Module 5: Introduction to Monte Carlo

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Announcements

- Please make sure that your .Rmd files for homework compile to .pdf format moving forward
- If you're having an issue with this, please talk to any member of the teaching team moving forward

Agenda

- Motivation
- Monte Carlo (The Classical or Naive Method)
- Inverse CDF Method
- Rejection Sampling

Sampling Methods

In this module, we will talk about ways of approximating

$$\mathbb{E}_X[h(x)] = \int_X h(x) f(x)\, dx$$

which is *intractable*. This means that we cannot compute the integral in closed form.

Why? This means h(x) is a complicated function or we cannot evaluate $f(x)$.

Sampling Methods

$$\mathbb{E}_X[h(x)] = \int_X h(x)f(x)\,dx$$

which is *intractable*. This means that we cannot compute the integral in closed form.

Example: Suppose the $h(x) = 1$ for all x.

$$\mathbb{E}_f[h(x)] = \mathbb{E}_f[X] = \int_X xf(x)\,dx$$

Monte Carlo Sampling

Suppose that we wish to find

$$\mathbb{E}_f[X].$$

Solution:

1. Draw samples $X_1, \ldots, X_N \overset{iid}{\sim} f$.
2. Let $\frac{1}{N} \sum_{i=1}^{N} X_i$ approximate $\mathbb{E}_f[X]$

This is called **Monte Carlo sampling** (and is the simplest way of producing samples).

Generalization

Suppose we want to estimate $\mathbb{E}[h(Y) \mid Z = z]$.

Solution:

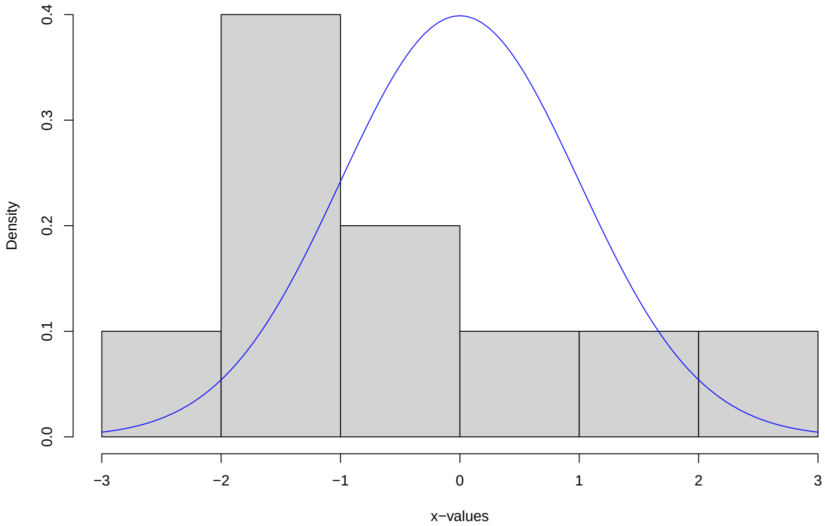
1. Draw samples $Y_1, \ldots, Y_N \overset{iid}{\sim} Y \mid Z = z$.
2. Let $\frac{1}{N} \sum_{i=1}^{N} h(Y_i)$ approximate $\mathbb{E}[h(Y) \mid Z = z]$.

Remark: The generalization is equivalent to the special case by letting X have distribution $h(Y) \mid Z = z$.

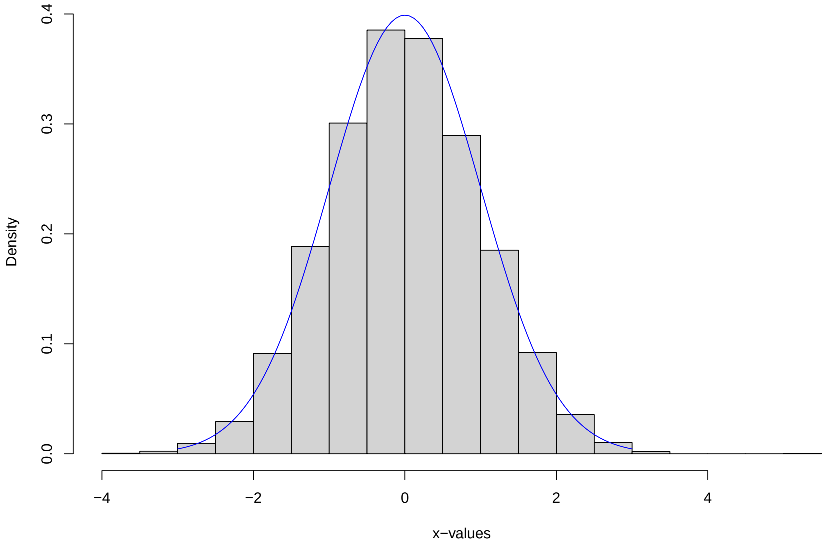
Monte Carlo Illustration

Simulate a N(0,1) histogram using Monte Carlo samples. Compare it to the standard normal density in R. Provide 10 and 10,000 simulations.

Monte Carlo Illustration



Monte Carlo Illustration



Monte Carlo Properties

Suppose that $\mathbb{E}|X| < \infty$.

Then

$$\frac{1}{N}\sum_{i=1}^{N} X_i \to \mathbb{E}[X] \quad \text{as} \quad N \to \infty.$$

Why? This is true by the Strong Law of Large Numbers. It ensures that our approximation converges to the "true value."

