Monte Carlo Methods Homework 4

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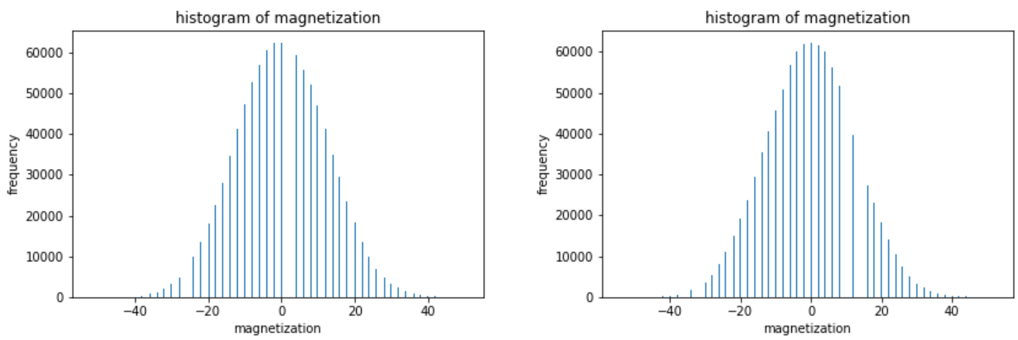
Exercise 39. *Write a routine that uses a Gibbs sampler to generate samples of the Ising model. Plot a histogram of the values of the magnetization*

$$f(\sigma) = \sum_{\vec{i} \in \mathbb{Z}_L^2} \sigma_{\vec{i}}.$$

Compute the integrated autocorrelation time for the magnetization. Do you find it better to select $\vec{i}_t$ randomly, or to sweep through the lattice deterministically? What happens to the integrated autocorrelation time when you change the temperature? What happens to the integrated autocorrelation time when you change the size of the lattice?

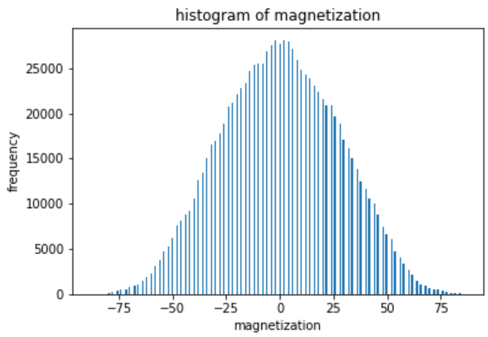
WARNING: integrated autocorrelation times are notoriously difficult to estimate. You should check that your estimate has converged by computing it on a few trajectories of increasing length.

Let the size of lattice $L = 10$, times of iteration $\max_{itr} = 10^6$. Histogram plots of magnetization for several choives of $\beta = \frac{1}{k_b T}$ are shown as below.

