uc3m | Universidad **Carlos III** de Madrid

Master Degree in Statistics for Data Science

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Resampling and Simulation

Worksheet 2

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EXERCISE 1

The time T, measured in days, during which a manufacturing system remains non-operational each time it breaks down, is described by a cumulative distribution function (cdf) given by:

$$F_T(t) = \begin{cases} 1 - \left(\frac{2}{t}\right)^3 & \textbf{if } t > 2 \\ 0 & \textbf{if } t \leq 2 \end{cases}$$

Apply the inverse transform method and write a function that simulates samples from the above cdf.

Given the previous CDF, we are asked to simulate samples using the inverse transform method. The inverse transform method involves finding the inverse of the CDF. To simulate samples, we can use the following steps:

1. Set $U \sim U(0, 1)$, a uniform random variable.
2. Solve for t in terms of U using the inverse of the CDF.

Inverse CDF:

We can start with:

$$U = 1 - \left(\frac{2}{t}\right)^3,$$

Rearranging for t:

$$t = \frac{2}{(1 - U)^{(1/3)}}.$$

Now, we are in disposition for writing a function in R that simulates samples based on the given CDF.

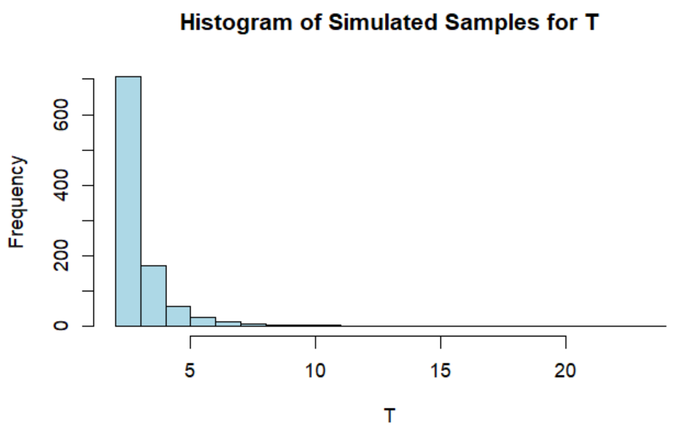
R

CODE 1. Simulating samples from the CDF using the inverse transform method

```r
# Function to simulate samples from the CDF using the inverse
    transform method
simulate_T <- function(n) {
  # Generate uniform random variables
  U <- runif(n)
  # Apply the inverse CDF
  T_samples <- 2 / (1 - U)^(1 / 3)
  return(T_samples)
}

# Test the function by generating 1000 samples
set.seed(123)
samples_T <- simulate_T(1000)
hist(samples_T, breaks = 30, main = "Histogram of Simulated Samples
    for T", xlab = "T", col = "lightblue")
```

Figure 1

Histogram of Simulated Samples for T



R Outcome

```
## First 10 simulated samples
[1] 3.285212 2.151949 7.139156 2.155628 2.322301 3.144130 7.218222
2.516681 2.008957 2.211103
```

Rcpp

We can do this exercise with Rcpp too, that it is useful in a lot of circunstances when R is slow (e.g. loops), Rcpp is the package that allows us to integrate C++ inside of R.

CODE 2. Simulating samples from the CDF using the inverse transform method

```
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector simulate_T_rcpp(int n) {
  NumericVector samples(n);
  for (int i = 0; i < n; ++i) {
    // Generate a random number U ~ U(0, 1)
    double U = R::runif(0, 1);
    // Apply the inverse of CDF
    samples[i] = 2 / pow(1 - U, 1.0/3.0);
  }
  return samples;
}

// Use the function to simulate 1000 samples from the CDF using Rcpp
library(Rcpp)
sourceCpp("Exercise1_Worksheet2.cpp")
set.seed(123)
samples_T <- simulate_T_rcpp(1000)
hist(samples_T, breaks = 30, main = "Histogram of Simulated Samples
    for T", xlab = "T", col = "lightblue")
```

```
## First 10 simulated samples
[1] 3.285212 2.151949 7.139156 2.155628 2.322301 3.144130 7.218222
2.516681 2.008957 2.211103
```