Monte Carlo Properties

$\frac{1}{N}\sum_{i=1}^{N} X_i$ is an **unbiased estimator** of $\mathbb{E}[X]$.

Proof:

$$\mathbb{E}[\frac{1}{N}\sum_{i=1}^{N} X_i] = \frac{1}{N} \times N \times \mathbb{E}[X_i] = \mathbb{E}[X].$$

Monte Carlo Properties

The **variance** of $\frac{1}{N}\sum_{i=1}^{N} X_i$ is

$$\mathbb{V}(\frac{1}{N}\sum_{i=1}^{N} X_i) = \frac{1}{N^2}\mathbb{V}(\sum_{i=1}^{N} X_i) = \frac{1}{N^2}\sum_{i=1}^{N}\mathbb{V}(X_i) = \frac{1}{N}\mathbb{V}(X).$$

Monte Carlo Properties

Because our estimator is unbiased, the **Root Mean Squared Error** (RMSE) is

$$\begin{aligned}
\text{RMSE} &=: \left[\mathbb{E}(|\tfrac{1}{N}\sum X_i - \mathbb{E}X|^2)\right]^{1/2} \\
&= \left[\mathbb{V}(\tfrac{1}{N}\sum X_i)\right]^{1/2} \\
&= \frac{1}{\sqrt{N}}\mathbb{V}(X)^{1/2} = \sigma(X)/\sqrt{N}. \qquad (1)
\end{aligned}$$

The RMSE tells us how far the approximation will be from the true value, on average.

Remark:

$$\text{MSE} = [\sigma(X)/\sqrt{N}]^2 = \frac{1}{N}V(X).$$

Return of IQ Scores

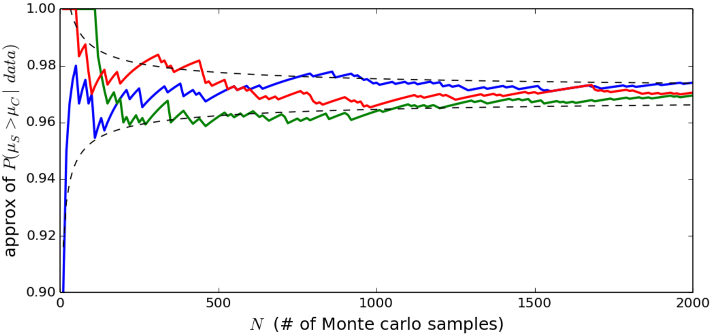


Figure 1: Monte Carlo approximations for an increasing number of samples, N. The red, blue, and green lines indicate three repetitions of the procedure, using different sequences of samples. The dotted lines indicate the true value $\pm$ the RMSE of the Monte Carlo estimator.

Return of IQ Scores

In Module 4, we saw an example involving the mean change in IQ score μ_S and μ_C of two groups of students (spurters and controls). To compute the posterior probability that the spurters had a larger mean change in IQ score, we drew $N = 10^6$ samples from each posterior:

$$(\boldsymbol{\mu}_S^{(1)}, \boldsymbol{\lambda}_S^{(1)}), \ldots, (\boldsymbol{\mu}_S^{(N)}, \boldsymbol{\lambda}_S^{(N)}) \sim \text{NormalGamma}(24.0, 8, 4, 855.0)$$
$$(\boldsymbol{\mu}_C^{(1)}, \boldsymbol{\lambda}_C^{(1)}), \ldots, (\boldsymbol{\mu}_C^{(N)}, \boldsymbol{\lambda}_C^{(N)}) \sim \text{NormalGamma}(11.8, 49, 24.5, 6344.0)$$

and used the Monte Carlo approximation

$$\mathbb{P}(\boldsymbol{\mu}_S > \boldsymbol{\mu}_C \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}\left(\boldsymbol{\mu}_S^{(i)} > \boldsymbol{\mu}_C^{(i)}\right).$$

Return of IQ Scores

- To visualize this, consider the sequence of approximations $\frac{1}{N}\sum_{i=1}^{N} \mathbb{1}(\boldsymbol{\mu}_S^{(i)} > \boldsymbol{\mu}_C^{(i)})$ for $N = 1, 2, \ldots$.
- Figure 1 shows this sequence of approximations for three different sets of random samples from the posterior.
- We can see that as the number of samples used in the approximation grows, it appears to be converging to around 0.97.

To visualize the theoretical rate of convergence, the figure also shows bands indicating the true value $\alpha = \mathbb{P}(\boldsymbol{\mu}_S > \boldsymbol{\mu}_C \mid \text{data}) =??$ plus or minus the RMSE of the Monte Carlo estimator, that is, from Equation 1:

$$\alpha \pm \sigma(X)/\sqrt{N} =??$$

Simpify this as much as possible for an ungraded exercise (exam II).

Solution to the ungraded exercise

$$
\begin{aligned}
\alpha \pm \sigma(X)/\sqrt{N} &= \alpha \pm \sqrt{\alpha(1-\alpha)/N} \\
&= 0.97 \pm \sqrt{0.97(1-0.97)/N}
\end{aligned}
$$

where X has the posterior distribution of $\mathbb{1}(\boldsymbol{\mu}_S > \boldsymbol{\mu}_C)$ given the data, in other words, X is a Bernoulli(α) random variable. Recall that the variance of a Bernoulli(α) random variable is $\alpha(1-\alpha)$.

