Sampling Methods

Nipun Batra

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IIT Gandhinagar

Topics

1. Monte Carlo Simulation

2. Rejection Sampling

Monte Carlo Simulation

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:

$$f(x) = \begin{cases} \text{Green}(1), & \text{if } x \text{ falls inside the quarter circle,} \\ \text{Red}(0), & \text{otherwise.} \end{cases}$$
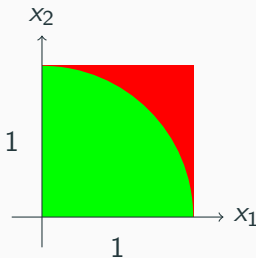
- Or, we can write $f(x)$ to be the following:

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

- 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 $\theta_i \sim p(\theta)$.
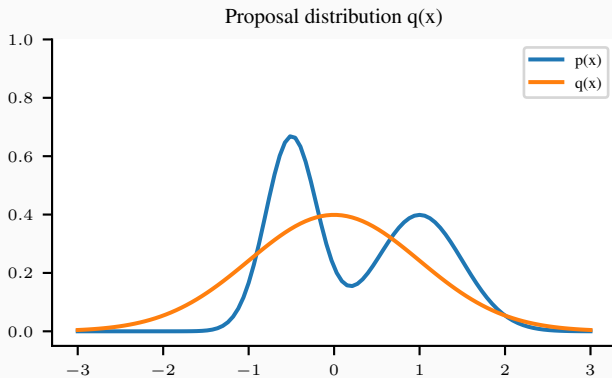
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Rejection Sampling

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 $\frac{p(x)}{Mq(x)}$.
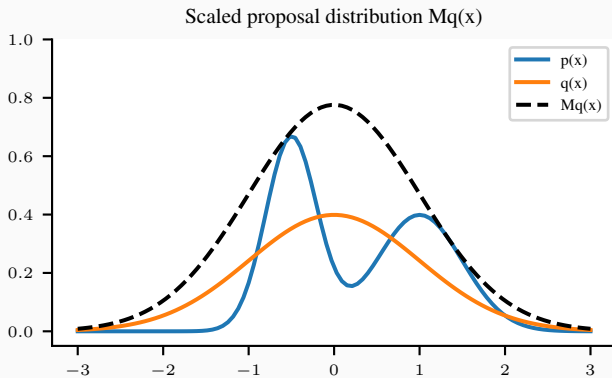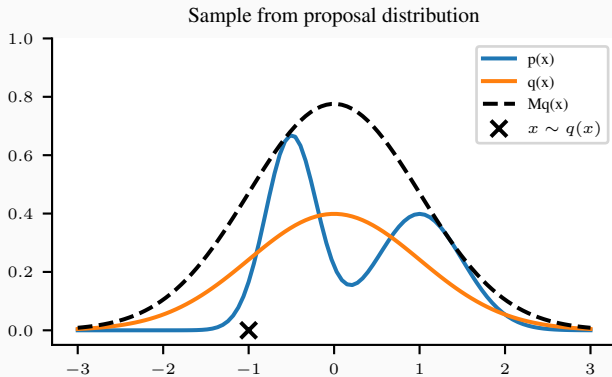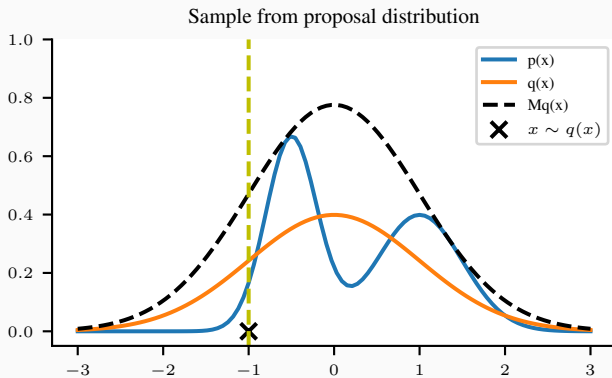
Rejection Sampling
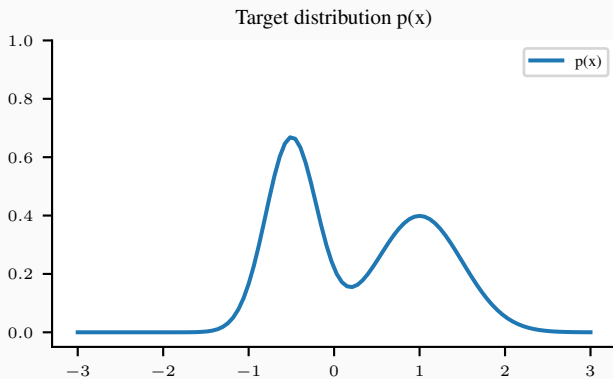
Target distribution p(x)

