Sampling Methods

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Topics

1. Monte Carlo Simulation

    General Form

    Applications

    Bias and Variance of Monte Carlo

2. Sampling from common probability distributions

    PRNG

    Inverse CDF Sampling

    Sampling from Normal Distribution

    Rejection Sampling

The Discovery That Transformed Pi

Monte Carlo Simulation

General Form

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

where $x_i \sim p(x)$.

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- 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:

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

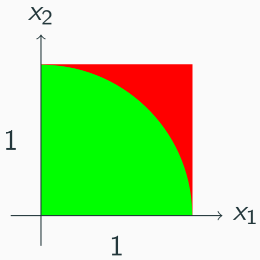
Estimating Pi using Monte Carlo (Part 1)

- 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:

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

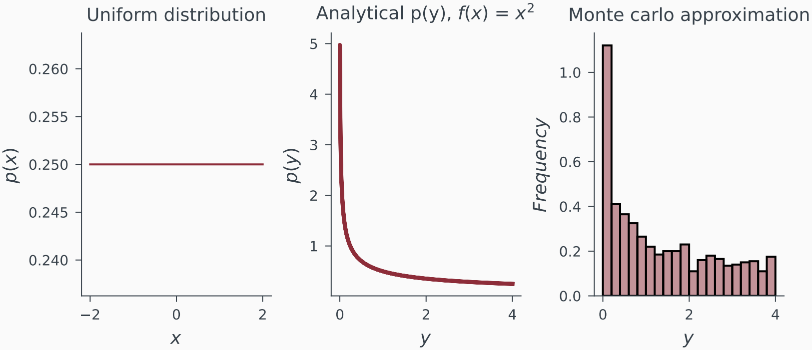


$$\frac{\pi}{4} \approx \frac{\text{Green area}}{\text{Green area} + \text{Red area}}$$

Notebook: `mc_sampling_intro.ipynb`

Estimating a function using Monte Carlo

Let $x \in \mathcal{U}(-1,1)$ and $y = f(x) = x^2$.



Estimating prior predictive distribution

- Let $p(\theta)$ be the prior distribution of parameter $\theta \in \mathbb{R}^2$. 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 $\theta_i \sim p(\theta)$.

Estimating posterior predictive distribution

Extending for posterior predictive distribution, we have:

$$p(y|x, D) = \int p(y|\theta, x)p(\theta|D)d\theta \tag{5}$$

$$p(y|x, D) \approx \frac{1}{N}\sum_{i=1}^{N} p(y|\theta_i, x) \tag{6}$$

Unbiased Estimator?

Is Monte Carlo Sampling a biased or unbiased estimator?

We know:

$$\mathbb{E}_{x \sim p(x)}[f(x)] = \int f(x)p(x)dx = \phi \tag{7}$$

Let $x_i \in 1, \ldots, N$ be i.i.d samples:

$$\hat{\phi} = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

$$\mathbb{E}(\hat{\phi}) = \int \frac{1}{N} \sum_{i=1}^{N} f(x_i)p(x_i)dx = \frac{1}{N} \sum_{i=1}^{N} \int f(x_i)p(x_i)dx$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}(f(x_i)) = \phi$$

Thus, it is an unbiased estimator!

Sampling converges slowly

The expected square error of the Monte Carlo estimate is given by:

$$\mathbb{E}\left(\hat{\phi} - \mathbb{E}(\hat{\phi})\right)^2 = \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N}(f(x_i) - \phi)\right]^2$$

$$= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\mathbb{E}(f(x_i)f(x_j)) - \phi\mathbb{E}(f(x_i)) - \mathbb{E}(f(x_j))\phi + \phi^2$$

$$= \frac{1}{N^2}\sum_{i=1}^{N}\left(\left(\sum_{i\neq j}\phi^2 - 2\phi^2 + \phi^2\right) + \mathbb{E}(f^2) - \phi^2\right) = \frac{1}{N}\mathbb{V}(f)$$

$$\therefore \mathbb{E}\left(\hat{\phi} - \mathbb{E}(\hat{\phi})\right)^2 = \mathcal{O}(N^{-1})$$

Thus, the expected error drops as $\mathcal{O}(N^{-\frac{1}{2}})$.

