Computer Projects: Applied Stochastic Analysis

Tiejun Li

There are 2 computer projects. The final project reports must be carefully written with LaTeX to include the following points:

- The detailed setup of the problem.
- The procedure you take to do the computation and analysis of the numerical results.
- The issues you encounter and how you overcome.
- Possible discussion about the results and further thinking.

Please submit the hardcopy/e-copy to our TA. The reports could be composed in either Chinese or English.

1. Metropolis algorithm: Potts model.

   Problem. Apply the Monte Carlo simulations to study the phase transition behavior of the 2D Potts model on the $N \times N$ square lattice with periodic boundary condition. The Hamiltonian of the q-state Potts model is defined as

   $$H(\sigma) = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j} - h \sum_i \sigma_i, \quad i = 1, 2 \ldots, N^2$$

   where $\sigma_i = 1, 2, \ldots, q$, $\delta_{\sigma_i \sigma_j} = 1$ if $\sigma_i = \sigma_j$ and 0 otherwise. Take $q = 3$ or $q = 10$ as concrete examples to explore the following problems.

   (a) Take $J = 1$, $k_B = 1$ and $h = 0$. Plot the internal energy u

   $$u = \frac{U}{N^2} \quad \text{where} \quad U = \langle H \rangle = \frac{1}{Z} \sum_\sigma H(\sigma) \exp(-\beta H(\sigma))$$

   and the specific heat

   $$c = \frac{C}{N^2} \quad \text{where} \quad C = k_B \beta^2 \mathrm{Var}(H)$$

   as the function of temperature T, where $\beta = (k_B T)^{-1}$ and $Z = \sum_\sigma \exp(-\beta H(\sigma))$ is the partition function. Identify the critical temperature T_* of the phase transition when N is sufficiently large.

(b) For different temperature T, plot the magnetization

$$m = \frac{M}{N^2} \quad \text{where} \quad M = \Big\langle \sum_i \sigma_i \Big\rangle$$

as the function of h. Can you say something from these plots?

(c) Define the spatial correlation function

$$C(i,j) = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$$

and the correlation length ξ as the characteristic length that $\Gamma(k) = C(i,j)|_{|i-j|=k}$ decays to 0. One can approximate $\Gamma(k)$ by computing the average

$$\Gamma(k) \approx \frac{1}{4N^2} \sum_i \sum_{j \in S_i} C(i,j),$$

where i is taken with respect to the whole N^2 lattice points, and the set

$$S_i = \{j | i - j = \pm(k,0) \text{ or } \pm(0,k)\},$$

the constant 4 in $\Gamma(k)$ is from four points $j \in S_i$. (The above approximation can be similarly extended to the average with respect to all point pairs with distance k.) The correlation length can then be defined through

$$\Gamma(k) \propto \Gamma_0 \exp(-k/\xi), \qquad k \gg 1.$$

Study the correlation length ξ as the function of T when $h = 0$.

(d) When $h = 0$, investigate the behavior of c and ξ around the critical temperature T_* if we assume the limiting behavior

$$c \sim c_0 \epsilon^{-\gamma} \text{ and } \xi \sim \xi_0 \epsilon^{-\delta},$$

where $\epsilon = |1 - T/T_*|$. That is, you need to numerically find the scaling exponents γ and δ through the linear fitting to the log-log plot of the obtained points in ϵ-c or ϵ-ξ space.

(e) (*optional*) Study the above problems in the 3D case.

2. Exit time: Numerical SDEs

Denote the pdfs

$$p_+(x,y) = \mathcal{N}\big((+1,0), I_2\big), \; p_-(x,y) = \mathcal{N}\big((-1,0), I_2\big).$$

Define $p(x,y) = \big(p_+(x,y) + p_-(x,y)\big)/2$, and the potential $V(x,y) := -\ln p(x,y)$. Consider the SDEs

$$d\boldsymbol{X}_t = -\nabla V(\boldsymbol{X}_t)dt + \sqrt{2\epsilon} d\boldsymbol{W}_t$$

where $\boldsymbol{X}_t := (X_t, Y_t)$ and $\boldsymbol{W}_t$ is the standard Wiener process in $\mathbb{R}^2$.

(a) For a fixed ϵ, compute the quantity $T(\epsilon, \boldsymbol{x}_0) = \mathbb{E}^{\boldsymbol{x}_0}\tau_b^\epsilon$ through the simulation of the above SDEs, where $\boldsymbol{x}_0 = (1, 0)$, and the stopping time

$$\tau_b^\epsilon := \inf\{t \geq 0 : X_t = 0\}.$$

(b) Investigate the function $T(\epsilon, \boldsymbol{x}_0)$ numerically for different ϵ when ϵ is varied from large to small. What can you infer from these results?

(c) Investigate the function $T(\epsilon, \boldsymbol{x}_0)$ numerically for different $\boldsymbol{x}_0$. What can you infer from these results?