Problem Set 4

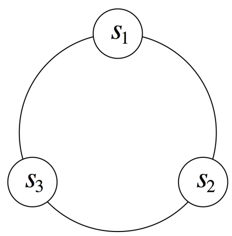
YSC4204 – Statistical Computing

Due on: Sunday, 16 October, 23:59

Problem 1

Convergence to the stationary distribution

Consider again the three-site Ising model. We call the two ground states "$+++$" and "$---$".



In class, we convinced ourselves that an MCMC simulation with the following transition probabilities must, in the long run, sample the states with Boltzmann probabilities (provided that $\beta > \frac{\ln 3}{4}$).

- If $\mu \neq +++$ and $\mu \neq ---$,

$$P(\mu \to \nu) = \begin{cases} \frac{1}{2} & \text{if } \nu = +++ \text{ or } \nu = ---, \\ 0 & \text{otherwise.} \end{cases}$$

- If $\mu = +++$ or $\mu = ---$,

$$\begin{aligned} P(+++ \to \nu) &= P(--- \to \nu) \\ &= \begin{cases} \frac{1}{2}e^{-4\beta} & \text{if } \nu \neq +++ \text{ and } \nu \neq ---, \\ \frac{1}{2}(1 - 3e^{-4\beta}) & \text{otherwise.} \end{cases} \end{aligned}$$

(a) Write R code to perform the MCMC simulation. Start the Markov chain in the state $+++$ at time $t = 0$.

(b) For $\beta = \frac{1}{3}$, estimate the probability distribution $p_\mu(t)$ of being in any of the states μ at $t = 1, 2, 5, 10, 100$ by repeatedly running the MCMC simulation. Compare with the exact Boltzmann probabilities.

(6 points total. 3 for (a), 3 for (b).)

Problem 2

MCMC with a non-Boltzmann target distribution (Rizzo 9.4)

"Implement a random walk Metropolis sampler for generating the standard Laplace distribution (see Exercise 3.2). For the increment, simulate from a normal distribution. Compare the chains generated when different variances are used for the proposal distribution. Also, compute the acceptance rates of each chain."

Rizzo refers here to the material from pages 253–256. Show your code, acceptance rates, plots similar to those in Figure 9.3 and a table similar to Table 9.1. Also briefly comment on your results.

(6 points.)

Problem 3

Correlation times and magnetization in the Ising model

Below are two figures from the book by Newman and Barkema. Repeat the measurements displayed in these figures and prepare your own plots. Show your code. (You can quote from the code we have discussed in class.)

Note that the variable on the horizontal axis is in both plots kT, not T.

For temperatures below $kT \approx 2.0$, our criterion for equilibration in principle still works (i.e. we wait until an initially aligned system is for the first time less magnetized than an initially random system). However, for low temperatures, the initial 50:50 random spin configuration can take unrepresentatively long to equilibrate. In these cases it is advisable to break the initial symmetry and start with a random 60:40 random configuration.

For temperatures below $kT \approx 0.5$, it is difficult to obtain correlation times because there are essentially no fluctuations. You can skip these data points.

(8 points.)

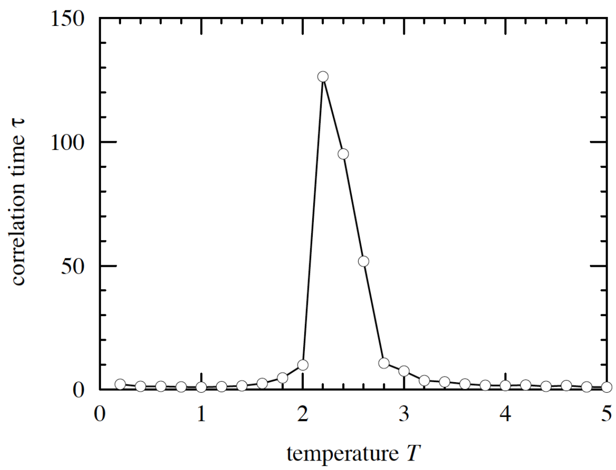


FIGURE 3.8 The correlation time for the 100×100 Ising model simulated using the Metropolis algorithm. The correlation time is measured in Monte Carlo steps per lattice site (i.e., in multiples of 10 000 Monte Carlo steps in this case). The straight lines joining the points are just to guide the eye.

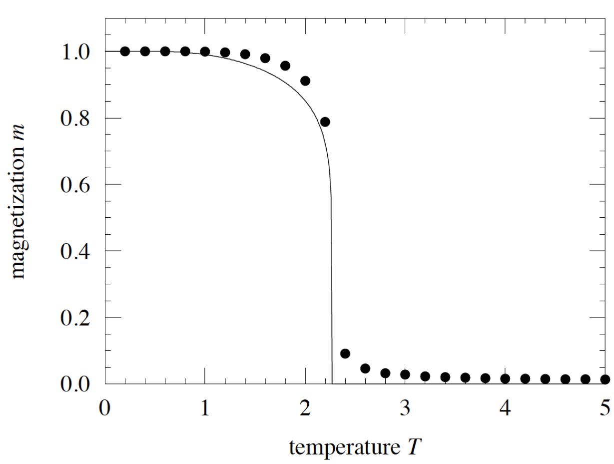


FIGURE 3.9 The magnetization per spin of the two-dimensional Ising model. The points are the results from our Monte Carlo simulation using the Metropolis algorithm. The errors are actually smaller than the points in this figure because the calculation is so accurate. The solid line is the known exact solution for the Ising model on an infinite two-dimensional square lattice.