Monte Carlo Methods Homework 5

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Exercise 64. *Consider a set of 2-dimensional vectors, $\vec{\sigma}_i \in \mathbb{R}^2$ indexed by the 1-dimensional periodic lattice $\mathbb{Z}_L$ and with $\|\vec{\sigma}_i\|_2 = 1$. The nearest neighbor XY model of statistical physics assigns to these vectors the density*

$$\pi(\vec{\sigma}) = \frac{e^{\beta \sum_{i \leftrightarrow j} \vec{\sigma}_i \cdot \vec{\sigma}_j}}{\mathcal{Z}}.$$

In terms of the angles $\theta_i \in [-\pi, \pi)$ of the vectors $\vec{\sigma}_i$, this density becomes

$$\pi(\theta) = \frac{e^{\beta \sum_{i \leftrightarrow j} \cos(\theta_i - \theta_j)}}{\mathcal{Z}}.$$

Write a routine to sample the XY model using both (5.8) and a Metropolized version of (5.8). Compare the Metropolized and un-Metropolized schemes for different values of h (but note that the total number of time-steps you use should scale like h^{-1}). Make your comparisons in terms of the integrated autocorrelation time of the variable

$$\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$$

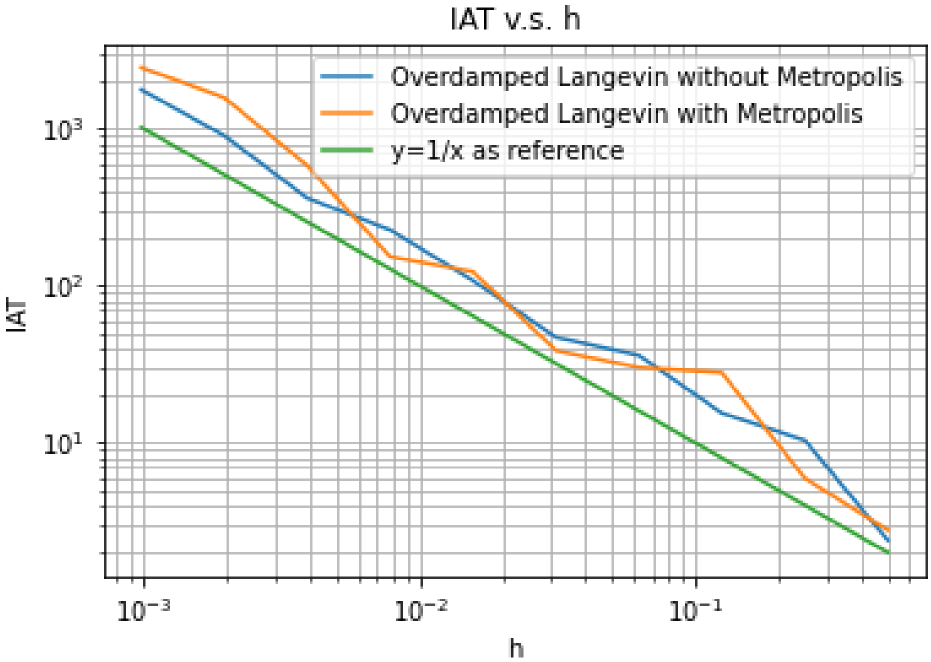
which is the cosine of the angle of the magnetization vector,

$$M(\sigma) = \sum_{i=0}^{L-1} \vec{\sigma}_i \in \mathbb{R}^2.$$

What do you observe when L increases.

