Lecture 3: Rejection Sampling

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MATH60047/70047 – Stochastic Simulation

October 17, 2022

Imperial College London

Announcements

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  - HXLY 414 - Mathematics Learning Centre

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- Python
  - Tell us if you cannot run Python (email me)
- Assignment
  - We will require a report written in Latex with figures (page limit to be announced with the assignment)

Lecture summary

Recap

The Fundamental Theorem of Simulation

Rejection Sampling

Recap: We have seen

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- Uniform random variate generation

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  - Transformation method.
    - Draw $U \sim \text{Unif}(0, 1)$,
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However, those methods required a quite specific structure for us to be able to sample.

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What if we cannot evaluate $p(x)$ – only evaluate an unnormalised density $\bar{p}(x)$

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What if we cannot evaluate $p(x)$ – only evaluate an unnormalised density $\bar{p}(x)$

Can we still do *exact* sampling?

The Fundamental Theorem of Simulation

Is there a more general structure?

Theorem 1 (Theorem 2.2, Martino et al., 2018)

Drawing samples from one dimensional random variable X with a density $p(x)$ is equivalent to sampling uniformly on the two dimensional region defined by

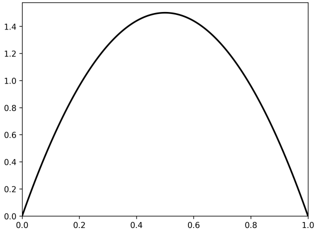
$$\mathsf{A} = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq p(x)\}. \tag{1}$$

In other words, if (x', y') is uniformly distributed on A*, then x' is a sample from $p(x)$.*

Let

$$p(x) = \mathsf{Beta}(\alpha, \beta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha) + \Gamma(\beta)} x^{\alpha - 1}(1 - x)^{\beta - 1},$$

where $\Gamma(n) = (n-1)!$ for integers. For Beta$(2, 2)$:



Its maximum is 1.5 in this specific case. Can we sample uniformly?

Sampling Beta density

Testing the theorem

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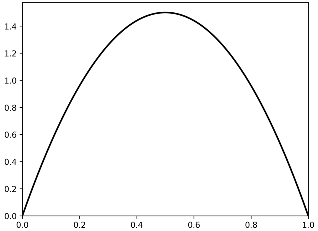

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- Sample from the box $[0,1] \times [0,1.5]$ and keep the ones inside.

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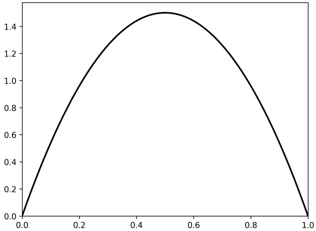

Its maximum is 1.5 in this specific case. Can we sample uniformly?

- Sample from the box $[0, 1] \times [0, 1.5]$ and keep the ones inside.
- Note though our aim is to 'test the x-marginal'

Sampling Beta density

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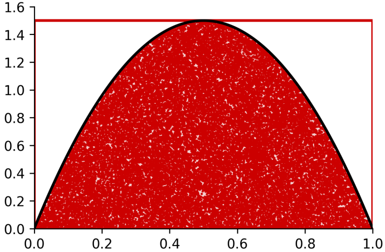

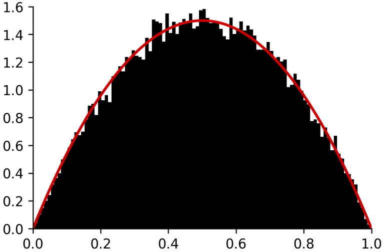

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    - We have used the expression of $p(x)$

We will see that we can get away with an unnormalised expression of $p(x)$ (later)

Rejection sampling

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Using a box wrapping the density is very inefficient:

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  which could be as hard as the sampling problem!
- For densities that are peaky, this could be wildly inefficient

Idea: Design a *proposal* density that tightly wraps the target density

Rejection sampling

Choice of the proposal

Consider a (target) density $p(x)$ and a *proposal* density $q(x)$.

Rejection sampling

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For rejection sampling, we always choose a proposal such that

$$p(x) \leq Mq(x),$$

for $M \geq 1$.

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For rejection sampling, we always choose a proposal such that

$$p(x) \leq Mq(x),$$

for $M \geq 1$. Intuitively, the $Mq(x)$ curve should be **above** $p(x)$.

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The rejection sampler:

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How does this relate to the Fundamental Theorem of Simulation?

Rejection sampling

The algorithm: A closer look

To implement the method:

- Sample $x' \sim q(x)$,

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This is how it is generally implemented!

