Sampling Methods

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Topics

Rejection Sampling

Importance Sampling

1. Markov Chains
2. Importance Sampling
3. Gibbs Sampling
4. Markov Chain Monte Carlo

Main Goal

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- Goal: sample from $p(x)$.

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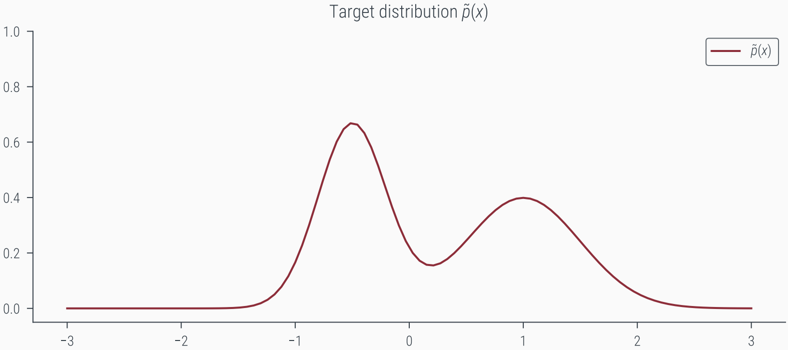
- Let M be a constant such that $M \geq \frac{\tilde{p(x)}}{q(x)}$ for all x.
- Then, we can sample from $p(x)$ by sampling from $q(x)$ and accepting the sample with probability $\frac{p(x)}{Mq(x)}$.

Notebook: `rejection-sampling.ipynb`

Rejection Sampling



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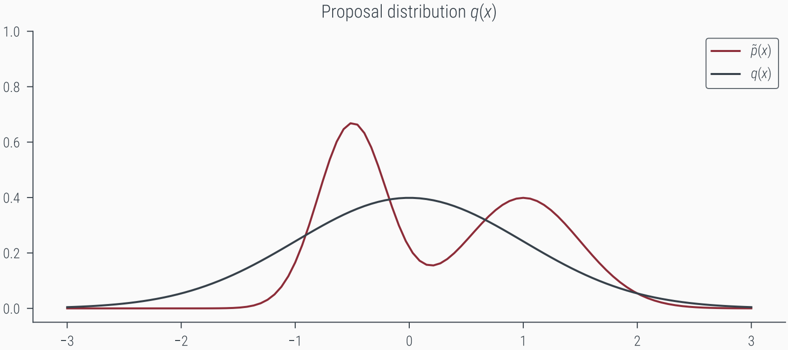

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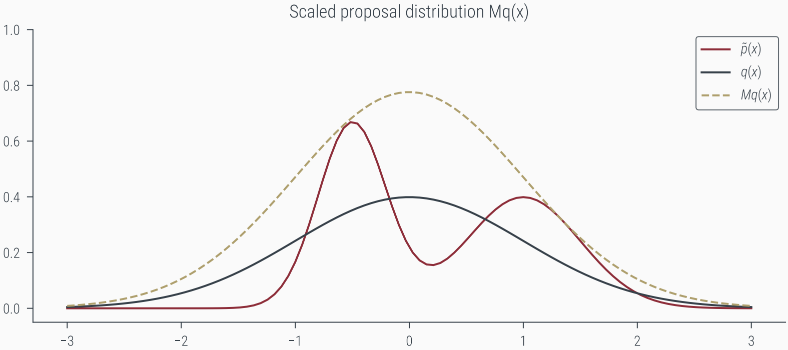

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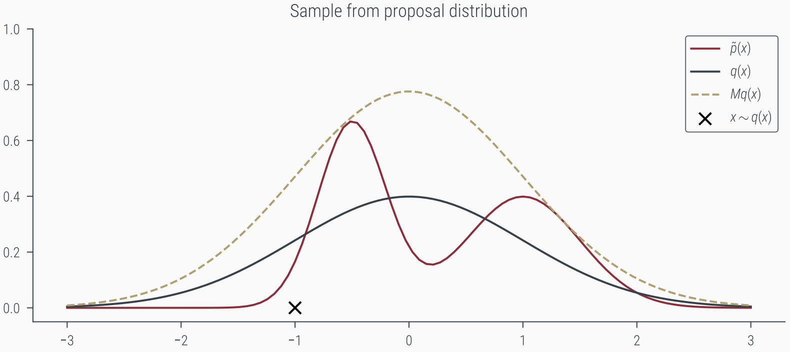

