Sampling Methods

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Topics

1. Monte Carlo Simulation
2. Rejection Sampling
3. Inverse CDF
4. Importance Sampling
5. Gibbs Sampling
6. Markov Chain Monte Carlo

Monte Carlo Simulation

The idea behind MC Simulation

- We often want to compute expected value of some function of a random variable, which turns into the integral,

$$\mathbb{E}\left[f(x)\right] = \int f(x)p(x)dx$$

where $x \in \mathbb{R}^n, f : \mathbb{R}^n \to \mathbb{R}^m$ and $p(x)$ is the target distribution.

- In low dimensions, we can use numerical integration techniques to compute the above integral. However, in high dimensions, this is not feasible.
- Alternative approach is to draw multiple random samples, $x_i \sim p(x)$ and compute

$$\mathbb{E}\left[f(x)\right] \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

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 $x_i \sim p(x)$.

Unbiased Estimator?

Is Monte Carlo Sampling a biased or unbiased estimator?

We know:

$$\mathbb{E}_{x\sim p(x)}[f(x)] = \int f(x)p(x)dx = \phi \tag{3}$$

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!

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:

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

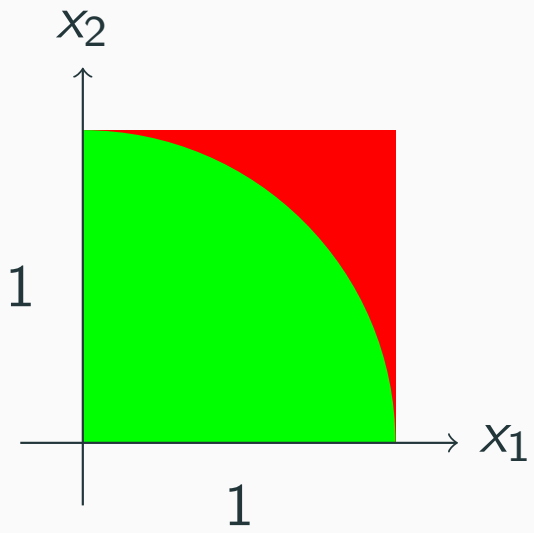
Estimating Pi using Monte Carlo (Part 1)

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

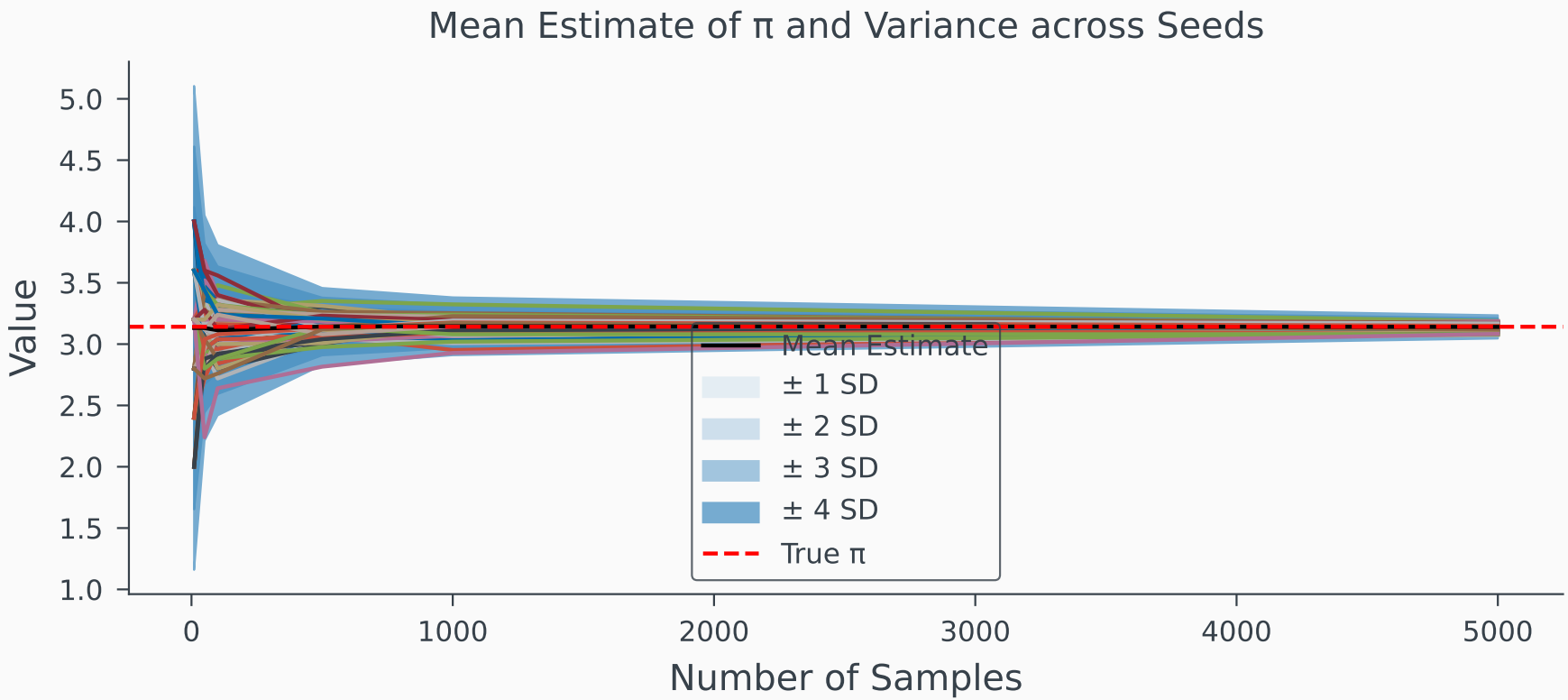
$$f(x) = \begin{cases} 1, & \text{if } x_1^2 + x_2^2 \leq 1, \\ 0, & \text{otherwise.} \end{cases}$$

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

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

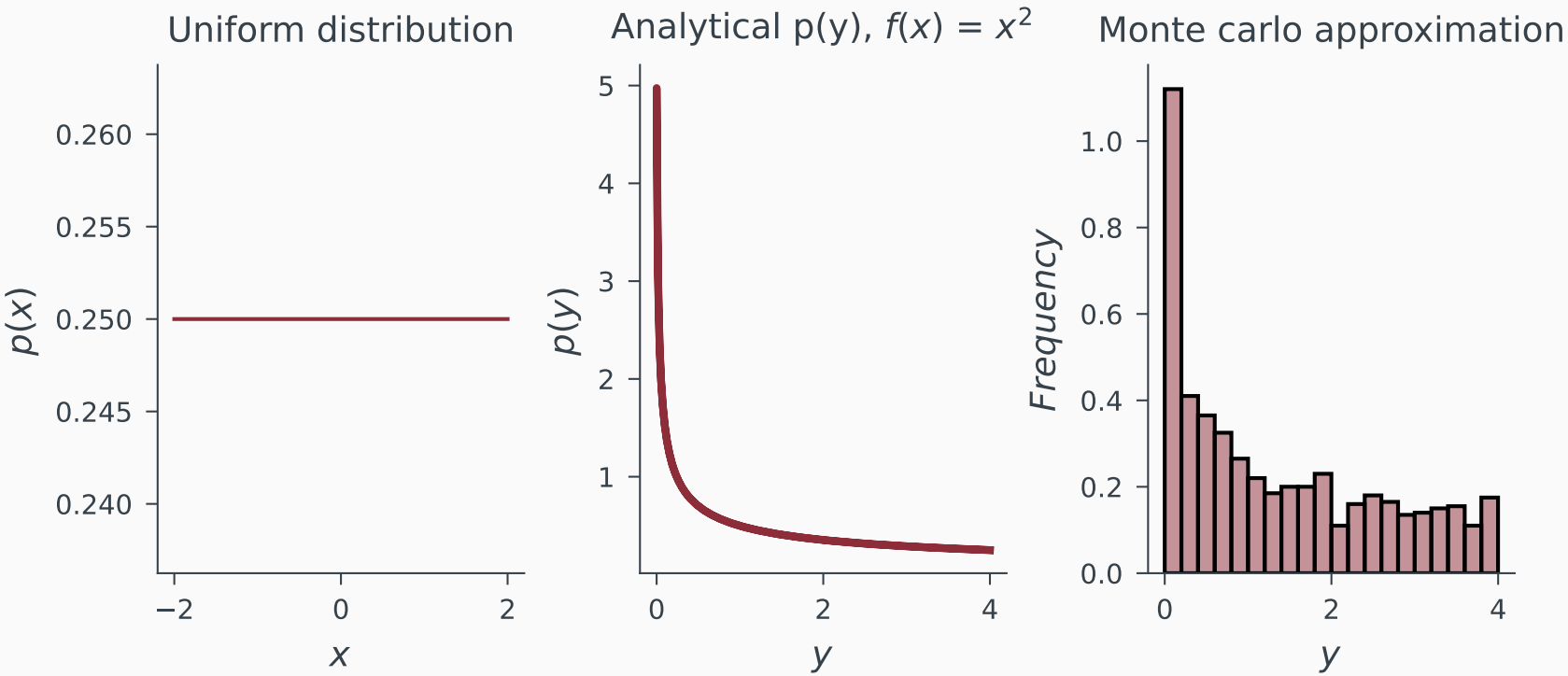


$$\frac{\pi}{4} \approx \frac{\text{Green area}}{\text{Green area} + \text{Red area}}$$