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- Accept

$$u' \leq p(x'),$$

This would give us (x', u') uniformly under the curve! (hence x' samples would be distributed w.r.t. $p(x)$)

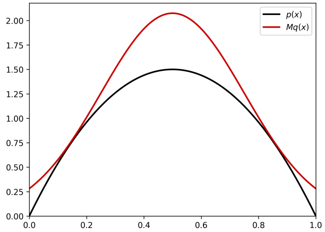
Rejection sampling

Examples: Same Beta$(2, 2)$, better proposal

Choose

$$q(x) = \mathcal{N}(0.5, 0.25),$$

with $M = 1.3$.



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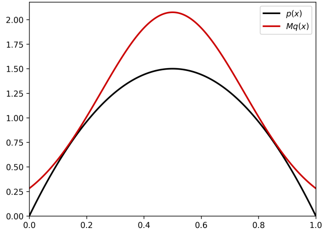

Simulation.

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- Z is called the normalising constant
  - It is a super important quantity for many other purposes
- We write $p(x) \propto \bar{p}(x)$ to say p is proportional to $\bar{p}(x)$ but normalised to integrate (or sum) to one.

The fundamental theorem of simulation is better than it looks. It works with unnormalised densities (recap, unnormalised version)

Theorem 2 (Theorem 2.2, Martino et al., 2018)

Drawing samples from one dimensional random variable X with a density $p(x) \propto \bar{p}(x)$ is equivalent to sampling uniformly on the two dimensional region defined by

$$\mathsf{A} = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \bar{p}(x)\}. \tag{2}$$

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Exactly same – $\bar{p}$ used instead of p provided that $\bar{p}(x) \leq Mq(x)$

Unnormalised densities

Why would you have them?

Easy to imagine the discrete case: Imagine you want to obtain the probability of observing something discrete

- People with black jumpers: 530
- People with red jumpers: 403
- People with yellow jumpers: 304

In order to talk about 'probability of seeing a black jumper', you'd normalise this numbers (normalisation is easy to compute here).

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f usually comes from a rule which determines how probability mass should be spread . Ising model:

$$p_\beta(\sigma) = \frac{e^{-\beta H(\sigma)}}{Z_\beta},$$

where $H(\sigma)$ defines the energy of a spin configuration of a magnetic material. The normalising constant is

$$Z_\beta(\sigma) = \sum_\sigma e^{-\beta H(\sigma)}.$$

All configurations for atomic spins!

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- $p(y)$ is the normalising constant

$$p(y) = \int p(y|x)p(x)\mathrm{d}x,$$

we do not know.

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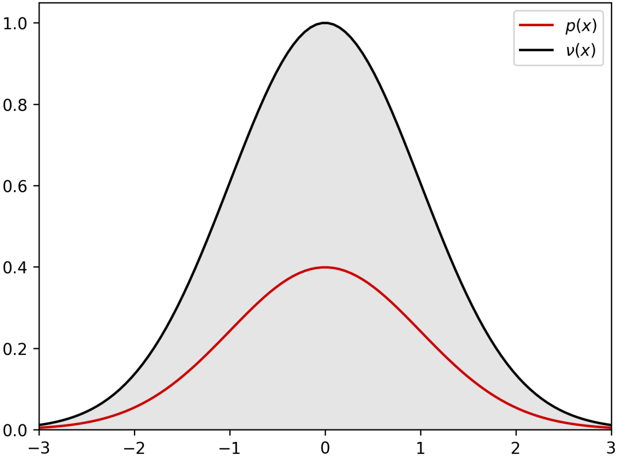
  we do not know.

Therefore, we can evaluate the posterior density only in unnormalised way:

$$p(x|y) \propto p(y|x)p(x).$$

An example of an unnormalised density.

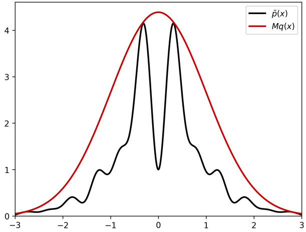


Consider (Robert and Casella, 2004)

$$p(x) \propto \exp(-x^2/2)(\sin^2(6x) + 3\cos^2(x)\sin^2 4x + 1)$$

and

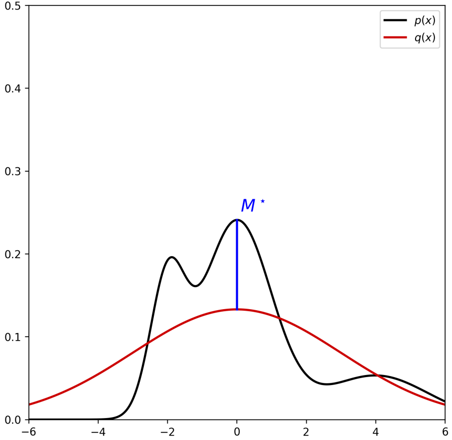
$$q(x) = \mathcal{N}(0,1) = \exp(-x^2/2)/\sqrt{2\pi}.$$



