Exercise 1

TMA4300 Computer Intensive Statistical Models

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Problem A: Stochastic simulation by the probability integral transform and bivariate techniques

Subproblem 1.

Let $X \sim \text{Exponential}(\lambda)$, with the cumulative density function

$$F_X(x) = 1 - e^{-\lambda x}, \quad x \ge 0.$$

Then the random variable $Y := F_X(X)$ has a Uniform (0,1) distribution. The probability integral transform becomes

$$Y = 1 - e^{-\lambda X} \quad \Leftrightarrow \quad X = -\frac{1}{\lambda} \ln(1 - Y).$$

It is clear that if $U \sim \text{Uniform}(0,1)$, then $1-U \sim \text{Uniform}(0,1)$, and therefore we may as well say that

$$X = -\frac{1}{\lambda}\ln(Y). \tag{1}$$

Thus, we sample Y from runif() and transform it using Equation (1), to sample from the exponential distribution. Figure 1 shows one million samples drawn from the generate_from_exp() function defined in the code chunk below. It also shows the theoretical PDF of the exponential distribution with rate parameter $\lambda = 2$.

```
#set.seed(123)

generate_from_exp <- function(n, rate = 1) {
    Y <- runif(n)
    X <- -(1 / rate) * log(Y)
    return(X)
}

# sample
n <- 1000000 # One million samples
lambda <- 2
exp_samp <- generate_from_exp(n, rate = lambda)

# plot
ggplot() +
geom_histogram(</pre>
```

```
data = as.data.frame(exp_samp),
  mapping = aes(x = exp_samp, y = ..density..),
  binwidth = 0.05,
  boundary = 0
) +
stat_function(
  fun = dexp,
  args = list(rate = lambda),
  aes(col = "Theoretical density")
ylim(0, lambda) +
xlim(0, 2) +
ggtitle("Simulating from an exponential distribution") +
xlab("x") +
ylab("Density") +
theme_minimal() +
theme(plot.title = element_text(hjust = 0.5))
```

Simulating from an exponential distribution

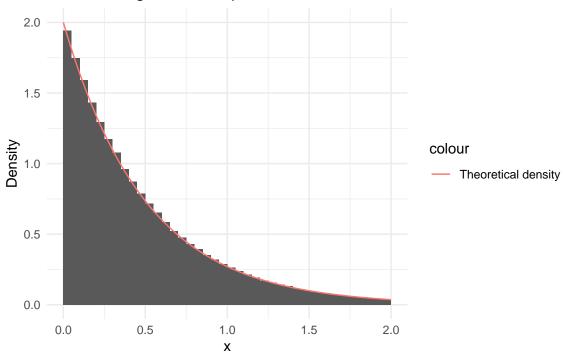


Figure 1: Normalized histogram of one million samples drawn from the exponential distribution, together with the theoretical PDF, with $\lambda = 2$.

Theoretically, the mean and variance of $X \sim \text{Exponential}(\lambda)$ is $\mathrm{E}(X) = \lambda^{-1}$ and $\mathrm{Var}(X) = \lambda^{-2}$. So for $\lambda = 2$ we would expect $\mathrm{E}(X) = 1/2$ and $\mathrm{Var}(X) = 1/4$. For the simulation we get the mean and variance as calculated in the code block below, showing what we would expect.

```
mean(exp_samp)
```

[1] 0.499487

var(exp_samp)

[1] 0.24952

Subproblem 2.

Subsubproblem (a)

We are considering the probability density function

$$g(x) = \begin{cases} cx^{\alpha - 1} & \text{if } 0 < x < 1, \\ ce^{-x} & \text{if } x \ge 1, \\ 0 & \text{otherwise,} \end{cases}$$
 (2)

where c is a normalizing constant and $\alpha \in (0,1)$. If $x \leq 0$ the cumulative distribution function is zero. In the interval 0 < x < 1 it becomes

$$G(x) = \int_{-\infty}^{x} g(\xi) d\xi = \int_{0}^{x} c\xi^{\alpha - 1} d\xi = \frac{c}{\alpha} [\xi^{\alpha}]_{0}^{x} = \frac{c}{\alpha} x^{\alpha},$$

