

Fall 2022: Monte Carlo Methods Homework 6

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Exercise 71 and **Exercise 75** asked us to generate samples from Rosenbrock density.

$$\pi(x) \propto \exp\left(-\frac{100(x_2 - x_1^2)^2 + (1 - x_1)^2}{20}\right)$$

In **Exercise 71** we are asked to generate samples using the Stochastic Newton Method and Overdamped Langevin Scheme. While solving the equation

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

This algorithm was implemented such that when method was passed as newton,

$$S = -(D^2 \log \pi(x))^{-1}$$

While solving for S analytically, a region was found where Hessian was not invertible. So, calculation of S was modified to

$$S = -(D^2 \log \pi(x) + \eta * I)^{-1}$$

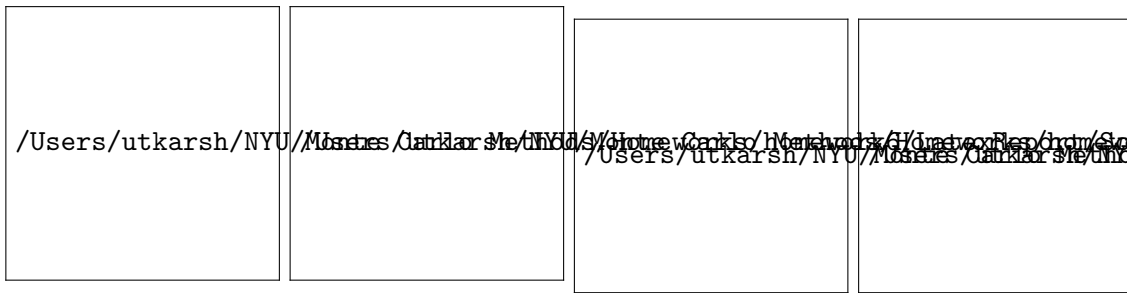
Here, η is small scalar in order to facilitate inversion and I is the identity matrix.

Also, since matrix S is the function of x_1 and x_2 , care was taken while writing metropolization step. Therefore proposal distribution was selected as

$$q(y|x) = \exp\left(-\frac{(y - x - hS(x)\nabla^T \log \pi(x))^T S(x)^{-1}(y - x - hS(x)\nabla^T \log \pi(x))}{4h}\right)$$

For the measure of performance, quantity of measure that was chosen was x_1 . So IAT was measured for the same. Total samples generated were 2million points.

Implementing these following are the results obtained for Overdamped Stochastic Newton Scheme



(a) Scatter Plot of Generated Samples

(b) Plot of IAT vs Generated Samples Count

(c) Time series of x_1

(d) Time series of x_2

Figure (1) Plots generated for Overdamped Stochastic Newton Scheme

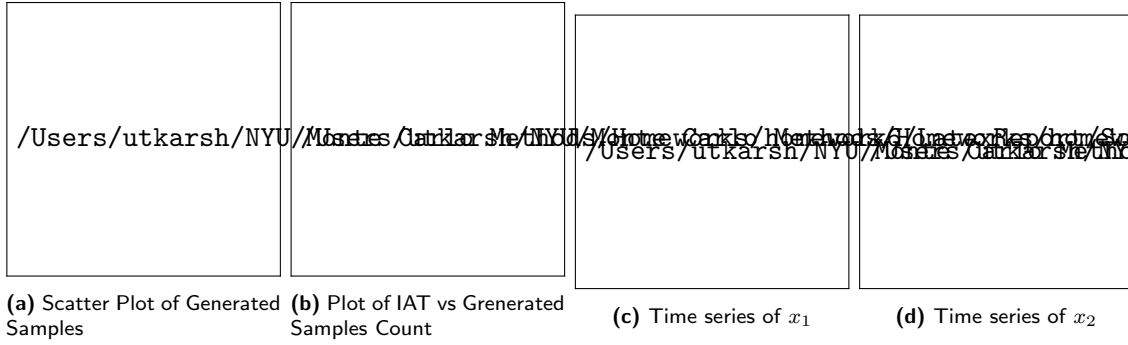


Figure (2) Plots generated for Overdamped Stochastic Newton Scheme with $S = I$

Following are the observations that could be made from ?? and ??

1. As we are already aware of contours for Rosenbrock Function, we can easily infer that these scatter plots are far from true values. For ?? Markov Chain have explored smaller region of the x_1 coordinate axis.
2. Those its IAT looks converging but the reason is that in that region it doesn't know much about the Banana Shape of the density.
3. While looking at the scatter plot of ??, generated points are having a lot of noise in them but they do have covered a larger region in space.
4. We can infer that if we increase the generated samples count, Stochastic Newton would perform better because of less noise being generated than the Overdamped Langevin Scheme

Exercise 75 asked us to implement the Ensemble Monte Carlo and compare its performance for various values of α . I experimented with values of $\alpha = \{1.5, 2, 2.5, 3\}$. For all the below figures, number of Markov chains are $L = 10$.