Pop Quiz

How many samples (N) do we need to reach single-precision (i.e., $\sim 10^{-7}$)?

Is sampling easy?

Many reasons contribute to sampling not always being easy in higher dimensions. For example,

- need a global description of the entire function
- need to know probability densities everywhere
- need to know regions of high density

Sampling from common probability distributions

Sampling from uniform U(0, 1)

- Question: How can you generate samples from the uniform distribution in $[0, 1]$?

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- where, a, c, m are constants and x_0 is the seed
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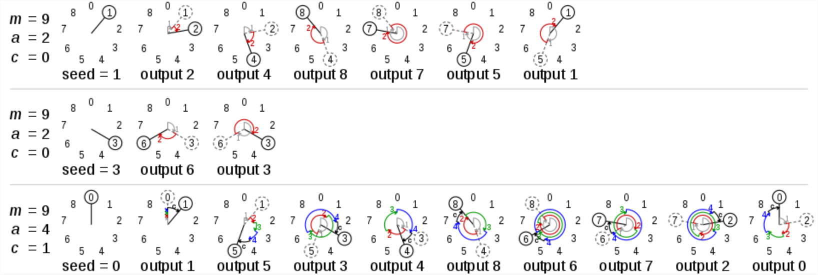
- $\frac{x_{n+1}}{m}$ is the next random number between 0 and 1

Sampling from uniform U(0, 1)

From Wikipedia page on LCG



Sampling from uniform U(0, 1)

Notebook: random-uniform.ipynb

Sampling from uniform U(a, b)

- Assume we have $X \sim U(0, 1)$

Sampling from uniform U(a, b)

- Assume we have $X \sim U(0, 1)$
- Then, $Y = a + (b - a)X \sim U(a, b)$

Inverse CDF sampling

[Inspired by content from Ben Lambert and Phillip Hennig]

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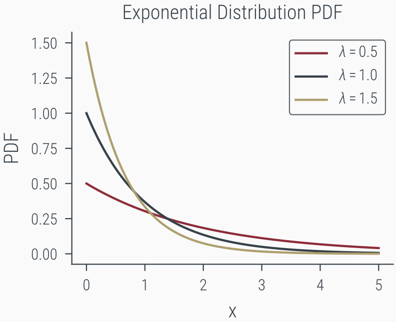
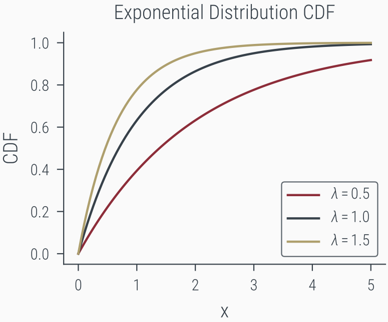
- The PDF of the exponential distribution is given by:
- $$p(x) = \lambda e^{-\lambda x} \tag{9}$$

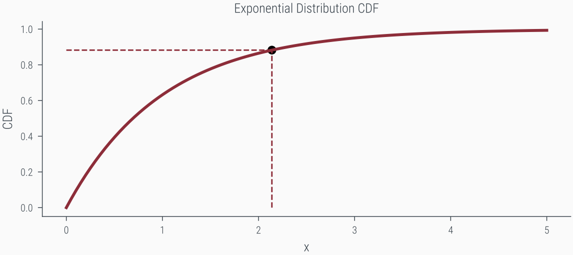




Notebook: inverse-cdf.ipynb

Inverse CDF Sampling for Number of samples = 1

- Let us consider the CDF ($F(x)$) of the exponential distribution ($\lambda = 1$) and try to generate samples from it.
- We generate a random number $u \sim U(0, 1)$.
- We then find the value of x such that $F(x) = u$.