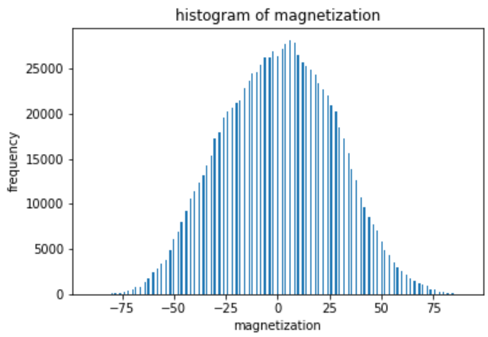


(a) Random Gibbs sampler, $\beta = 0.1$

(b) Deterministic Gibbs sampler, $\beta = 0.1$

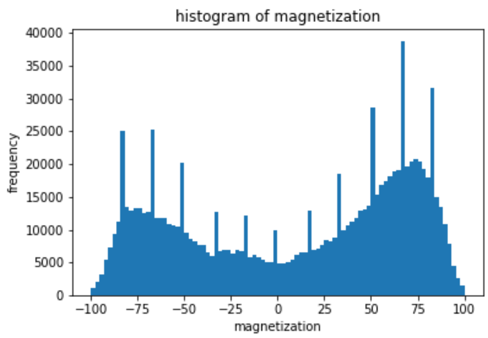


(c) Random Gibbs sampler, $\beta = 0.3$

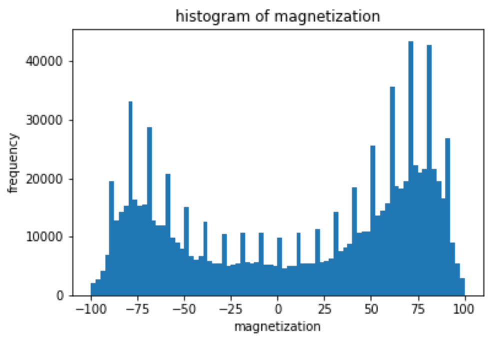


(d) Deterministic Gibbs sampler, $\beta = 0.3$

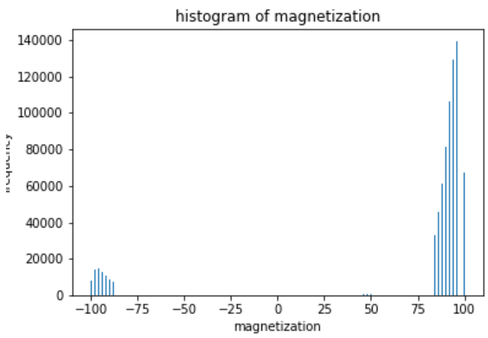
We can see that for $\beta < 0.4$, the magnetization of lattice is distributed as Gaussian random variables. However, for $\beta \geq 0.4$, indicating lower temperature, we observe closer to bi-Gaussian distribution.



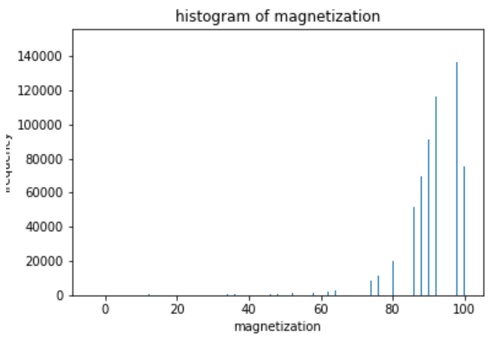
(e) Random Gibbs sampler, $\beta = 0.4$



(f) Deterministic Gibbs sampler, $\beta = 0.4$

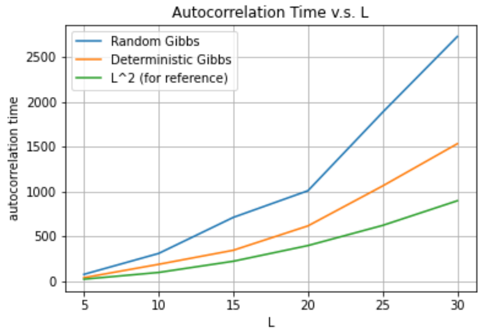


(g) Random Gibbs sampler, $\beta = 0.5$

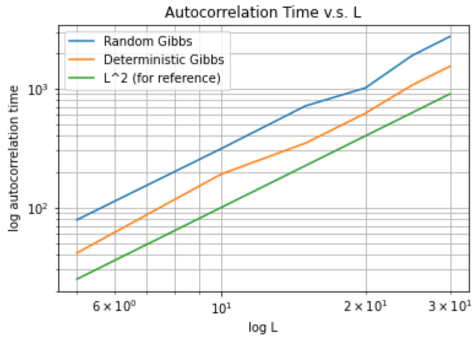


(h) Deterministic Gibbs sampler, $\beta = 0.5$

To observe how the integrated autocorrelation time change with lattice size L, we fix the temperature by letting $\beta = 0.1$ and L in list [5, 10, 15, 20, 25, 30].



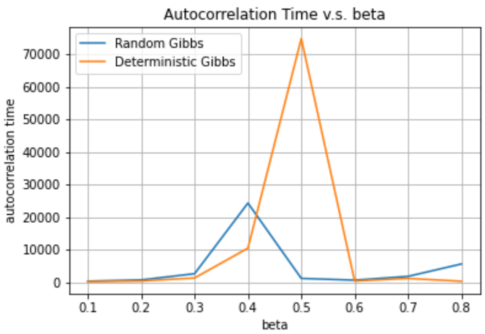
(i) Autocorrelation time v.s. L plot, $\beta = 0.1$



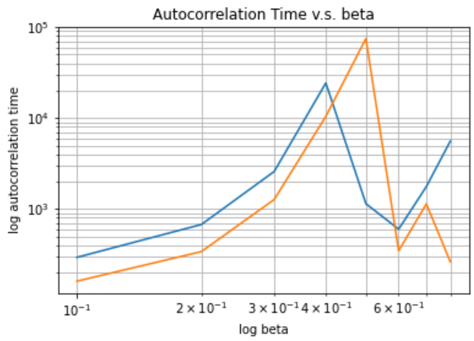
(j) Log-log autocorrelation time v.s. L plot, $\beta = 0.1$

We could see that the integrate autocorrelation time is growing superlinearly with Lattice size L for both random Gibbs sampler and deterministic Gibbs sampler. The convergence is quadratic in L; deterministic Gibbs sampler converges faster than random Gibbs sampler by a constant factor.

To observe how the integrated autocorrelation time change with temperature, we fix the size of lattice $L = 10$ and β in list [[0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8].