and finally for $x \geq 1$ we have

$$G(x) = \int_{-\infty}^{x} g(\xi) \, d\xi = \int_{0}^{1} c\xi^{\alpha - 1} \, d\xi + \int_{1}^{x} c e^{-\xi} \, d\xi = \left[\frac{c}{\alpha} \xi^{\alpha} \right]_{0}^{1} - \left[c e^{-\xi} \right]_{1}^{x} = c \left(\frac{1}{\alpha} - e^{-x} + \frac{1}{e} \right),$$

for $\alpha \in (0,1)$. That is, the cumulative density function is

$$G(x) = \begin{cases} 0 & \text{if } x \le 0, \\ \frac{c}{\alpha} x^{\alpha} & \text{if } 0 < x < 1, \\ c\left(\frac{1}{\alpha} - e^{-x} + \frac{1}{e}\right) & \text{if } x \ge 1. \end{cases}$$

In this case it is trivial to find c. We solve

$$1 = \int_{\mathbb{R}} g(x) dx = \int_{0}^{1} cx^{\alpha - 1} dx + \int_{1}^{\infty} ce^{-x} dx = \frac{c}{\alpha} + \frac{c}{e},$$

which gives that

$$c = \frac{\alpha e}{\alpha + e}.$$

Writing the cumulative density function using this as c we obtain

$$G(x) = \begin{cases} 0 & \text{if } x \le 0, \\ \frac{e}{\alpha + e} x^{\alpha} & \text{if } 0 < x < 1, \\ 1 - \frac{\alpha}{\alpha + e} e^{1 - x} & \text{if } x \ge 1, \end{cases}$$

for $\alpha \in (0,1)$.

We may then find the inverse cumulative function. For $x \le 0$ this is just zero, and for 0 < x < 1, that is $0 < G(x) < \frac{\mathrm{e}}{\alpha + \mathrm{e}}$, we solve $x = \frac{\mathrm{e}}{\alpha + \mathrm{e}} y^{\alpha}$ for y giving $G^{-1}(x) = \left(\frac{\alpha + \mathrm{e}}{\mathrm{e}} x\right)^{1/\alpha}$. Similarly for $x \ge 1$, that is $G(x) \ge 1 - \frac{\alpha}{\alpha + \mathrm{e}} = \frac{\mathrm{e}}{\alpha + \mathrm{e}}$, we solve $x = 1 - \frac{\alpha}{\alpha + \mathrm{e}} \mathrm{e}^{1-y}$ for y, such that

$$G^{-1}(x) = \begin{cases} \left(\frac{\alpha + e}{e}x\right)^{1/\alpha} & \text{if } 0 \le x < \frac{e}{\alpha + e}, \\ \ln\left[\frac{\alpha e}{(1 - x)(\alpha + e)}\right] & \text{if } \frac{e}{\alpha + e} \le x \le 1, \end{cases}$$

for $\alpha \in (0,1)$.

Subsubproblem (b)

Using what we found in (a) we may use the inversion method to sample from g(x) given in Equation (2), as shown in the code block beneath. Figure 2 shows one million samples drawn from generate_from_gx() and also the theoretical PDF.

```
generate_from_gx <- function(n, alpha) {</pre>
  U <- runif(n) # Generate n Uniform(0, 1) variables
  bound \leftarrow exp(1) / (alpha + exp(1)) # Boundary where G^{(-1)} changes
  left <- U < bound # The left of the boundary</pre>
  U[left] <- (U[left] / bound)^(1 / alpha)</pre>
                                                # Left CDF
  U[!left] \leftarrow 1 + log(alpha) - log(1 - U[!left]) - log(alpha + exp(1)) # Right CDF
  return(U)
}
# Sample
n \leftarrow 1000000 # One million samples
alpha <- 0.75
gx_samp \leftarrow generate_from_gx(n, alpha) # Generating n samples from g(x)
# The theoretically correct PDF
theo gx <- function(x, alpha) {
  const <- alpha * exp(1) / (alpha + exp(1)) # Normalizing constant</pre>
  func <- rep(0, length(x)) # Vector of zeros of same length as x
  left \langle -x \rangle 0 \& x \langle 1 \rangle # The PDF has one value for 0 \langle x \langle 1 \rangle
  right \langle -x \rangle = 1 # ... and one value for x \geq 1
  func[left] <- const * x[left]^(alpha - 1) # The value to the left</pre>
  func[right] <- const * exp(-x[right]) # The value to the right</pre>
  return(func)
# Plot
ggplot() +
  geom_histogram(
    data = as.data.frame(gx_samp),
    mapping = aes(x = gx_samp, y = ..density..),
    binwidth = 0.05,
    boundary = 0
  ) +
  stat_function(
    fun = theo_gx,
    args = list(alpha = alpha),
    aes(col = "Theoretical density")
  ) +
  xlim(0, 5) +
  ggtitle("Simulating from g(x) given in Equation (2)") +
  xlab("x") +
  ylab("Density") +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5))
```

