Physics > Data Analysis, Statistics and Probability

On Stochastic Error and Computational Efficiency of the Markov Chains Monte Carlo Method

J. Li, P. Vignal, S. Sun, V. M. Calo

(Submitted on 14 Apr 2012)

In Monte Carlo simulations, the thermal equilibria quantities are estimated by ensemble average over a sample set containing a large number of correlated samples. As the stochastic error of the simulation results is significant, it is desirable to understand the variance of the estimation by ensemble average, which depends on the sample size (i.e., the total number of samples in the set) and the sampling interval (i.e., cycle number between two consecutive samples). Although large sample sizes reduce the stochastic error, they increase the computational cost of the simulation. In this work, we report a few general rules that relate the variance with the sample size and the sampling interval. These relations were observed in our numerical results. The main contribution of this work is the theoretical proof of these numerical observations and the set of assumptions that lead to them.

Comments: {\em Journal of Computational Physics}, submitted, 2012
Subjects: **Data Analysis, Statistics and Probability (physics.data-an)**
Cite as: **arXiv:1204.3176 [physics.data-an]**
(or **arXiv:1204.3176v1 [physics.data-an]** for this version)

Submission history

From: Jun Li [view email]
[v1] Sat, 14 Apr 2012 14:37:26 GMT (804kb,D)

Which authors of this paper are endorsers?