Inverse CDF Sampling for Number of samples = 2

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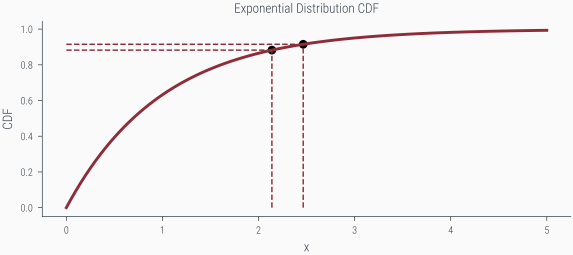

Inverse CDF Sampling for Number of samples = 3

- Let us consider the CDF ($F(x)$) of the exponential distribution ($\lambda = 1$) and try to generate samples from it.
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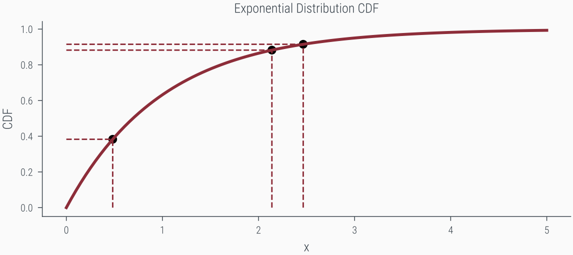

Inverse CDF Sampling for Number of samples = 4

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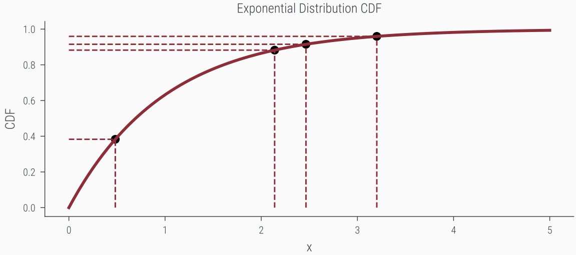

Inverse CDF Sampling for Number of samples = 5

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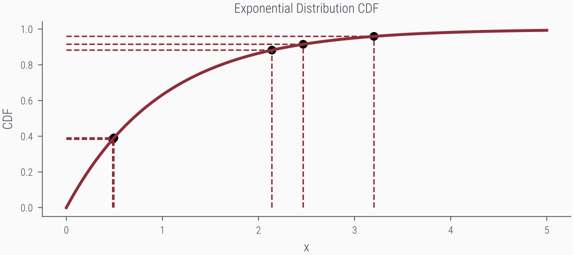

Inverse CDF Sampling for Number of samples = 6

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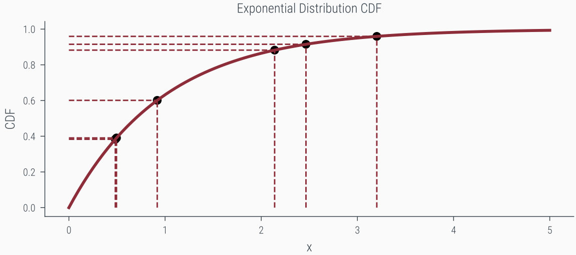

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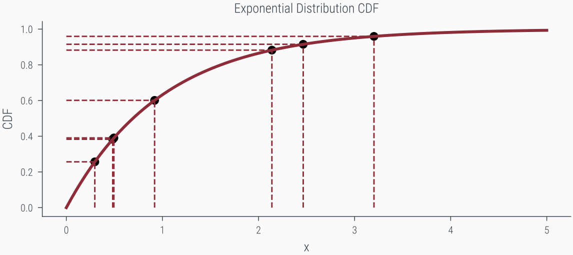

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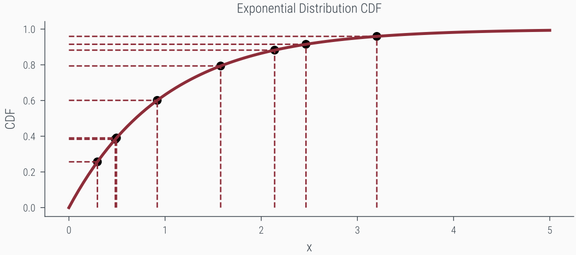

