Monte Carlo Methods

Univariate

Nipun Batra

June 14, 2023

IIT Gandhinagar

Introduction

General Form

The general form of Monte Carlo methods is: The expectation of a function $f(x)$ with respect to a distribution $p(x)$ is given by:

$$\mathbb{E}_{x \sim p(x)}[f(x)] = \int f(x)p(x)dx \tag{1}$$

Using Monte Carlo methods, we can estimate the above expectation by sampling x_i from $p(x)$ and computing the average of $f(x_i)$.

$$\mathbb{E}_{x \sim p(x)}[f(x)] \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i) \tag{2}$$

where $x_i \sim p(x)$.

Estimating Pi using Monte Carlo (Part 1)

We can estimate the value of pi using Monte Carlo methods by considering a unit square with a quarter circle inscribed within it.

- Let $p(x)$ be defined over the unit square using the uniform distribution in two dimensions, i.e., $p(x) = U(x) = 1$ for $x \in [0, 1]^2$.
- Let $f(x)$ be the indicator function defined as follows:

$$f(x) = \begin{cases} \text{Green}(1), & \text{if } x \text{ falls inside the quarter circle,} \\ \text{Red}(0), & \text{otherwise.} \end{cases}$$

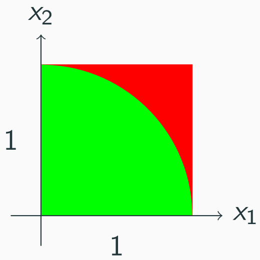
Estimating Pi using Monte Carlo (Part 1)

- Or, we can write $f(x)$ to be the following:

$$f(x) = \begin{cases} 1, & \text{if } x_1^2 + x_2^2 \leq 1, \\ 0, & \text{otherwise.} \end{cases}$$

- Or, using the indicator function, we can write $f(x)$ to be the following:

$$f(x) = \mathbb{I}(x_1^2 + x_2^2 \leq 1)$$



$$\frac{\pi}{4} \approx \frac{\text{Green area}}{\text{Green area} + \text{Red area}}$$

Estimaing prior predictive distribution

- Let $p(\theta)$ be the prior distribution of parameter $\theta \in R^2$. Say, for example, $p(\theta_i) = \mathcal{N}(0,1) \forall i$.
- Let $p(y|\theta, x)$ be the likelihood function. Say, for example, $p(y|\theta, x) = \mathcal{N}(\theta_0 + \theta_1 x, 1)$.
- Then, the prior predictive distribution is given by:

$$p(y|x) = \int p(y|\theta, x)p(\theta)d\theta \tag{3}$$

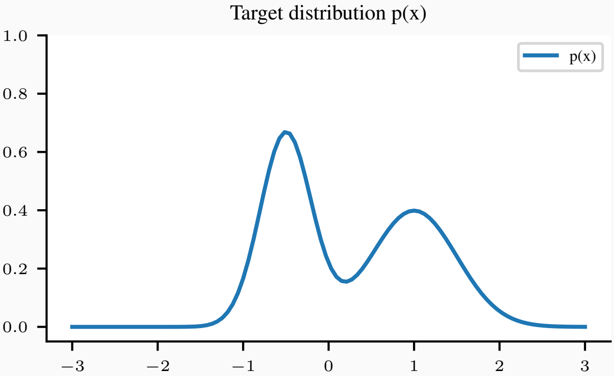
$$p(y|x) \approx \frac{1}{N}\sum_{i=1}^{N} p(y|\theta_i, x) \tag{4}$$

where $\theta_i \sim p(\theta)$.

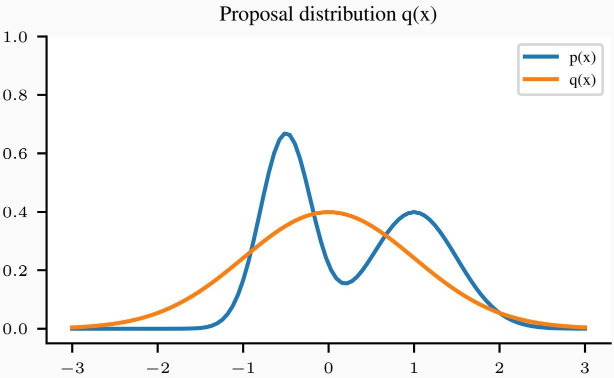
Rejection Sampling

- Let $p(x)$ be the target distribution from which we want to sample.
- Let $q(x)$ be a proposal distribution from which we can sample.
- Let M be a constant such that $M \geq \frac{p(x)}{q(x)} \forall x$.
- Then, we can sample from $p(x)$ by sampling from $q(x)$ and accepting the sample with probability $\frac{p(x)}{Mq(x)}$.

