

Advanced Computational Methods in Statistics

Lecture 1

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LTCC Advanced Course

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Imperial College
London

Computational Statistics

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- ▶ Expectations with respect to intractable distributions
- ▶ Tail probabilities
- ▶ Sampling from posterior distributions of Bayesian models

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 - ▶ Gaussian distribution
 - ▶ Exponential distribution

and others.

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 - ▶ Gaussian distribution
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and others.

These random number generation techniques are at the core of many fields, e.g., statistical inference and generative models.

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Then finally, we will finalize with sequential Monte Carlo (if time permits).

Computational Statistics

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In computational Bayesian statistics, we are interested in synthesising *the model* and *the data* (among other things).

One very effective way is to use Bayesian statistical methodology.

For this, we are often interested in sampling from posterior distributions of the form

$$p(x|y) \propto p(y|x)\pi(x), \quad (1)$$

and estimating expectations w.r.t. them.

Computational Statistics

Generative models



Computational Statistics

Generative models



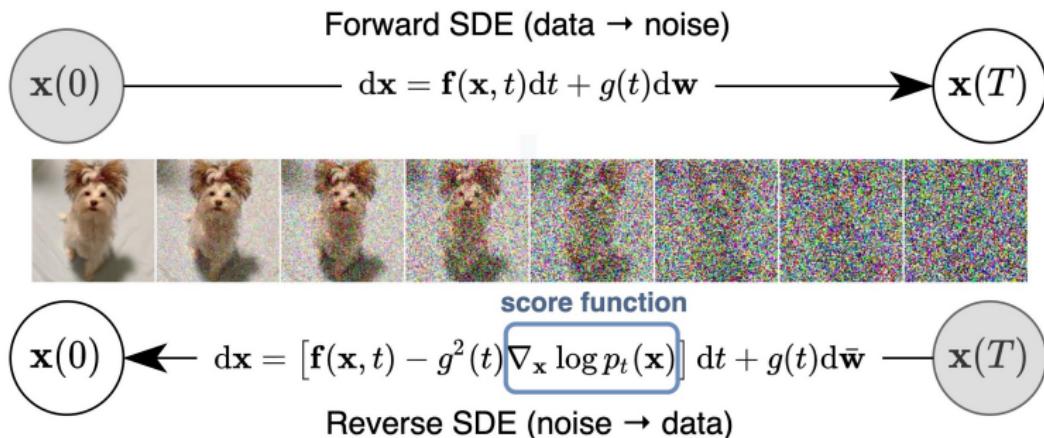
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Goal: Sample from p_{data} by only accessing data $\{Y_i\}_{i=1}^n$.

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¹Figure from: <https://yang-song.net/blog/2021/score/>

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Let's get to our first motivating example.

Estimating π

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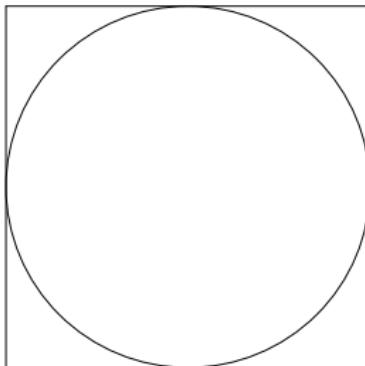
Let's try to solve a simple problem to illustrate the methodology:
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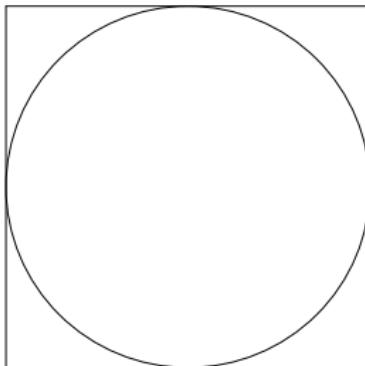
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Estimating π .

Can we estimate π using sampling? Any ideas?

Estimating π 

Given the knowledge that:

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Can we phrase this question probabilistically?

What does this mean?

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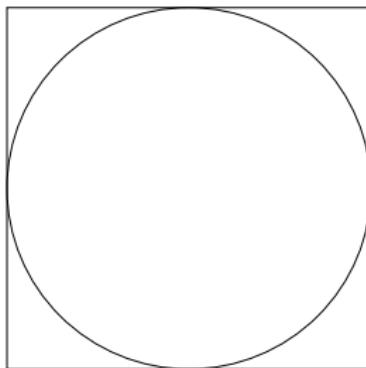
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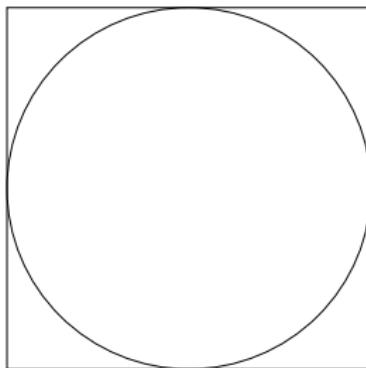
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Most of the time, expectation is the most general way.