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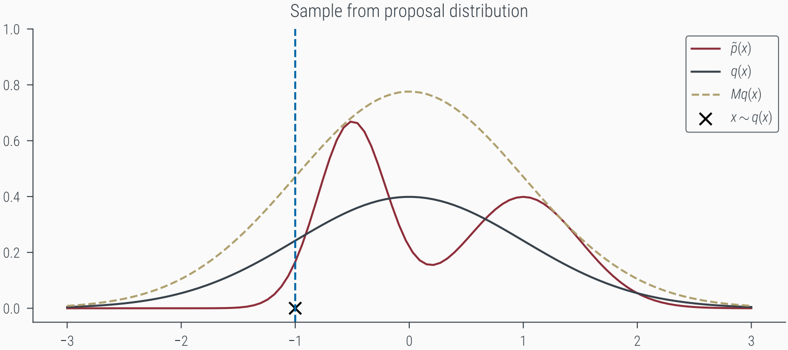

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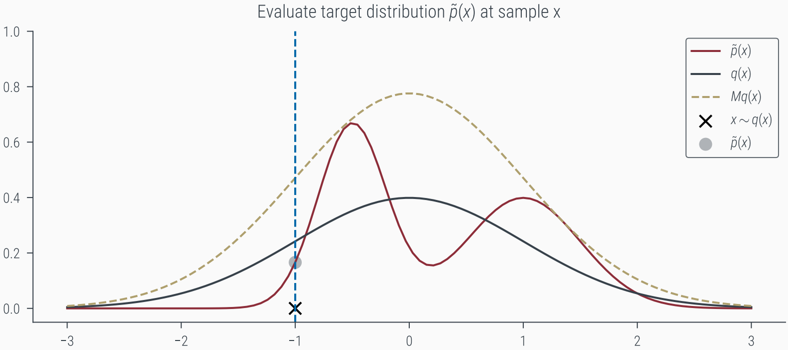

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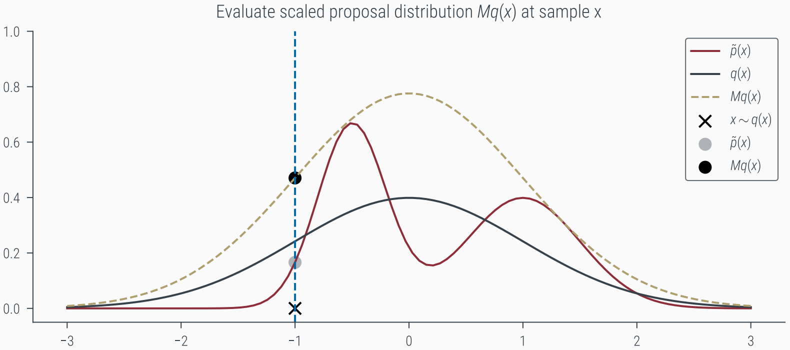

