Advanced Simulation

Problem Sheet 1

Exercise 1 (Inversion and Rejection)

1. Let $Y \sim \mathcal{E}xp(\lambda)$ and let $a > 0$. We consider the variable after restricting its support to be $[a, +\infty)$. That is, let $X = Y | Y \geq a$, i.e. X has the law of Y conditionally on being in $[a, +\infty)$. Calculate $F_X(x)$, the cumulative distribution function of X, and $F_X^{-1}(u)$, the quantile function of X. Describe an algorithm to simulate X from $U \sim \mathcal{U}_{[0,1]}$.

2. Let a and b be given, with $a < b$. Show that we can simulate $X = Y | a \leq Y \leq b$ from $U \sim \mathcal{U}_{[0,1]}$ using

$$X = F_Y^{-1}(F_Y(a)(1-U) + F_Y(b)U),$$

i.e. show that if X is given by the formula above, then $\Pr(X \leq x) = \Pr(Y \leq x | a \leq Y \leq b)$. Apply the formula to simulate an exponential random variable conditioned to be greater than a, as in the previous question.

3. Here is a simple algorithm to simulate $X = Y | Y > a$ for $Y \sim \mathcal{E}xp(\lambda)$:

   (a) Let $Y \sim \mathcal{E}xp(\lambda)$. Simulate $Y = y$.

   (b) If $Y > a$ then stop and return $X = y$, and otherwise, start again at step (a).

   Show that this is just a rejection algorithm, by writing the proposal and target densities π and q, as well as the bound $M = \max_x \pi(x)/q(x)$. Calculate the expected number of trials to the first acceptance. Why is inversion to be preferred for $a \gg 1/\lambda$?

Exercise 2 (Rejection)

Consider the following "squeeze" rejection algorithm for sampling from a distribution with density $\pi(x) = \widetilde{\pi}(x)/Z_\pi$ on a state space $\mathbb{X}$ such that

$$h(x) \leq \widetilde{\pi}(x) \leq M\widetilde{q}(x)$$

where h is a non-negative function, $M > 0$ and $q(x) = \widetilde{q}(x)/Z_q$ is the density of a distribution that we can easily sample from. The algorithm proceeds as follows.

- **(a)** Draw independently $X \sim q$, $U \sim \mathcal{U}_{[0,1]}$.
- **(b)** Accept X if $U \leq h(X) / (M\widetilde{q}(X))$.
- **(c)** If X was not accepted in step (b), draw an independent $V \sim \mathcal{U}_{[0,1]}$ and accept X if

$$V \leq \frac{\widetilde{\pi}(X) - h(X)}{M\widetilde{q}(X) - h(X)}.$$

1. Show that the probability of accepting a proposed $X = x$ in either step (b) or (c) is

$$\frac{\widetilde{\pi}(x)}{M\widetilde{q}(x)}.$$

2. Deduce from the previous question that the distribution of the samples accepted by the above algorithm is π.

3. Show that the probability that step (c) has to be carried out is

$$1 - \frac{\int_{\mathbb{X}} h(x)\,dx}{M Z_q}.$$

4. Let $\widetilde{\pi}(x) = \exp\left(-x^2/2\right)$ and $\widetilde{q}(x) = \exp(-|x|)$. Using the fact that

$$\widetilde{\pi}(x) \geq 1 - \frac{x^2}{2}$$

for any $x \in \mathbb{R}$, how could you use the squeeze rejection sampling algorithm to sample from $\pi(x)$. What is the probability of not having to evaluate $\widetilde{\pi}(x)$? Why could it be beneficial to use this algorithm instead of the standard rejection sampling procedure?

Exercise 3 (Transformation)

Consider the following algorithm known as Marsaglia's polar method.