Inverse CDF Sampling for Number of samples = 9

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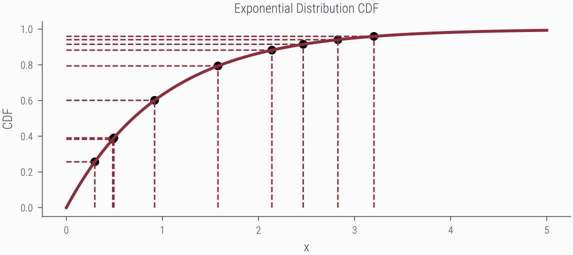

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- $$u = 1 - e^{-x} \tag{10}$$
- $$x = -\log(1 - u) \tag{11}$$

Inverse CDF sampling

[From Wikipedia page on Inverse Transform Sampling] From $U \sim \text{Unif}[0,1]$, we want to generate X with CDF $F_X(x)$. We assume $F_X(x)$ to be a continuous, strictly increasing function, which provides good intuition.

We want to see if we can find some strictly monotone transformation $T : [0,1] \mapsto \mathbb{R}$, such that $T(U) \overset{d}{=} X$. We will have

$$F_X(x) = \Pr(X \leq x) = \Pr(T(U) \leq x) = \Pr\left(U \leq T^{-1}(x)\right) = T^{-1}(x), \text{ fo}$$

where the last step used that $\Pr(U \leq y) = y$ when U is uniform on $[0,1]$. So we got F_X to be the inverse function of T, or, equivalently $T(u) = F_X^{-1}(u), u \in [0,1]$. Therefore, we can generate X from $F_X^{-1}(U)$.

Generating samples from $\mathcal{N}(0,1)$ using Box-Muller Transform

[From Wikipedia page on Box-Muller Transform]

- Let $U_1, U_2 \sim U(0,1)$ be two independent random variables.

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- Then, $Z_0 = R \cos \Theta$ and $Z_1 = R \sin \Theta$ are independent random variables.
- Z_0 and Z_1 are independent and identically distributed (i.i.d) $\mathcal{N}(0,1)$ random variables.

Notebook: sampling-normal.ipynb

Generating samples from $\mathcal{N}(\mu, \sigma)$

- Let $Z_0 \sim \mathcal{N}(0, 1)$ be independent random variables.

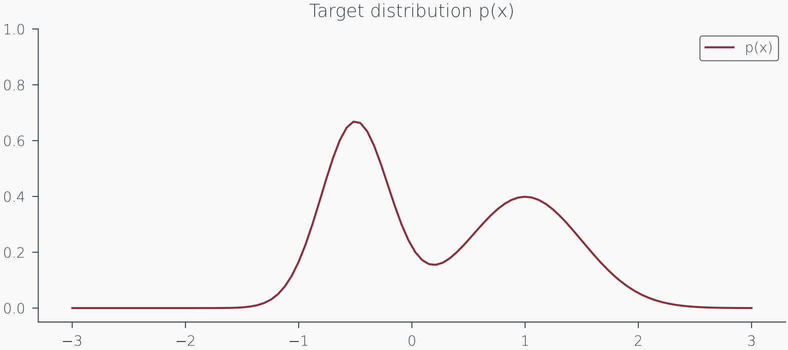
Generating samples from $\mathcal{N}(\mu, \sigma)$

- Let $Z_0 \sim \mathcal{N}(0, 1)$ be independent random variables.
- Then, $X = \mu + \sigma Z_0$ is a random variable with $\mathcal{N}(\mu, \sigma)$ distribution.

