Physics of Complex Systems

Université Pierre et Marie Curie (Paris VI)

Advanced simulation techniques and mathematical tools

(19 December 2012 - duration: 3h)

The exam consists of three independent parts. The questions of each part are also independent and can be solved by using previous results. It is not necessary to answer all questions to obtain full credit.

Lecture notes are allowed.

1 Balance and detailed balance

The detailed balance fulfills the condition of convergence towards equilibrium for a stochastic process illustrated by the Monte Carlo method. One considers here a new algorithm based on the balance equation which provides a better convergence towards equilibrium. For a lattice model, one considers that by starting from a given configuration, n **configurations are available** (including the current one) for the next configuration. The equilibrium weight of a configuration i is given by p_i.

▷ **1-1** By introducing the raw stochastic flow (probability current in the space of configurations visited by the algorithm) from the state i to j, $v(i \to j) = p_i w(i \to j)$ where $w(i \to j)$ is the transition matrix element between states i and j, and by using the probability conservation, show that

$$p_i = \sum_{j=1}^{n} v(i \to j), \ \forall i \tag{1}$$

▷ **1-2** By using the fact that p_i is a stationary solution of the problem and that $w(i \to j)$ can be interpreted as a conditional probability distribution, show that

$$p_i = \sum_{j=1}^{n} v(j \to i), \ \forall i \tag{2}$$

▷ **1-3** Show that the Metropolis algorithm can be reexpressed as

$$v(i \to j) = \frac{1}{n-1} min(p_i, p_j) \text{ for } i \neq j \tag{3}$$

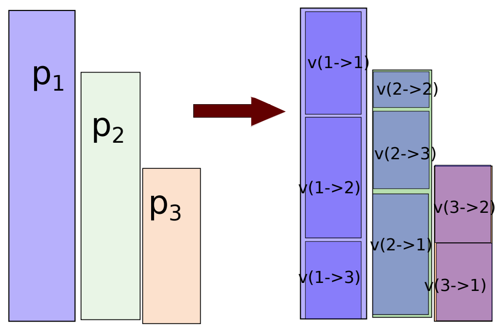

Figure 1: Metropolis algorithm: 3 configuration weights (left side) and rate stochastic flows (right side) .

▷ **1-4** How is the detailed balance expressed in terms of raw stochastic flow?

▷ **1-5** Figure 1 shows the interpretation of the Metropolis algorithm in terms of raw stochastic flows for 3 configurations. The area of each box (p_1, p_2, p_3) corresponds to the weights of the three configurations. Explain why the flow stochastic rate fills each box and why the right box does not contain $v(3 \to 3)$.

▷ **1-6** The average rejection rate R corresponds to the ratio of the number of rejected configurations over the total number of configurations, show that R can be expressed as a function of all $v(i \to i)$ and p_i.

▷ **1-7** Draw a similar figure with 4 configurations such that $p_1 = 3p_4$, $p_2 = p_3 = 2p_4$. Hint: Consider first the box 4 and draw the figure such that p_4 is corresponds to 3 unit lengths..

A new algorithm is proposed (see Fig. 2): first the maximum weight (p_1) is allocated to the second box. It saturates the second box, and the remainder is all put into the third one. Next, p_2 is allocated to the partially filled box and the box 1. The same procedure is repeated for p_3.

▷ **1-8** Why is this algorithm rejection free?

▷ **1-9** Why the detailed balance is broken and what about the balance condition?

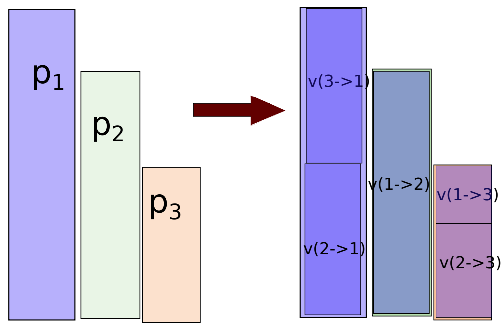

Figure 2: New algorithm :3 configuration weights (left side) and rate stochastic flows (right side) .