Return of IQ Scores

Using the same approach, we could easily approximate any number of other posterior quantities as well, for example,

$$\mathbb{P}(\boldsymbol{\lambda}_S > \boldsymbol{\lambda}_C \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}(\boldsymbol{\lambda}_S^{(i)} > \boldsymbol{\lambda}_C^{(i)})$$

$$\mathbb{E}(|\boldsymbol{\mu}_S - \boldsymbol{\mu}_C| \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^{N} |\boldsymbol{\mu}_S^{(i)} - \boldsymbol{\mu}_C^{(i)}|$$

$$\mathbb{E}(\boldsymbol{\mu}_S / \boldsymbol{\mu}_C \mid \text{data}) \approx \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{\mu}_S^{(i)} / \boldsymbol{\mu}_C^{(i)}.$$

Background: inverse CDF method

For a random variable X with c.d.f. F, define the generalized CDF as

$$F^{-1}(u) = \min\{x : F(x) \geq u\}.$$

If

$$U \sim \mathit{Uniform}(0, 1)$$

then

$$F^{-1}(U) \sim X.$$

Illustration

$$X \sim Exponential(1).$$ [1]

Then

$$f(x) = \exp(-x) \implies F(x) = 1 - \exp(-x).$$

Let $u = 1 - \exp^{-x}$ and solve for u. Then $x = -log(1 - u)$.

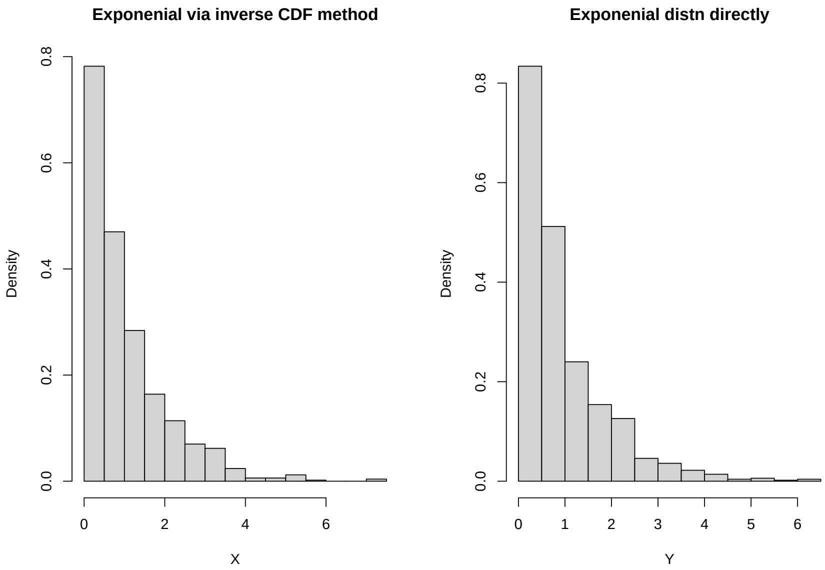
Let $U \sim Uniform(0, 1) \implies 1 - U \sim Uniform(0, 1)$.

Thus,

$$X \sim -log(U).$$

[1] Applications include the length of time, in minutes, of long distance business telep

Illustration



Rejection Sampling

Rejection sampling is a method for drawing random samples from a distribution whose p.d.f. can be evaluated up to a constant of proportionality.

Compared with the inverse c.d.f. method, rejection sampling has the advantage of working on complicated multivariate distributions. (see homework)

Difficulties? You must design a good proposal distribution (which can be difficult, especially in high-dimensional settings).

Uniform Sampler

Goal: Generate samples from Uniform(A), where A is complicated.

- $X \sim Uniform(Mandelbrot)$.
- Consider $I_{X(A)}$.

The Mandelbrot

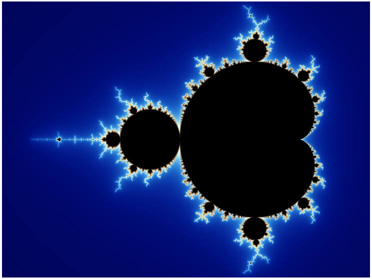


Figure 2: A complicated function A, called the Mandelbrot!

The Mandelbrot

The Mandelbrot set is a set of points in the complex plane.[2]

A point in this plane can be defined using a complex number $c \in C$ such that

$$c = a + bi,$$

where a,b are real numbers and $i = \sqrt{-1}$.

Formally, $c \in C$ belongs to the Mandelbrot set iff

$$lim_{n\to\infty}||z_{n+1} = z_n^2 + c|| \nrightarrow \infty \quad \text{where} \quad z_o = 0.$$

- Note that $||\cdot||$ is the Euclidean norm[3]

[2] The complex plane is a two-dimensional space with the a vertical imaginary axis, and a horizontal real axis.

[3] This measures how far a point is from it's origin.

The Mandelbrot

Formally, $c \in C$ belongs to the Mandelbrot set iff

$$lim_{n \to \infty} ||z_{n+1} = z_n^2 + c|| \nrightarrow \infty \quad \text{where} \quad z_o = 0.$$

- We have a re-cursive function.[4]
- Conjugate distributions – out the window!
- We're going to need to do something numerical!

[4] To read more about fractals, see https://www.kth.se/social/files/5504b42ff276543e4aa5f5a1/An_introduction_to_the_Mandelbrot_Set.pdf.

