Optimally adjusted mixture sampling and locally weighted histogram analysis

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Consider the two problems of simulating observations and estimating expectations and normalizing constants for multiple distributions. First, we present a self-adjusted mixture sampling method, which accommodates both adaptive serial tempering and a generalized Wang-Landau algorithm. We propose two stochastic approximation schemes by Rao-Blackwellization of the scheme commonly used, and derive the optimal choice of a gain matrix, resulting in the minimum asymptotic variance for free energy estimation, in a simple and feasible form. Second, we develop an offline method, locally weighted histogram analysis, for estimating free energies and expectations, using all the simulated data from multiple distributions by either self-adjusted mixture sampling or other schemes. This method can be computationally much cheaper, with little sacrifice of statistical efficiency, than a global method currently used, especially with a large number of distributions. We provide both theoretical results and numerical studies to demonstrate the advantages of the proposed methods.

Keywords: Markov chain Monte Carlo; Normalizing constant.