Mean Estimate of π and Variance across Seeds
Value
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0
1000
2000
3000
4000
5000
Number of Samples
Mean Estimate
± 1 SD
± 2 SD
± 3 SD
± 4 SD
True π

Estimating a function using Monte Carlo

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



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

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:

$$p(y|x) = \int p(y|\theta, x)p(\theta)d\theta \tag{4}$$

$$p(y|x) \approx \frac{1}{N} \sum_{i=1}^{N} p(y|\theta_i, x) \tag{5}$$

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

Estimating posterior predictive distribution

Extending for posterior predictive distribution, we have:

$$p(y|x, D) = \int p(y|\theta, x)p(\theta|D)d\theta \tag{6}$$

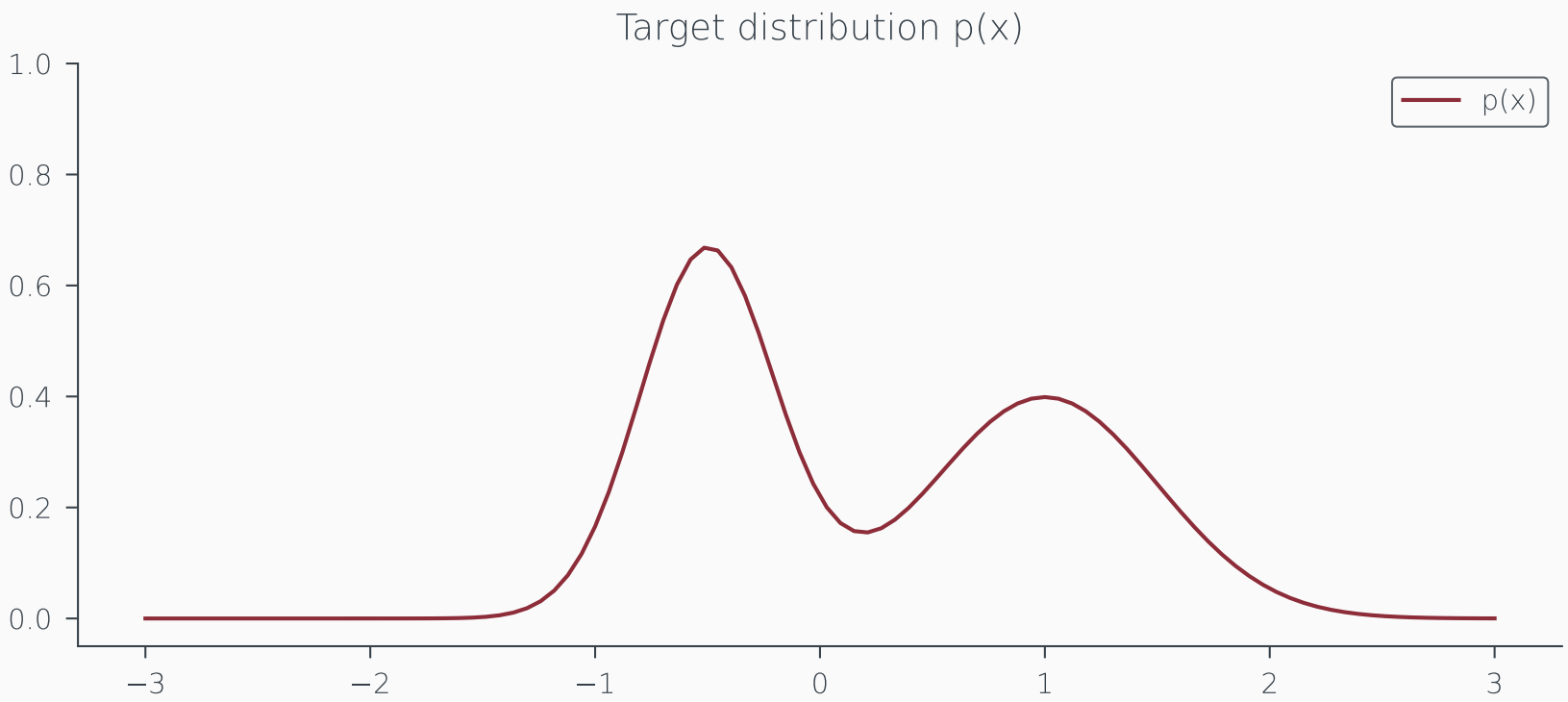
$$p(y|x, D) \approx \frac{1}{N}\sum_{i=1}^{N} p(y|\theta_i, x) \tag{7}$$

Rejection Sampling

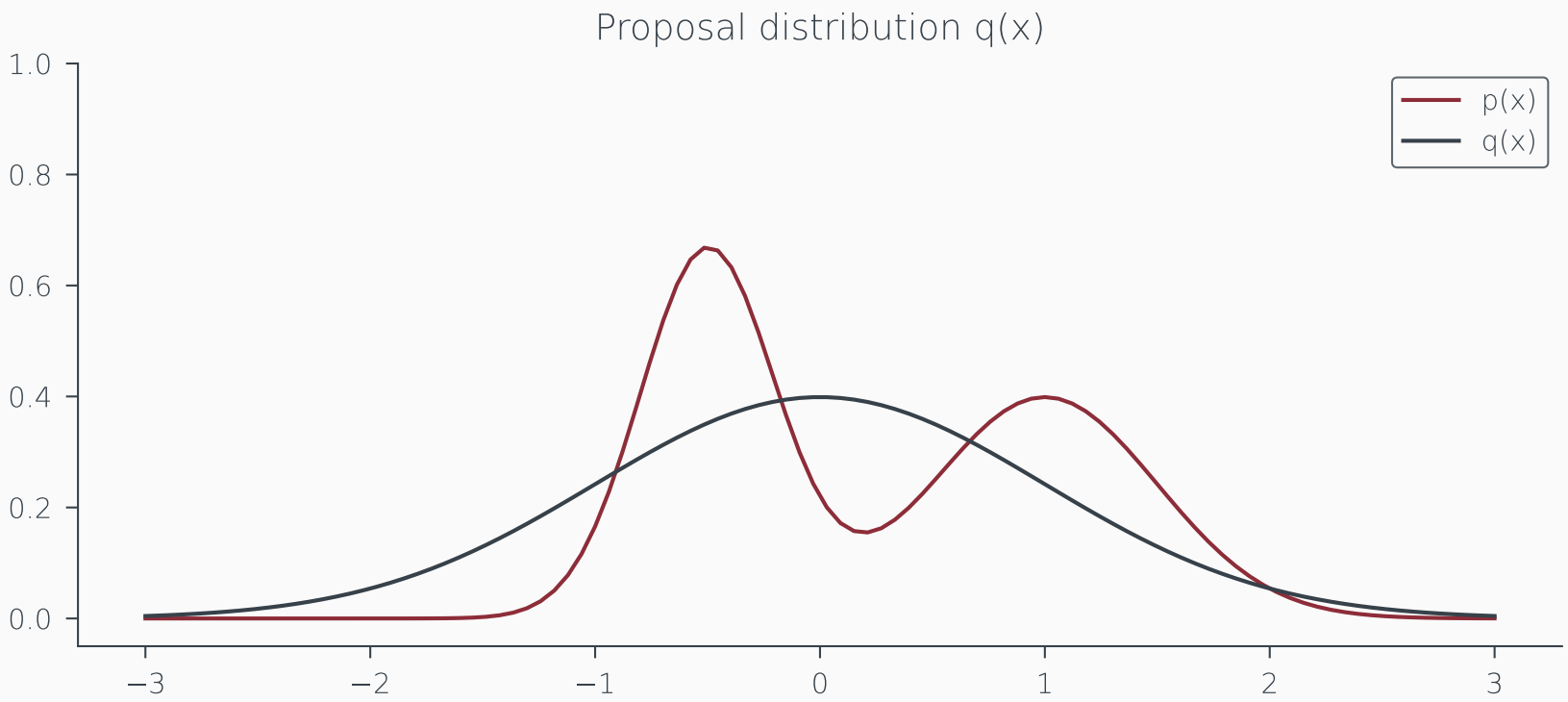
Rejection Sampling

- 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 $\frac{p(x)}{Mq(x)}$.