Exercise

- Suppose $A \subset B$.
- Let $Y_1, Y_2, \ldots \sim \text{Uniform(B)}$ iid and
- $X = Y_k$ where $k = \min\{k : Y_k \in A\}$,

Then it follows that

$$X \sim \text{Uniform}(A).$$

Drawing Uniform Samples

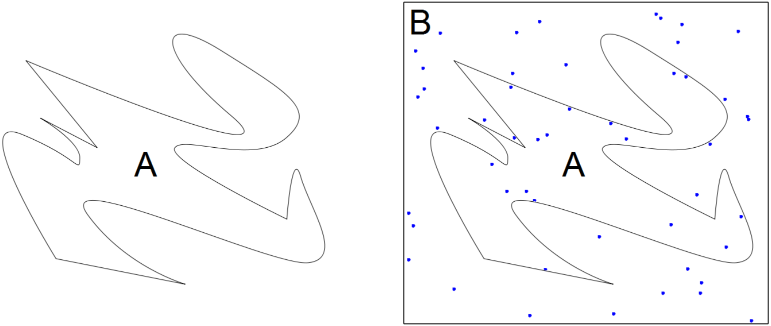


Figure 3: (Left) How to draw uniform samples from region A? (Right) Draw uniform samples from B and keep only those that are in A.

General Rejection Sampling Algorithm

Goal: Sample from a complicated pdf $f(x)$.

Suppose that

$$f(x) = \tilde{f}(x)/\alpha, \alpha > 0$$

.

Assumption: f is difficult to evaluate, $\tilde{f}$ is easy! Why? α may be very difficult to calculate even computationally.

1. Choose a proposal distribution q such that $c > 0$ with

$$cq(x) \geq \tilde{f}(x).$$

2. Sample $X \sim q$, sample $Y \sim \text{Unif}(0, c\, q(X))$ (given X)
3. If $Y \leq \tilde{f}(X), Z = X$, otherwise we reject and return to step (2).

Output: $Z \sim f(x)$

Visualizing just f

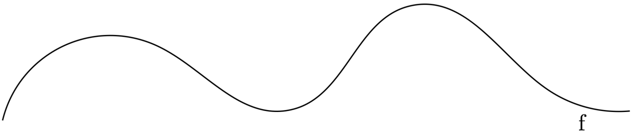


Figure 4: Visualizing just f.

Visualizing just f and $\tilde{f}$

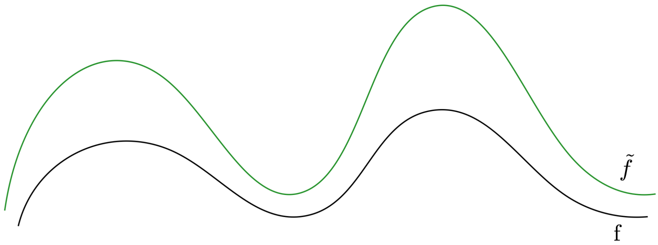


Figure 5: Visualizing just f and $\tilde{f}$.

Enveloping q over f

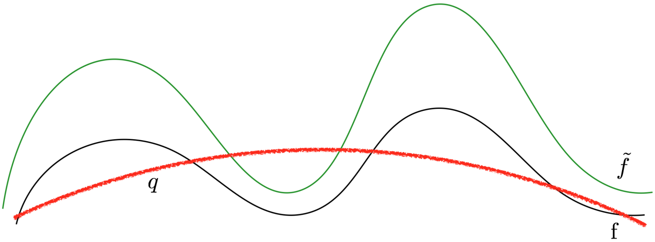


Figure 6: Visualizing f and $\tilde{f}$. Now we look at enveloping q over f.

Enveloping cq over $\tilde{f}$

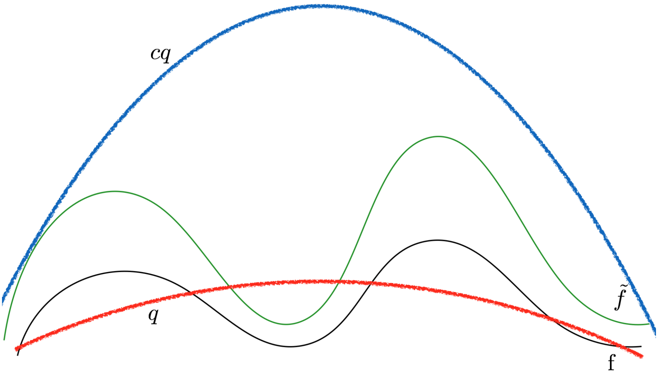


Figure 7: Visualizing f and $\tilde{f}$. Now we look at enveloping cq over $\tilde{f}$.

Recalling the sampling method and accept/reject step

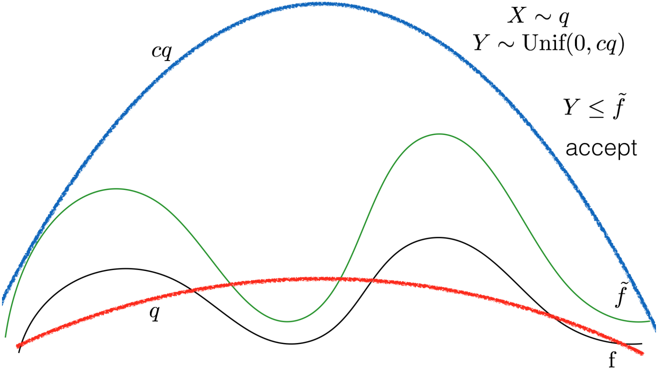


Figure 8: Recalling the sampling method and accept/reject step.