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



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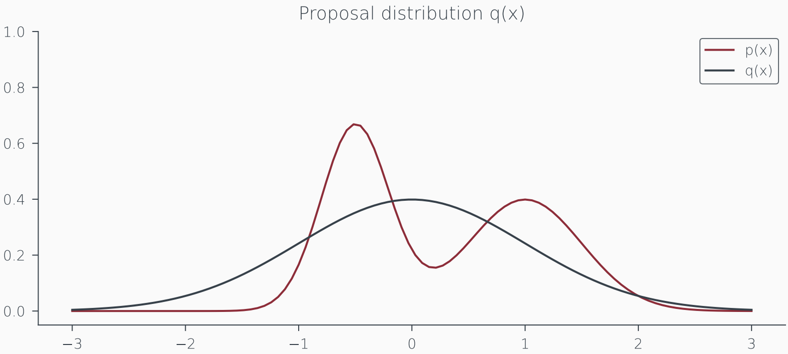

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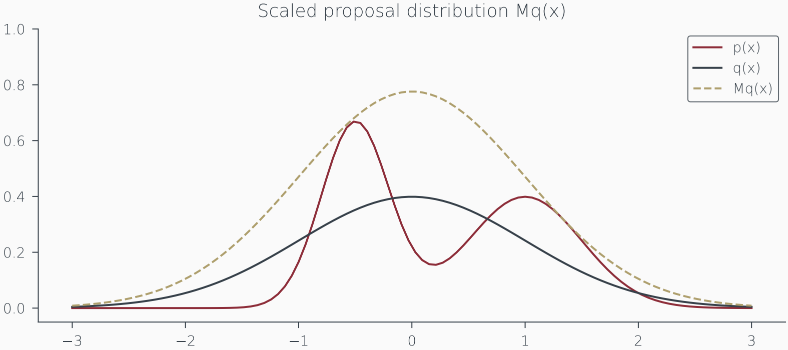

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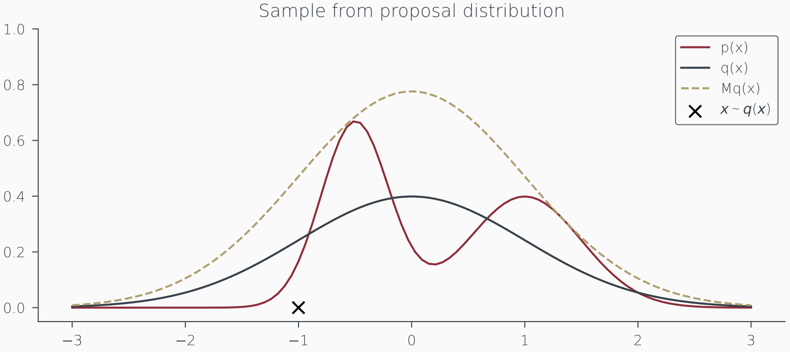

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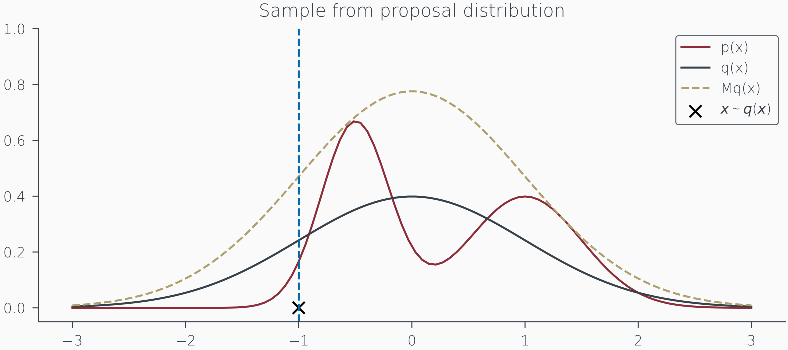