We obtain the same samples as expected, because we are using a random seed for reproducibility. And now, we can finally compare the performance in terms of computational cost between R and C++ (Rcpp). To perform this comparison we apply the library `microbenchmark` as follows:

Comparing the performance R vs. Rcpp:

CODE 3. Comparing the speed of the 2 functions

```
library(microbenchmark)
Comparison1 <- microbenchmark(simulate_T(1000), simulate_T_rcpp
    (1000), times = 1000)
print(Comparison1)
```

```
Unit: microseconds
                 expr   min    lq     mean median    uq    max neval
     simulate_T(1000) 105.0 107.5 116.9555  109.2 111.5 2942.9  1000
 simulate_T_rcpp(1000)  77.8  79.8  85.0483   81.0  82.5  564.5  1000
```

Looking to the previous output, we can observe the remarkable difference in the speed between the two different ways of solving this exercise. Continuing with this exercise, we have improve it with a possible code to do the same but in Python:

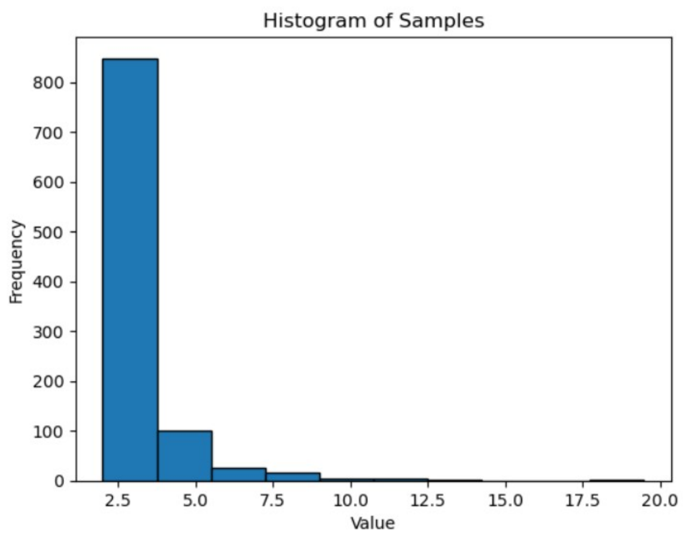
Python

CODE 4. Proposal for exercise 1 in Python

```python
import numpy as np
import matplotlib.pyplot as plt

np.random.seed(123)

# sample from inverse
def sample_from_cdf(n=1):
    U = np.random.uniform(0, 1, n)
    T = 2 * (1 - U) ** (-1/3)
    return T

# generate & plot samples
samples = sample_from_cdf(1000)

plt.hist(samples, edgecolor='black')
plt.title('Histogram of Samples')
plt.xlabel('Value')
plt.ylabel('Frequency')
plt.show()
```

Figure 2

Histogram of Simulated Samples for T



Python Outcome

And we can observe how the histogram of samples performed in Python is basically the same as the histogram of samples from R.

EXERCISE 2

A random variable T follows a Pareto distribution with scale parameter equal to 2 and shape parameter equal to 3. We can use its density function as an instrumental density function to simulate samples from another Pareto model whose tail is not as heavy. Consider now a random variable S (Pareto with scale parameter 2 and shape parameter 4) with cdf

$$F_S(t) = \begin{cases} 1 - \left(\frac{2}{t}\right)^4 & \textbf{if } t > 2 \\ 0 & \textbf{if } t \leq 2 \end{cases}$$

(a) Determine M such that $f_S(t) \leq M f_T t$, where f_s and f_t are the density functions of S and t.

We are given two Pareto distributions:

- A random variable T with the CDF $F_T(t) = 1 - \left(\frac{2}{t}\right)^3$ for $t > 2$.
- A random variable S with the CDF $F_S(t) = 1 - \left(\frac{2}{t}\right)^4$ for $t > 2$.

The density functions for S and T are the derivatives of their respective CDFs:

$$f_T(t) = \frac{6}{t^4}, \text{for } t > 2,$$
$$f_S(t) = \frac{8}{t^5}, \text{for } t > 2,$$

We want to find M such that:

$$\frac{8}{t^5} \leq M \leq \frac{6}{t^4},$$

Simplifying this inequality:

$$\frac{8}{6} \leq Mt$$
$$M \geq \frac{4}{3} \text{ for all } t > 2,$$

Thus, $M = \frac{4}{3}$ works.