Entire picture and an example point X and Y

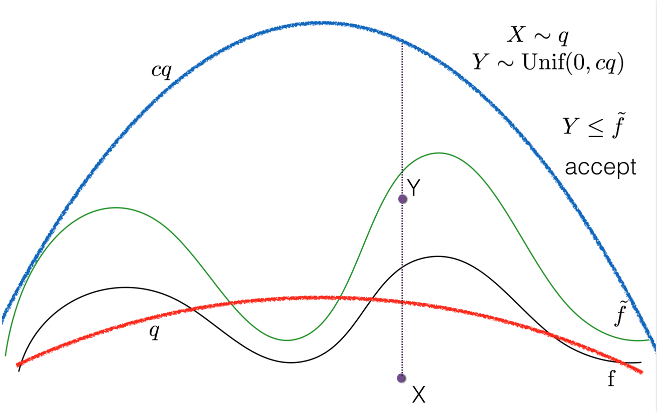


Figure 9: Entire picture and an example point X and Y.

Efficiency of the Rejection Sampler

Recall:

$$f(x) = \frac{\tilde{f}(x)}{\alpha}, \alpha > 0$$

(typically don't know α in practice.)

Constraint:

$$cq(x) \geq \tilde{f}(x).$$

(We can choose c to make our rejection sampler efficient.)

Recall: $q(x)$ is our **proposal distribution** or **enveloping function** (Uniform, Beta, etc.).

Efficiency of the Rejection Sampler

Result: The **acceptance ratio** is inversely proportional to c.

$$
\begin{aligned}
\mathrm{eff}(q(x)) &= Pr(\text{samples accepted}) && (2)\\
&= \int Pr(x \text{ accepted}) \times q(x)\, dx && (3)\\
&= \int \frac{\tilde{f}(x)}{cq(x)} \times q(x) dx && (4)\\
&= \frac{1}{c} \int \tilde{f}(x) dx && (5)\\
&= \frac{\alpha}{c} && (6)\\
&\propto \frac{1}{c}. && (7)
\end{aligned}
$$

Efficiency of the Rejection Sampler

Note that for all $x \in \mathcal{X}$:

$$cq(x) \geq \tilde{f}(x) \implies \tag{8}$$
$$c \geq \frac{\tilde{f}(x)}{q(x)}. \tag{9}$$

It follows that the optimal value of c, denoted by $\hat{c}$ is

$$\hat{c} = \max_x \frac{\tilde{f}(x)}{q(x)}. \tag{10}$$

Takeaways

- What is Monte Carlo (The naive method)
- Rejection sampling
- Inverse CDF method

Detailed Takeaways

- Why do we use Monte Carlo?
- Why do we use rejection sampling?
- In the next modules, we will learn about Markov chain Monte Carlo algorithms (MCMC), which are used for working in high dimensional parameters spaces.

Exercise (Lab 5)

Consider the function

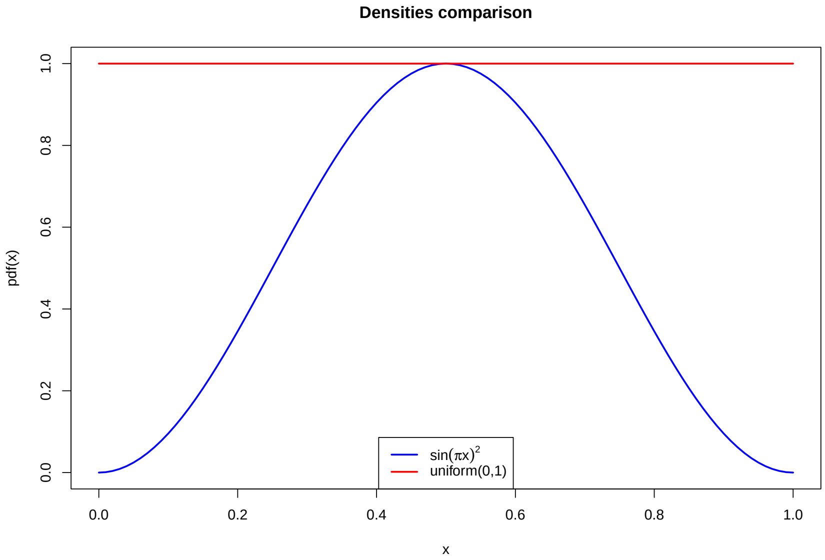
$$f(x) \propto \sin^2(\pi x), x \in [0, 1]$$

1. Plot the densities of $f(x)$ and the Unif(0,1) on the same plot.
2. According to the rejection sampling approach sample from $f(x)$ using the Unif(0,1) pdf as an enveloping function.
3. Plot a histogram of the points that fall in the acceptance region. Do this for a simulation size of 10^2 and 10^5 and report your acceptance ratio. Compare the ratios and histograms.
4. Repeat Tasks 1 - 3 for Beta(2,2) as an enveloping function. Compare your results with results in Task 3.
5. Do you recommend the Uniform or the Beta(2,2) as a better enveloping function (or are they about the same)? If you were to try and find an enveloping function that had a high acceptance ratio, which one would you try and why?

