FICS COMP-IT Summer School August 16-20, 2010: "Markov Chains and Monte Carlo Simulations Without Detailed Balance"

Problem description and background

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1 Introduction

One of the most powerful simulation methods in physics, namely the Monte Carlo (MC) simulation method, is based on the theory of Markov chains. In virtually all practically applied simulation algorithms, the convergence of the Markov chain to its equilibrium distribution is guaranteed by enforcing the so-called detailed balance condition (DBC) between the transition rates. However, while DBC is sufficient, it is not necessary for the convergence of the chain to its equilibrium distribution. Can Monte Carlo be done more efficiently by not imposing the detailed balance condition?

2 Markov Chain and Detailed Balance

Let us consider a system with a discrete and finite number of states $\{r_i\}$, where $i = 1, 2, 3, ..., N$. A Markov Chain is a stochastic process, where the probability to be in state r_i only depends on the probability (density) p of being in a previous state r_{i-1}, and not on the other states, i.e.

$$p(r = r_i | r_1, r_2, r_3, ..., r_{i-1}) = p(r_i | r_{i-1}), \tag{1}$$

where $p(\cdot|\cdot)$ denotes the usual conditional probability density. Thus, Markov chains have no memory beyond their present state, and from this follows a number of powerful mathematical results concerning their properties.

If we consider a discrete, homogenous Markov chain in a configuration space Ω, we can define the (normalized) transition probabilities between states r_i and r_j to be given by $P_{ij} = P(r_i, r_j)$. If these are represented as the elements of a $N \times N$ transition matrix $\mathbf{P}$, an equilibrium or steady-state configuration of the Markov chain can be defined by the condition

$$\mathbf{P} \cdot \mathbf{p}_{eq} = \mathbf{p}_{eq}, \tag{2}$$

where the vector $\mathbf{p}_{eq} = [p_1^{eq} p_2^{eq} p_3^{eq} ... p_N^{eq}]^T$ contains all the elements of the state probability densities p_i. In particular, if the Markov chain is finite ($N < \infty$) and regular ($\mathbf{P}^n > 0 \ \forall \ n$), the steady-state is unique. If we assume that temporally the Markov chain evolves from some initial state $\mathbf{p}_0$ by constant rate of transitions from each state i to state j, the rate of change of the probability densities follows the Master equation

$$\frac{\partial p_i}{\partial t} = -\sum_{j=1}^{N} [w_{ij} p_i - w_{ji} p_j]. \tag{3}$$

The quantities w_{ij} are the transition rates, defined by $w_{ij} = P_{ij}/\tau$, where τ is some (arbitrary) transition time. From the last equation follows the usual DBC as

$$P_{ij} p_i^{eq} = P_{ji} p_j^{eq}. \tag{4}$$

Obviously, this condition is sufficient but *not necessary*, since there's no fundamental reason why each transition should pairwise satisfy Eq.(4).

3 Boltzmann Distribution

If the detailed balance condition is enforced, it is easy to use it to construct any desired equilibrium probability distribution. For example, in a canonical Monte Carlo simulation, we require the distribution to be of Boltzmann type

$$p_i^{eq} = \exp(-\beta E_i)/Z, \tag{5}$$

where E_i is the energy (function) associated with state i, Z is the partition function (normalization constant), and $\beta = 1/k_B T$ the inverse temperature (thermal energy). Using DBC gives simply that

$$\frac{P_{ij}}{P_{ji}} = \exp[-\beta(E_j - E_i)]. \tag{6}$$

Thus, any Markov chain where the ratio of the transition probabilities satisfies Eq.(6), converges to the unique canonical Boltzmann distribution at fixed temperature T. One such simple choice is given by the form

$$\begin{aligned} w_{ij} &= \frac{1}{\tau} e^{-\beta(E_j - E_i)}, \text{ for } E_j - E_i > 0; \\ &= \frac{1}{\tau}, \text{ for } E_j - E_i \leq 0. \end{aligned} \tag{7}$$

This forms the basis of the Metropolis Monte Carlo simulation method.

4 Formulation of the Research Problem

The research problem formulated here concentrates on studying alternative schemes for realizing a Monte Carlo Markov chain without having to evoke DBC. While such alternative schemes may be relatively easy to construct, the essential question is their performance as compared to the usual DBC Monte Carlo schemes, such as the Metropolis scheme. To this end, it may be useful to apply and test such alternative schemes in the context of a simple model, such as the 2D ferromagnetic Ising model, for which an exact solution is know for its critical properties. The Ising model has served as a generic test bench model in the literature for new simulation algorithms, and it should be well suited for the present purposes, too.