(b) Write an acceptance-rejection algorithm to simulate from F_S.

Our proposal for the acceptance-rejection algoritm to simulate from F_S is the following:

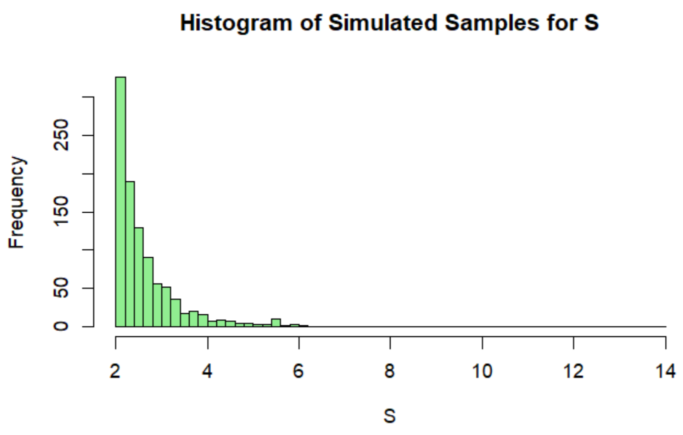
R

CODE 5. Acceptance-Rejection algorithm to simulate from F_S

```r

# Function for acceptance-rejection sampling
simulate_S <- function(n) {
  samples_S <- numeric(n)
  i <- 1
  while (i <= n) {
    # Propose a sample from T using its PDF
    T_candidate <- 2 / (1 - runif(1))^(1/3)
    # Generate a uniform random number for acceptance
    U <- runif(1)

    # Accept with probability proportional to the ratio of densities
    if (U <= (8/6) * (T_candidate^(-5)) / (T_candidate^(-4))) {
      samples_S[i] <- T_candidate
      i <- i + 1
    }
  }
  return(samples_S)
}

# Generate samples and check the first 10
set.seed(123)
samples_S <- simulate_S(10000)
hist(samples_S, breaks = 50, main = "Histogram of Simulated Samples
    for S", xlab = "S", col = "lightgreen")
```

Figure 3

Histogram of Simulated Samples for S



R Outcome

As before, we can solve this statement in other languages as Python, and this is what we are going to do:

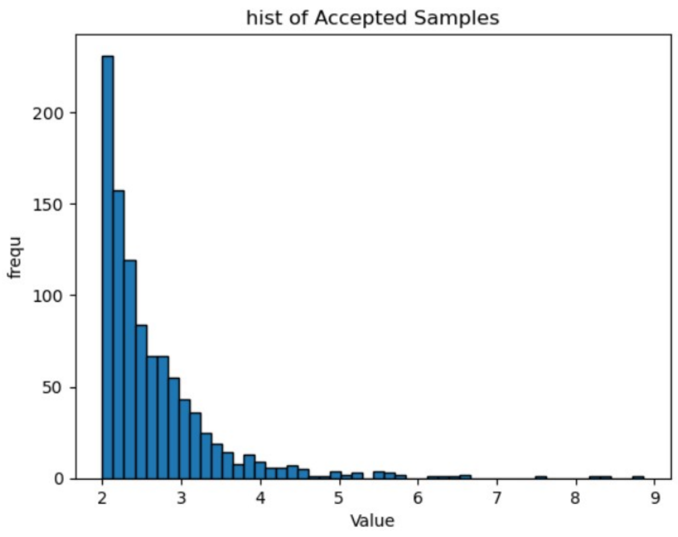
CODE 6. Acceptance-Rejection algorithm to simulate from F_S in Python

```python
import numpy as np
import scipy.stats as stats

# Sample generation algo
def sample_pareto_s(n):

    # params
    x_m = 2
    alpha_T = 3
    alpha_S = 4
    M = 4/3

    samples = []
    samples_rejected = []
    while len(samples) < n:
        T = (np.random.pareto(alpha_T, 1) + 1) * x_m  # sample
        U = np.random.uniform(0, 1)

        # acceptance ratio
        acceptance_ratio = (8 / T**5) / (M * (6 / T**4))

        if U <= acceptance_ratio:
            samples.append(T[0])
        else:
            samples_rejected.append(T[0])
    return np.array(samples),np.array(samples_rejected)

# run Monte Carlo
MC = 1000
samples, samples_rejected = sample_pareto_s(MC)

plt.hist(samples, bins=50, edgecolor='black')
plt.title('hist of Accepted Samples')
plt.xlabel('Value')
plt.ylabel('frequ')
```

