Singapore-MIT Alliance, CME5233 – Particle Methods and Molecular Dynamics

Tutorial 5, Monday 2:30 – 4:00, 4 Dec 2006

1. Write down the transition matrix W for a one-dimensional 3-spin Ising system with periodic boundary condition using Metropolis flip rate, where a spin is picked at random, and flip is accepted with probability min$[1, \exp(-\Delta E/(kT))]$. What is W if site is scanned sequentially? The energy function of a one-dimensional Ising model is

$$E(\sigma) = -J\sum_{i=0}^{N-1} \sigma_i \sigma_{(i+1) \bmod N}, \quad \sigma_i = \pm 1.$$

   Note that N=3 system has 2^3 possible states.

2. Consider the Ising model. One way to simulate the Ising model is to pick a site at random and flip the spin with probability min$[1, \exp(-\Delta E/(kT))]$. Show that the detailed balance is satisfied also for
   (a) (Glauber dynamics) Flip the spin with probability

$$\frac{1}{2}\left[1-\sigma_i \tanh\left(\frac{J}{kT}\sum_{\langle i,j\rangle}\sigma_j\right)\right],$$

   where site i is the center site whose spin is to be flipped; the summation is over the nearest neighbors of the center site.
   (b) (Heat-bath algorithm) Reset of the center spin as

$$\sigma_i = \mathrm{sign}\left(\xi - \frac{e^{-\Delta}}{1+e^{-\Delta}}\right), \quad \Delta = \frac{2J}{kT}\sum_{\langle i,j\rangle}\sigma_j$$

   where ξ is a uniformly distributed random number between 0 and 1.

3. Consider the ratio of two-dimensional integrations:

$$\frac{\int_0^1 dx \int_{-\infty}^{+\infty} dy \, \log(x+1)\, e^{-xy^2}}{\int_0^1 dx \int_{-\infty}^{+\infty} dy \, e^{-xy^2}}.$$

   Design a complete pseudo-code of a Metropolis algorithm for the numerical evaluation of the expression.