Proposal distribution q(x)

Scaled proposal distribution Mq(x)

Sample from proposal distribution

Sample from proposal distribution

Evaluate target distribution p(x) at sample x

Evaluate scaled proposal distribution Mq(x) at sample x

Draw a uniform u between 0 and 1 and evaluate uMq(x) at sample x

Reject sample as uMq(x) > p(x)
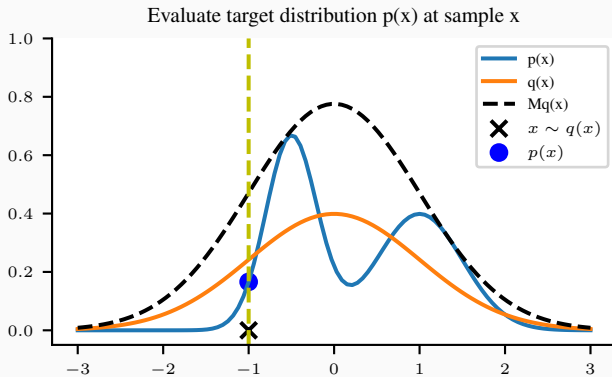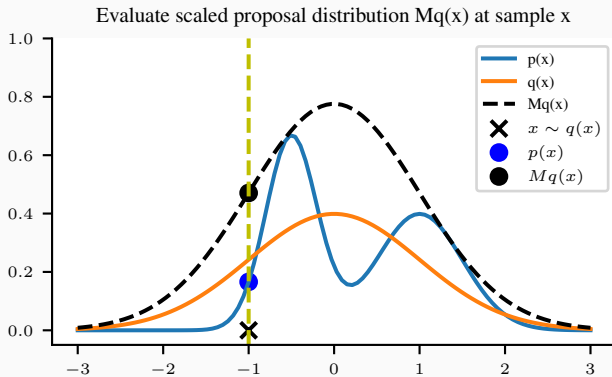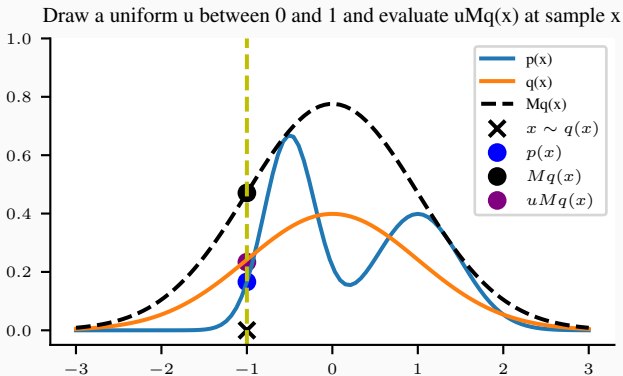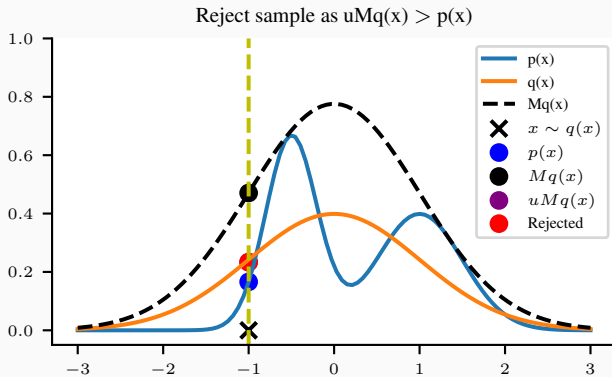
Proof of Rejection Sampling

