Fall 2022: Monte Carlo Methods
Homework 5

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We are given a 2-dimensional set of vectors $\overrightarrow{\sigma_i} \in R^2$ indexed by 1 dimensional periodic lattice Z_L and with $||\overrightarrow{\sigma_i}||_2 = 1$. The nearest neighbor XY model of statistical physics assigns these vectors the density

$$\pi(\overrightarrow{\sigma}) = \frac{\exp\left(\beta \sum_{i \leftrightarrow j} \sigma_{\overrightarrow{i}} \sigma_{\overrightarrow{j}}\right)}{Z}$$

The above expression can also be simplified and written As

$$\pi(\overrightarrow{\theta}) = \frac{\exp\left(\beta \sum_{i \leftrightarrow j} \cos(\theta_i - \theta_j)\right)}{Z}$$

Here, θ is a scaler following the given density.

We have been asked to compute the consine of the angle of magnetization vector. Magnetization is defined as

$$M(\overrightarrow{\sigma}) = \sum_{i=0}^{L-1} \overrightarrow{\sigma_i}$$

Therefore cosine of angle of magnetization is

$$f(\overrightarrow{\sigma}) = \frac{(\overrightarrow{\sigma})_x}{(||\overrightarrow{\sigma})||}$$

In terms of angle this will be written as

$$M(\overrightarrow{\theta}) = \sum_{i=0}^{L-1} \cos\theta_i \hat{\mathbf{i}} + \sin\theta_i \hat{\mathbf{j}}$$

Therefore cosine of angle of magnetization in terms of theta is

$$f(\overrightarrow{\theta}) = \cos\left(\arctan\left(\frac{\sum_{i=0}^{L-1} \sin\theta_i}{\sum_{i=0}^{L-1} \cos\theta_i}\right)\right)$$

Exercise 64 asked to implement an Overdamped Langevian MCMC Secheme for both with and without metropolization step.

$$\theta_h^{k+1} = \theta_h^k + hS(\theta_h^k)\nabla^T \log \pi(\theta_h^k) + h\,\mathsf{div}S(\theta_h^k) + \sqrt{2hS(\theta_h^k)}\zeta^{k+1}$$

So on choosing $S(\theta) = \mathbf{I}$ (Identity Matrix), above equation can be simplified into

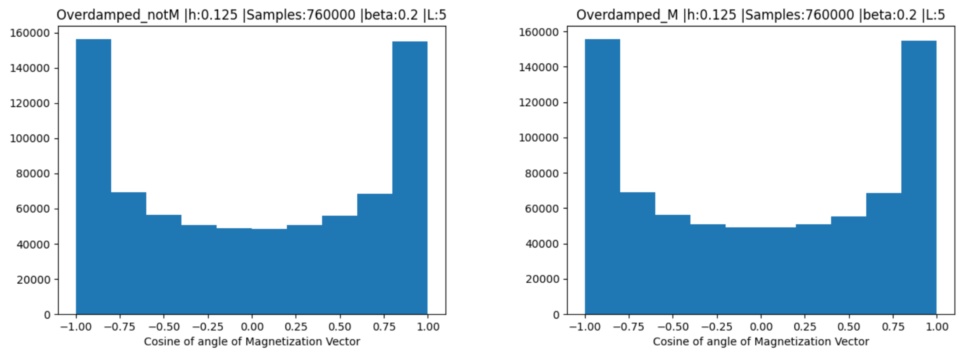
$$\theta_h^{k+1} = \theta_h^k + h\nabla^T \log \pi(\theta_h^k) + h\,\mathsf{div}\mathbf{I} + \sqrt{2h}\mathbf{I}\zeta^{k+1}$$

Since, divergence of a constanct is 0, it can be further simplified into

$$\theta_h^{k+1} = \theta_h^k + h\nabla^T \log \pi(\theta_h^k) + \sqrt{2h}\mathbf{I}\zeta^{k+1}$$

Here, ζ are generated using Multivarite Gaussian Distribution with Covariance as $IdentityMatrix$