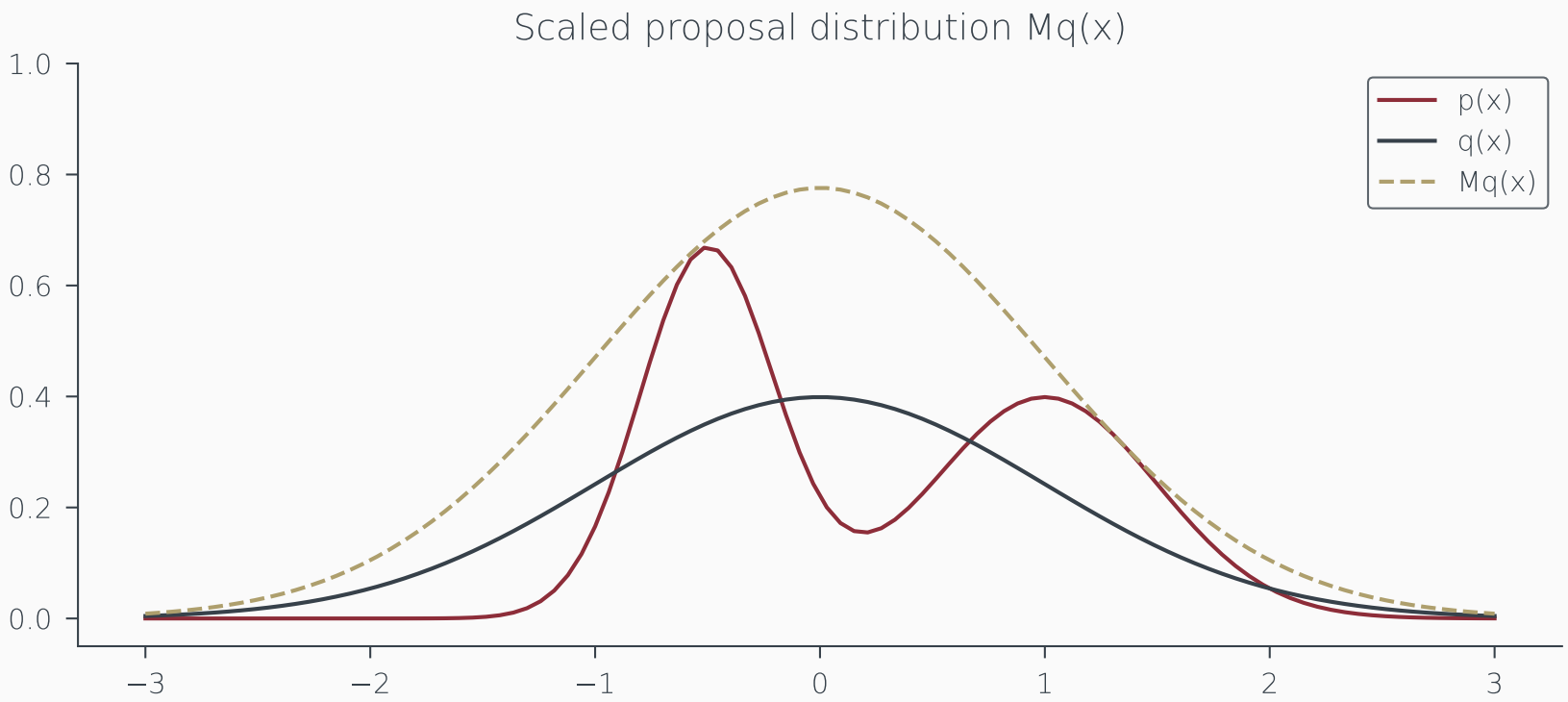
Rejection Sampling



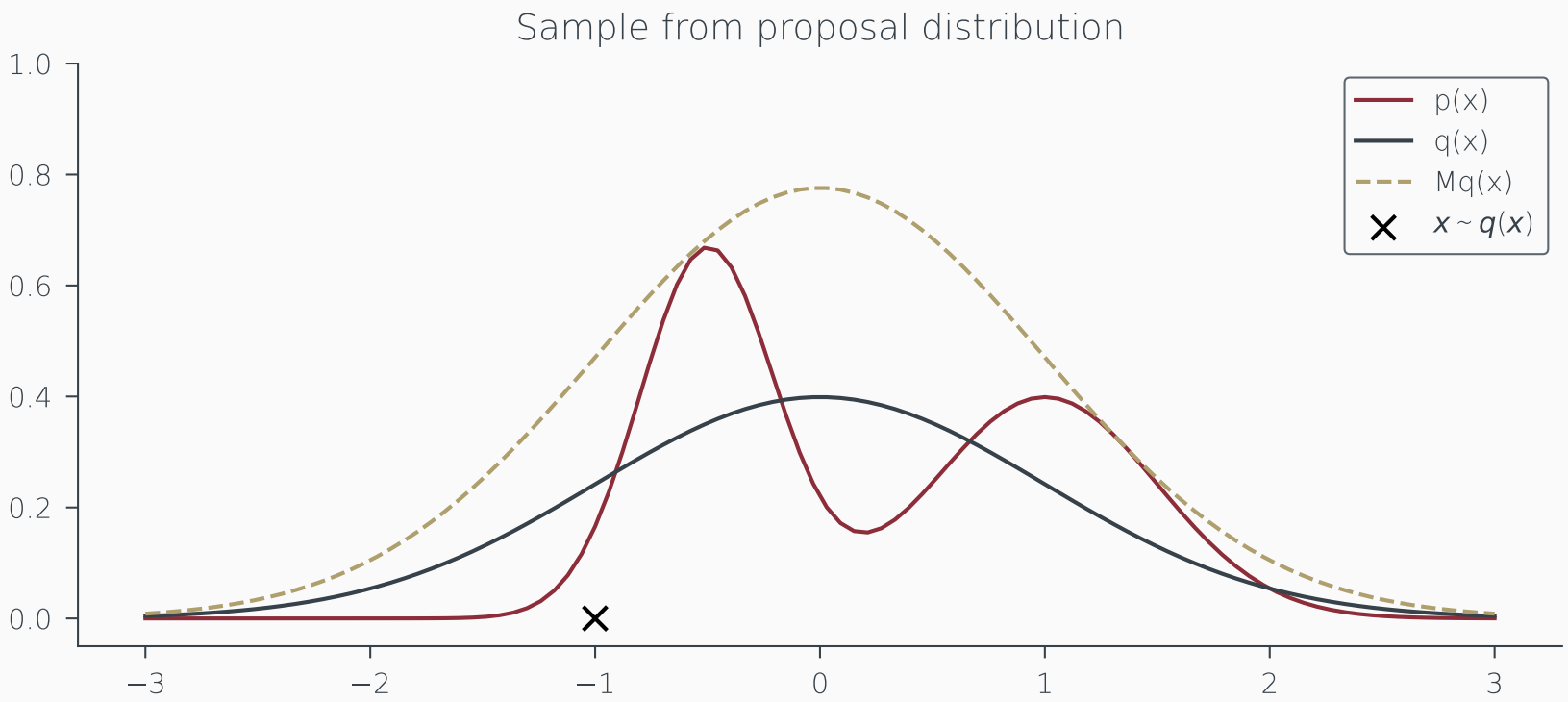
Rejection Sampling



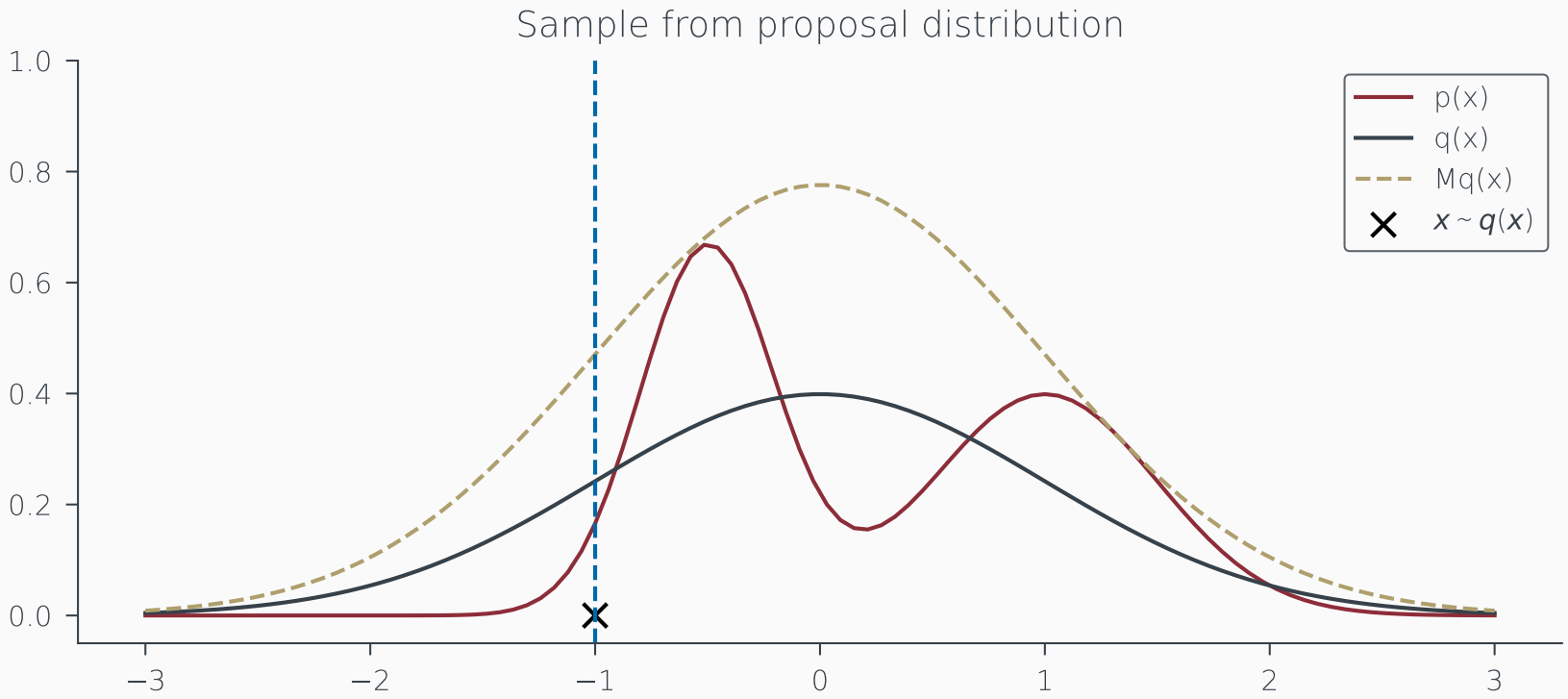
Rejection Sampling



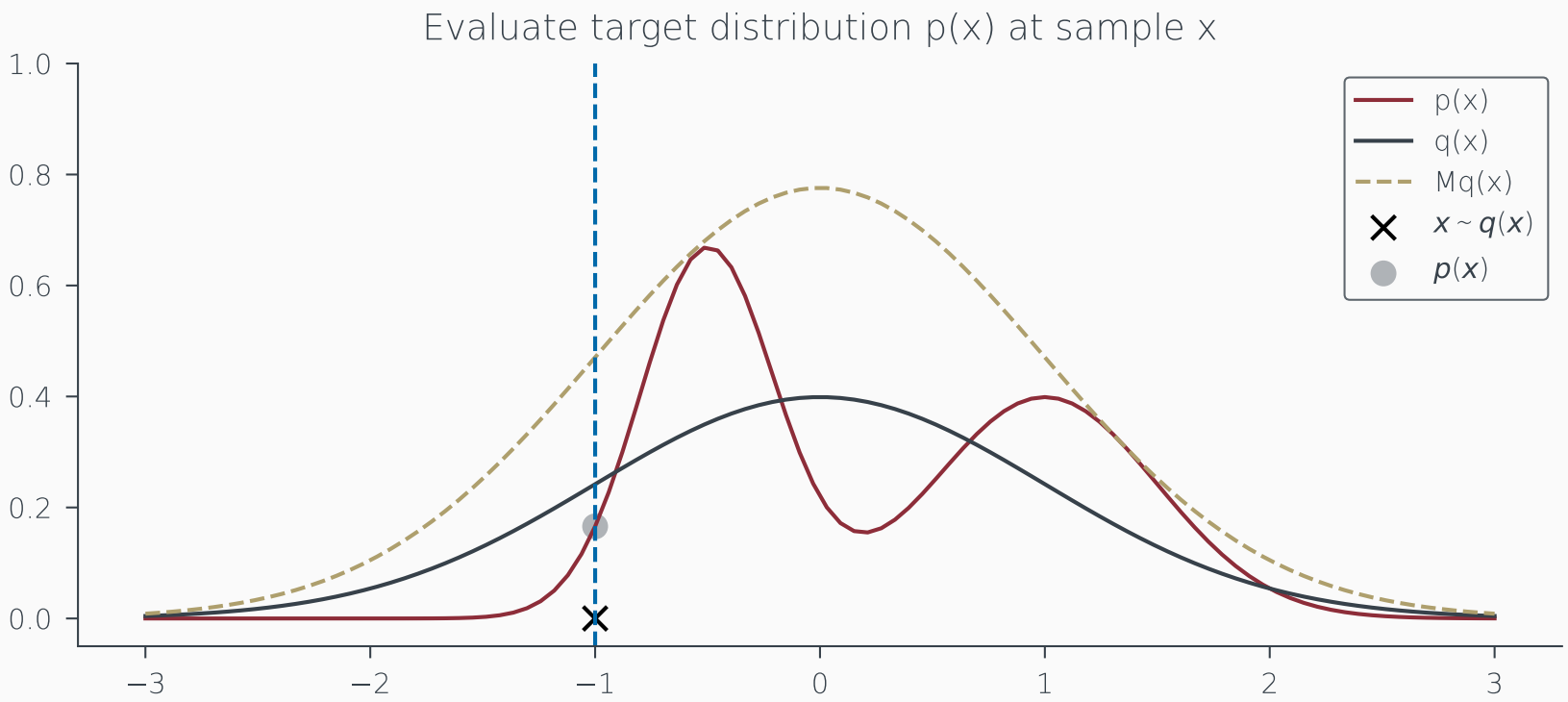
Rejection Sampling



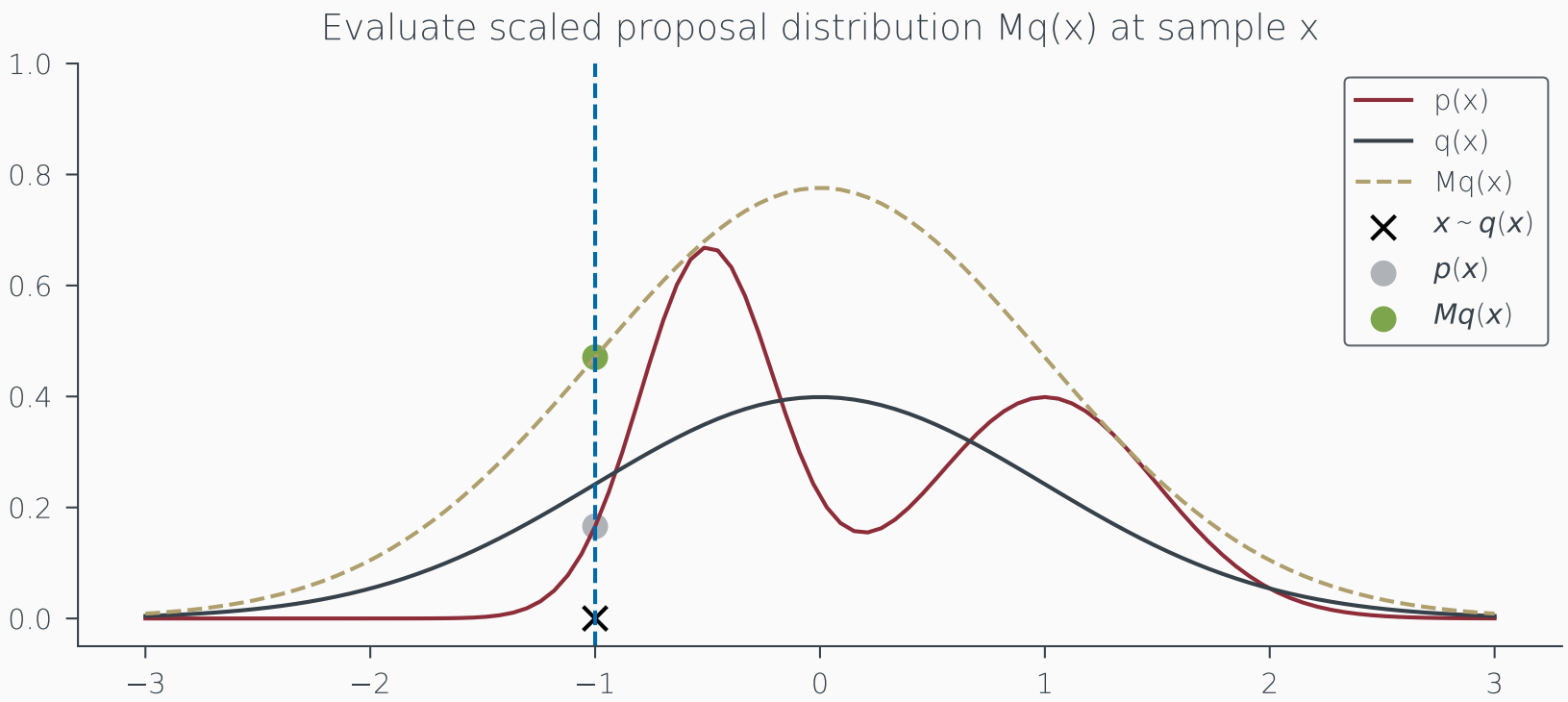
Rejection Sampling



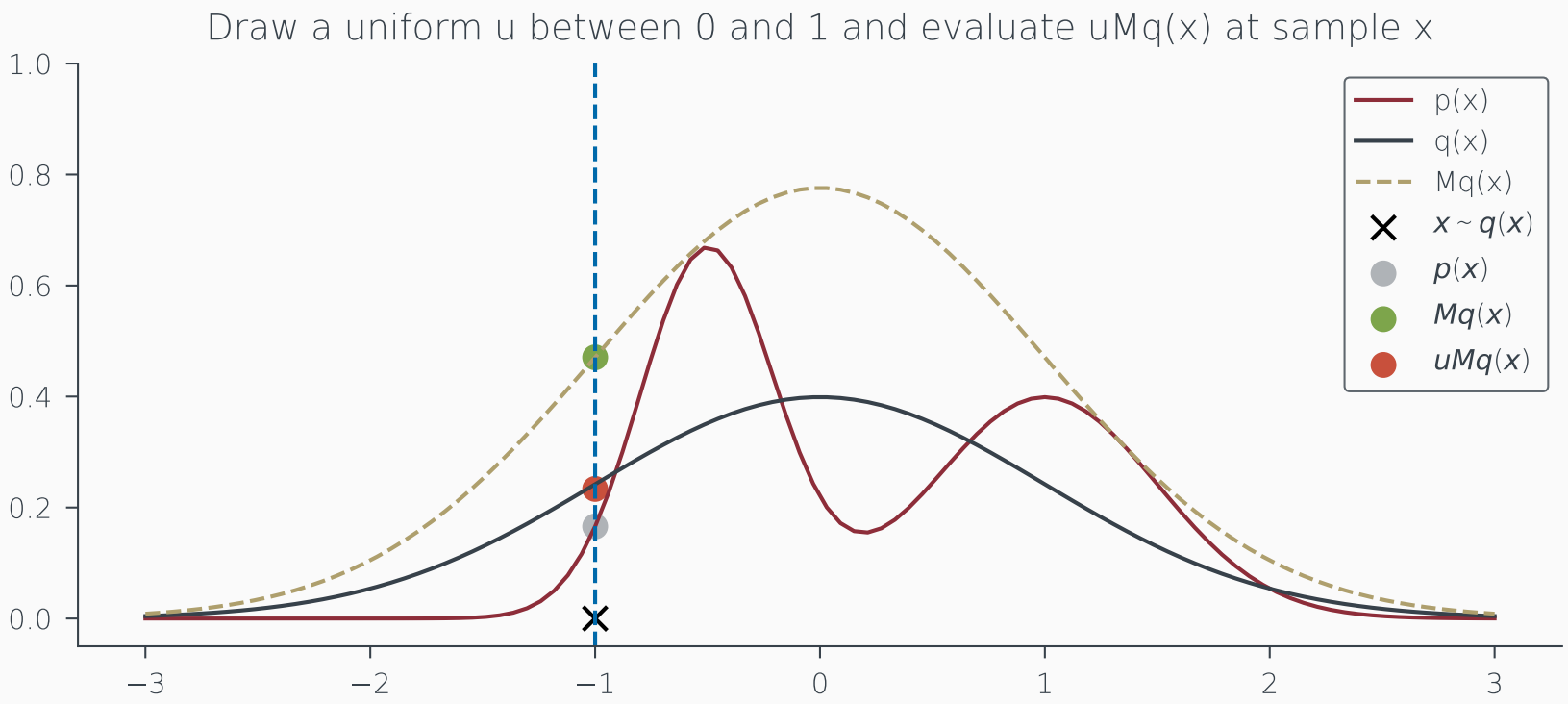
Rejection Sampling



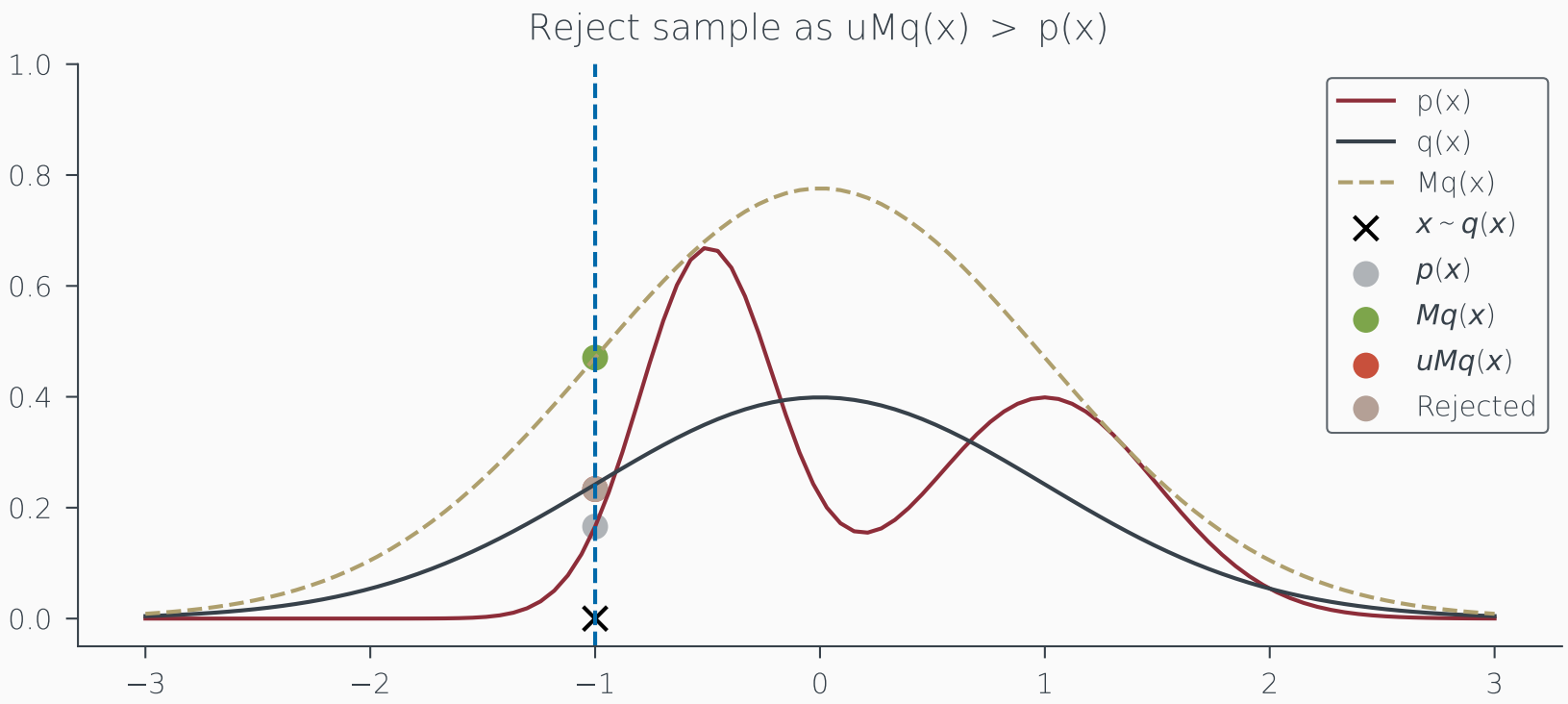
Rejection Sampling



Rejection Sampling



Rejection Sampling



Proof of Rejection Sampling

Acceptance Probability $\alpha(x)$

$$\alpha(x) = \frac{p(x)}{Mq(x)} \tag{8}$$

Bayes Rule for Acceptance

$$P(Sample|Accept) = \frac{P(Accept|Sample)P(Sample)}{P(Accept)} \tag{9}$$

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)

$$P(Accept) = \frac{1}{M} \tag{10}$$

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.

Inverse CDF

General Form

Inverse Cumulative Distribution Function (Inverse CDF) sampling is a technique used to generate random numbers from a given probability distribution.

Particularly useful when sampling from distributions lacking a straightforward analytical method for direct sampling.

A method of sampling from the distribution is sampling $u \in \mathcal{U}(0,1)$ and find $x = F_X^{-1}(u)$. The cumulative probability distribution (cdf) of X is:

$$F_X(x) = \mathbb{P}(X <= x) = \int_{-\infty}^{\infty} \pi(u) I(u <= x) du = \int_{-\infty}^{\infty} \pi(u) du \tag{11}$$

Thus, Sample $u \in \mathcal{U}(0,1)$ and set $Y = F_\pi^{-1}(u)$.