- **Step a**: Generate independent U_1, U_2 according to $\mathcal{U}_{[-1,1]}$ until $Y = U_1^2 + U_2^2 \leq 1$.
- **Step b**: Define

$$Z = \sqrt{-2\log(Y)}$$

and return

$$X_1 = Z\frac{U_1}{\sqrt{Y}},\ X_2 = Z\frac{U_2}{\sqrt{Y}}.$$

1. Define $\vartheta = \arctan(U_2/U_1)$. Show that the joint distribution of Y and ϑ has density

$$f_{Y,\vartheta}(y,\theta) = \mathbb{1}_{[0,1]}(y)\,\frac{\mathbb{1}_{[0,2\pi]}(\theta)}{2\pi}.$$

2. Show that X_1 and X_2 are independent standard normal random variables.
3. What are the potential benefits of this approach over the Box-Muller algorithm?

Exercise 4 (Transformation)

1. Let $\pi(x) = \widetilde{\pi}(x)/Z_\pi$ be any probability density function on $\mathbb{R}$. Prove that if (U,V) is uniformly distributed on $G = \left\{(u,v); 0 \leq u \leq \sqrt{\widetilde{\pi}(v/u)}\right\}$, then V/U is distributed according to π, i.e. admits π as a probability density function.
2. In order to use the result of (1) in practice, we need to be able to sample uniformly from G. Show that if $\sup_x \sqrt{\widetilde{\pi}(x)} < \infty$ and $\sup_x |x| \sqrt{\widetilde{\pi}(x)} < \infty$, then $G \subseteq R$ where

$$R = \left[0, \sup_x \sqrt{\widetilde{\pi}(x)}\right] \times \left[\inf_x x\sqrt{\widetilde{\pi}(x)}, \sup_x x\sqrt{\widetilde{\pi}(x)}\right].$$

Suggest a way to sample uniformly from G.

3. Let $\widetilde{\pi}(x) = \exp\left(-x^2/2\right)$. Using results from (1) and (2), propose a method to sample from $\pi(x)$.

Exercise 5 (Rejection and Importance Sampling)

Consider two probability densities π, q on $\mathbb{X}$ such that $\pi(x) > 0 \Rightarrow q(x) > 0$ and assume that you can easily draw samples from q. Whenever $\pi(x)/q(x) \leq M < \infty$ for any $x \in \mathbb{X}$, it is possible to use rejection sampling to sample from π. When M is unknown or when this condition is not satisfied, we can use importance sampling techniques to approximate expectations with respect to π. However it might be the case that most samples from q have very small importance weights.

Rejection control is a method combining rejection and importance weighting. It relies on an arbitrary threshold value $c > 0$. We introduce the notation $w(x) = \pi(x)/q(x)$ and

$$Z_c = \int_{\mathbb{X}} \min\{1, w(x)/c\}\, q(x)\, dx.$$

Rejection control proceeds as follows.

- **Step a.** Generate independent $X \sim q$, $U \sim \mathcal{U}_{[0,1]}$ until $U \leq \min\{1, w(X)/c\}$.
- **Step b**. Return X.

1. Give the expression of the probability density $q^*(x)$ of the accepted samples.
2. Prove that
$$\mathbb{E}_{q^*}\left([w^*(X)]^2\right) = Z_c \mathbb{E}_q(\max\{w(X), c\}\, w(X))$$
where $w^*(x) = \pi(x)/q^*(x)$.
3. Establish that
$$\mathbb{E}_q(\min\{w(X), c\})\, \mathbb{E}_q(\max\{w(X), c\}\, w(X)) \leq \mathbb{E}_q(\min\{w(X), c\} \max\{w(X), c\}\, w(X))$$
(Hint. Show first that for any $c > 0, w_1 > 0, w_2 > 0$
$$h(w_1, w_2) = [\min\{w_1, c\} - \min\{w_2, c\}]\,[w_1 \max\{w_1, c\} - w_2 \max\{w_2, c\}] \geq 0.$$
This is related to the Harris inequality).
4. Deduce from the results established in (2) and (3) that
$$\mathbb{V}_{q^*}(w^*(X)) \leq \mathbb{V}_q(w(X)).$$

Exercise 6 (Rejection and Importance Sampling)

We want to use Monte Carlo methods to approximate the integral

$$I = \int_{\mathbb{X}} \phi(x)\, \pi(x)\, dx$$

where $\phi : \mathbb{X} \to \mathbb{R}$ and π is a probability density on $\mathbb{X}$. Assume we have access to a proposal probability density q such that $w(x) = \pi(x)/q(x) \leq M < \infty$ for any $x \in \mathbb{X}$.