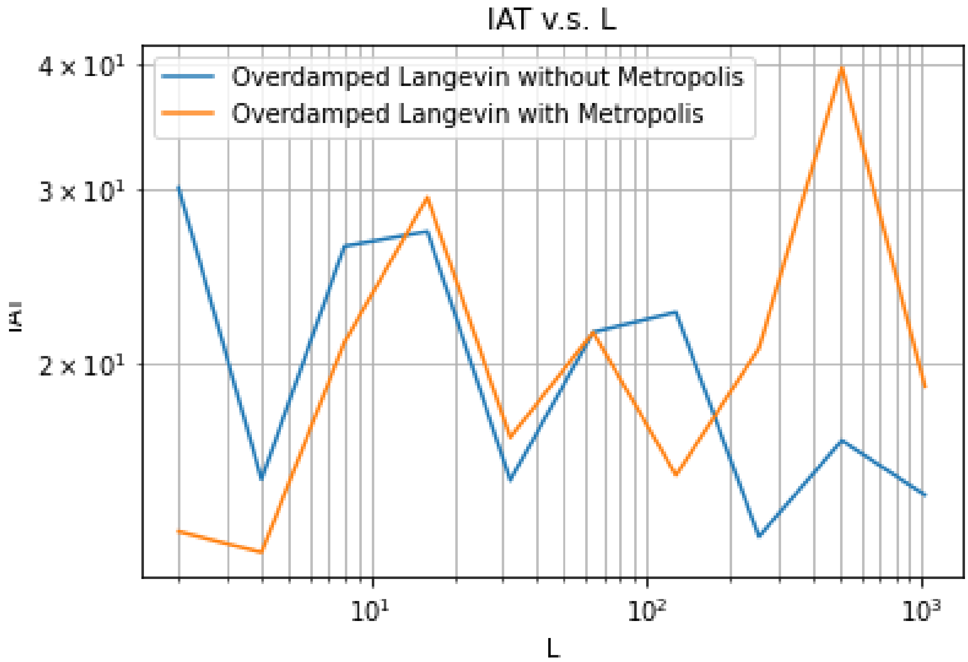
We choose S = identity, $P(\xi = -1) = P(\xi = 1) = \frac{1}{2}$ for the Overdamped Langevin scheme.

Let the size of lattice $L = 10$, $\beta = 0.1$. We vary the step size h from 2^{-10} to 2^{-1}, and plotted the integrated automatic time (IAT) of $\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$.



We observe that, as h increases, the IAT decreases proportionally to $\frac{1}{h}$, both the Overdamped Langevin with Metropolis and without Metropolis. Also, the Metropolis doesn't not cause significant and clear influence on the IAT. This encourages us to use a bigger step size for better efficiency.

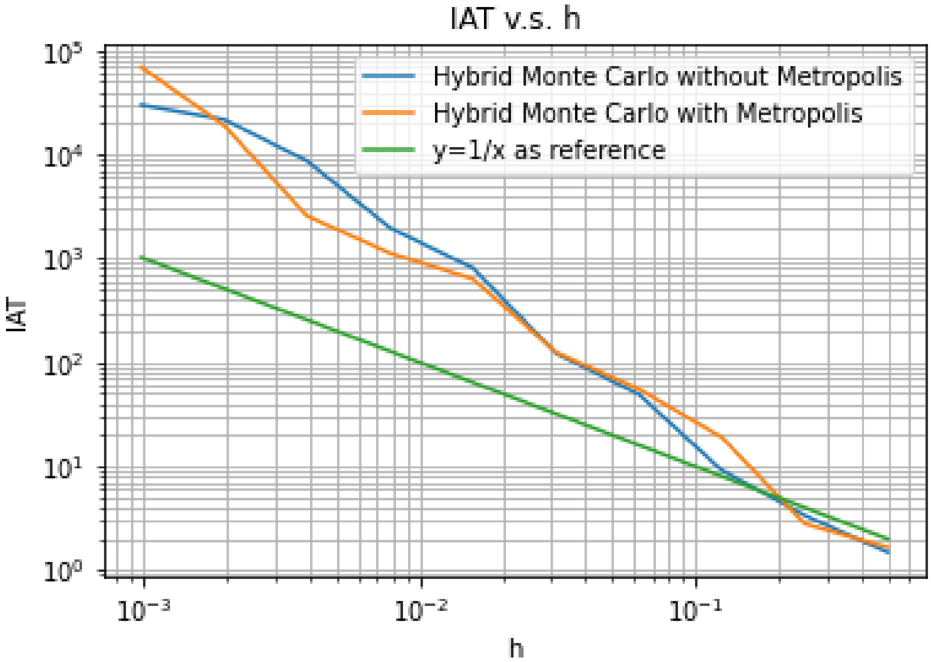
Let the step size $h = 0.1$, $\beta = 0.1$. We vary the size of lattice L from 2^1 to 2^{10}, and plotted the integrated automatic time (IAT) of $\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$.



We observe that, as h increases, the IAT does not show significant decreasing or increasing pattern. Thus, we conclude that both the Overdamped Langevin with Metropolis and without Metropolis is robust against the object size.