Proof

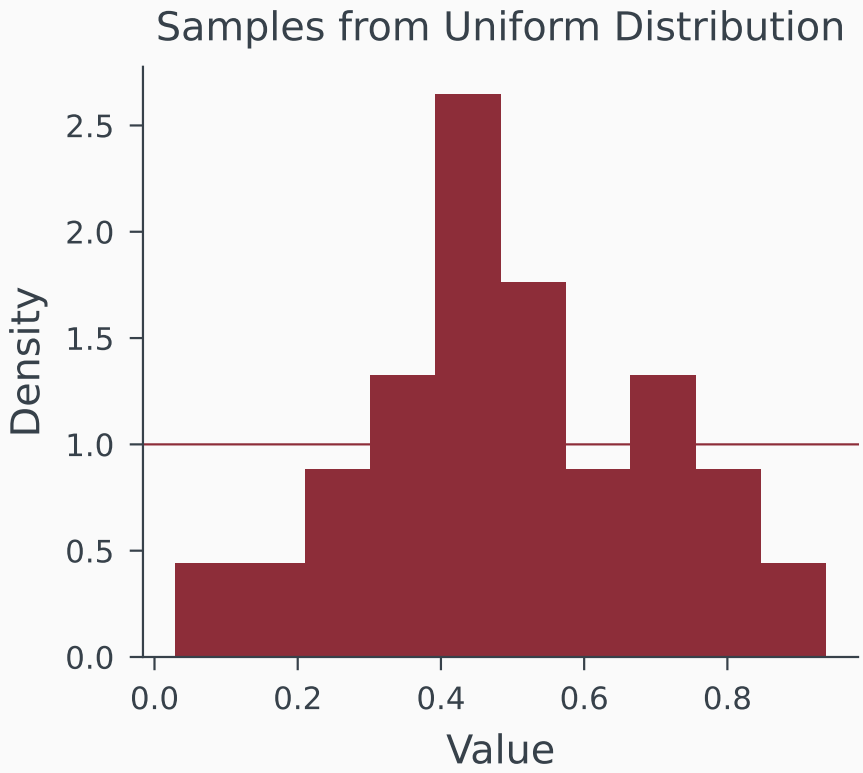
We need to prove that the algorithm mentioned above produces samples from π. We calculate the cdf of X produced by the algorithm above. For any $y \in X$ we have:

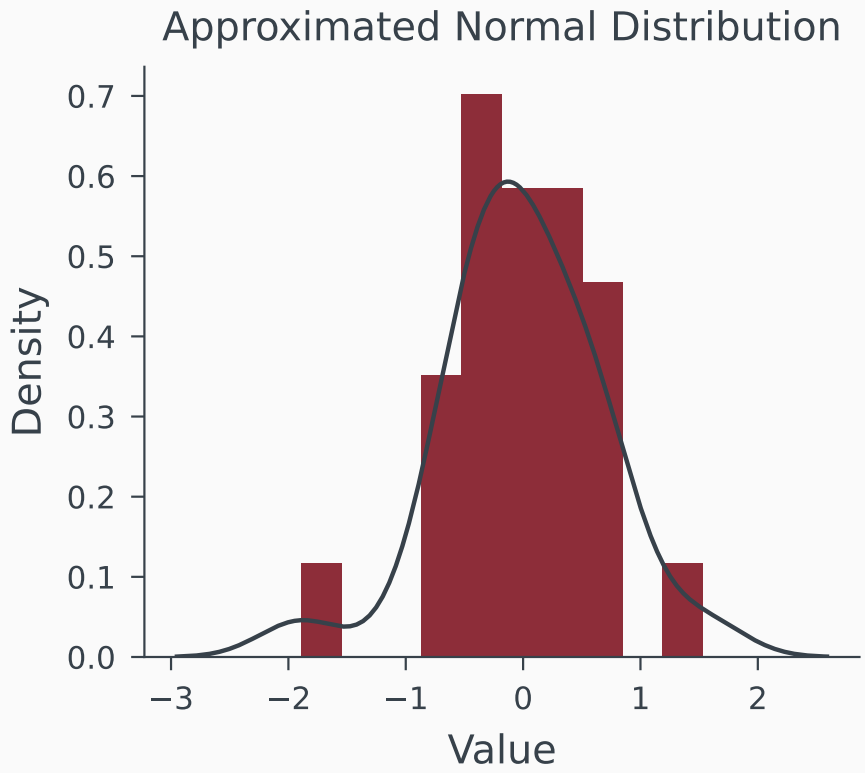
$$\begin{aligned}\mathbb{P}(Y <= y) &= \mathbb{P}(Y = F_X^{-1}(u) <= y) \\ &= \mathbb{P}(u <= F_X(y)) \\ &= \int_0^1 I(u <= F_X(y)).1 du = \int_0^{F_X(y)} du = F_X(y)\end{aligned}$$

This shows that the cdf of Y produced by the algorithm is the same as cdf of $X \sim \pi$.

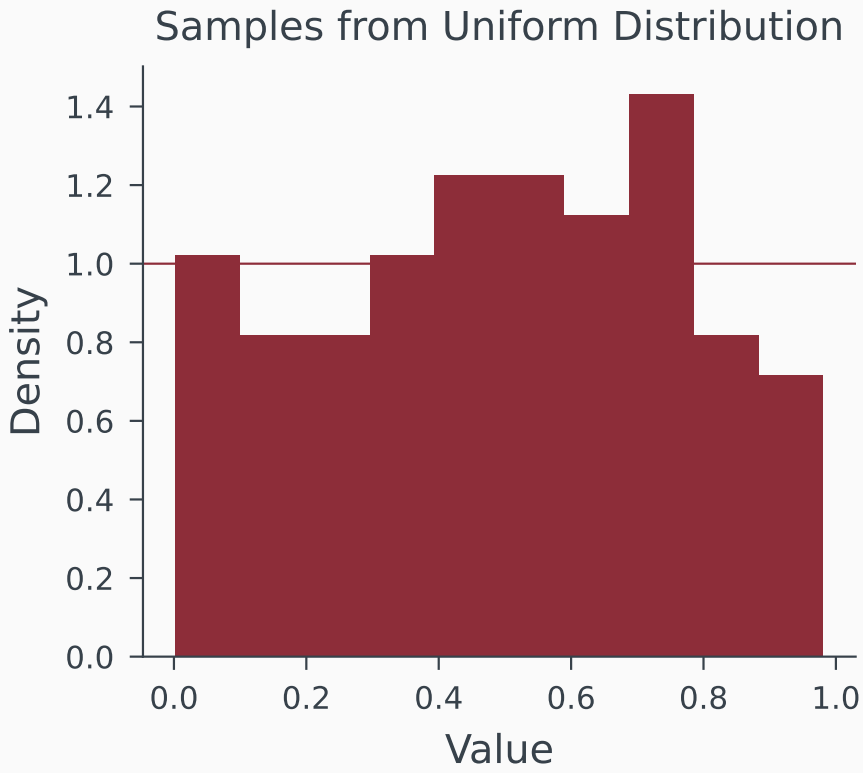
Example of Normal distribution

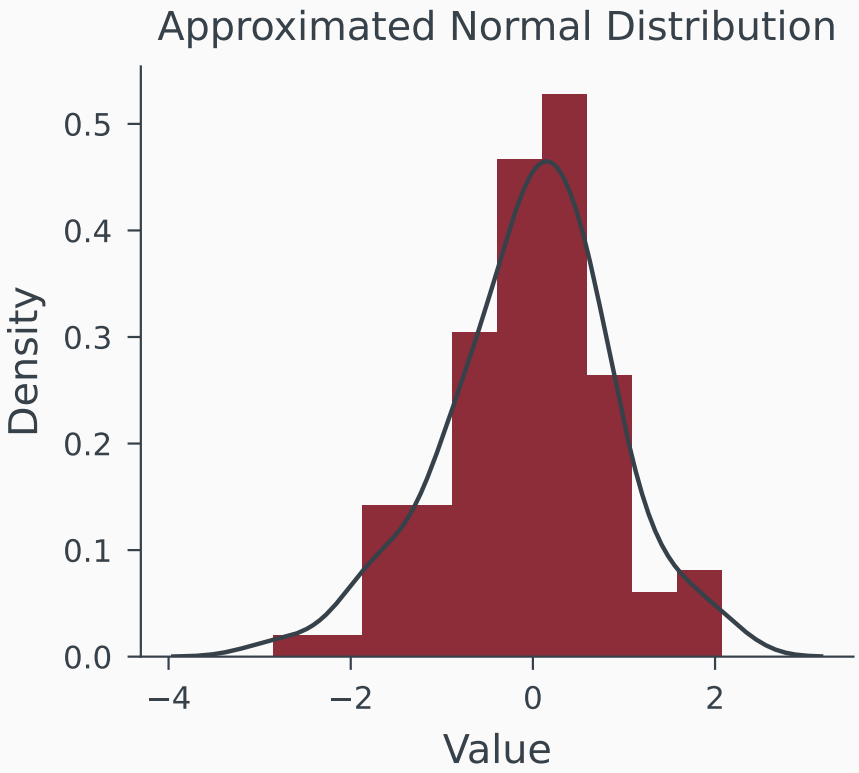
Number of samples = 25:



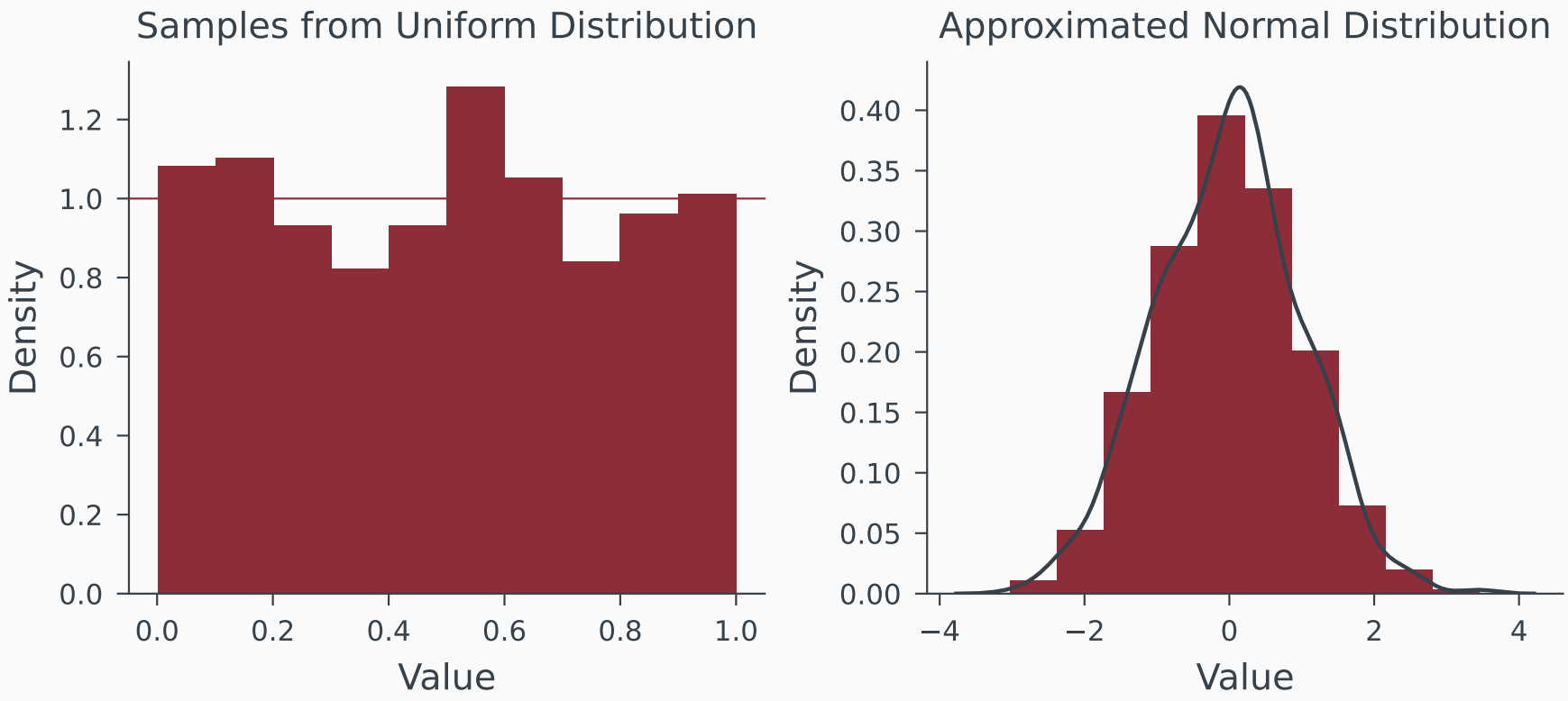


Number of samples = 100:





Number of samples = 1000:



We see that as the number of samples increases, we are able to approximate the induced distribution which is the normal distribution for this example.

Limitations:

- Limited Distribution Complexity: It relies on having an analytically calculable cumulative distribution function (CDF) and an invertible CDF function.
- Numerical Inversion Challenges: When the inverse of the CDF cannot be expressed analytically, numerical methods introduce numerical errors and slow down the sampling process.
- Efficiency and Multivariate Distributions: It can be resource-intensive for high-dimensional multivariate distributions.

Importance Sampling

General Form

In rejection sampling, we saw that due to less acceptance probability, a lot of samples were wasted leading to more time and higher complexity to approximate a distribution.

Computing $p(x), q(x)$ thus seems wasteful. Let us rewrite the equation as:

$$\phi = \int f(x)p(x)dx = \int f(x)\frac{p(x)}{q(x)}q(x)dx$$
$$\sim \frac{1}{N}\sum_{i=1}^{N} f(x_i)\frac{p(x_i)}{q(x_i)} = \frac{1}{N}\sum_{i=1}^{N} f(x_i)w_i$$

Here, $x_i \sim q(x)$. w_i is known as the importance(weight) of sample i.

However the normalization constant Z is generally not known to us. Thus writing:

$$p(x) = \frac{\tilde{p}(x)}{Z} \tag{12}$$

Now inserting this in earlier equations, we get:

$$\begin{aligned}\phi &= \frac{1}{Z}\int f(x)\tilde{p}(x)dx = \frac{1}{Z}\int f(x)\frac{\tilde{p}(x)}{q(x)}q(x)dx \\ &\sim \frac{1}{NZ}\sum_{i=1}^{N} f(x_i)\frac{\tilde{p}(x_i)}{q(x_i)} = \frac{1}{NZ}\sum_{i=1}^{N} f(x_i)w_i\end{aligned}$$

We know that:

$$\begin{aligned}Z &= \int_{\infty}^{\infty}\tilde{p}(x)dx = \int_{\infty}^{\infty}\frac{\tilde{p}(x)}{q(x)}q(x)dx \\ &= \frac{1}{N}\sum_{i=1}^{N} w_i\end{aligned}$$

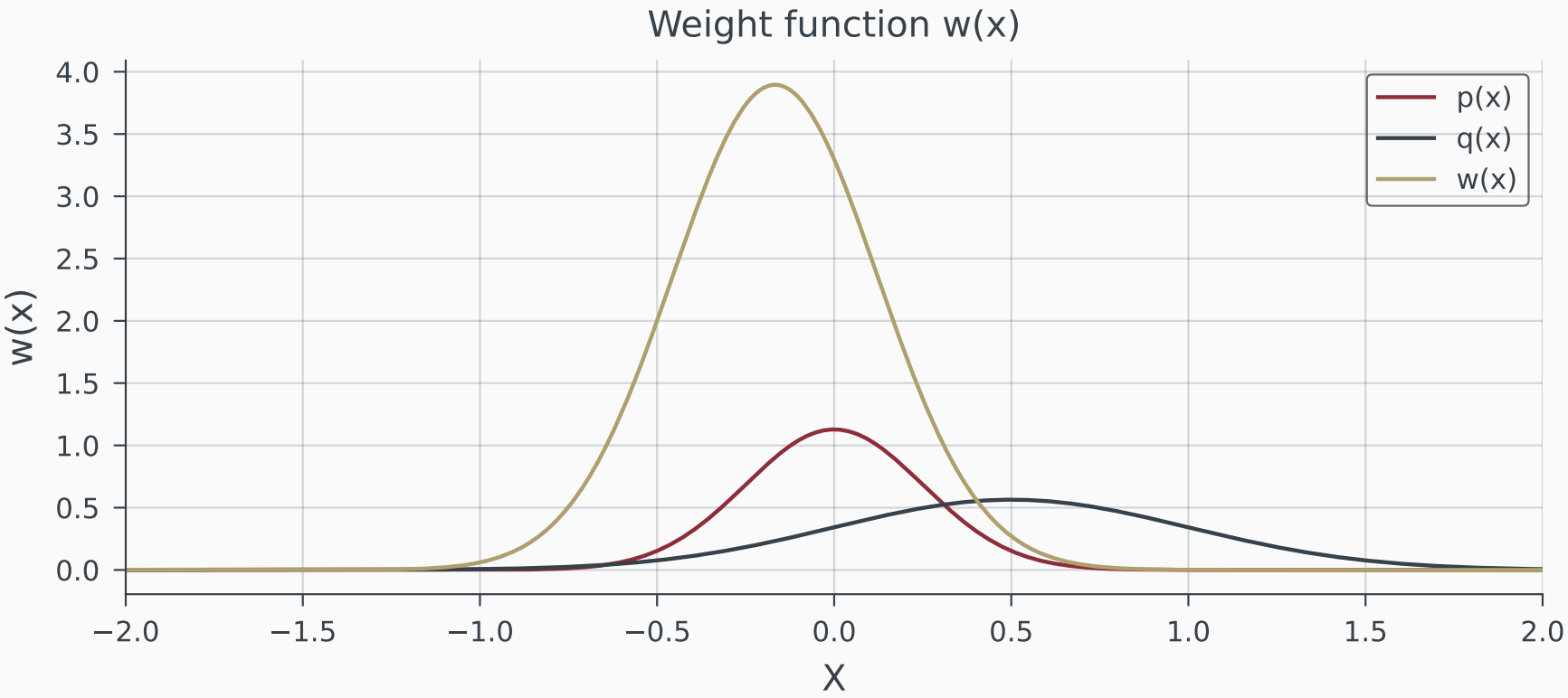
Substuting this value of Z in the equation above, we get:

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

Here $W_i = \frac{w_i}{\sum_{i=1}^{N} w_i}$ are the normalized weights.

Limitations

- Recall that Var $\hat{\phi} = \frac{var(f)}{N}$. Importance sampling replaces $var(f)$ with $var(f\frac{p}{q})$. At positions where $p >>> q$, the weight can tend to ∞!



Gibbs Sampling

General Form

Suppose we wish to sample $\theta_1, \theta_2 \sim p(\theta_1, \theta_2)$, but cannot use:

- direct simulation
- accept-reject method
- Metropolis-Hasting

But we can sample using the conditionals i.e.:

- $p(\theta_1|\theta_2)$ and
- $p(\theta_2|\theta_1)$,

then we can use Gibbs sampling.