On using this equation to generate the samples from distribution π and plotting the histogram we are getting



(a) Without Metropolization

(b) With Metropolization

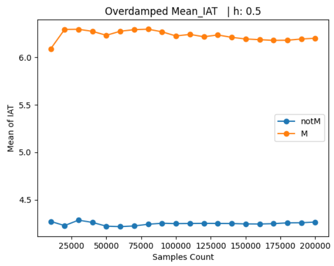
Figure (1) Histograms for magnetization samples generated for Overdamped Langevian MCMC Schemes

Looking, at the histogram we can validate the implementation as the the cosine of magnetization should either transitioing between $+1$ and -1 with almost equal probability. And we can see that maximum sampled points are lying at the two ends of the histogram.

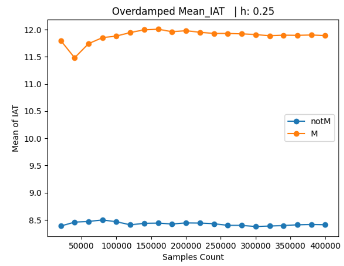
We can compare the quality of the samples with the IAT value of the cosine angle of magnetization. Since IAT are notoriously hard to accurately compute, I ran independent simulations on M parallel chains, with other parameters as constant. And after computing IAT, took a mean of them.

From figure 2 it we can conclude the following

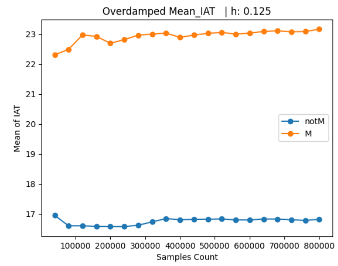
- As we decrease the value of h by a factor of 2 meant value of the IAT also increases by the same factor of 2. From the above figure we can see that h decreases from 0.5 to 0.25 to 0.125 the IATs for both wit and without metropolization incases in the same proportion.
- IAT of Overdamped Langevian with metropolization is more than the IAT without metropolization. This is because of the accept reject step in metropolization method.
- Due to smaller size of lattice, IAT converges even for samller sample count.
- There is not much of the difference in the IAT values with the variation in L. So we could infer that L is independent of the cosine of magnetization.