Assuming $X \sim g(x)$ we may find the expectation to be

$$E(X) = \int_{\mathbb{R}} xg(x) dx = \int_{0}^{1} cx^{\alpha} dx + \int_{1}^{\infty} cxe^{-x} dx = \frac{\alpha e}{(\alpha + 1)(\alpha + e)} + \frac{2\alpha}{\alpha + e} \approx 0.768,$$

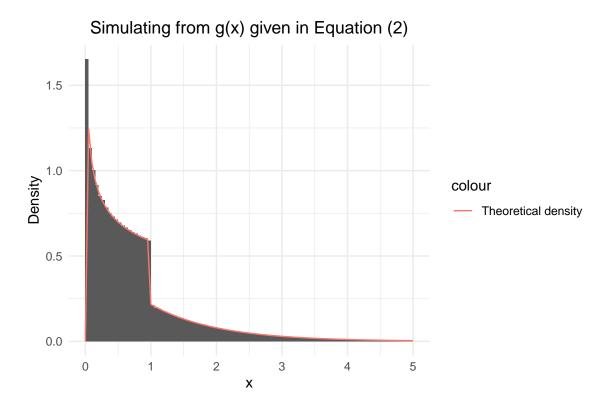


Figure 2: Normalized histogram of one million samples drawn from g(x) given in Equation (2), together with the theoretical PDF, with $\alpha = 0.75$.

when $\alpha = 0.75$. This corresponds approximately to the sample mean shown in the following code block.

mean(gx_samp)

[1] 0.76749

Similarly we may find the theoretical variance to be

$$Var(X) = E(X^2) - E(X)^2 \approx 0.705,$$

also for $\alpha=0.75$, corresponding approximately to the sample variance given in the code block below. var(gx_samp)

[1] 0.703663

Subproblem 3.

Subsubproblem (a)

We consider the probability density function

$$f(x) = \frac{ce^{\alpha x}}{(1 + e^{\alpha x})^2},$$

for $-\infty < x < \infty$ and $\alpha > 0$. To find the normalizing constant c we make sure that the integral over \mathbb{R} of f(x) is one. That is

$$1 = \int_{\mathbb{R}} f(x) dx = c \int_{\mathbb{R}} \frac{e^{\alpha x}}{(1 + e^{\alpha x})^2} dx,$$

and letting $u = 1 + e^{\alpha x}$, it follows that

$$1 = \frac{c}{\alpha} \int_{1}^{\infty} \frac{\mathrm{d}u}{u^{2}} = \frac{c}{\alpha} \left[-\frac{1}{u} \right]_{1}^{\infty} = \frac{c}{\alpha}.$$

That is, the normalizing constant is $c = \alpha$, for $\alpha > 0$. We may then write the probability density function as

$$f(x) = \frac{\alpha e^{\alpha x}}{(1 + e^{\alpha x})^2},\tag{3}$$

for $-\infty < x < \infty$ and $\alpha > 0$.