And the output is the following histogram:

Figure 4

Histogram of Simulated Samples for S



Python Outcome

With this histogram in python we have finished this statement.

(c) Use your simulation algorithm to check that $E[S] = 8/3 = 2.6667$. Show a 99% confidence interval algorithm based on MC = 10000 observations.

To check the expectation $E[S] = 8/3$, we can compute the sample mean of the generated values.

R

CODE 7. Checking the expectation is equal to 8/3

```r
# Compute the sample mean
mean_S <- mean(samples_S)
mean_S  # Should be close to 8/3 = 2.6667
```

```
The mean of S is: 2.674881
```

The result is very near to the theoretical value. Now, we can also compute a 99% confidence interval using the standard error.

CODE 8. Computing the 99% confidence interval

```r
# 99% Confidence interval
stderr_S <- sd(samples_S) / sqrt(length(samples_S))
```

```
ci_lower <- mean_S - 2.576 * stderr_S
ci_upper <- mean_S + 2.576 * stderr_S
c(ci_lower, ci_upper)  # 99% confidence interval
```

```
[1] 2.601231 2.748532
```

This is the final result for the exercise 2. The confidence interval is narrow, so we have done a good job estimating the expectation of S.

We are going to propose a solution for this exercise in Rcpp:

Rcpp

CODE 9. Proposal in Rcpp for exercise 2

```
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector simulate_S_rcpp(int n) {
  NumericVector samples(n);
  int i = 0;
  while (i < n) {
    // Propose a sample from T using the inverse CDF
    double T_candidate = 2 / pow(1 - R::runif(0, 1), 1.0/3.0);

    // Generate a random number U ~ U(0, 1)
    double U = R::runif(0, 1);

    // Accept with proportional probability to the ratio of the
        density functions
    if (U <= (8.0 / 6.0) * pow(T_candidate, -5.0) / pow(T_candidate,
        -4.0)) {
      samples[i] = T_candidate;
      ++i;
    }
  }
  return samples;
}

// Use the function to simulate 1000 samples from the CDF using Rcpp
library(Rcpp)
sourceCpp("Exercise2_Worksheet2.cpp")
set.seed(666)
samples_S_rcpp <- simulate_S(1000)
hist(samples_S_rcpp, breaks = 50, main = "Histogram of Simulated
    Samples for S", xlab = "S", col = "lightgreen")

```

```
// Compute the sample mean
mean_S_rcpp <- mean(samples_S_rcpp)
print(mean_S_rcpp)  # Should be close to 8/3 = 2.6667

// 99% Confidence interval
stderr_S_rcpp <- sd(samples_S_rcpp) / sqrt(length(samples_S_rcpp))
ci_lower_rcpp <- mean_S_rcpp - 2.576 * stderr_S_rcpp
ci_upper_rcpp <- mean_S_rcpp + 2.576 * stderr_S_rcpp
c(ci_lower_rcpp, ci_upper_rcpp)  # 99% confidence interval
```

```
The mean of S is: 2.674881
[1] 2.601231 2.748532
```

We obtain the same result as before, now we can compare again the performance between R and C++, we apply the `microbenchmark` library.

Comparing performances R vs. Rcpp

CODE 10. Comparing the speed of the 2 functions

```
library(microbenchmark)
## Compare the results of the two methods
Comparison2 <- microbenchmark(simulate_S(1000), simulate_S_rcpp
    (1000), times = 1000)
print(Comparison2)
```

```
Unit: microseconds
            expr    min      lq      mean   median    uq     max
      simulate_S 2403.4 2714.65 3379.7160 2870.5 3127.95 28825.0
 simulate_S_rcpp  220.8  236.50  282.0873  245.7  263.75  1210.4
```

From the previous output, we can observe how the difference in the speed between R and C++ in microseconds is huge, with C++ obtaining an outstanding performance.