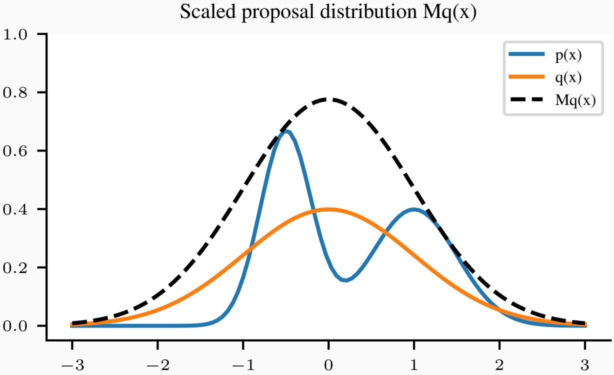
Rejection Sampling



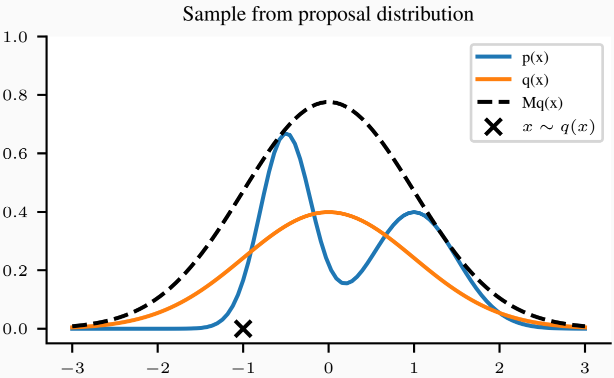
Rejection Sampling



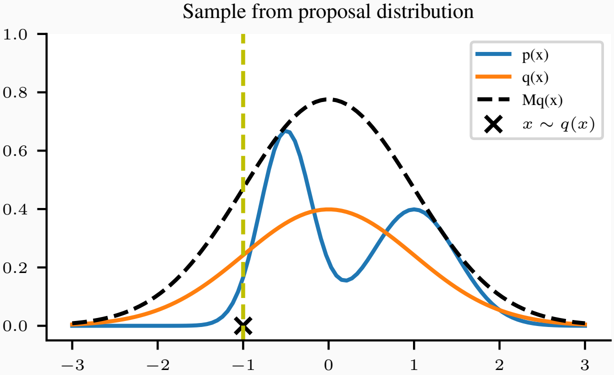
Rejection Sampling



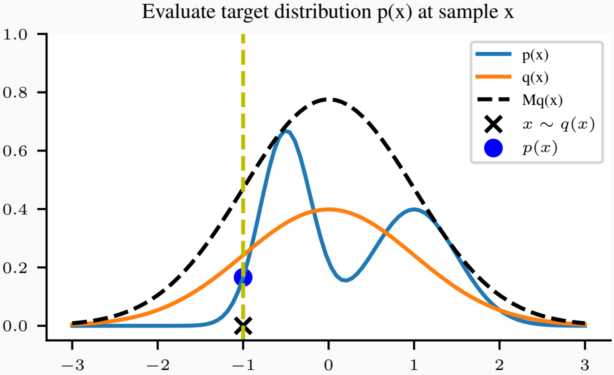
Rejection Sampling



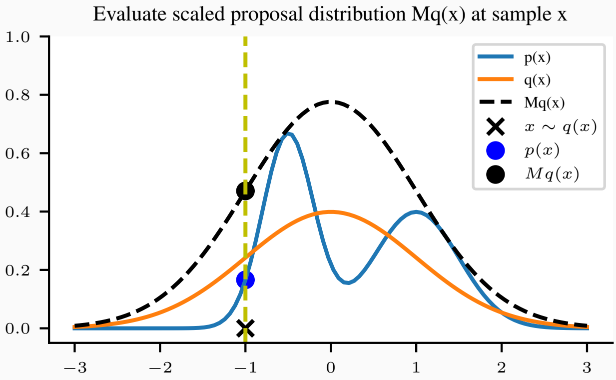
Rejection Sampling



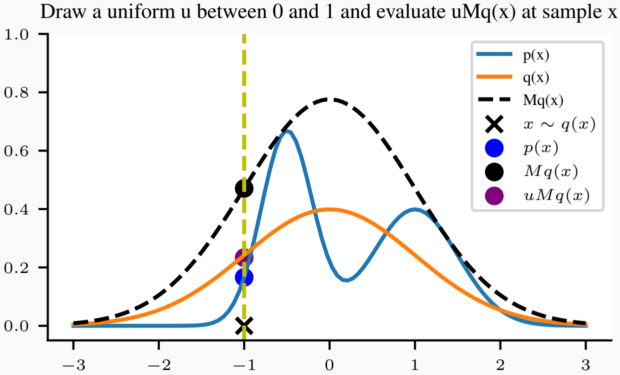
Rejection Sampling



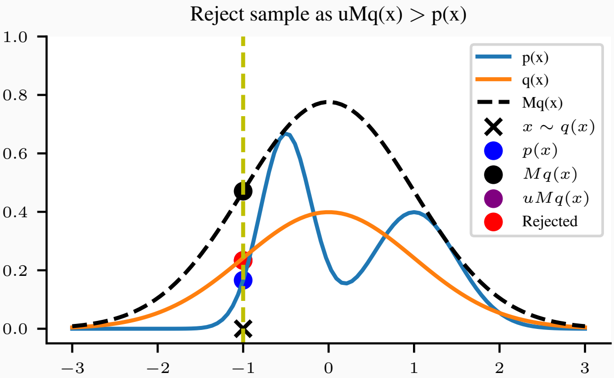
Rejection Sampling



Rejection Sampling



Rejection Sampling



Proof of Rejection Sampling

Acceptance Probability $\alpha(x)$

$$\alpha(x) = \frac{p(x)}{Mq(x)} \tag{5}$$