2 Optimal finite time process in thermodynamics

We consider below a system which is driven through the application of an external time-dependent control parameter $\lambda(\tau)$. The following Langevin equation describes the driven over-damped motion of a single degree of freedom x in a 1D potential $V(x, \lambda)$,

$$\dot{x}(\tau) = -\mu \frac{\partial V(x, \lambda(\tau))}{\partial x} + \xi(\tau), \tag{4}$$

where $\xi(\tau)$ is a Gaussian white noise such that $\langle \xi(\tau) \rangle = 0$ and $\langle \xi(\tau)\xi(\tau') \rangle = 2\mu k_B T \delta(\tau - \tau')$. For the sake of simplicity, one set $\mu = k_B T = 1$. Initially, the system is in equilibrium in the potential $V(x, \lambda_0)$, and we choose $\lambda_0 = 0$. During the interval $0 \leq \tau \leq t$, the control parameter is varied from λ_0 at the initial time to $\lambda_f \neq 0$ at the final time $\tau = t$. Below, we are particularly interested in the optimal protocol $\lambda^*(\tau)$ which minimizes the mean work for an imposed finite duration t of the process.

▷ **2-1** Write the expression of the work for an arbitrary potential which corresponds to a realization of this process. Explain why the work is in fact a stochastic variable, and give the expression of the mean work.

In the following, we assume that the potential is harmonic of the form

$$V(x, \tau) = \frac{1}{2}\left(x - \lambda(\tau)\right)^2. \tag{5}$$

Let us first consider two simple cases where: (i) the control parameter is varied infinitely slowly, corresponding to the quasi-static limit when $t \to \infty$ and (ii) the control parameter is varied very fast, corresponding to the limit $t \to 0$.

▷ **2-2** For both cases, obtain the expression of the mean work $\langle W \rangle$ and the variation of free energy ΔF. Why can one say that the results are compatible with the second law of thermodynamics.

▷ **2-3** Let us now return to the general problem of determining the optimal the control parameter $\lambda(\tau)$ which optimizes the mean work in a fixed given time t. To progress, introduce the variable $u(t) = \langle x(t) \rangle$ and obtain an evolution equation for this variable using the Langevin equation.

▷ **2-4** With the equation obtained above, write the mean work in terms of only $u(t)$ and its derivatives. This mean work should have the form of a sum of a boundary term plus an integral of the form $\int_0^t d\tau \dot{u}^2$, where the dot means the time derivative.

▷ **2-5** In order to optimize the mean work, one should solve the Euler-Lagrange equations associated with the mean work obtained above. In the present case, the Euler-Lagrange equation is very simple $\ddot{u} = 0$. What is the solution of this equation compatible with the boundary conditions ?

▷ **2-6** Minimize the mean work for fixed λ_f and t, and deduce from this that the optimal protocol has the form

$$\lambda^*(\tau) = \lambda_f \frac{1+\tau}{2+t}. \tag{6}$$

▷ **2-7** Deduce from the above, the expression of the optimal mean work. The result should have a compact simple form. Verify that the results obtained in question 2 for cases (i) and (ii) are recovered when $t \to \infty$ and $t \to 0$ respectively.

▷ **2-8** The optimal protocol differs from the simple linear protocol $\lambda(\tau) = \lambda_f \tau / t$. Verify that the mean work associated with that protocol is not optimal in the sense that

$$W^{lin} = (\lambda_f^2/t)^2 (t + e^{-t} - 1) > W^*, \tag{7}$$

where W^* is the optimal mean work found previously.

3 Equilibrium properties of a fully-connected Ising model

One considers an Ising model of N spins ($\sigma_i = \pm 1$) whose Hamiltonian is given by

$$H = -\frac{J_0}{N} \sum_{i<j} \sigma_i \sigma_j \tag{8}$$

where $J_0 > 0$ is the ferromagnetic strength.

▷ **3-1** By introducing the intensive variable $m = \frac{\sum_{i=1}^N \sigma_i}{N}$, express the Hamiltonian in terms of m, J_0 and N. Justify that the energy of the system is extensive in the thermodynamic limit.

▷ **3-2** Show that the ground states (corresponding to the lowest energy) are given when $\sigma_i = +1$ or $\sigma_i = -1$ for $i \in [1, n]$.

▷ **3-3** By using the formula section, show that the canonical partition function is given by

$$Z = \exp(-\beta J_0) \sqrt{\beta \frac{J_0 N}{2\pi}} \sum_{\{\sigma_i\}} \int_{-\infty}^{+\infty} dx \exp\left(-\frac{\beta J_0 N}{2} x^2 + \sum_i x \beta J_0 \sigma_i\right) \tag{9}$$

where $\{\sigma_i\}$ denotes all configurations of the system.

