Markov Chain Monte Carlo

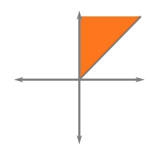
Homework

Gibbs Sampling

(i) From Exam 2018

Consider the 2D joint probability distribution (jPDF) defined over the triangular domain:

$$\pi(x, y) = \begin{cases} e^{-y} & 0 \leq x \leq y \\ 0 & \text{otherwise.} \end{cases}$$



(a) Find the marginal distributions of x and y, $\pi(x) = \int \pi(x, y)\, dy$ and $\pi(y) = \int \pi(x, y)\, dx$. **Note**: Take care to integrate over the correct domain for x and y. You may verify your setup by ensuring that $\iint \pi(x, y)\, dx\, dy = 1$.

(b) For independent distributions, the joint distribution is the product of the marginals. Test whether $\pi(x, y) = \pi(x)\pi(y)$ and show that x and y are not independent.

(c) Suppose we decide to sample the jPDF using Metropolis MCMC.[1] From a "current" point (x, y) in the domain, we propose a symmetric move,

$$\begin{aligned} x' &\sim U[x - \delta, x + \delta] \\ y' &\sim U[y - \delta, y + \delta]. \end{aligned}$$

Write pseudocode/algorithm to decide whether or not to accept the proposed move. What happens if $x' > y'$?

(d) Show that the conditional distributions $\pi(x|y)$ and $\pi(y|x)$ are uniform and exponential, respectively.

(e) Use direct Monte Carlo algorithms to sample 10000 random numbers from $\pi(x|y = 1)$ and $\pi(y|x = 1)$. You may use built-in functions, if convenient. Plot normalized histograms for both cases.[2]

(f) Starting from $(x, y) = (1, 2)$, write a Gibbs sampler to sample 10000 points from the jPDF $\pi(x, y)$. For burn-in, disregard the first 10% of the samples. Produce a scatter plot of the remaining points. Plot histograms of $\pi(x)$ and $\pi(y)$ and compare with the theoretically derived marginals in part (i).

(ii) Radius of Gyration of a Nonuniform Sphere

The density of a sphere Ω of radius $R = 1$ is given by $\rho(r) = R - r$. The radius of gyration R_g is defined by,

$$R_g^2 = \frac{\int_\Omega \rho(r) r^2 dA}{\int_\Omega \rho(r) dA}$$

[1] You don't have to actually perform the simulation.

[2] Use 30 bins for all histograms requested for this question.

We can use MC to estimate R_g^2 by sampling points (x, y, z) from a uniform distribution on the domain Ω.[3]

(a) Find the conditional distributions, $\pi(x|y, z)$, $\pi(y|x, z)$, and $\pi(z|x, y)$.

(b) Use Gibbs sampling to uniformly sample $N = 5000$ points inside the sphere.

(c) Draw traceplots of the sampled x, y, and z coordinates. Find the autocorrelation of the samples. Show the autocorrelation of x, y, z on the same plot.

(d) Estimate the radius of gyration. Use block-averaging to find the associated uncertainty.

[3] For a uniform sphere $\rho =$ constant, $R_g^2 = 3/5R^2$. You can use this to test your answers.