Task 1

```r
# density function for f(x)
densFun <- function(x) {
  return(sin(pi*x)^2)
}
x <- seq(0, 1, 10^-2)
```

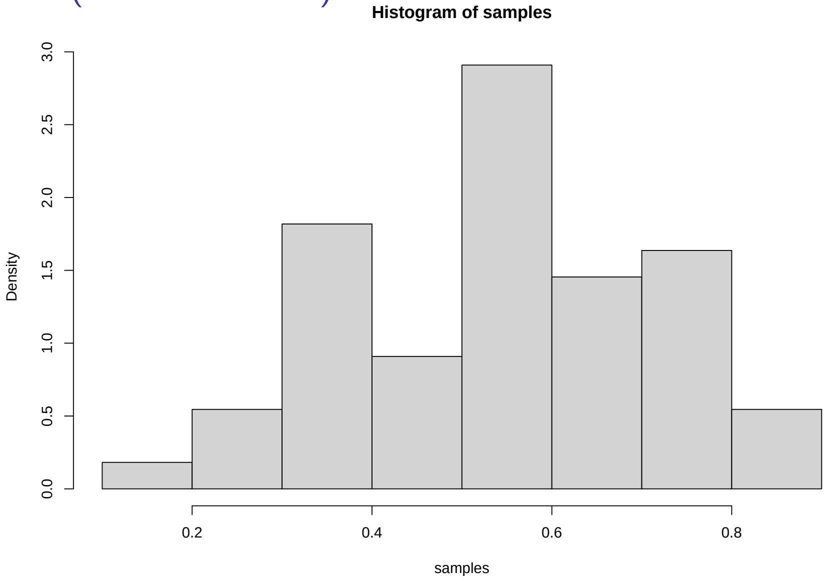
Task 1


Densities comparison
pdf(x)
x
0.0
0.2
0.4
0.6
0.8
1.0
0.0
0.2
0.4
0.6
0.8
1.0
$\sin(\pi x)^2$
uniform(0,1)

Task 2

```r
numSim=10^2
samples = NULL
for (i in 1:numSim) {
  # get a uniform proposal
  proposal <- runif(1)
  # calculate the ratio
  densRat <- densFun(proposal)/dunif(proposal)
  #accept the sample with p=densRat
  if ( runif(1) < densRat ){
    #fill our vector with accepted samples
    samples <- c(samples, proposal)
  }
}
```

Task 3 (Partial solution)




```
## [1] "Acceptance Ratio: 0.55"
```

Task 2 – 4 (Partial Solution)

```
sim_fun <- function(f, envelope = "unif", par1 = 0,
                    par2 = 1, n = 10^2, plot = TRUE){

  r_envelope <- match.fun(paste0("r", envelope))
  d_envelope <- match.fun(paste0("d", envelope))
  proposal <- r_envelope(n, par1, par2)
  density_ratio <- f(proposal) / d_envelope(proposal, par1, par2)
  samples <- proposal[runif(n) < density_ratio]
  acceptance_ratio <- length(samples) / n
  if (plot) {
    hist(samples, probability = TRUE,
         main = paste0("Histogram of ", n, " samples from ",
                       envelope, "(", par1, ",", par2, ").\n
                       Acceptance ratio: ",
                       round(acceptance_ratio,2)), cex.main = 0.75)
  }
  list(x = samples, acceptance_ratio = acceptance_ratio)
}
```

Task 2 – 4 (Partial Solution)

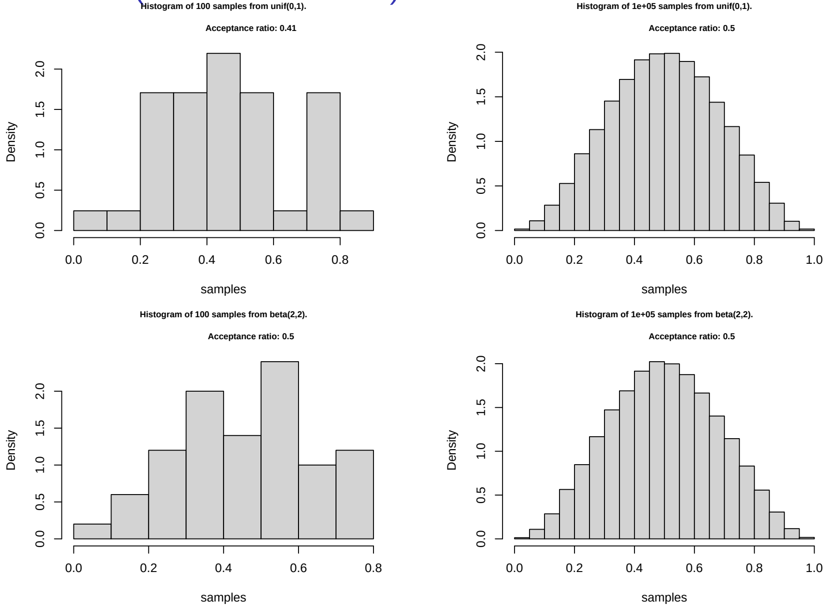


Figure 2: Rejection sampling for 100 versus 100,000 simulations

Takeaways

1. What do you notice about the enveloping functions and the acceptance ratio as the number of samples is large?
2. What does this tell you about the uniform proposal versus the beta proposal in this specific application?

Exercise (Lab 6)

Consider

$$I = \int_{-\infty}^{\infty} \exp(-x^4)\, dx.$$

Tasks (Lab 6)

1. Task 1: Find a closed form solution to I and evaluate this.
2. Task 2: Approximate I using Monte carlo.
3. Task 3: Approximate I using importance sampling.