▷ **3-4** Summing over all configurations, show that the partition function in the large N limit is given by

$$Z = \exp(-\beta J_0) \sqrt{\frac{\beta J_0 N}{2\pi}} \int_{-\infty}^{+\infty} \exp(-N\beta f(\beta, x)) \tag{10}$$

▷ **3-5** By using the formula section, justify that $f(\beta) = min_x(f(\beta, x))$ represents the free energy per spin in the themodynamic limit.

▷ **3-6** By minimizing $f(\beta, x)$ and assuming that the value of x corresponds to the mean magnetization per spin, show that the system has a nonzero magnetization for $\beta < 1$ and equal to 0 for $\beta \geq 1$. Infer that the phase transition is continuous.

The dynamics of the system is a Markovian process which is the Glauber dynamics: The transition rate of a spin flip $\sigma_i \to -\sigma_i$ is given by

$$\pi(\sigma_i \to -\sigma_i) = \frac{1}{2}(1 - \sigma_i \tanh(\beta h_i)) \tag{11}$$

where $h_i = \frac{1}{N} \sum_{j \neq i} \sigma_i$.

▷ **3-7** Show that the dynamics satisfies the detailed balance.

One can show that the dynamics obeys

$$\frac{\partial}{\partial t} \langle \sigma_i(t) \rangle = \langle t_i(t) - \sigma_i(t) \rangle \tag{12}$$

$$\frac{\partial}{\partial t} \langle \sigma_i(t) \sigma_j(t) \rangle = \langle (t_i(t) - \sigma_i(t)) \sigma_j(t) \rangle + \langle (t_j(t) - \sigma_j(t)) \sigma_i(t) \rangle \text{ for } i \neq j \tag{13}$$

where the brackets denotes over the thermal history of the system and over initial conditions, and $t_i(t) = \tanh(\beta J_0 h_i(t))$.

The equal time correlation function between i and j is defined as

$$C_{ij}(t,t) =< \sigma_i(t) \sigma_j(t) > - < \sigma_i(t) >^2 \tag{14}$$

$$=< \Delta\sigma_i(t) \Delta\sigma_i(t) > \tag{15}$$

where $\Delta\sigma_i = \sigma_i - < \sigma_i >$ and the global correlation function as

$$C_g(t,t) = \frac{1}{N} \sum_{ij} C_{ij}(t,t) \tag{16}$$

▷ **3-8** Due to the permuation invariance between spins, there are only two different correlation functions, one local and one nonlocal $C_{ii} = C_{loc} + O(N)$ and $C_{ij} = \frac{C_{nl}}{N} + O(N^2)$, show that $C_g(t,t)$ is the sum of C_{loc} and C_{nl}.

▷ **3-9** Show that $C_{local} = 1 - m^2(t)$

▷ **3-10** By using that $< t_i > \simeq \tanh[\beta J_0 m]$, show that

$$\frac{\partial m}{\partial t} = -m + \tanh(\beta J_0 m) \tag{17}$$

▷ **3-11** Show that, for $i \neq j$

$$< \Delta h_i \Delta \sigma_j > = \frac{C_g(t,t)}{N} + O(N^{-2}) \tag{18}$$

▷ **3-12** Infer that

$$\frac{\partial C_g(t,t)}{\partial t} = -2a(t) C_g(t,t) + b(t) \tag{19}$$

where $a(t) = 1 - \beta J_0 [1 - \tanh^2(\beta J_0 m)]$ and $b = 2(1 - m \tanh(\beta J_0 m))$.

▷ **3-13** Show that the global correlation function is given as

$$C_g(t,t) = r^2(t) \left(C_g(0,0) + \int_0^t dt' \frac{b(t')}{r^2(t')} \right) \tag{20}$$

where $r(t) = \exp(\int_0^t dt' a(t))$

4 Formula

The Gaussian identity gives

$$\exp(bm^2) = \sqrt{\frac{b}{\pi}} \int_{-\infty}^{+\infty} dx \exp(-bx^2 + 2bmx) \tag{21}$$

also called the Hubbard-Stratonovitch transformation. For a given function g, the saddle-point method states that for large N

$$\int_{-\infty}^{+\infty} dx \exp(-Ng(x)) \simeq \exp(-N min_x(g(x))) \tag{22}$$