Just as another option, the result for this statement in Python is the following:

CODE 11. Proposal in Python for exercise 2c

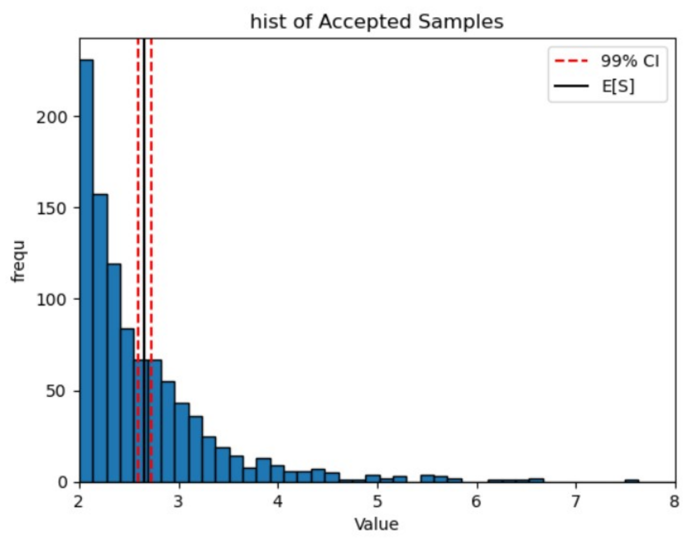
```
# Exp of S
E_S = np.mean(samples)
print(f"E[S]: {E_S:.4f}")

# CI 99% of S
std_dev = np.std(samples, ddof=1)
z_alpha = 2.576  # z for 99% CI
```

```python
CI_lower = E_S - z_alpha * (std_dev / np.sqrt(MC))
CI_upper = E_S + z_alpha * (std_dev / np.sqrt(MC))

print(f"99% Confidence Interval: ({CI_lower:.4f}, {CI_upper:.4f})")

# plot
plt.hist(samples, bins=50, edgecolor='black')
plt.axvline(CI_lower, color='red', linestyle='--', label='99% CI')
plt.axvline(CI_upper, color='red', linestyle='--')
plt.axvline(E_S, color='black', linestyle='-', label='E[S]')
plt.title('hist of Accepted Samples')
plt.xlabel('Value')
plt.ylabel('frequ')
plt.xlim(2, 8)
plt.legend()
```

```
E[S]: 2.6598
99% Confidence Interval: (2.5953, 2.7243)
```

Figure 5

Histogram of Simulated Samples for S with 99% Confidence Interval



Python Outcome

We obtain very similar results, but they are not equal (R vs Python), as we know from exercises in class or as we could see from the first task.

EXERCISE 3

A random variable X follows a truncated normal distribution within the interval [a,b] characterized by the parameters μ (mean) and σ (standard deviation). Thus, X can be denoted as TN (μ, σ, a, b) if its probability density function $f_X(x)$ is defined as:

$$f_X(x) = \frac{\frac{1}{\sigma}\phi\left(\frac{x-\mu}{\sigma}\right)}{\Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)}$$

where $a \leq x \leq b$ holds and $\phi(\cdot)$ represents the normal density function, while $\Phi(\cdot)$ represents the cumulative distribution function (cdf) of a standard normal distribution. To simulate observations from a truncated normal random variable TN(0,1;-1,1), write functions utilizing:

(a) Rejection sampling algorithm with the density function of a standard normal distribution as a candidate function.

For the truncated normal distribution TN(μ, σ, a, b), we are asked to simulate samples using different methods.

We use the standard normal distribution as a candidate function for rejection sampling. The algorithm is as follows:

- Propose a sample from the normal distribution $N(\mu, \sigma)$.
- Reject samples outside the range [a,b].
- Accept the sample if it lies within [a,b].