1. Consider the extended probability density $\overline{\pi}_{X,U}$ on $\mathbb{X} \times [0,1]$ defined as
$$\overline{\pi}_{X,U}(x, u) = \begin{cases} Mq(x) & \text{for } x \in \mathbb{X}, u \in \left[0, \frac{w(x)}{M}\right] \\ 0 & \text{otherwise.} \end{cases}$$
Verify that $\overline{\pi}_X(x) = \pi(x)$.

2. Using the identity

$$I = \int_0^1 \int_{\mathbb{X}} \phi(x) \overline{\pi}_{X,U}(x,u)\, dx du,$$

give the expression of the normalised importance sampling estimate $\widehat{I}_n$ of I when using n independent samples (X_i, U_i) such that $(X_i, U_i) \sim \overline{q}_{X,U}$ where $\overline{q}_{X,U}(x,u) = q(x) \times \mathbb{I}_{[0,1]}(u)$ (that is under $\overline{q}_{X,U}$ we have $X \sim q$, $U \sim \mathcal{U}_{[0,1]}$ and X and U are independent). Express this estimate as a function the importance weight function

$$\overline{w}(x,u) = \frac{\overline{\pi}_{X,U}(x,u)}{\overline{q}_{X,U}(x,u)}.$$

Show that this estimate is equivalent to the estimate one would obtain by sampling from π using rejection sampling using n proposals from q.

3. Show that

$$\mathbb{V}_q(w(X)) \leq \mathbb{V}_{\overline{q}_{X,U}}(\overline{w}(X,U)).$$

4. Show similarly that can one reinterpret the rejection control procedure introduced in Exercise 5 as a standard importance sampling procedure on the extended space $\mathbb{X} \times [0,1]$. Give the expressions of the extended "target" probability density $\widetilde{\pi}_{X,U}$ on $\mathbb{X} \times [0,1]$, the associated importance density $\widetilde{q}_{X,U}(x,u)$ and show that

$$\mathbb{V}_q(w(X)) \leq \mathbb{V}_{\widetilde{q}_{X,U}}(\widetilde{w}(X,U)),$$

where $\widetilde{w}(x,u) = \widetilde{\pi}_{X,U}(x,u) / \widetilde{q}_{X,U}(x,u)$.

Simulation question (Rejection)

The simulation questions are optional and should not be handed back. However, the material covered in these questions is instrumental for a precise understanding of the lecture content. The solution will not be covered in the classes, but will be directly posted on the course's website.

1. Reproduce the figures on the estimation of the number π in the slides of Lecture 2.
2. Implement the Box-Muller algorithm from Lecture 2.
3. Consider the genetic linkage model as in the slides of Lecture 3. Sample some simulated data with a fixed value of θ of your choice. Implement rejection sampling and reproduce the histograms of the posterior of θ and the waiting time before acceptance. Experiment with different proposal distributions.
4. Implement a sampler to draw from a mixture of Gaussians

$$\pi(x) = \omega_1 \phi(x; \mu_1, \sigma_1^2) + \omega_2 \phi(x; \mu_2, \sigma_2^2),$$

where ϕ is the Gaussian pdf. You are allowed to use R's Gaussian generator (but feel free to reimplement Box-Muller from Lecture 3 or Marsaglia's method from Question 1 of this sheet, just for fun).

5. Let

$$h(x) = [\cos(50x) + \sin(20x)].$$

We consider estimating $\int_0^1 h(x)dx$ through Monte Carlo methods.

- First of all, what is the exact answer, to accuracy within 10^{-4}?
- Can you implement rejection sampling with a uniform proposal?
- Find a way to assess how good you are doing.
- Implement an importance sampling solution with a smart proposal (*hint: plot h and find a matching q*).