Suppose $\theta_1, \theta_2 \sim p(\theta_1, \theta_2)$ and we can sample from $p(\theta_1, \theta_2)$. We begin with an initial value (θ_1^0, θ_2^0), the workflow for Gibbs algorithm is:

1. sample $\theta_1^j \sim p(\theta_1 | \theta_2^{j-1})$ and then
2. sample $\theta_2^j \sim p(\theta_2 | \theta_1^j)$.

One thing to note here is that the sequence in which the theta's are sampled are not independent!

Bivariate Normal Example

Suppose

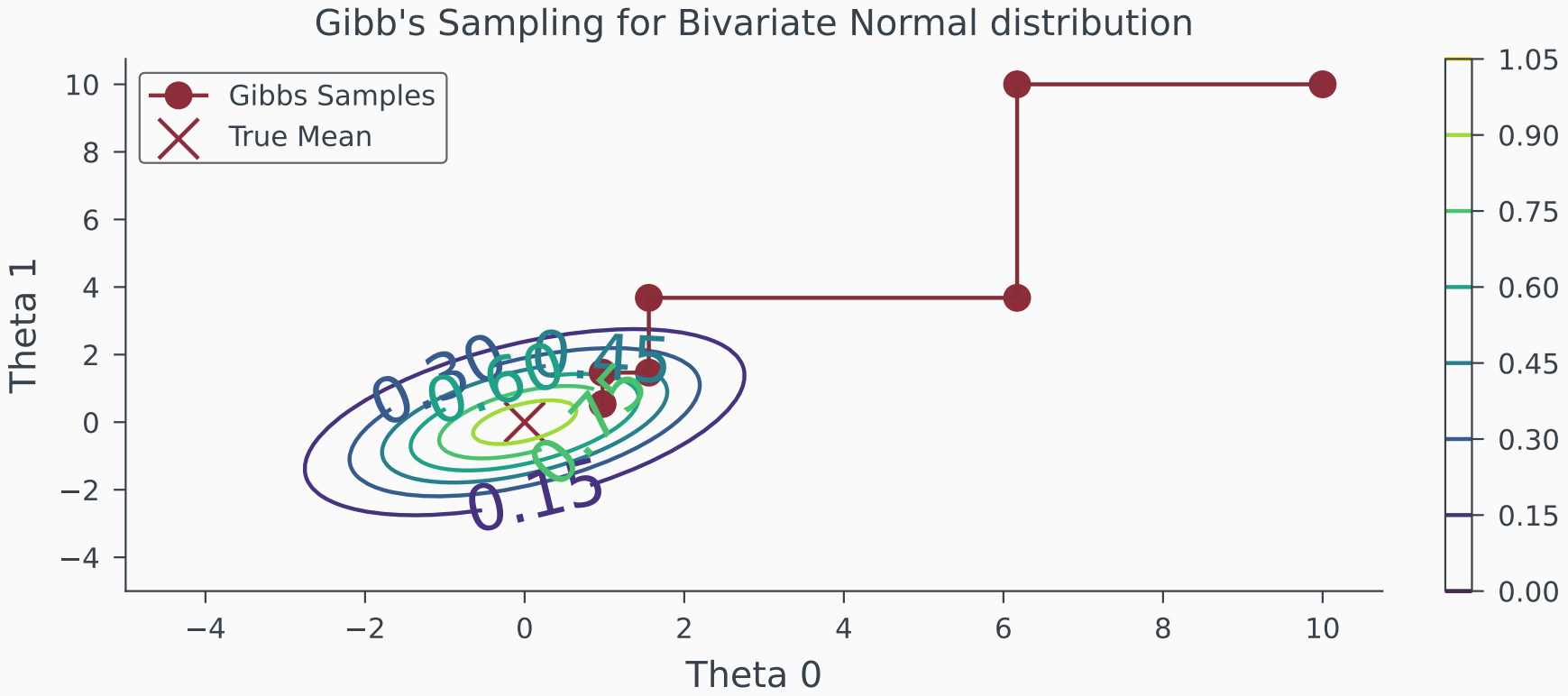
$\theta \sim N_2(0, \Sigma)$ and $\Sigma = \begin{matrix} 1 & \rho \\ \rho & 1 \end{matrix}$

Then, we have:

$\theta_1|\theta_2 \sim N(\rho\theta_2, [1-\rho^2])$

$\theta_2|\theta_1 \sim N(\rho\theta_1, [1-\rho^2])$ are the conditional distributions. The Gibbs sampling proceeds as follows:

Iteration	Sample θ_1	Sample θ_2
1	$\theta_1 \sim N(\rho\theta_2^0, [1-\rho^2])$	$\theta_2 \sim N(\rho\theta_1^1, [1-\rho^2])$
	.	
	.	
k	$\theta_1 \sim N(\rho\theta_2^{k-1}, [1-\rho^2])$	$\theta_2 \sim N(\rho\theta_1^k, [1-\rho^2])$


Gibb's Sampling for Bivariate Normal distribution
Gibbs Samples
True Mean
Theta 1
Theta 0
10
8
6
4
2
0
−2
−4
−4
−2
0
2
4
6
8
10
1.05
0.90
0.75
0.60
0.45
0.30
0.15
0.00

Multivariate case

Suppose $\theta = (\theta_1, \theta_2, \ldots, \theta_K)$, the Gibbs workflow is as follows:

$\theta_1^j = p(\theta_1 | \theta_2^{j-1}, \ldots, \theta_K^{j-1})$

$\theta_2^j = p(\theta_2 | \theta_1^j, \theta_3^{j-1}, \ldots, \theta_K^{j-1})$

.

.

$\theta_k^j = p(\theta_k | \theta_1^j, \ldots, \theta_{k-1}^j, \theta_{k+1}^{j-1}, \ldots, \theta_K^{j-1})$

.

.

$\theta_K^j = p(\theta_K | \theta_1^j, \ldots, \theta_{K-1}^j)$

The distributions above are call the full conditional distributions.

Advantages

Gibbs sampling can be used to draw samples from $p(\theta)$ when:

- Other methods don't work quite well in higher dimensions.
- Draw samples from the full conditional distributions is easy, $p(\theta_k|\theta_{-k})$.

Markov Chain Monte Carlo

Limitations of basic sampling methods

- *Transformation based methods*: Usually limited to drawing from standard distributions.
- *Rejection and Importance sampling*: Require selection of good proposal distirbutions.

In high dimensions, usually most of the density $p(x)$ is concentrated within a tiny subspace of x. Moreover, those subspaces are difficult to be known a priori.

A solution to these are MCMC methods.

Markov Chain

- **Markov Chain**: A joint distribution $p(X)$ over a sequence of random variables $X = \{X_1, X_2, \ldots, X_n\}$ is said to have the Markov property if

$$p(X_i|X_1, \ldots, X_{i-1}) = p(X_i|X_{i-1})$$

  The sequence is then called a Markov chain.
- The idea is that the estimates contain information about the shape of the target distribution p.

Metropolis Hastings

- The basic idea is propose to move to a new state x_{i+1} from the current state x_i with probability $q(x_{i+1}|x_i)$, where q is called the proposal distribution and our target density of interest is $p(= \frac{1}{Z}\tilde{p})$.
- The new state is accepted with probability $\alpha(x_i, x_{i+1})$.
  - If $p(x_{i+1}|x_i) = p(x_i|x_{i+1})$, then $\alpha(x_i, x_{i+1}) = \min(1, \frac{p(x_{i+1})}{p(x_i)})$.
  - If $p(x_{i+1}|x_i) \neq p(x_i|x_{i+1})$, then $\alpha(x_i, x_{i+1}) = \min(1, \frac{p(x_{i+1})q(x_i|x_{i+1})}{p(x_i)q(x_{i+1}|x_i)}) = \min(1, \frac{\tilde{p}(x_{i+1})q(x_i|x_{i+1})}{\tilde{p}(x_i)q(x_{i+1}|x_i)})$
- Evaluating α, we only need to know the target distribution up to a constant of proportionality or without normalization constant.

Algorithm: Metropolis Hastings

1. Initialize x_0.
2. for $i = 1, \ldots, N$ do:
3. Sample $x^* \sim q(x^*|x_{i-1})$.
4. Compute $\alpha = \min(1, \frac{\tilde{p}(x^*)q(x_{i-1}|x^*)}{\tilde{p}(x_{i-1})q(x^*|x_{i-1})})$
5. Sample $u \sim \mathcal{U}(0, 1)$
6. if $u \leq \alpha$:

   $x_i = x^*$

   else:

   $x_i = x_{i-1}$

Pop Quiz

How do we choose the initial state x_0?

Pop Quiz

How do we choose the initial state x_0?

1. Start the Markov Chain at an initial x_0.
2. Using the proposal $q(x|x_i)$, run the chain long enough, say N_1 steps.
3. Discard the first $N_1 - 1$ samples (called 'burn-in' samples).
4. Treat x_{N_1} as first sample from $p(x)$.

MCMC demo

https://chi-feng.github.io/mcmc-demo/app.html