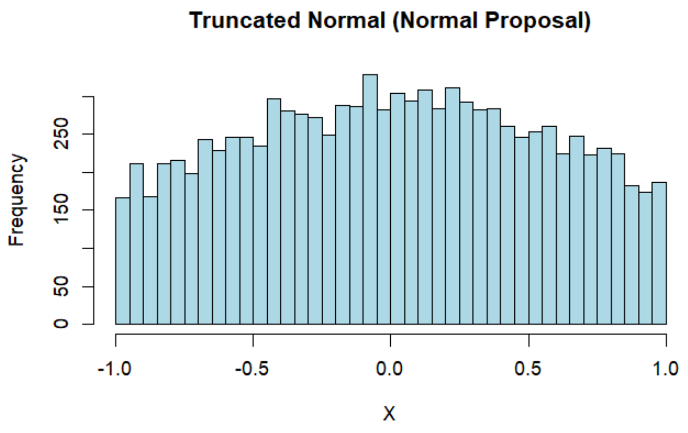
R

CODE 12. Function for rejection sampling with normal distribution as candidate

```r
# Function for rejection sampling with normal distribution as
    candidate
simulate_truncated_normal_normal <- function(n, mu, sigma, a, b) {
  samples <- numeric(n)
  i <- 1
  while (i <= n) {
    # Propose a sample from normal distribution
    candidate <- rnorm(1, mu, sigma)
    # Reject if the candidate is outside [a, b]
    if (candidate >= a && candidate <= b) {
      samples[i] <- candidate
      i <- i + 1
    }
  }
  return(samples)
}

# Simulate from TN(0, 1; -1, 1)
set.seed(666)
samples_trunc_normal <- simulate_truncated_normal_normal(10000, 0,
    1, -1, 1)
hist(samples_trunc_normal, breaks = 50, main = "Truncated Normal (
    Normal Proposal)", xlab = "X", col = "lightblue")
```

Figure 6

Truncated Normal (Normal Proposal)



R Outcome

As can be seen, the histogram is between -1 and 1, as we were requested and the form is as expected a gaussian bell.

(b) A rejection sampling algorithm with the density function of a uniform distribution $U(-1, 1)$ as the candidate function.

We can use a uniform distribution as the proposal distribution. The process is similar, but now we generate uniform samples instead of normal ones.

R

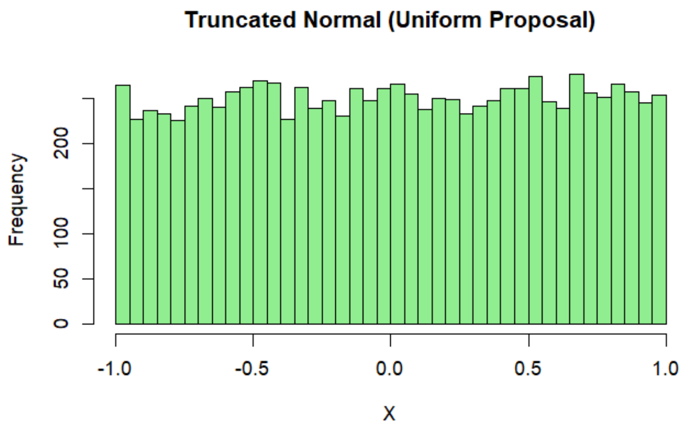
CODE 13. Function for rejection sampling with uniform distribution as candidate

```r
# Function for rejection sampling with normal distribution as
    candidate
```

```r
simulate_truncated_normal_normal <- function(n, mu, sigma, a, b) {
  samples <- numeric(n)
  i <- 1
  while (i <= n) {
    # Propose a sample from normal distribution
    candidate <- rnorm(1, mu, sigma)
    # Reject if the candidate is outside [a, b]
    if (candidate >= a && candidate <= b) {
      samples[i] <- candidate
      i <- i + 1
    }
  }
  return(samples)
}

# Simulate from TN(0, 1; -1, 1)
set.seed(666)
samples_trunc_normal <- simulate_truncated_normal_normal(10000, 0, 1, -1, 1)
hist(samples_trunc_normal, breaks = 50, main = "Truncated Normal (Normal Proposal)", xlab = "X", col = "lightblue")


# Function for rejection sampling with uniform distribution as candidate
simulate_truncated_normal_uniform <- function(n, mu, sigma, a, b) {
  samples <- numeric(n)
  i <- 1
  while (i <= n) {
    # Propose a sample from uniform distribution
    candidate <- runif(1, a, b)
    # Accept the candidate
    samples[i] <- candidate
    i <- i + 1
  }
  return(samples)
}

# Simulate from TN(0, 1; -1, 1)
set.seed(666)
samples_trunc_normal_uniform <- simulate_truncated_normal_uniform(10000, 0, 1, -1, 1)
hist(samples_trunc_normal_uniform, breaks = 50, main = "Truncated Normal (Uniform Proposal)", xlab = "X", col = "lightgreen")
```