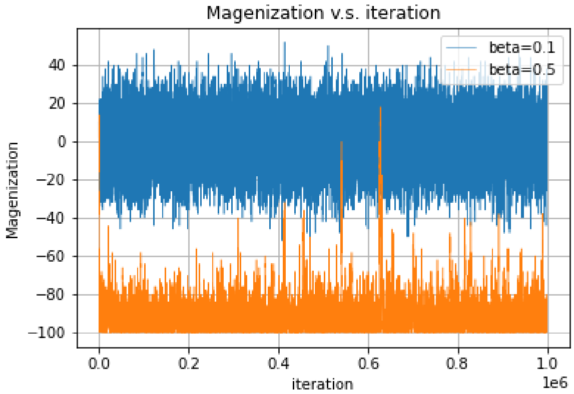


(k) Autocorrelation time v.s. β plot, $L = 10$



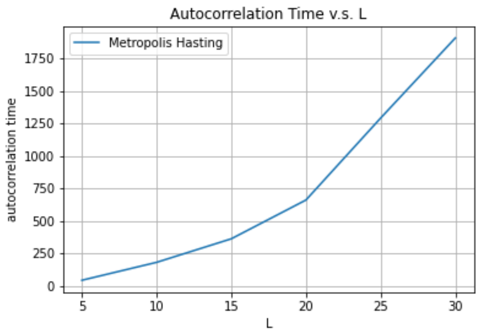
(l) Log-log autocorrelation time v.s. β plot, $L = 10$

We could see that the integrate autocorrelation time is growing superlinearly with β for $\beta \leq 0.4$, which is a scaled inverse of the temperature, for both random Gibbs sampler and deterministic Gibbs sampler. Deterministic Gibbs sampler converges faster than random Gibbs sampler by a constant factor. However, when $\beta > 0.4$, the integrated autocorrelation time decreases, instead of increasing exponentially. This is because it becomes extremely hard for the chain to jump from one magnetization to the other, as illustrated in the figure below.

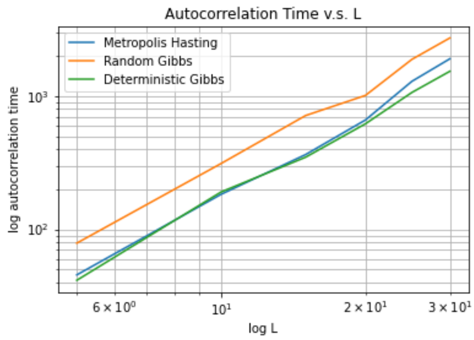

Magenization v.s. iteration
beta=0.1
beta=0.5
Magenization
iteration
1e6
40
20
0
−20
−40
−60
−80
−100
0.0
0.2
0.4
0.6
0.8
1.0

Exercise 42. *Write a Metropolis based scheme to sample the 2d-Ising model. Compare the magnetism integrated autocorrelation time for this scheme to the one you computed for the Gibbs sampler.*

To observe how the integrated autocorrelation time change with lattice size L, we fix the temperature by letting $\beta = 0.1$ and L in list [5, 10, 15, 20, 25, 30].



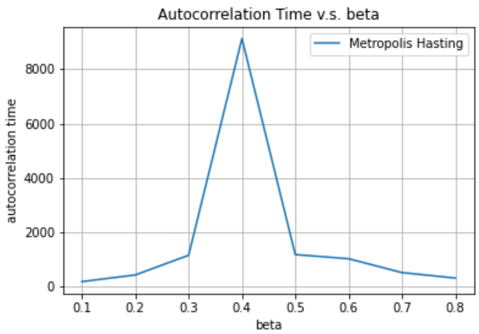
(m) Autocorrelation time v.s. L plot, $\beta = 0.1$



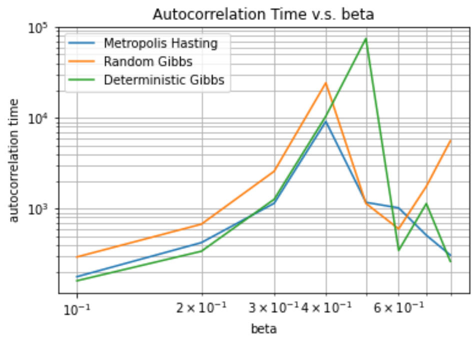
(n) Log-log autocorrelation time v.s. L plot, $\beta = 0.1$

We could see that the integrate autocorrelation time is growing superlinearly with Lattice size L for Metropolis Hasting sampler. The convergence is quadratic in L; Metropolis Hasting sampler converges similarly as deterministic Gibbs sampler, faster than random Gibbs sampler by a constant factor.

To observe how the integrated autocorrelation time change with temperature, we fix the size of lattice $L = 10$ and β in list [[0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8].