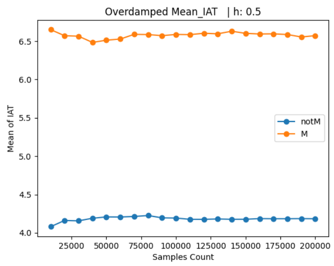
(a) $h = 0.5$ and $L = 5$



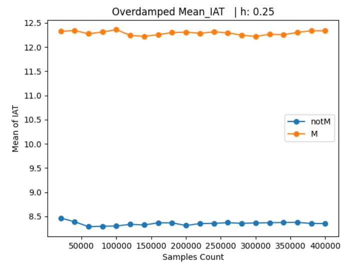
(b) $h = 0.25$ and $L = 5$



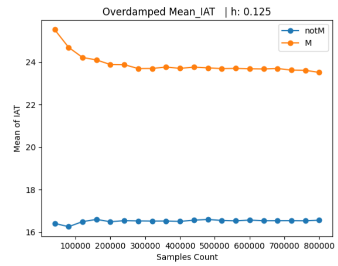
(c) $h = 0.125$ and $L = 5$



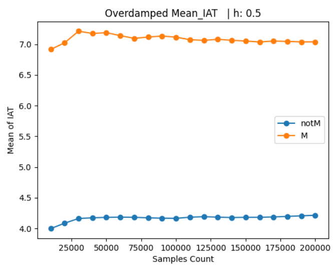
(d) $h = 0.5$ and $L = 10$



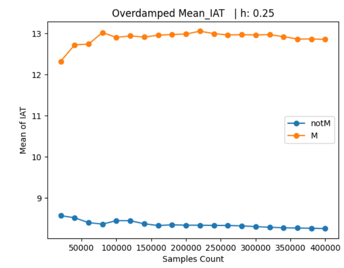
(e) $h = 0.25$ and $L = 10$



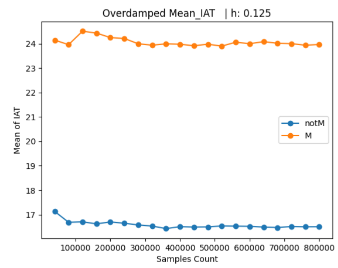
(f) $h = 0.125$ and $L = 10$



(g) $h = 0.5$ and $L = 15$



(h) $h = 0.25$ and $L = 15$



(i) $h = 0.125$ and $L = 15$

Figure (2) Plots of IAT with samples generated for Overdamped Langevian MCMC for both with and without metropolization for different values of h and L

Exercise 65 asked to implement an Hybrid Monte Carlo Scheme for both with and without metropolization step using Equation (5.26) and Algorithm 4 from the notes.

Following are the expressions chosen for solving Velocity Verlet Scheme

$$\hat{d} = L \text{ and } \tilde{d} = L$$

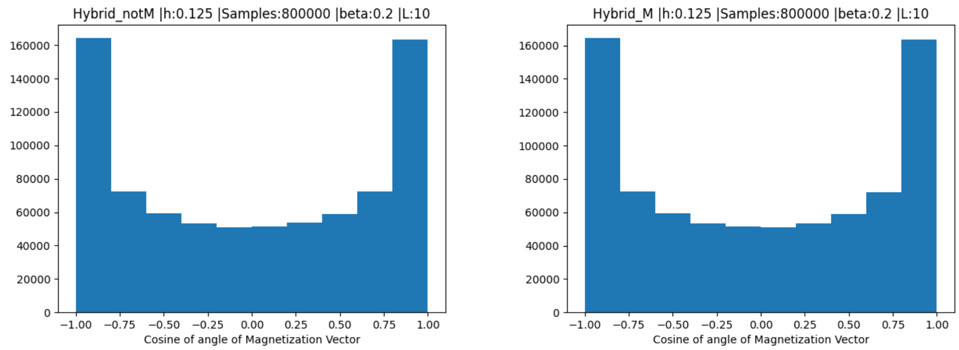
$$J(\hat{x}) = \mathbf{I}_{\hat{d} \times \hat{d}}$$

$$K(\tilde{x}) = \frac{||\tilde{x}|_2^2}{2}$$

$$n = 10$$

Figure 3 contains the histogram of the generated samples.

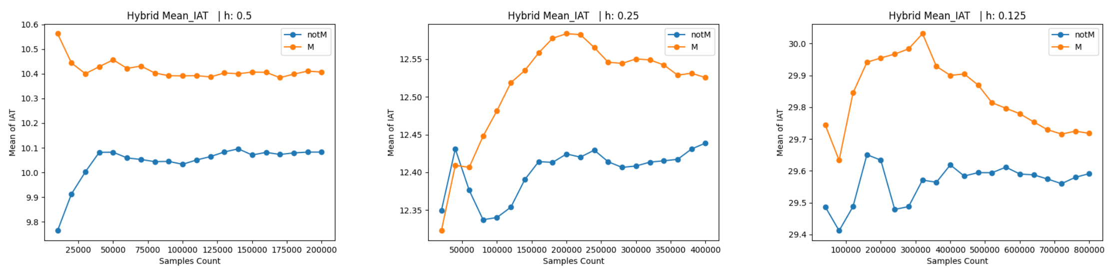
On using this equation to generate the samples from distribution π and plotting the histogram we are getting



(a) Without Metropolization **(b)** With Metropolization

Figure (3) Histograms for magnetization samples generated for Overdamped Langevian MCMC Schemes

Now, while measuring the IAT we need to take care of multiplication by the factor of n, since for generating 1 sample we generated n points using Velocity Verlet and this was taken into accounting. 4 contains the plots of IATs for different value of h.