Bayes Rule for Acceptance

$$P(Sample|Accept) = \frac{P(Accept|Sample)P(Sample)}{P(Accept)} \tag{6}$$

P(Sample)

We draw samples from $q(x)$, so $P(Sample) = q(x)$.

Proof of Rejection Sampling

Further, $P(Accept|Sample) = \alpha(x) = \frac{p(x)}{Mq(x)}$.

Finally, $P(Accept) = \int P(Accept|Sample)P(Sample)dSample = \int \alpha(x)q(x)dx = \frac{1}{M}\int p(x)dx = \frac{1}{M}$.

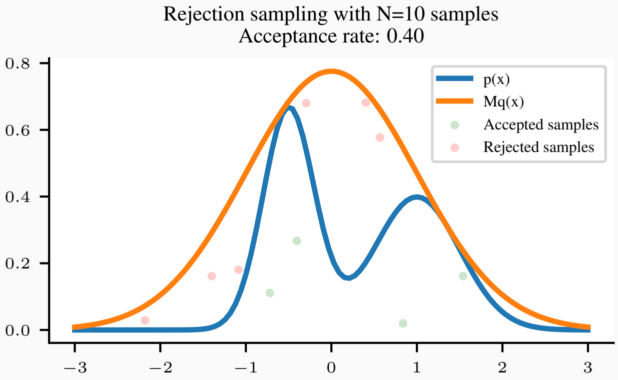
P(Accept)

$$P(Accept) = \frac{1}{M} \tag{7}$$

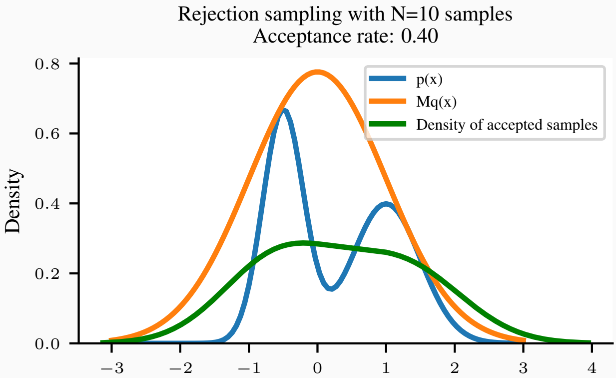
Thus, $P(Sample|Accept) = \frac{p(x)}{Mq(x)} \times \frac{q(x)}{1/M} = p(x)$.