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

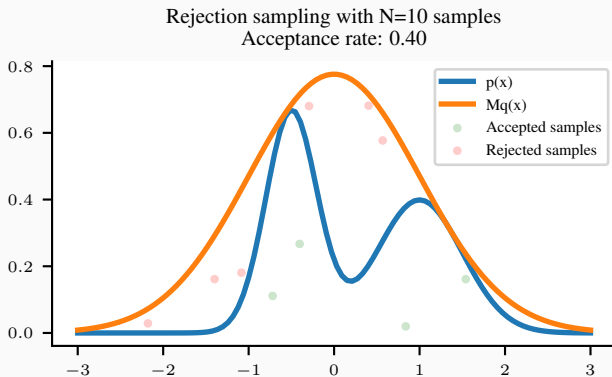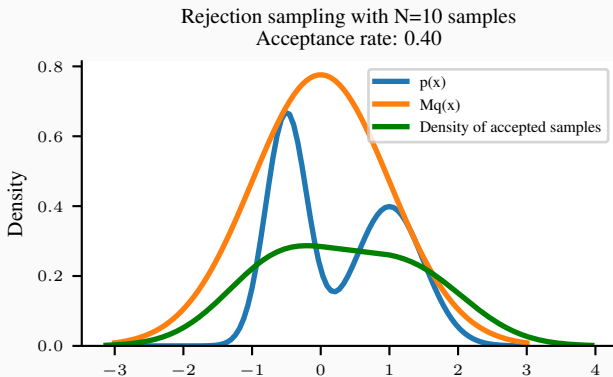### P(Accept)

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

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

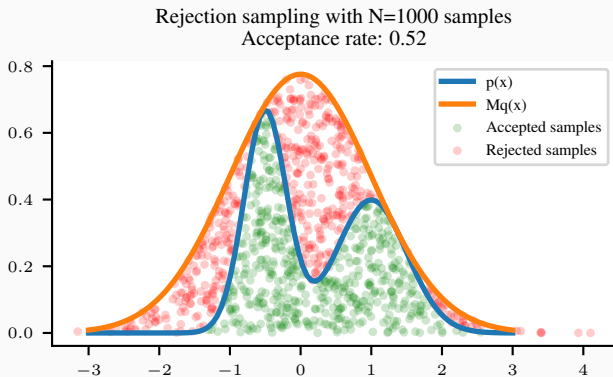Thus, we have shown that the samples we accept are distributed according to $p(x)$.
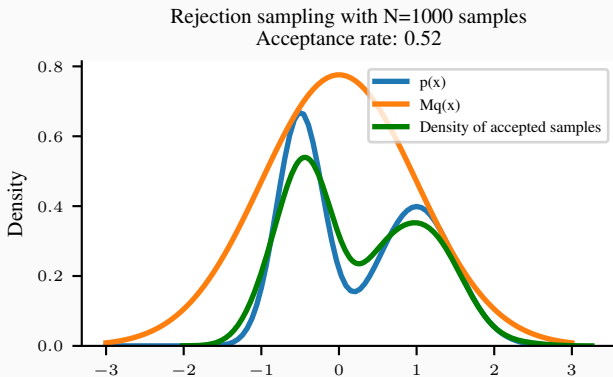
Rejection sampling with N=10 samples
Acceptance rate: 0.40

Rejection sampling with N=10 samples
Acceptance rate: 0.40

Rejection sampling with N=1000 samples
Acceptance rate: 0.52

Rejection sampling with N=1000 samples
Acceptance rate: 0.52

Legend:
- p(x)
- Mq(x)
- Density of accepted samples

Rejection sampling with N=10000 samples
Acceptance rate: 0.51

Rejection sampling with N=10000 samples
Acceptance rate: 0.51
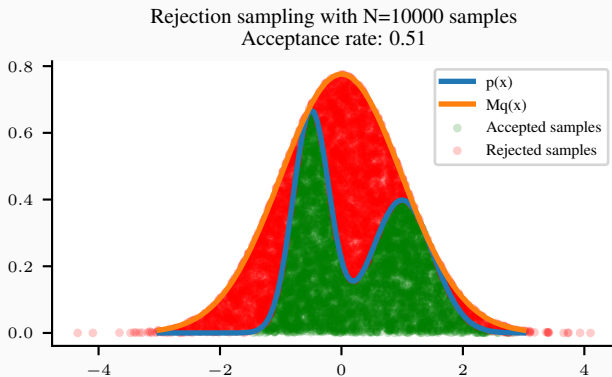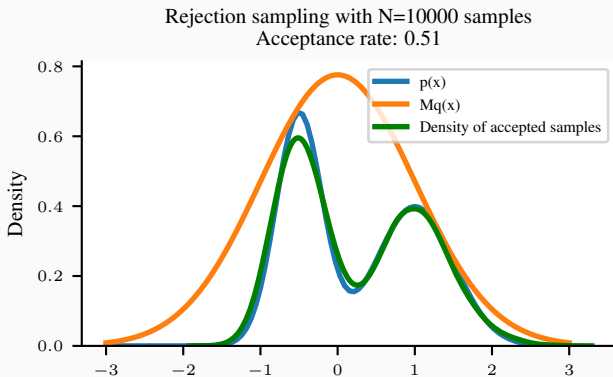
Challenges with Rejection Sampling

- 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.