Subsubproblem (b)

The cumulative distribution function is given as

$$F(x) = \int_{-\infty}^{x} f(\xi) d\xi = \int_{-\infty}^{x} \frac{\alpha e^{\alpha \xi}}{(1 + e^{\alpha \xi})^2} d\xi.$$

Again letting $u = 1 + e^{\alpha \xi}$ it follows that

$$F(x) = \int_{1}^{1 + e^{\alpha x}} \frac{\alpha e^{\alpha \xi}}{u^2} \frac{du}{\alpha e^{\alpha \xi}} = \int_{1}^{1 + e^{\alpha x}} \frac{du}{u^2} = \left[\frac{1}{u}\right]_{1 + e^{\alpha x}}^{1} = 1 - \frac{1}{1 + e^{\alpha x}} = \frac{e^{\alpha x}}{1 + e^{\alpha x}},$$

which holds for $-\infty < x < \infty$ and $\alpha > 0$.

Solving $x = e^{\alpha y}/(1 + e^{\alpha y})$ for y then gives us the inverse cumulative distribution function. Some algebra then gives that

$$F^{-1}(x) = \frac{1}{\alpha} \ln \left(\frac{x}{1-x} \right) = \frac{1}{\alpha} \left[\ln (x) - \ln (1-x) \right],$$

for 0 < x < 1 and $\alpha > 0$.

Subsubproblem (c)

Simulating from f(x) given in Equation (3) is shown in the code block below, and the result is shown in Figure 3. The sampling is done by letting $U \sim \text{Uniform}(0,1)$ and using inversion sampling.

```
generate_from_fx <- function(n, alpha) {</pre>
  U <- runif(n) # Generate n Uniform(0, 1) variables
  X \leftarrow 1 / alpha * (log(U) - log(1 - U)) # Using the inverse CDF
 return(X)
}
# Sample
n <- 1000000 # One million samples
alpha <- 100 # Letting alpha be 100
fx_samp \leftarrow generate_from_fx(n, alpha) # Generating n samples from f(x)
# The theoretically correct PDF
theo_fx <- function(x, alpha) {</pre>
  return(alpha * exp(alpha * x) / (1 + exp(alpha * x))^2)
# Plot
ggplot() +
  geom histogram(
   data = as.data.frame(fx samp),
```

```
mapping = aes(x = fx_samp, y = ..density..),
binwidth = 0.001,
boundary = 0
) +
stat_function(
  fun = theo_fx,
    args = list(alpha = alpha),
    aes(col = "Theoretical density")
) +
ggtitle("Simulating from f(x) given in Equation (3)") +
xlab("x") +
ylab("Density") +
theme_minimal() +
theme(plot.title = element_text(hjust = 0.5))
```

Simulating from f(x) given in Equation (3) 25 20 Colour Theoretical density

Figure 3: Normalized histogram of one million samples drawn from f(x) given in Equation (3), together with the theoretical PDF, with $\alpha = 100$.

0.1

Letting $X \sim f(x)$ we may find the expected value to be

-0.1

0.0

Х

$$\mathrm{E}(X) = \int_{\mathbb{R}} x f(x) \, \mathrm{d}x = \int_{\mathbb{R}} \frac{\alpha x \mathrm{e}^{\alpha x}}{(1 + \mathrm{e}^{\alpha x})^2} \, \mathrm{d}x = 0,$$

because of symmetry. This is confirmed in the following code block where we see that the sample mean is approximately zero. This also holds for all $\alpha > 0$.

```
mean(fx_samp)
```

[1] 2.957973e-05

We may also find the variance of X to be

$$Var(X) = E(X^2) = \int_{\mathbb{R}} \frac{\alpha x^2 e^{\alpha x}}{(1 + e^{\alpha x})^2} dx \approx 0.000329,$$

for $\alpha = 100$. This also corresponds to the sample variance as shown in the code block below.

```
var(fx_samp)
```

[1] 0.0003288562

Subproblem 4.