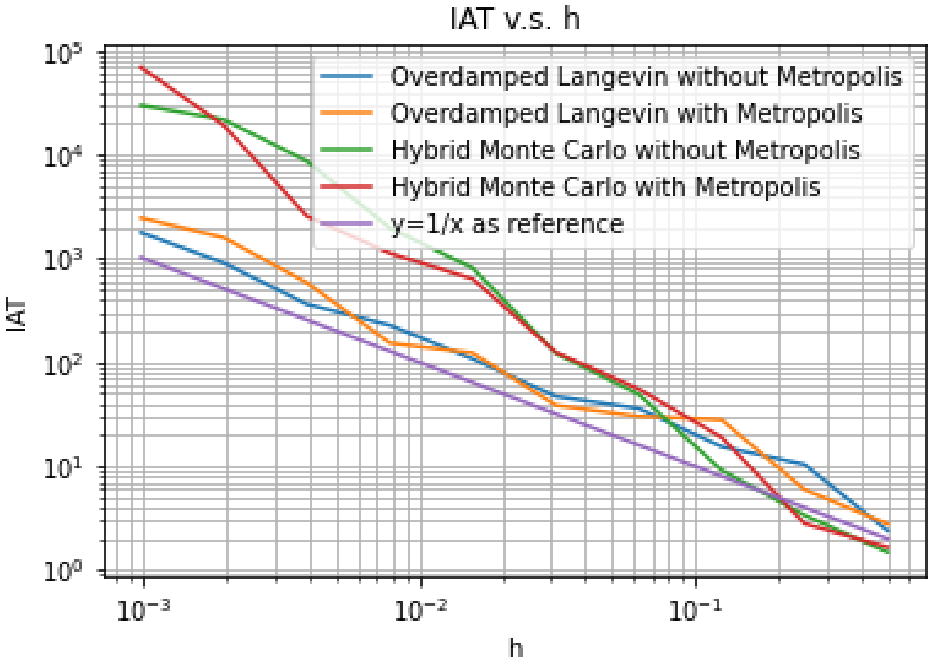
Exercise 65. *Write a routine to sample the XY model described in Exercise 64 using Algorithm 4 both with and without the Metropolis accept/reject step. You're free to choose the other parameters of the algorithm (K, J, n, and h) as you like (but be clear about your choices). Compare the results to those of Exercise 64 using integrated autocorrelation time of the cosine of the angle of magnetization as your measure of efficiency. Make sure you are accounting correctly for the cost to generate each step of the chain (e.g. as measured by the number of evaluations of $\nabla \log \pi$.*

Let $K = \frac{\|x\|^2}{2}$, $J = I$, $n = 5$, $h = 0.1$. We vary the size of lattice L from 2^1 to 2^{10}, and plotted the integrated automatic time (IAT) of $\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$.



We observe that, as h increases, the IAT decreases proportionally to $O(h^{-2})$, both the Hybrid Monte Carlo with Metropolis and without Metropolis. Also, the Metropolis doesn't not cause significant and clear influence on the IAT. This encourages us to use a bigger step size for better efficiency.

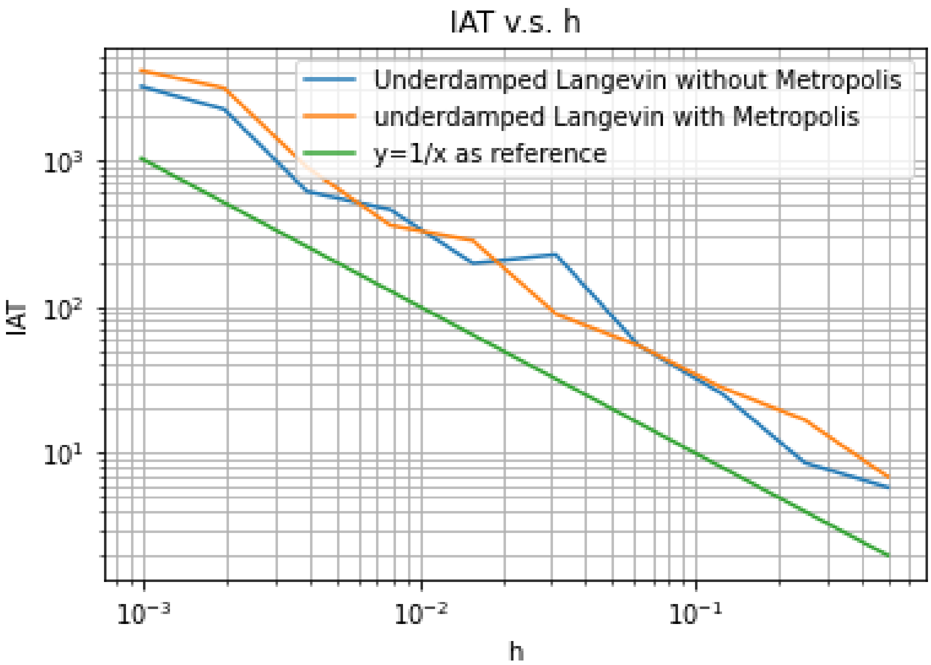
We compare the IAT of Overdamped Langevin and Hybrid Monte Carlo.