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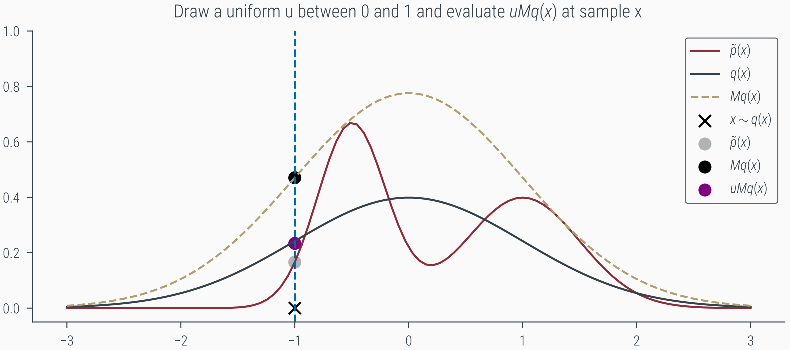
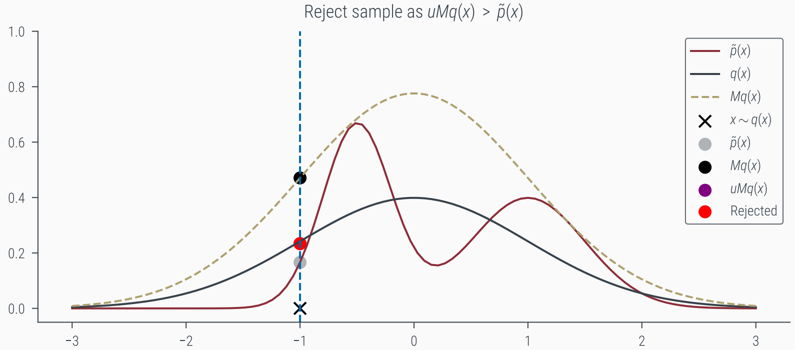
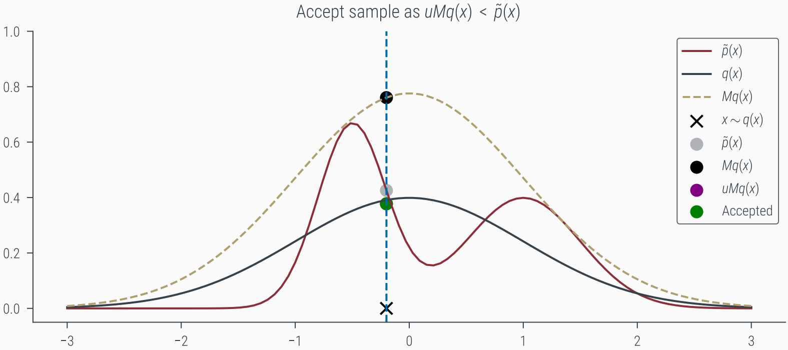


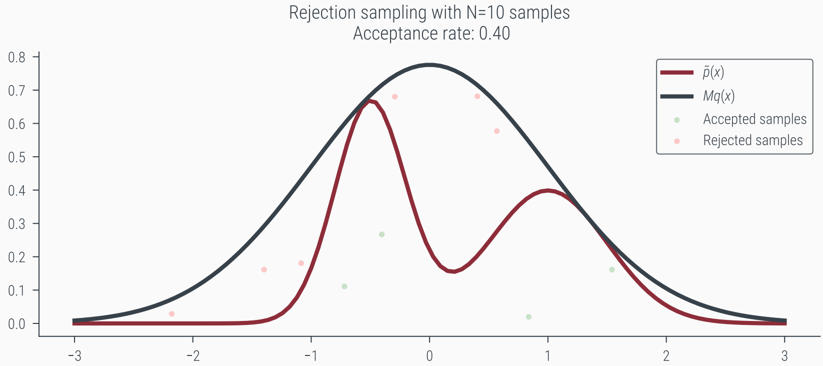
Rejection Sampling (Rejected Sample)



Rejection Sampling (Accepted Sample)



Rejection Sampling (10 samples)



