Practical Numerical Simulation Homework 4

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1 Markov Chain

A Markov chain is a sequence of N states $\mu_1, ..., \mu_N$ where the system in state μ_k depends only on μ_{k-1} and no others. We can require that all the states of the system follow any fixed point distribution p_μ. It is useful to require that $p_\mu P(\mu \to \nu) = p_\nu P(\nu \to \mu)$. This is detailed balance and will ensure that we approach the fixed point distribution.

2 Metropolis

1. We propose a new state of the system ν in a reversible way, ie.

$$P(\mu \to \nu) = P(\nu \to \mu)$$

2. We accept new state ν with probability P:

$$P = min[1, \frac{p_\nu}{p_\mu}]$$

3. If accepted we add ν to our Markov chain, if rejected we add μ to the markov chain.

3 Part 1

We define one Monte Carlo step as an entire Metropolis 'sweep' through the lattice. That is when we've performed a metropolis action on each lattice site. For this part our proposed change per site was changing to a random angle $\theta' \in [-\pi, \pi]$. We could choose this selection probability arbitrarily as we adapt the acceptacne probability accordingly. We calculate average acceptance ratio of the proposed θ' over many Monte Carlo steps at each temperature in the range $0 \leq \beta \leq 1.5$ normalised by the size of the lattice (so that $<$ Acceptance ratio $>$ of 1 implied that every site was change during the Monte Carlo step.). The results are shown in figure 1.

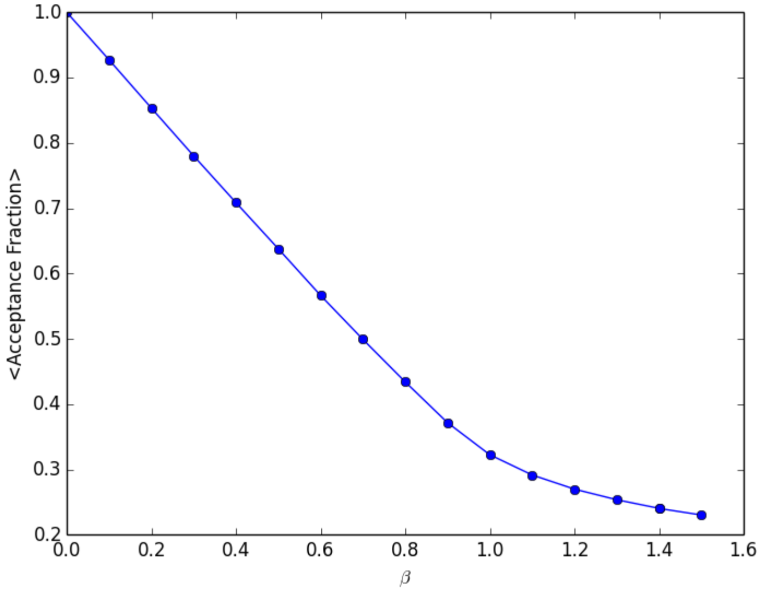

Figure 1: Acceptance ratio as a function of β.

As we can see the probably of the selection being accepted falls off at low temperatures (high β) which implies that we may take a long time to reach a state representative of the system at that temperature.

4 Part 2

For this part we change our selection of a new angle theta to a shift of η, $\theta' + \eta$, $\eta \in [-\delta, \delta]$. As we saw from part 1; the major problem in computation time is around $\beta = 1$. Thus we need to determine a range for the shift that maximises acceptance in this region. To find optimum δ we set $\beta = 1$ and changed the β 'for loop' which can be seen in the program to a delta 'for loop' of the form (double delta = 0; delta $<=$ pi; delta += 0.01) which was subsequently removed from the program. We included delta as another argument to the function and wrote it to file so that we could plot acceptance ratio as a function of δ.

We tested the acceptance ratio for 315 values of $\delta \in [0, \pi]$. This can be seen in figure 2.

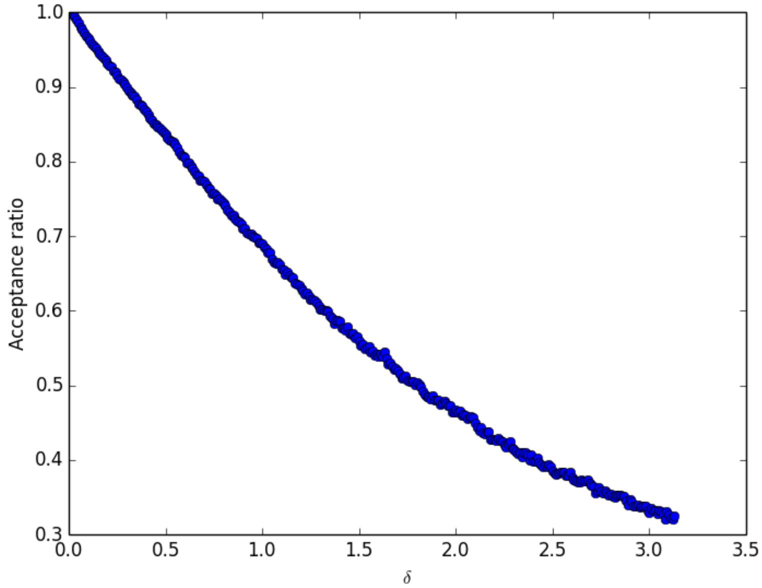

Figure 2: Acceptance ratio as a function of δ. $\beta = 1$

We may also see that our desired accpetance percentage (50%) is approximately $\delta = 1.8$. Therefore choose this to be the appropriate *delta* for subsequent parts.

