESIAN INFERENCE AND STATISTICAL MECHANICS

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Abstract

The Bayesian and statistical mechanical communities often share the same objective in their work – estimating and integrating probability distribution functions (pdfs) describing stochastic systems, models or processes. Frequently, these pdfs are complex functions of random variables exhibiting multiple, well separated local minima. Conventional strategies for sampling such pdfs are inefficient, sometimes leading to an apparent non-ergodic behavior. Several recently developed techniques for hadling this problem have been successfully applied in statistical mechanics.

In the multicanonical and Wang-Landau Monte Carlo (MC) methods, the correct pdfs are recovered from uniform sampling of the parameter space by iteratively establishing proper weighting factors connecting these distributions. Trivial generalizations allow for sampling from any chosen pdf. The closely related transition matrix method relies on estimating transition probabilities between different states. All these methods proved to generate estimates of pdfs with high statistical accuracy. In another MC technique, parallel tempering, several random walks, each corresponding to a different value of a parameter (e.g. "temperature"), are generated and occasionally exchanged using the Metropolis criterion. This method can be considered as a statistically correct version of simulated anneling.

An alternative approach is to represent the set of independent variables as a Hamiltonian system. Considerable progress has been made in understanding how to ensure that the system obeys the equipartition theorem or, equivalently, that coupling between the variables is correctly described. Then a host of techniques developed for dynamical systems can be used. Among them, probably the most powerful is the Adaptive Biasing Force method, in which thermodynamic integration and biased sampling are combined to yield very efficient estimates of pdfs.

The third class of methods deals with transitions between states described by rate constants. These problems are isomorphic with chemical kinetics problems. Recently, several efficient techniques for this purpose have been developed based on the approach originally proposed by Gillespie.

Although the utility of the techniques mentioned above for Bayesian problems has not been determined, further research along these lines is warranted.