# Analysis and optimization of certain parallel Monte Carlo methods in the low temperature limit

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**Abstract**

Metastability is a formidable challenge to Markov chain Monte Carlo methods. In this talk we present methods for algorithm design to meet this challenge. The design problem we consider is temperature selection for the infinite swapping scheme, which is the limit of the widely used parallel tempering scheme obtained when the swap rate tends to infinity. We use a recently developed tool for the large deviation properties of the empirical measure of a metastable small noise diffusion to transform the variance reduction problem into an explicit graph optimization problem. The nodes in the graph optimization problem correspond to metastable states of the noiseless dynamics. Our first analysis of the optimization problem is in the setting of a double well model, and it shows that the optimal selection of temperature ratios is a geometric sequence except possibly the highest temperature. In the same setting we identify two different sources of variance reduction, and show how their competition determines the optimal highest temperature. In the general multi-well setting we prove that the same geometric sequence of temperature ratios as in the two-well case is always nearly optimal, with a performance gap that decays geometrically in the number of temperatures. Moreover, this optimal placement of temperatures is explicit and independent of the particular functional being integrated on the potential.

**Keywords:** large deviations, metastability, Monte Carlo, parallel tempering, infinite swapping, Gibbs measures, variance reduction

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