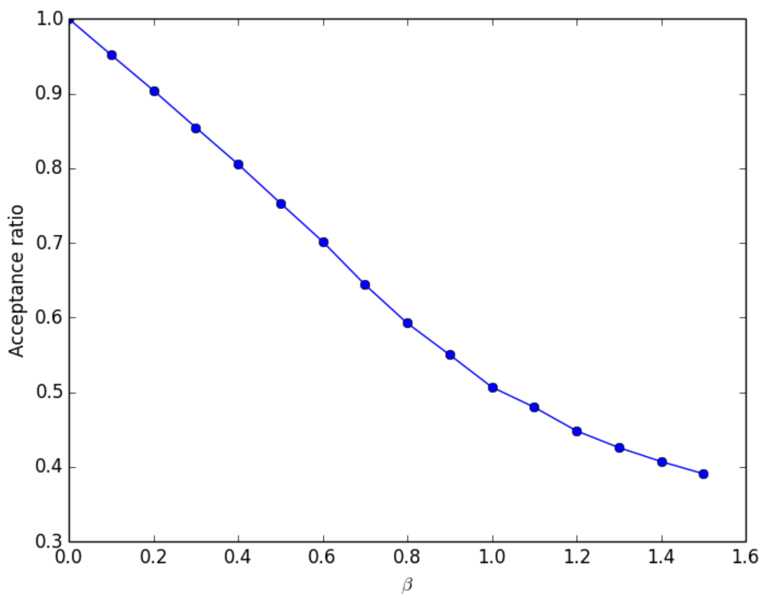

Figure 3: Acceptance ratio as a function of β. $\delta = 1$

This provided much better acceptance ratio especially in the region $\beta \approx 1$. This can be sen from figure 3 which should be compared to figure 1. We can see that the acceptance ratio is much higher at lower temperatures that with a random shift and we may conclude that we have improved the algorithm by restricting our shifts within one radian.

5 Part 3

We wish to determine spin stiffness

$$C(\beta) = \langle cos(\theta_{x,y} - \theta_{x+L/2,y})$$

20,000 timesteps were used for each value of β. We generally discarded the first 1,000 steps in each case to account for thermalisation. We then took the average of the C computed at the other timesteps and we took this to be our expectation value. This high number of timesteps was particularly important at around $\beta = 1$. The results are shown in figure 4.

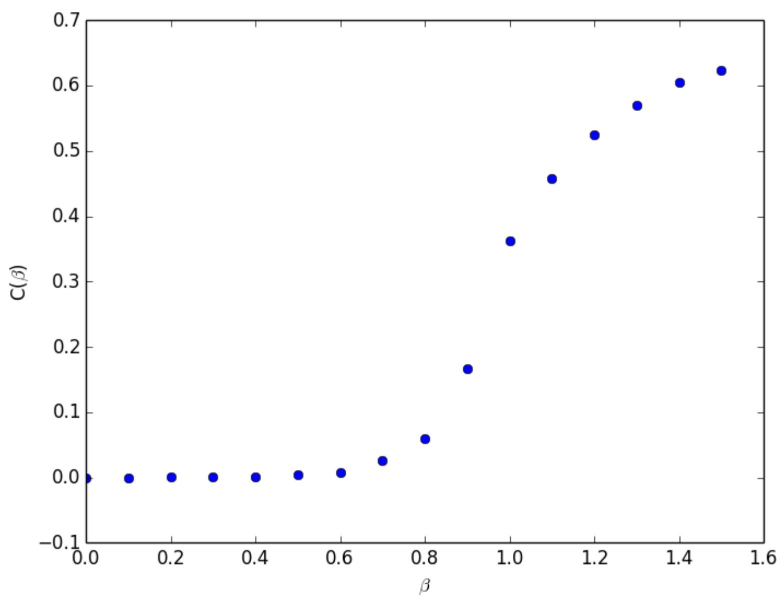

Figure 4: $C(\beta)$. $\delta = 1.8$

We also include error bars which were taken from the standard deviation of the the values of C at all timesteps for each temperature. These account only for statistical error due to flucttutation around the expected value of C and fell of with $\frac{1}{\sqrt{N}}$ where N is sample size. The sample size was generally $\approx 19,000$ so these error bars are tiny and in fact are not visable on the graph. Note they account only for the statistical fluctuation of the data about the average and does not relate to systematic error.