Gamma density

Before proceeding with the tasks, let's recall that one variant of the Gamma(a,b) density can be written as follows:

$$\text{Gamma}(x|a, b = \text{rate}) = \frac{b^a}{\Gamma(a)} x^{a-1} e^{-bx}\, \mathbb{1}(x > 0)$$

for $a, b > 0$,

Task 1

For the sake of comparison, we can derive the true value using substitution and the gamma function. We will use the substitution $u = x^4$ and $\text{Gamma}(x|a, b = \text{rate}) = \frac{b^a}{\Gamma(a)} x^{a-1} e^{-bx} \mathbb{1}(x > 0)$ for $a, b > 0$,

$$
\begin{aligned}
\int_{-\infty}^{\infty} \exp(-x^4)\, dx &= 2 \int_0^{\infty} \exp(-x^4)\, dx \\
&= 2 \int_0^{\infty} \frac{\exp(-u)}{4u^{3/4}}\, du \\
&= 2^{-1} \int_0^{\infty} u^{1/4-1} e^{-u}\, du \\
&= \frac{\Gamma(1/4)}{1^{1/4}} \times 2^{-1} \int_0^{\infty} u^{1/4-1} e^{-u} \times \frac{1^{1/4}}{\Gamma(1/4)}\, du \\
&= \frac{\Gamma(1/4)}{2} \\
&= 1.813.
\end{aligned}
$$

Task 2 (Monte Carlo)

In this task, we perform Monte carlo. Let $y = \sqrt{2}x^2$. We will perform u-substitution to evaluate the integral with Monte Carlo (verify this calculation on your own)[5]

$$I = 2^{-5/4} \int_0^\infty \sqrt{\frac{2\pi}{y}} 2\phi(y)\, dy.$$

The function $2\phi(y)$ is the density of the normal distribution truncated (or folded) at zero. We can sample from this distribution by taking samples from the standard normal distribution and then taking their absolute value. Note that if $X \sim N(0,1)$ we see for any $c > 0$

$$\begin{aligned} P(|X| < c) &= P(-c < X < c) \\ &= 2(\Phi(c) - 1/2) \\ &= 2\Phi(c) - 1, \end{aligned}$$

Task 3 (Importance Sampling)

We can multiply and divide the integral by a density that has a support equal to the area over which we are integrating. An obvious and easy choice is the standard normal density, ϕ:

$$\int_{-\infty}^{\infty} \exp(-x^4)\, dx = \int_{-\infty}^{\infty} \frac{\exp(-x^4)}{\phi(x)} \phi(x)\, dx.$$

We can therefore evaluate the integral by sampling from a standard normal and averaging the values evaluated in $\exp(-x^4)/\phi(x)$. Thus, we will perform re-weighting, and thus, utilizing importance sampling.

Comparison of Methods

The results of 10,000 simulations using the three methods described above are summarized in Table 1; the true value is included for comparison. Of these methods, multiplying and dividing by the standard normal density and then sampling from this density seems to yield the best estimate, which is both closer to the true value and has lower standard error. The other two methods are comparable in both their estimates and standard errors.

	Mean	SE
True value	1.81	
Truncated Normal (Monte Carlo)	1.79	0.06
Full Normal (IS)	1.81	0.01

Table 1: Comparison of the Monte Carlo estimate for the value of the integral using various methods with 10,000 draws for each method. As we can see under importance sampling, the estimate is closer to the true value and the SE is also lower.

Comparison of Methods

```
## pdf
##   2

## pdf
##   2

## pdf
##   2

## % latex table generated in R 4.4.1 by xtable 1.8-4 packa
## % Wed Sep 17 08:48:29 2025
## \begin{table}[ht]
## \centering
## \begin{tabular}{rrr}
##   \hline
##  & Mean & SE \\
##   \hline
## True value & 1.81 &  \\
##   row.names
##                                       Normal & 1.79 & 0.06
```

Histograms

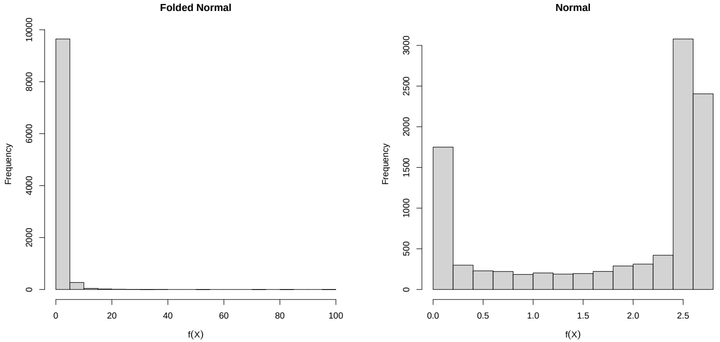


Figure 10: Histograms for the various Monte Carlo simulations.

An ideal histogram would be highly centered around the true value of 1.81. For the folded normal, we see that there are some very large observations that skew the distribution. The normal method also results in a strange histogram, with values concentrated near the edges.

Module I (Recap)

- Bayes Theorem
- Cast of characters
- Conjugacy
- Marginal and posterior predictive distributions
- Here, we looked at very simple applied examples regarding polling and sleep to motivate the use of conjugacy.

Module II (Recap)

- Decision Theory
- Loss functions
- Bayes Risk
- Frequentist Risk
- Integrated Risk
- Here, we looked at a resource allocation problem with a non-trivial loss function.