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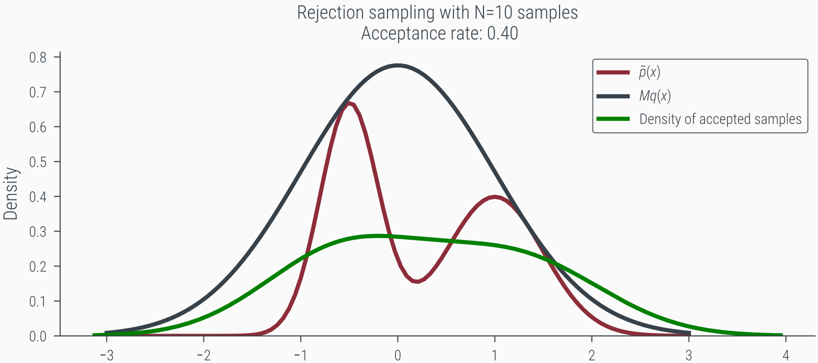
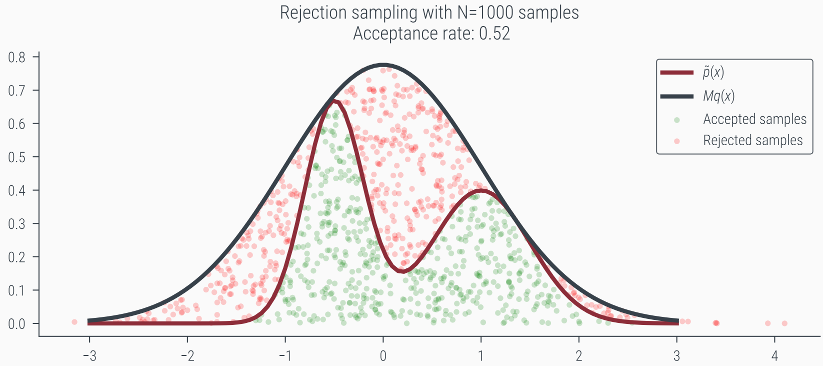


Rejection Sampling (1000 samples)



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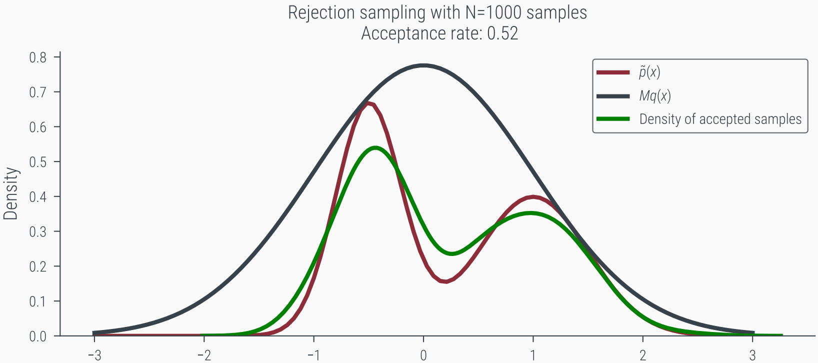

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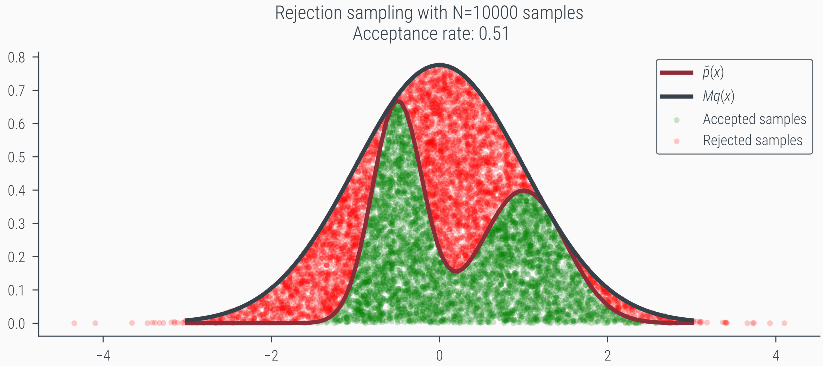