(o) Autocorrelation time v.s. β plot, $L = 10$



(p) Log-log autocorrelation time v.s. β plot, $L = 10$

We could see that the integrate autocorrelation time is growing superlinearly with β for $\beta \leq 0.4$, which is a scaled inverse of the temperature, for Metropolis Hasting sampler. Metropolis Hasting sampler converges similarly as deterministic Gibbs sampler, faster than random Gibbs sampler by a constant factor.

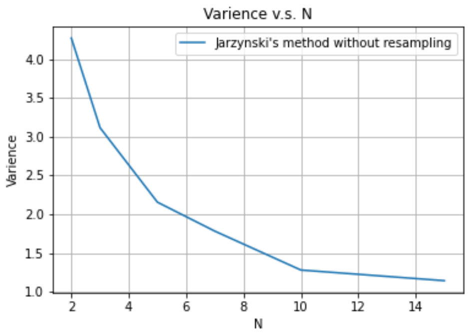
Exercise 43. *Use Jarzynski's method (without resampling) to generate weighted samples from the* $2d$*-Ising model. Choose*

$$\pi_k = \pi^{\frac{k}{N}}$$

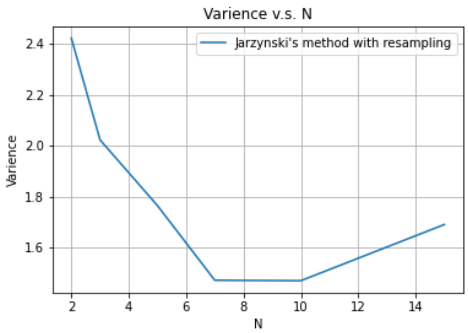
and try defining the transition operators $\mathcal{T}_k$ *for the Markov chain to be the ones you used in Exercises 39 and 42 with* π *in those exercises by* π_{k-1}*. Note that this means that* $X^{(0)}$ *is drawn from the distribution with independent spins (i.e.* $\beta = 0$*). Evaluate the performance of the estimator of the magnetization. How does the variance change when you increase* N*? What seems to be the optimal choice of* N *(considering variance and effort) for this problem? Try Jarzynski's method with resampling. Does resampling help? How would you compare Jarzynski's method to Gibbs or Metropolis sampling for this problem?*

For Gibbs sampler, the transition operators T_k equals to the original transition matrix with $\beta_k = \frac{k-1}{N}\beta$. For Metropolis Hasting sampler, the proposal is symmetric with accepting rate $p_k = p^{\frac{k-1}{N}}$, which is also equivalent to using $\beta_k = \frac{k-1}{N}\beta$.

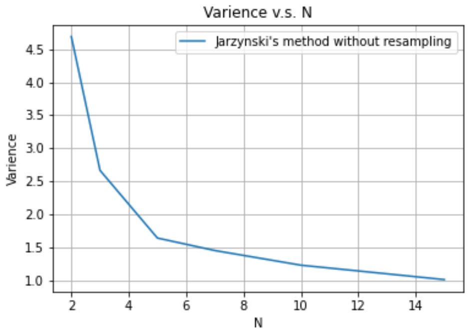
Here, the number of samples in ensemble is 100, and the number of runs to calculate the variance is 500, the interpolation N is in list [2, 3, 5, 7, 10, 15].



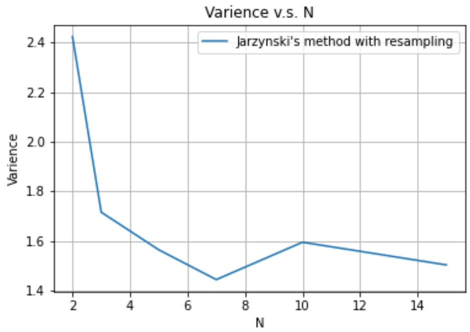
(q) Variance v.s. N using Gibbs without resampling



(r) Variance v.s. N using Gibbs with resampling



(s) Variance v.s. N using Metropolis without resampling



(t) Variance v.s. N using Metropolis with resampling

We observe that without resampling, the variance decreases as N increases. With resampling, the variance decreases even faster as N increases where $N \leq 7$. However,for $N > 7$, the variance increases at some point. The reason may be the accuracy harmed by two parameters, ensemble size and interpolating step N, not large enough.

The variance when using Jarzynski's method is expected to vanish for large enough k. However, for small k, variance may be large and dominate the error. On the other hand, Metropolis or Gibbs may be biased unless we run the chain longer. However, when the size of lattice or beta is large, the integrated autocorrelation time will be large and dominate the error. Thus, when the size is relatively small, partial resampling with Metropolis-Hasting or Gibbs is better since the bias can be small enough using longer chain; when the size is very large, it is better to use Jarzynski's method (with resampling) to suffer less from bias.