We wish to simulate from a Normal(0,1) distribution using the Box-Muller algoritm. If $X_1 \sim \text{Uniform}(0,\pi)$ and $X_2 \sim \text{Exponential}(1/2)$, then $Y_1 = \sqrt{X_2}\cos(X_1)$ and $Y_2 = \sqrt{X_2}\sin(X_1)$ are standard normal distributed. We use $Z = \sqrt{X_2}\cos(X_1)$ in the following code block. The result of the simulation can be seen in Figure 4, and it also shows the theoretical probability density function.

```
std normal <- function(n) {</pre>
 X1 <- pi * runif(n) # n samples from Uniform(0, pi)</pre>
 X2 <- generate_from_exp(n, 1/2) # n samples from Exponential(1/2)</pre>
  Z \leftarrow X2^{(1/2)} * cos(X1)  # Z ~ Normal(0, 1)
  return(Z)
}
# Sample
n <- 1000000 # One million samples
Box_Muller <- std_normal(n)</pre>
                              # Generating n samples from Normal(0, 1)
# Plot
ggplot() +
  geom_histogram(
    data = as.data.frame(Box_Muller),
    mapping = aes(x = Box_Muller, y = ..density..),
    binwidth = 0.05,
    boundary = 0
  stat_function(
    fun = dnorm,
    aes(col = "Theoretical density")
  ggtitle("Simulating from standard normal distribution") +
  xlab("z") +
  ylab("Density") +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5))
```

We know that if $Z \sim \text{Normal}(0,1)$, then E(Z) = 0 and Var(Z) = 1, and this corresponds to the approximate sample mean and variance shown in the code block below.

```
mean(Box_Muller)

## [1] -0.0006589413

var(Box_Muller)

## [1] 1.002119
```

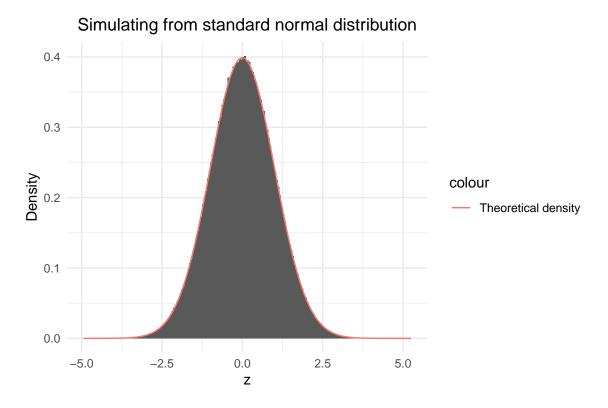


Figure 4: One million samples drawn from a standard normal distribution using the Box-Muller algorithm, together with the theoretical PDF.

Subproblem 5.

We wish to simulate from a d-variate normal distribution with mean vector μ and covariance matrix Σ . Let $Z \sim \text{Normal}_d(0, I_d)$, where I_d is the identity matrix in $\mathbb{R}^{d \times d}$ and 0 is the zero-vector in \mathbb{R}^d . Then

$$X = \mu + AZ \sim \text{Normal}_d(\mu, AA^\top)$$

such that we need to find A such that $\Sigma = AA^{\top}$, this is done using chol() in R, and we construct the function in the following code block.

```
d_variate_normal <- function(n, mu, Sigma) {
    d <- length(mu)  # The dimension d is the dimension of mu
    A <- t(chol(Sigma)) # Cholesky decomposition of Sigma. Transpose to get lower triangular
    Z <- matrix(0, d, n)
    for(i in 1:d) {  # Create d realizations of Normal(0, 1)
        Z[i, ] <- std_normal(n)  # Put realizations of Normal(0, 1) in row of Z
    }
    X <- mu + A %*% Z  # X ~ Normal_d(mu, Sigma)
    return(X)
}</pre>
```

We now test the implementation using one million samples in \mathbb{R}^3 , with

$$\mu = \begin{bmatrix} 1 \\ 7 \\ 2 \end{bmatrix}$$
 and $\Sigma = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}$.

We then expect the sample mean and sample covariance matrix to be approximately equal to these. In the following code block we see that this is indeed the case.

Problem B: The gamma distribution
1.
(a)
(b)
2.
(a)
(b)
3.
(a)
(b)
4.
5.
(a)
(b)
Problem C: Monte Carlo integration and variance reduction
1.
2.
3.
(a)
(b)
Problem D: Rejection sampling and importance sampling
1.
2.
3.
4.