Module III (Recap)

- Univariate Normal distribution
- Properties of the normal distribution
- Normal-Uniform
- The uniform is an example of an imporoper prior
- Normal-Normal conjugacy
- The precision
- What happens to the Normal-Normal posterior as the sample size gets large?
- The applied example here was about Dutch heights of women and men and looking at bi-modality.

Module IV (Recap)

- The Normal-Gamma conjugacy
- This module was the first time we saw a three-layer hierarhical model
- This was a very long derivation
- The applied example that went with this model was IQ scores since we had two different populations with different means and precisions.

Review Materials

- Practice exercises: https://github.com/resteorts/modern-bayes/tree/master/exercises
- Review homework exercises
- I highly recommend that you work all these problems on your own and make sure that you understand the solutions (which are provided).

In class notes

Derivation of bounds can be found here: https://github.com/resteorts/modern-bayes/blob/master/lecturesModernBayes20/lecture-5/05-class-notes/derivation-of-bounds.pdf

Notes on importance sampling can be found here: https://github.com/resteorts/modern-bayes/blob/master/lecturesModernBayes20/lecture-5/05-class-notes/importance-sampling.pdf

Appendix

The appendix sketches out a proof of the general rejection sampler, which you do not need to know for the exam.

Lemma 1

Lemma: If

$$X \sim q \quad Y \mid X \sim \text{Unif}(0, cq) \implies (X, Y) \sim Unif(B),$$

where $B = \{(x, y), \quad x \in R^d, \quad 0 < y < cq(x)\}$.

Proof:

a.) If $y \notin (0, cq)$, then $p(x, y) = p(y \mid x)p(x) = 0$.

b.) Else, $p(x, y) = p(y \mid x)p(x) = \frac{1}{cq(x)} \times q(x) = \frac{1}{c}$.

Lemma 2

If $(X, Y) \sim Unif(A)$, where $A = \{(x, y) : x \in R^d, 0 < y < \tilde{f}(x)\}$, then $X \sim f$.

Proof: It follows that $m(A) = \int \tilde{f}(x)dx = \int \alpha f(x)dx = \alpha$.

Consider $1 = \int_A b\ dxdy = b \int [\int_0^{\tilde{f}(x)} dy]dx = b \int \tilde{f}(x)dx = b\alpha \implies b = 1/\alpha$.

Then $p(x) = \int p(x, y)dy = \int \frac{1}{\alpha} I(0 < y < \tilde{f}(x))dy = \frac{1}{\alpha} \int_0^{\tilde{f}(x)} dy = \frac{1}{\alpha}\tilde{f}(x) = f(x)$.

Proposition

Suppose f and q are pdfs on $\mathbb{R}^d$ such that

$$f(x) = \tilde{f}(x)/\alpha, \alpha > 0$$

and

$$cq(x) \geq \tilde{f}(x) \forall x \in \mathbb{R}^d.$$

If

$$X_1, X_2, \ldots, \sim q,$$

$$Y_k \mid X_k \sim Unif(0, cq(X_k)),$$

and

$$Z = X_k \text{ where } K = min\{k : Y_k \leq \tilde{f}(X_k)\}$$

then

$$Z \sim f.$$

Proof of Proposition

The proposition follows by Lemma 1 and Lemma 2.

Lemma 3

Let

$$X \sim q \quad \text{and} \quad Y \mid X \sim \text{Uniform}(0, cq(x)).$$

Then

$$(X, Y) \sim \mathit{Uniform}(B), \quad \text{where} \quad B = \{(x, y) : x \in R^d, 0 < y < cq(x)\}.$$

Proof of Lemma 3

1. Suppose $y \notin (0, cq(x))$.

Then

$$p(x, y) = p(y \mid x)p(x) = 0.$$

2. Otherwise

$$p(x, y) = p(y \mid x)p(x) = \frac{1}{cq(x)} \times q(x) = \frac{1}{c}.$$

Lemma 4

If

$$(X, Y) \sim Uniform(A),$$

where

$$A = \{(x, y) : x \in R^d, 0 < y < \tilde{f}(x)\}$$

then

$$X \sim f.$$

Proof of Lemma 4

$$m(A) = \int \tilde{f}(x)dx = \int \alpha f(x)dx.$$

$$\begin{aligned}
p(x) &= \int p(x,y)dy && (11)\\
&= \int \frac{1}{\alpha} I(0 < y < \tilde{f}(x))dy && (12)\\
&= \frac{1}{\alpha} \int_0^{\tilde{f}(x)dy} && (13)\\
&= \frac{\tilde{f}(x)}{\alpha} = \frac{\alpha f(x)}{\alpha} = f(x). && (14)
\end{aligned}$$

Proposition

Suppose f and q are pdfs on R^d such that

$$f(x) = \frac{\tilde{f}(x)}{\alpha}, \alpha > 0$$

and $cq(x) \geq \tilde{f}(x)$ for all $x \in R^d, c > 0$.

If $X_1, X_2, \ldots q$ then

$$Y_k \mid X_k \sim Uniform(0, cq(X_k))$$

and

$$Z = X_K \quad \text{where} \quad K = \min\{k : Y_k \leq \tilde{f}(X_k)\}$$

then $Z \sim f$.

Proof of Proposition

The general rejection sampler proof follows directly from Lemma 3 – 4.

Video on Rejection Sampling

https://www.youtube.com/watch?v=OXDqjdVVePY

Thank you to Mona Su, Class of 2023 for the recommendation!