$M = 11.$

A standard choice for M is

$$M^\star = \sup_x \frac{p(x)}{q(x)}.$$



Rejection sampling

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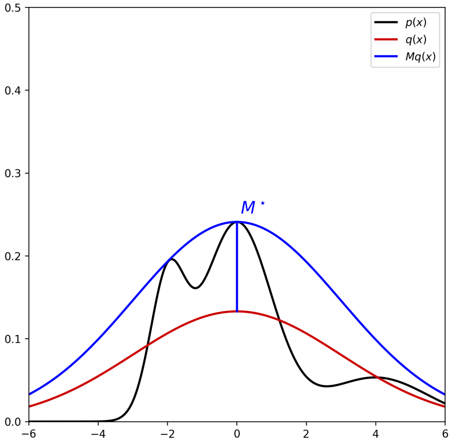

An important quantity for a rejection sampler is *the acceptance rate*. For the normalised case, it can be analytically derived:

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For the unnormalised case, similarly,

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We often would like to optimise our proposal q, such that the acceptance rate is maximised. $\implies$ Minimize M!

Assume that we would like to sample from

$$X \sim \Gamma(\alpha, 1),$$

for $\alpha > 1$. The density is given by

$$p(x) = \frac{x^{\alpha-1} e^{-x}}{\Gamma(\alpha)}, \qquad \text{for } x > 0,$$

where $\Gamma(\alpha)$ is the Gamma function. $\Gamma(n) = (n-1)!$

Choose as a *proposal*:

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$$M_\lambda = \sup_x \frac{p(x)}{q_\lambda(x)}.$$

Find M_λ for fixed λ first:

$$\frac{p(x)}{q_\lambda(x)} = \frac{x^{\alpha-1} e^{(\lambda-1)x}}{\lambda \Gamma(\alpha)}.$$

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Maximise this w.r.t. x?

How to compute a maximum? It is useful to take $\log$:

$$\arg\max_x f(x) = \arg\max_x \log f(x).$$

Take the $\log$ of

$$\frac{p(x)}{q_\lambda(x)} = \frac{x^{\alpha-1}e^{(\lambda-1)x}}{\lambda\Gamma(\alpha)}.$$

So we want to optimise

$$G(x) = \log\frac{p(x)}{q_\lambda(x)} = (\alpha-1)\log x + (\lambda-1)x - \log\lambda\Gamma(\alpha).$$

Set $\frac{\mathrm{d}G(x)}{\mathrm{d}x} = 0$.

The derivative

$$\frac{\mathrm{d}G(x)}{\mathrm{d}x} = \frac{\alpha - 1}{x} + (\lambda - 1) = 0$$

which implies

$$x^\star = \frac{\alpha - 1}{1 - \lambda}.$$

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$$x^{\star} = \frac{\alpha - 1}{1 - \lambda}.$$

How do we understand if this is a maximum? Compute

$$\frac{\mathrm{d}G^2(x)}{\mathrm{d}^2 x} = -\frac{\alpha - 1}{x^2},$$

plug $x^{\star}$ into this

$$\frac{\mathrm{d}^2 G(x^{\star})}{\mathrm{d}x^2} = -\frac{(\alpha - 1)(1 - \lambda)^2}{(\alpha - 1)^2} < 0,$$

as $\alpha > 1$ and $0 < \lambda < 1$.

Therefore,

$$
\begin{aligned}
M_\lambda &= \frac{p(x^\star)}{q_\lambda(x^\star)}, \\
&= \frac{{x^\star}^{\alpha-1} e^{(\lambda-1)x^\star}}{\lambda\Gamma(\alpha)}, \\
&= \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{(\lambda-1)\frac{\alpha-1}{1-\lambda}}}{\lambda\Gamma(\alpha)} \\
&= \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{-(\alpha-1)}}{\lambda\Gamma(\alpha)}.
\end{aligned}
$$

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Recall that, we are interested in the acceptance probability (or maximising it)

$$\frac{p(x)}{M_\lambda q_\lambda(x)} = \left(\frac{x(1-\lambda)}{\alpha - 1} \right)^{\alpha - 1} e^{(\lambda - 1)x + \alpha - 1}.$$

Now, the task is to minimise M_λ w.r.t. λ so we get the *optimal* proposal ($\hat{a} = 1/M_\lambda$ would be maximised).