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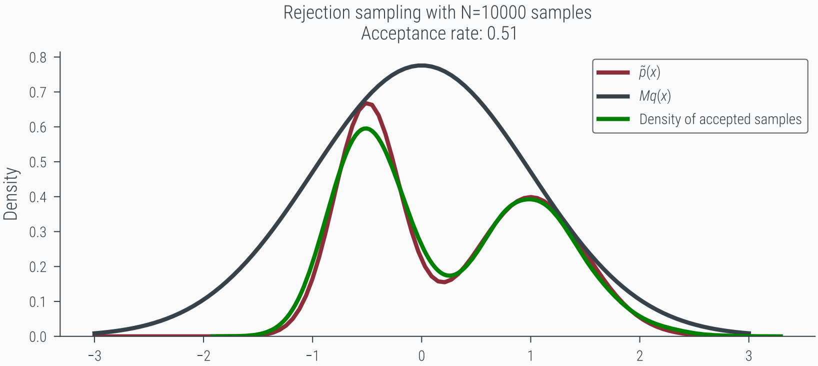

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- Acceptance Probability $\alpha(x)$: Probability that we accept a sample x_s generated from $q(x)$.

$$\alpha(x_s) = \frac{\tilde{p}(x_s)}{Mq(x_s)} = P(Accept|x_s) \tag{1}$$

Rejection Sampling Proof

- Bayes Rule for Acceptance:

$$P(x_s|Accept) = \frac{P(Accept|x_s)P(x_s)}{P(Accept)} \tag{2}$$

  - where $P(x_s|Accept)$ is the density of accepted sample x_s. We want to evaluate this and show this is $p(x_s)$.

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

where Z is the normalization constant of $\tilde{p}(x)$.

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- How to choose multiplier M?
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- $M = \frac{\tilde{p}(x)}{q(x)} = \frac{\sigma_q^D}{\sigma_p^D} = (\frac{\sigma_q}{\sigma_p})^D$

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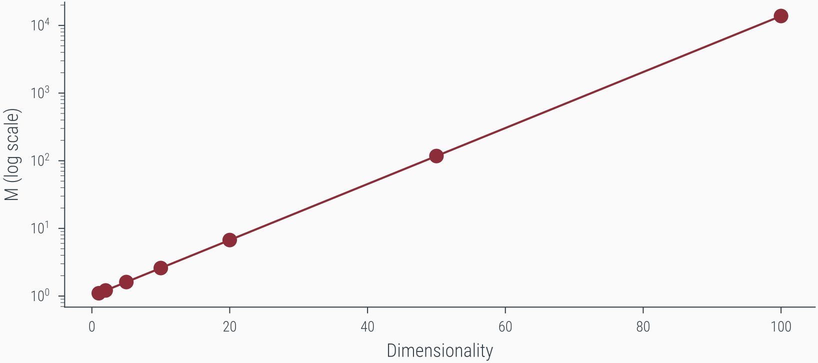
- Let us assume $\sigma_p = 1$ and $\sigma_q = 1.1$



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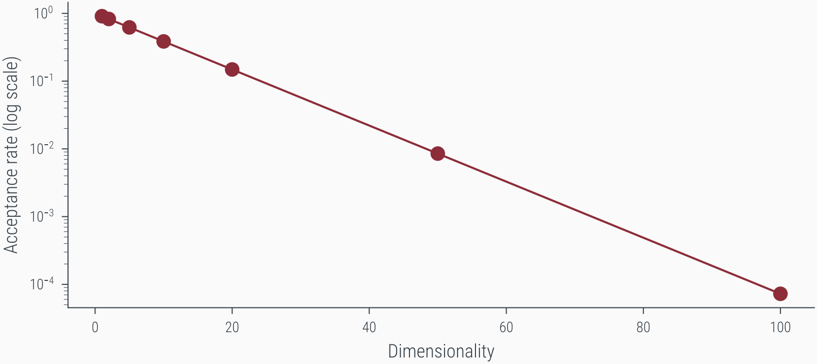

- Acceptance probability is very low as D increases.

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.