We observe that, as h shrinks to 0, IAT of Hybrid Monte Carlo grows faster than Overdamped Langevin. Thus, we conclude that Overdamped Langevin with is better than Hybrid Monte Carlo grows in terms of IAT here.

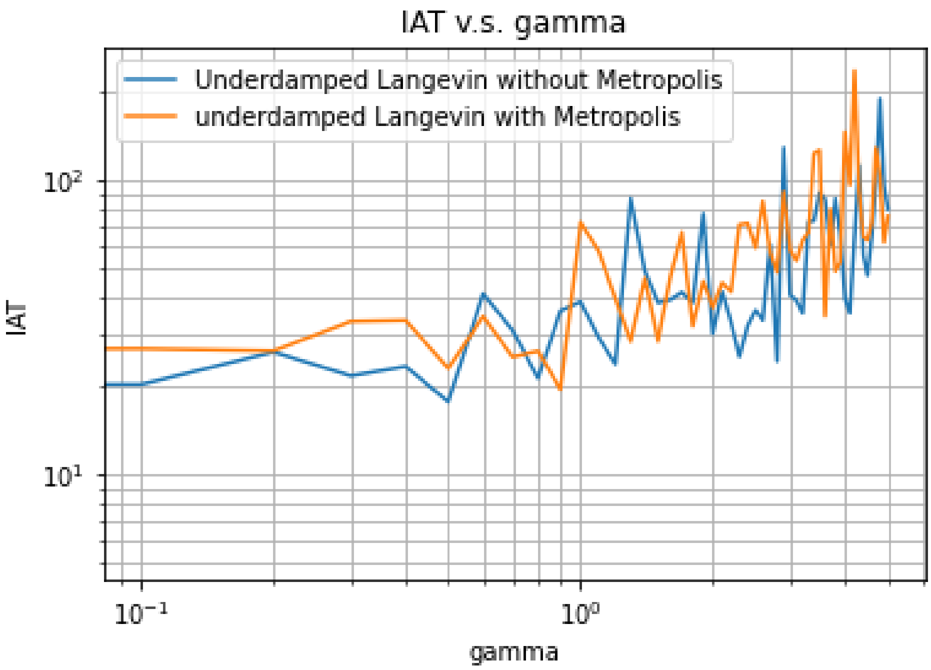
Exercise 66. *Sample the XY model described in Exercise 64 using* (5.30) *with* $\hat{J} = \hat{I}$. *Compare to the Metropolized scheme in Algorithm 6 for different values of* h *and for different values of* γ *using integrated autocorrelation time of the cosine of the angle of magnetization as your measure of efficiency. Compare to your results from Exercises 64 and 65. Which of the schemes do you prefer for sampling the XY model?*

Let $K = \frac{\|x\|^2}{2}$, $\hat{J} = I$. Let the size of lattice $L = 10$, $\beta = 0.1$. We vary the step size h from 2^{-10} to 2^{-1}, and plotted the integrated automatic time (IAT) of $\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$.



We observe that, as h increases, the IAT decreases proportionally to $\frac{1}{h}$, both the Underdamped Langevin with Metropolis and without Metropolis. Also, the Metropolis doesn't not cause significant and clear influence on the IAT. This encourages us to use a bigger step size for better efficiency.

Let the size of lattice $L = 10$, $\beta = 0.1$, $\gamma = 1$. We vary γ from 0 to 5, with a step size of 0.1, and plotted the integrated automatic time (IAT) of $\frac{M_1(\sigma)}{\|M(\sigma)\|_2}$.



We observe that, as γ increases, the IAT increases with disturbance, both the Underdamped Langevin with Metropolis and without Metropolis. Also, the Metropolis doesn't not cause significant and clear influence on the IAT. This encourages us to use a smaller step size for better efficiency.