Recall

$$M_\lambda = \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{-(\alpha-1)}}{\lambda\Gamma(\alpha)}.$$

Compute

$$\begin{aligned}\log M_\lambda = {} & (\alpha-1)\log(\alpha-1) - (\alpha-1)\log(1-\lambda) \\ & - (\alpha-1) - \log\lambda - \log\Gamma(\alpha).\end{aligned}$$

$$\frac{\mathrm{d}\log M_\lambda}{\mathrm{d}\lambda} = \frac{\alpha - 1}{1-\lambda} - \frac{1}{\lambda} = 0,$$

which implies

$$\lambda\alpha - \lambda = 1 - \lambda,$$

therefore

$$\lambda^\star = \frac{1}{\alpha}.$$

Finally we get the optimal M by computing

$$M_{\lambda^\star} = \frac{\alpha^\alpha e^{-(\alpha-1)}}{\Gamma(\alpha)}.$$

In order to sample from $\Gamma(\alpha, 1)$, we perform

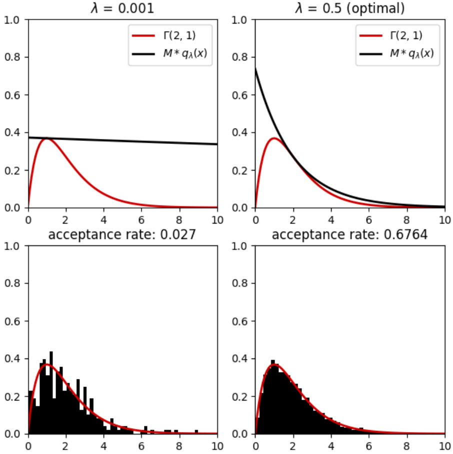
- Sample $X' \sim \mathsf{Exp}(1/\alpha)$ and $U \sim \mathsf{Unif}(0, 1)$
- If

$$U \leq (x/\alpha)^{\alpha-1} e^{(1/\alpha-1)x+\alpha-1},$$

accept X', otherwise start again.

Rejection sampling

Example: Optimising rejection sampling



Rejection Sampling

Example: Sampling truncated distributions

Given $\mathcal{N}(x; 0, 1)$, suppose we are interested in sampling this density between $[-a, a]$. We can write this truncated normal density as

$$p(x) = \frac{\bar{p}(x)}{Z} = \frac{\mathcal{N}(x; 0, 1)\mathbf{1}_{\{x:|x|\leq a\}}(x)}{\int_{-a}^{a} \mathcal{N}(y; 0, 1)\mathrm{d}y}.$$

We can choose $q(x) = \mathcal{N}(x; 0, 1)$ anyway, and we have $\bar{p}(x) \leq q(x)$ (i.e. we can take $M = 1$). The resulting algorithm is extremely intuitive: All you need is to sample from $q(x) = \mathcal{N}(x; 0, 1)$ and reject if this sample is out of bounds $[-a, a]$.

Rejection Sampling

Example: Beta$(2, 2)$

$$p(x) = \mathsf{Beta}(\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)+\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1},$$

Choose

$$\bar{p}(x) = x^{\alpha-1}(1-x)^{\beta-1},$$

Choose

$$q(x) = \mathsf{Unif}(0, 1)$$

What is

$$M = \sup_x \frac{\bar{p}(x)}{q(x)}$$

Rejection Sampling

Example: Beta$(2, 2)$

Compute

$$\log \bar{p}(x)/q(x) = (\alpha - 1)\log x + (\beta - 1)\log(1 - x)$$

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$$\log \bar{p}(x)/q(x) = (\alpha - 1)\log x + (\beta - 1)\log(1 - x)$$

The derivative

$$\frac{\mathrm{d}\log \bar{p}(x)/q(x)}{\mathrm{d}x} = \frac{\alpha - 1}{x} + \frac{1 - \beta}{1 - x}$$

Compute

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$$\frac{\mathrm{d}\log \bar{p}(x)/q(x)}{\mathrm{d}x} = \frac{\alpha - 1}{x} + \frac{1 - \beta}{1 - x}$$

The maximum is

$$x^\star = \frac{\alpha - 1}{\alpha + \beta - 2}.$$

Since

$$M = \frac{\bar{p}(x^\star)}{q(x^\star)}$$

We obtain

$$M = \frac{(\alpha-1)^{\alpha-1}(\beta-1)^{\beta-1}}{(\alpha+\beta-2)^{\alpha+\beta-2}}.$$

Rejection Sampling

Example: Beta$(2, 2)$

The algorithm:

- Sample $X' \sim q(x) = \text{Unif}(0, 1)$
- Sample $U \sim \text{Unif}(0, 1)$
- If $U \leq \bar{p}(X')/Mq(X')$,
  - Accept X'

See you tomorrow!

References I

- Martino, Luca, David Luengo, and Joaquín Míguez (2018). *Independent random sampling methods*. Springer.
- Robert, Christian P and George Casella (2004). *Monte Carlo statistical methods*. Springer.