Thus, we have shown that the samples we accept are distributed according to $p(x)$.

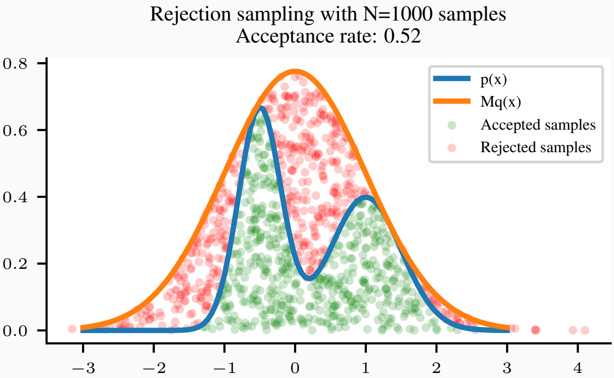
Rejection Sampling Completed Example



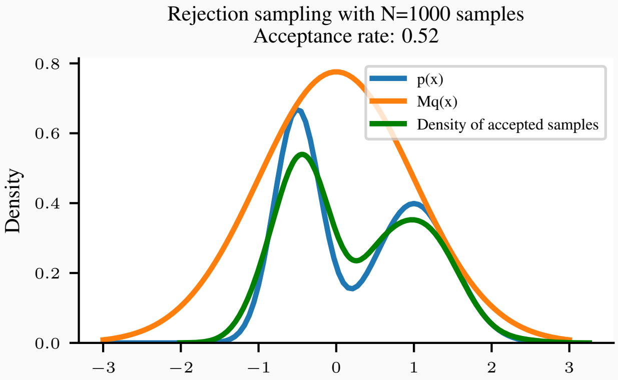
Rejection Sampling Completed Example



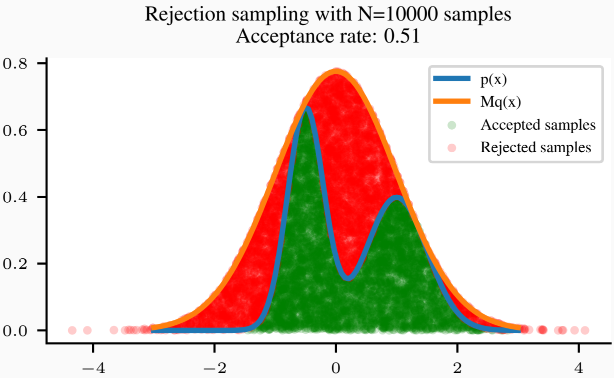
Rejection Sampling Completed Example



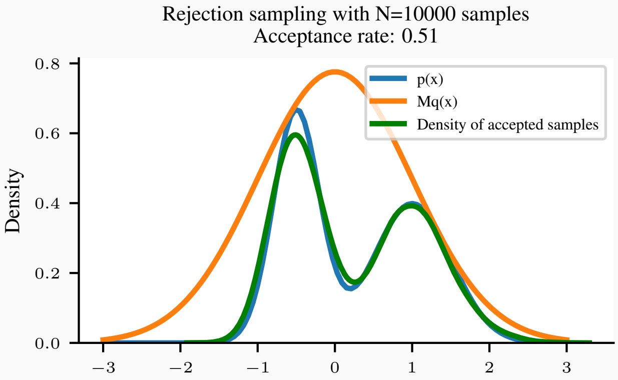
Rejection Sampling Completed Example



Rejection Sampling Completed Example



Rejection Sampling Completed Example



Challenges with Rejection Sampling

- Rejection sampling is inefficient when the target distribution is very different from the proposal distribution.
- In this case, we will reject a lot of samples.
- This is a problem when sampling from high-dimensional distributions.
- Acceptance probability $\alpha(x)$ is very low.