Figure 7

Truncated Normal (Uniform Proposal)



R Outcome

As can be observed, we obtained a uniform distribution in the interval [-1,1].

(c) An inverse transform technique.

For the inverse transform method, we generate a random number (U(0,1) and apply the inverse of the truncated CDF.

R

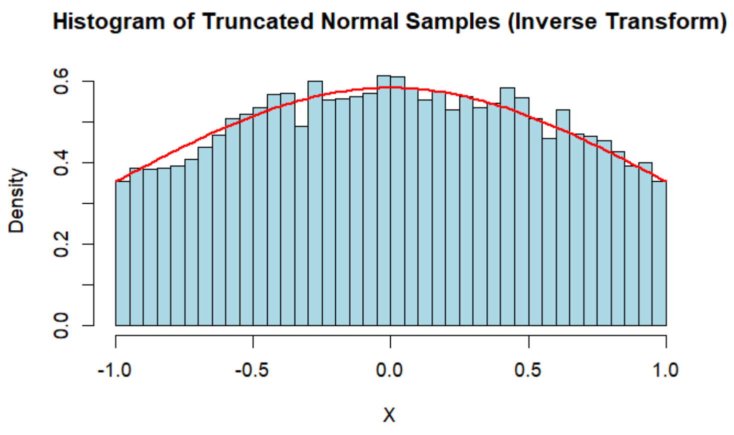
CODE 14. Function to generate truncated normal samples using the inverse transform method

```r

# Function to generate truncated normal samples using the inverse
    transform method
truncated_normal_inverse_transform <- function(n) {
  # Compute the CDF values at the truncation points
  Fa <- pnorm(-1, mean = 0, sd = 1)  # CDF at a = -1
  Fb <- pnorm(1, mean = 0, sd = 1)   # CDF at b = 1

  # Generate uniform samples
  U <- runif(n, Fa, Fb)

  # Apply the inverse normal CDF (qnorm) to transform the samples
  samples <- qnorm(U, mean = 0, sd = 1)

  return(samples)
}

# Example usage: Generate 10,000 samples
```

```r
set.seed(666)
samples <- truncated_normal_inverse_transform(10000)

# Plot the histogram
hist(samples, breaks = 50, probability = TRUE, col = "lightblue",
     main = "Histogram of Truncated Normal Samples (Inverse
        Transform)",
     xlab = "X")

# Overlay the true density of TN(0,1; -1,1)
curve(dnorm(x, 0, 1) / (pnorm(1, 0, 1) - pnorm(-1, 0, 1)),
      from = -1, to = 1, col = "red", lwd = 2, add = TRUE)
```

Figure 8

Truncated Normal (Inverse Transform)



R Outcome

Now, we are going to replicate the exercise 3 in Rcpp and finally, we will finish this task comparing the performance of the algorithms as before with `microbenchmark`.