(a) $h = 0.5$ and $L = 10$ **(b)** $h = 0.25$ and $L = 10$ **(c)** $h = 0.125$ and $L = 15$

Figure (4) Plots of IAT with samples generated for Hybrid Monte Carlo for both with and without metropolization for different values of h

From figure 4, we can conclude the following

- We don't observe much difference between the IAT values for both with and without Metropolization.
- On decreasing the value of h we observe that the value of IAT are increasing.
- Due to smaller size of lattice, IAT converges even for samller sample count.

On comparing the figure 2 and 4 we can compare Overdamped Langevian MC Schemes as well as Hybrid MC Schemes. Below are the comparision observations:

- In overdamped scheme there is huge difference with and without metropolization while in hybrid scheme we get almost same results with both the metropolization and without metropolization.
- In overdamped scheme decrease in the value of h by some factor increased the value of IAT by same factor. Whereas in the hybrid sceme with observe the increase but not by the same factor.

Exercise 66 asked us to implement Underdamped Langevian Monte Carlo Following are the expresions used various factors and matrices.

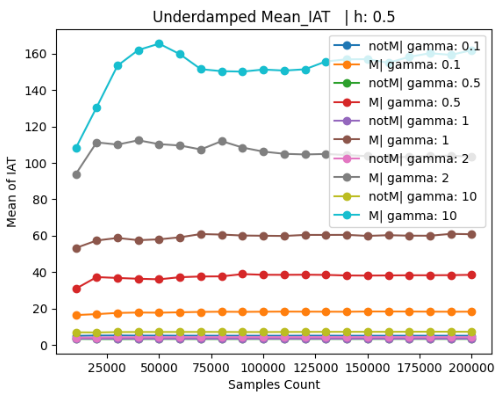
$$\hat{d} = L \text{ and } \tilde{d} = L$$

$$J(\hat{x}) = \mathbf{I}_{\hat{d} \times \hat{d}}$$

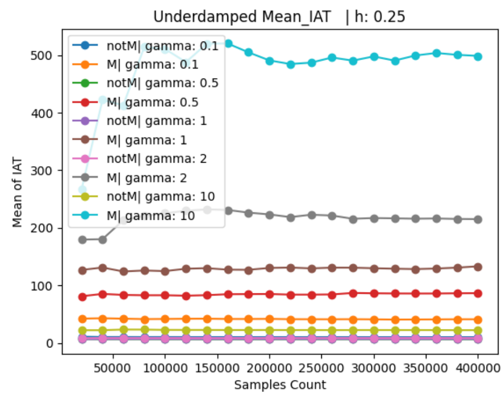
$$K(\tilde{x}) = \frac{||\tilde{x}|_2^2}{2}$$

$$H(\hat{x}, \tilde{x}) = -\log \pi(\hat{x}) + K(\tilde{x})$$

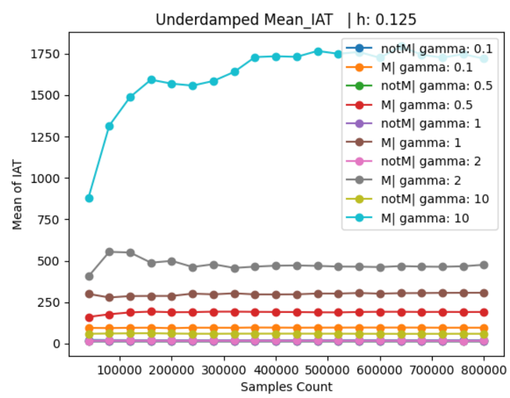
Implementation of the code was validated using the same mechanism of generating samples and plotting the histogram. It was similar in shape as previous two parts, hence the code was validated.



(a) $h = 0.5$ and $L = 10$



(b) $h = 0.25$ and $L = 10$



(c) $h = 0.125$ and $L = 15$

Figure (5) Plots of IAT with samples generated for Hybrid Monte Carlo for both with and without metropolization for different values of h

From figure 4, we can conclude the following

- On increasing the value of γ we see the increase in the value of IAT.
- Only reducing the value of h some factor, the value of IAT multiples by the same factor