Back to the main problem at hand

- We want to compute posterior predictive distribution (or something similar)
- We would typically use Monte Carlo methods to do this.
- $I = \int f(x)p(x)dx$ where $p(x)$ is the posterior distribution.
- We can approximate I by $\frac{1}{N}\sum_{i=1}^{N} f(x_i)$, where $x_i \sim p(x)$.
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- But, we do not have access to $p(x)$. Rather, we have access to $\tilde{p}(x)$, which is proportional to $p(x)$.
- In rejection sampling, we took a sample x_i from $q(x)$ and accepted it with probability $\frac{\tilde{p}(x_i)}{Mq(x_i)}$.
- Can we use all samples x_i from $q(x)$ without rejection?

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- In rejection sampling, we took a sample x_i from $q(x)$ and accepted it with probability $\frac{\tilde{p}(x_i)}{Mq(x_i)}$.
- Can we use all samples x_i from $q(x)$ without rejection?
- $I = \int f(x)p(x)dx \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$, where $x_i \sim p(x)$.
- Let us choose a proposal distribution $q(x)$ which has support over the entire domain of $p(x)$.
- $I = \int f(x)p(x)dx = \int f(x)\frac{p(x)}{q(x)}q(x)dx$
- $I = \int f(x)w(x)q(x)dx$, where $w(x) = \frac{p(x)}{q(x)}$. $w(x)$ is called the importance weight.
- $I = \mathbb{E}_q[f(x)w(x)] = \sum_{i=1}^{N} f(x_i)w(x_i)$, where $x_i \sim q(x)$.

Markov Chains

https://nipunbatra.github.io/hmm/

Global Optimization

Notebook: mcmc=optimization.ipynb

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:

$$p(x) = \frac{\tilde{p}(x)}{Z} \tag{13}$$

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:

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

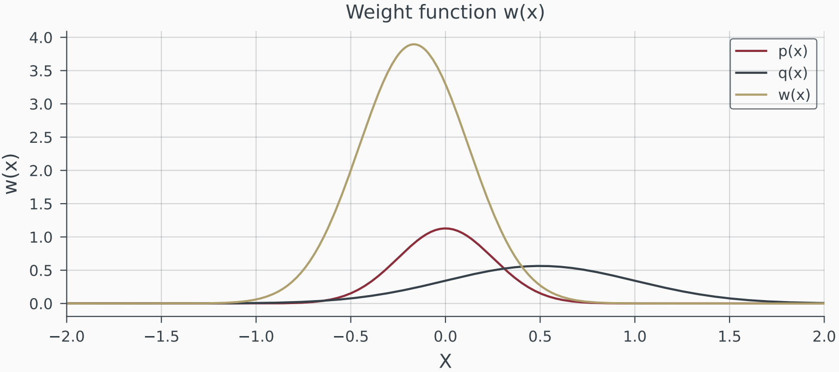
Substuting this value of Z in the equation above, we get:

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

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

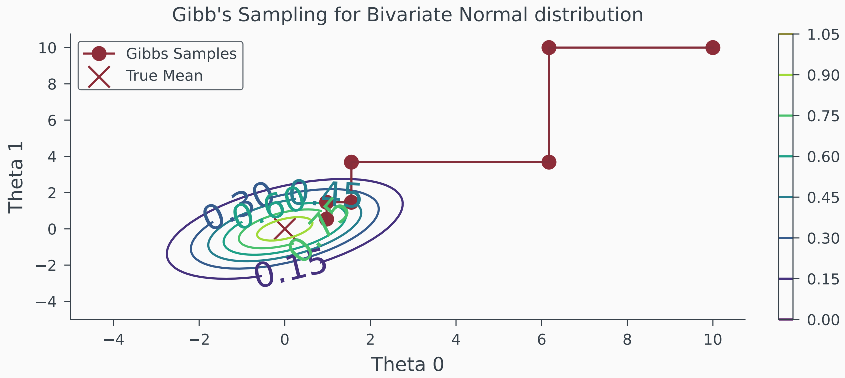
$\theta \sim N_2(0, \Sigma)$ and $\Sigma = \begin{matrix} 1 & \rho \\ \rho & 1 \end{matrix}$

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
0.15
0.30
0.45
0.60
0.75
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`