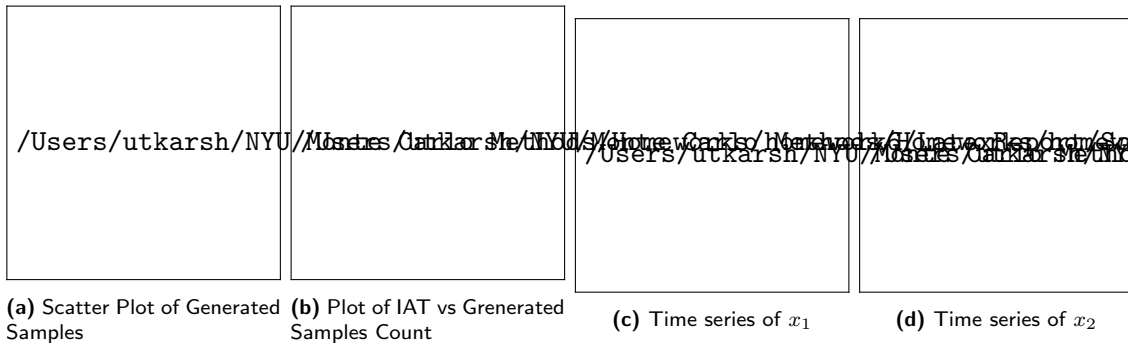


Figure (3) Plots generated for Ensemble Scheme with $\alpha = 1.5$ and $L = 10$

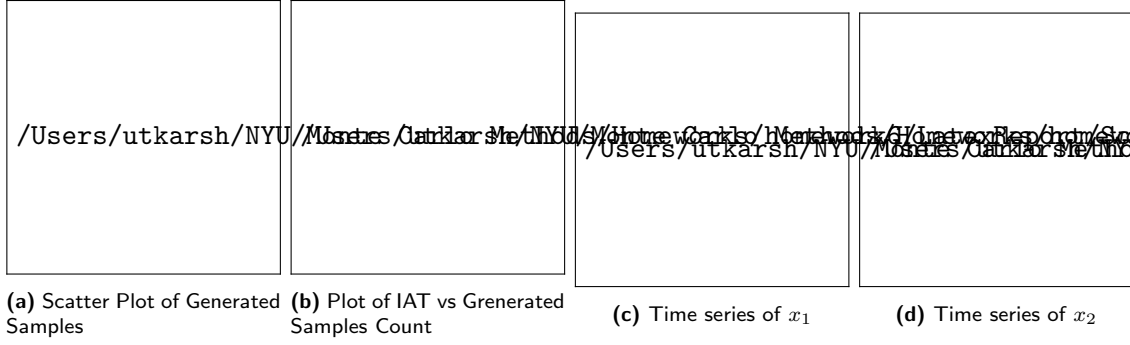


Figure (4) Plots generated for Ensemble Scheme with $\alpha = 2$ and $L = 10$

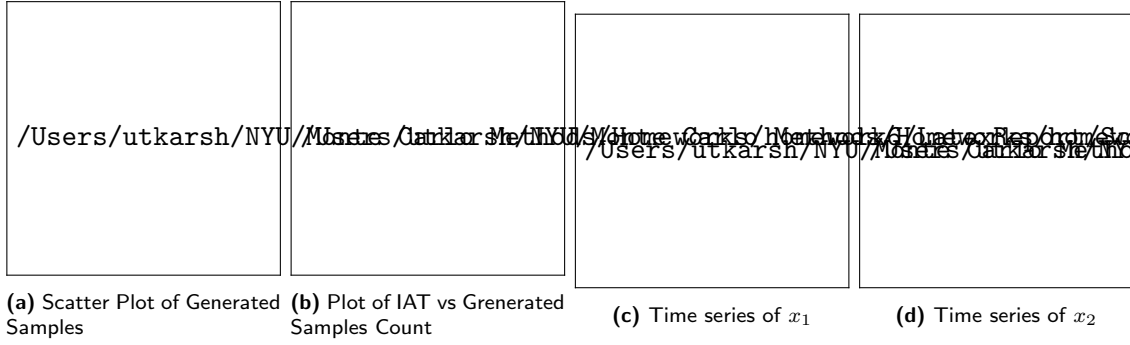


Figure (5) Plots generated for Ensemble Scheme with $\alpha = 2.5$ and $L = 10$

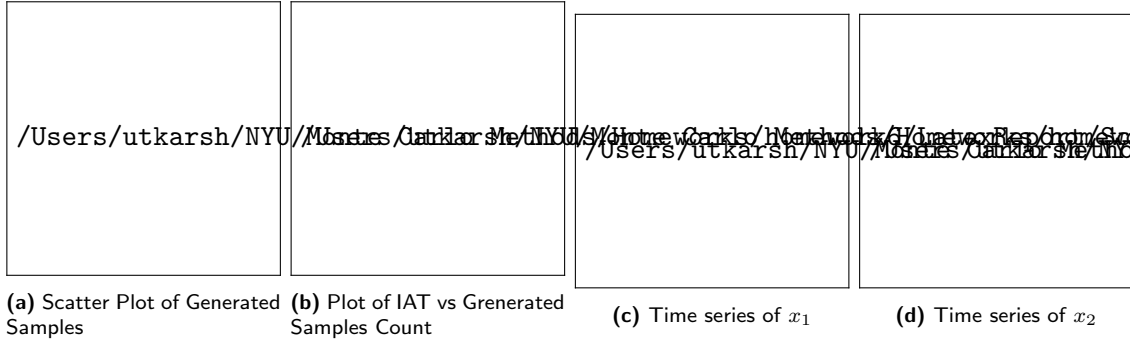


Figure (6) Plots generated for Ensemble Scheme with $\alpha = 3$ and $L = 10$

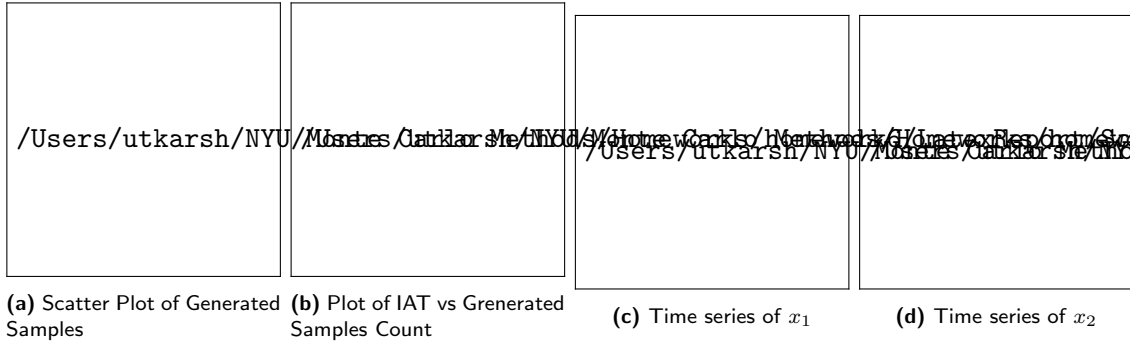


Figure (7) Plots generated for Ensemble Scheme with $\alpha = 1.5$ and $L = 20$

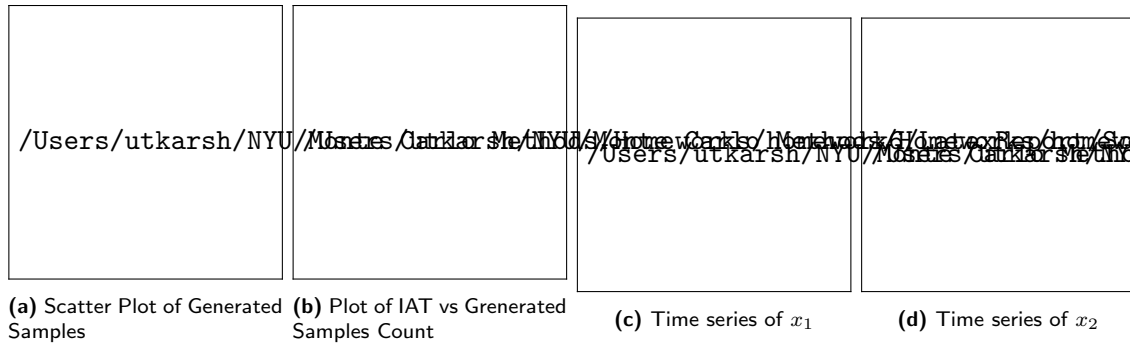


Figure (8) Plots generated for Ensemble Scheme with $\alpha = 2$ and $L = 20$

Following are the observations that could be made from ??, ??, ??, ??

1. Figure ?? shows the best generated plots for samples from the Rosenbrock density which is generate using $\alpha = 2$.
2. Figure ??, for $\alpha = 1.5$ genrated points, have losts of noise in it. While figure ??, for $\alpha = 2$ and figure ??, for $\alpha = 3$ have generated 2 million samples in a very confined region. So it could be inferred that there is surely an optimal value of α for which the markov chain is able entirely explore the region and in this case out of four choices, it is 2.
3. On increasing the number of trajectories L in Ensemble Methods, we can see from the plots ?? and ?? and from ?? and ?? that the IAT value decreases even for the same sample counts. So having more trajectories makes them iids quickly.
4. Ensemble Scheme is not only better in terms of reuslts (as evident from attached images), it is simpler to implement as well. We don't need a lot of information regarding the differential equation governing the generation proces.
5. Ensemble Schemes are much faster as well because of no need to compute hessian. Working with Hessian is a complex task, lot of thinks have to be taken care of like checkign for Symmetry, positive definiteness, invertibility, etc. Ensemble Scehems don't face such problems.

Hence, we can easily conclude that Ensemble Method with $\alpha = 2$ is the best method for generating points from Rosenbrock Density.