

Computer Projects: Applied Stochastic Analysis

Tiejun Li

There are 2 computer projects. The final project reports must be carefully written with L^AT_EX 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 to our TA. The reports could be composed in either Chinese or English.

1. 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

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

where $\sigma_i = 1, 2, \dots, q$. Take $q = 3$ or $q = 10$ as concrete example to explore the following problems.

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

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

and the specific heat

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

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

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

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 the set

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

the constant 4 is from four points $j \in S_i$. The correlation length can then be defined through

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

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

(d) When $h = 0$, investigate the behavior of c, m_+ 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 .

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

2. Numerical SDE: Exit problem.

Problem. Numerically solve the following boundary value problem via the simulation of SDEs

$$\begin{cases} b \cdot \nabla u + \frac{1}{2} \Delta u = f(x, y), & (x, y) \in B_1(0), \\ u = \frac{1}{2} \text{ on } (x, y) \in \mathbb{S}^1, \end{cases}$$

where $b = (x, y)$, $f(x, y) = x^2 + y^2 + 1$. We have exact solution $u(x, y) = (x^2 + y^2)/2$ for the model problem. Utilize the standard Euler-Maruyama scheme to do the simulation and check the numerical convergence order in time.

Investigate the multi-level Monte Carlo methodology to solve the above exit problem^(optional).