Rcpp

CODE 15. Exercise 3 in Rcpp

```cpp
// Simulation of TN(0,1; -1,1) using rejection with standard normal
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector truncated_normal_rejection_normal_RCPP(int n) {
  NumericVector samples(n);
  int i = 0;
  while (i < n) {
    double candidate = R::rnorm(0, 1); // Proposal from N(0,1)
    if (candidate >= -1 && candidate <= 1) { // Accept if within the interval
      samples[i] = candidate;
      i++;
    }
  }
  return samples;
}

// Simulation of TN(0,1; -1,1) using rejection with uniform distribution
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector truncated_normal_rejection_uniform_RCPP(int n) {
  NumericVector samples(n);
  int i = 0;
  while (i < n) {
    double candidate = R::runif(-1, 1); // Proposal U(-1,1)
    double accept_prob = R::dnorm(candidate, 0, 1, false) / 0.5; // Acceptance probability
    if (R::runif(0, 1) < accept_prob) {
      samples[i] = candidate;
      i++;
    }
  }
  return samples;
}

// Simulation of TN(0,1; -1,1) using inverse transform
#include <Rcpp.h>
using namespace Rcpp;

// [[Rcpp::export]]
NumericVector truncated_normal_inverse_transform_RCPP(int n) {
  NumericVector samples(n);
  double Fa = R::pnorm(-1, 0, 1, true, false);
  double Fb = R::pnorm(1, 0, 1, true, false);
  int i = 0;
  while (i < n) {
    double U = R::runif(0, 1);
    samples[i] = R::qnorm(Fa + U * (Fb - Fa), 0, 1, true, false);
    i++;
  }
  return samples;
}
```

Comparison between R and Rcpp

CODE 16. Comparison of algorithms

```r
library(Rcpp)
sourceCpp("Exercise3a_Worksheet2.cpp")
sourceCpp("Exercise3b_Worksheet2.cpp")
sourceCpp("Exercise3c_Worksheet2.cpp")
n <- 10000
set.seed(666)
samples_normal <- truncated_normal_rejection_normal_RCPP(n)
samples_uniform <- truncated_normal_rejection_uniform_RCPP(n)
samples_inverse <- truncated_normal_inverse_transform_RCPP(n)

library(microbenchmark)
Comparison3 <- microbenchmark(simulate_truncated_normal_normal
    (10000, 0, 1, -1, 1),
                              simulate_truncated_normal_uniform
                                  (10000, 0, 1, -1, 1),
                              truncated_normal_inverse_transform
                                  (10000),
                              truncated_normal_rejection_normal_RCPP
                                  (10000),
                              truncated_normal_rejection_uniform_
                                  RCPP(10000),
                              truncated_normal_inverse_transform_
                                  RCPP(10000),
                              times = 1000)
print(Comparison3)
```

```
Unit: microseconds
 expr          min       lq        mean    median       uq       max
 normal_R     9922.2 11067.70 11707.3875 11349.05 11683.50   49820.7
 uniform_R    6325.2   6933.55  7536.7495  7134.15  7394.80 110039.6
 inverse_R    277.9    300.00   324.0749   313.70   327.45    2533.5
 normal_Rcpp  492.9    530.55   552.0135   544.90   561.65    1117.1
 uniform_Rcpp 1011.4   1077.40  1118.2521  1108.40  1134.90    2550.1
 inverse_RCPP 182.9    196.95   209.2799   203.00   214.75    1008.9
```

Performance Analysis

The benchmark results indicate that the Rcpp implementations significantly improve performance. The inverse transform method in Rcpp is the fastest, with a mean execution time of only 209.3 microseconds. The rejection sampling methods using normal and uniform distributions are slower, especially in pure R implementations. The standard normal rejection method in R takes the longest time due to a lower acceptance rate. Therefore, for efficiency, the inverse transform method in Rcpp is recommended.

FINAL CONCLUSION

In this work, we explored different methods for simulating random variables with specific probability distributions. Using the inverse transform method, we generated samples from a given cumulative distribution function, demonstrating a fundamental technique in stochastic simulation. We also implemented an acceptance-rejection algorithm to simulate from a modified Pareto distribution, carefully selecting an instrumental density function to ensure efficiency. Finally, we examined the truncated normal distribution, implementing three different simulation approaches—rejection sampling with normal and uniform proposals, and the inverse transform method—allowing for a comparative analysis of their computational efficiency.

Our results show that the choice of simulation method significantly impacts computational performance. While the inverse transform method is often straightforward and efficient, rejection sampling can become computationally expensive depending on the acceptance rate. The use of Rcpp further enhanced efficiency, particularly in rejection sampling scenarios. These findings highlight the importance of selecting appropriate simulation techniques based on the characteristics of the target distribution and available computational resources.