Markov Chain Monte Carlo

Homework

Metropolis Monte Carlo and Analysis

Consider the "three-peaks" PDF discussed in the lecture notes on Metropolis Monte Carlo:

$$\begin{aligned}\pi(x,y) \sim \exp\left(-\frac{1}{10}(x^2+y^2)\right) &+ \\ \frac{1}{2}\exp\left(-\frac{1}{20}((x-20.)^2+(y-20.)^2)\right) &+ \\ \exp\left(-\frac{1}{200}((x-40.)^2+(y-40.)^2)\right)\end{aligned} \tag{1}$$

The domain $x, y \in \Omega = [-30, 100]^2$. Basic python code to sample from this distribution is provided at the end of the lecture notes.

(i) Use visualization/traceplots to estimate reasonable choices for (a) δ in the proposal step, (b) thinning frequency, (c) the length of the burn-in period, and (d) initial state.

(ii) According to the Gelman-Rubin heuristic, how long should you run the simulation to ensure convergence?

(iii) Let $R(x,y) = \sqrt{x^2+y^2}$ be a scalar of interest. Plot the auto-correlation function of the samples R? Estimate the decorrelation time in units of Monte Carlo Steps (MCS).

(iv) Let $\langle R \rangle = E_\pi[R]$ which is given by the integral,

$$\langle R \rangle = \iint_\Omega \sqrt{x^2+y^2}\ \pi(x,y)\ dx\, dy \tag{2}$$

where $\pi(x,y)$ is given by equation 1. Using importance sampling, the integral may be approximated by the simple average,

$$\langle R \rangle \approx \frac{1}{N}\sum_{i=1}^{N}\sqrt{x_i^2+y_i^2}, \tag{3}$$

where N samples of x_i, y_i are drawn from $\pi(x,y)$ given in equation 1.

Using block-averaging to estimate $\langle R \rangle$, and attach an errorbar to it.

Hint: Python code to compute the Gelman-Rubin diagnoistic, autocorrelation function, and block averaging are provided at the end of lecture notes.