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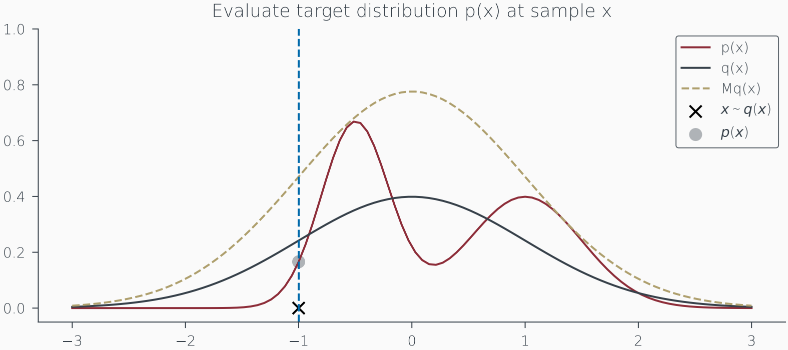

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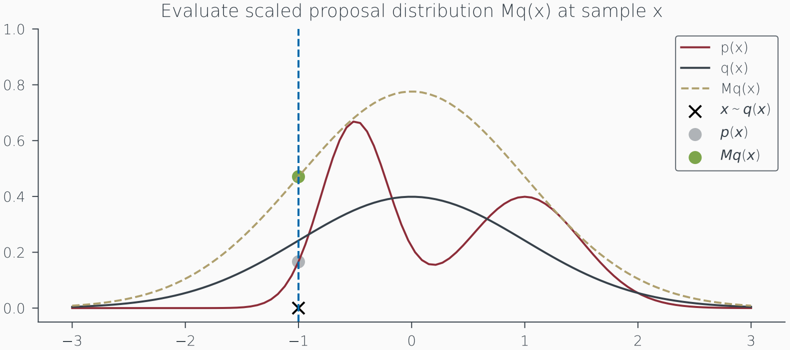

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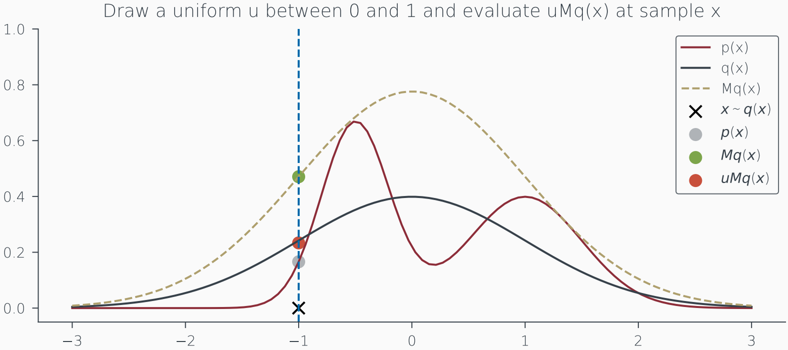

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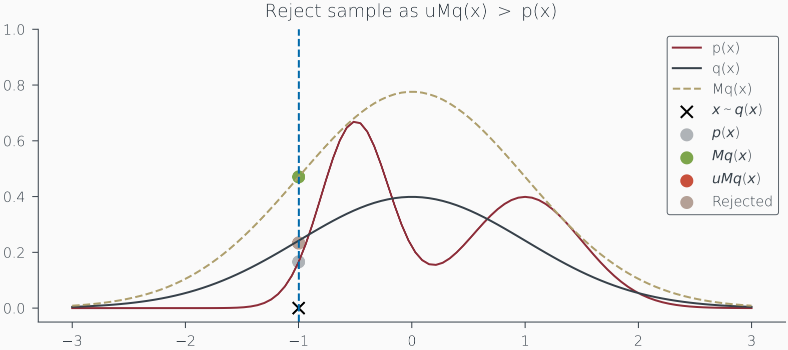

Proof of Rejection Sampling

Acceptance Probability $\alpha(x)$

$$\alpha(x) = \frac{p(x)}{Mq(x)} \tag{12}$$

Bayes Rule for Acceptance

$$P(Sample|Accept) = \frac{P(Accept|Sample)P(Sample)}{P(Accept)} \tag{13}$$

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)

$$P(Accept) = \frac{1}{M} \tag{14}$$

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

Note: Figures not on github.

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.