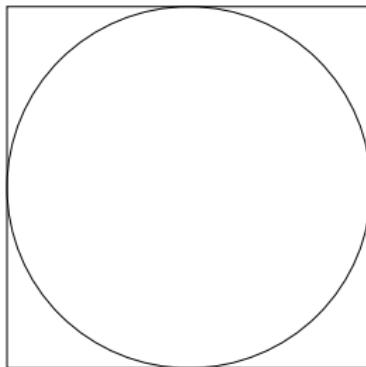


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- ▶ The 'probability' of the square (whole space) is 1.
- ▶ The 'probability of the circle' (set) is precisely the ratio of areas.

$$\mathbb{P}(\text{Circle}) = \frac{\pi}{4}.$$

Last question:

Can we estimate the probability of this set, if we had access to samples from $\text{Unif}([-1, 1] \times [-1, 1])$?

Estimating π

We have used here the most basic idea of estimating an integral (we will clarify shortly).

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Consider now a target measure $\pi(x)dx^3$ and a function $\varphi(x)$. If we have access to i.i.d samples from $X_i \sim \pi(x)$, then

$$(\varphi, \pi) := \int \varphi(x)\pi(x)dx \approx \frac{1}{N} \sum_{i=1}^N \varphi(X_i),$$

using a particle approximation

$$\pi^N(dx) = \frac{1}{N} \sum_{i=1}^N \delta_{X_i}(dx).$$

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Note by definition of the Dirac measure

$$\varphi(y) = \int \varphi(x) \delta_y(dx).$$

Therefore, given the approximation $\pi^N(dx) = \frac{1}{N} \sum_{i=1}^N \delta_{X_i}(dx)$, we have

$$(\varphi, \pi) \approx (\varphi, \pi^N) = \int \varphi(x) \frac{1}{N} \sum_{i=1}^N \delta_{X_i}(dx) = \frac{1}{N} \sum_{i=1}^N \varphi(X_i).$$

Estimating π

Special case

Let $X = [-1, 1] \times [-1, 1]$ and define the uniform measure such that $\mathbb{P}(X) = 1$.

Let A be the “circle” s.t. $A \subset X$. Now, the probability of A is given

$$\begin{aligned}\mathbb{P}(A) &= \int_A \mathbb{P}(\mathrm{d}x) \\ &= \int \mathbf{1}_A(x) \mathbb{P}(\mathrm{d}x), \\ &\approx \frac{1}{N} \sum_{i=1}^N \mathbf{1}_A(x_i) \rightarrow \frac{\pi}{4} \quad \text{as } N \rightarrow \infty.\end{aligned}$$

where $x_i \sim \mathbb{P}$.

In general, we will be interested in sampling from general (unnormalized) distributions:

$$\pi(x) \propto \frac{\gamma(x)}{Z},$$

where $Z = \int \gamma(x)dx$ is the normalizing constant. Our general aim throughout this course is to compute

$$(\varphi, \pi) = \int \varphi(x)\pi(x)dx,$$

for $\varphi : X \rightarrow \mathbb{R}$ a measurable function. $\varphi(x) = x^n$ for moments, $\varphi(x) = \mathbf{1}_A(x)$ for probabilities... In Bayesian inference

$$\gamma(x) = p(y|x)p(x),$$

Perfect Monte Carlo

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- ▶ CLT holds

$$\sqrt{N} ((\varphi, \pi^N) - (\varphi, \pi)) \rightarrow \mathcal{N}(0, \sigma^2(\varphi, \pi)) \quad \text{as } N \rightarrow \infty.$$

In terms of theoretical guarantees, we will favor L_p bounds, i.e., for perfect MC, one can show that

$$\|(\varphi, \pi) - (\varphi, \pi^N)\|_p \leq \frac{c_p \|\varphi\|_\infty}{\sqrt{N}},$$

for bounded test functions φ , i.e., $\|\varphi\|_\infty < \infty$.

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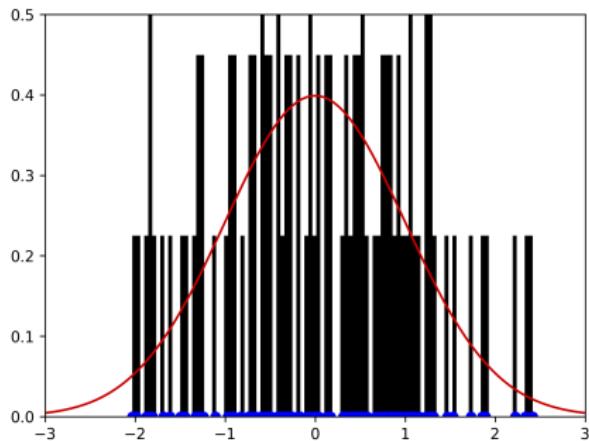
We are mostly interested in $p = 2$ case, which is square root of the MSE in general.

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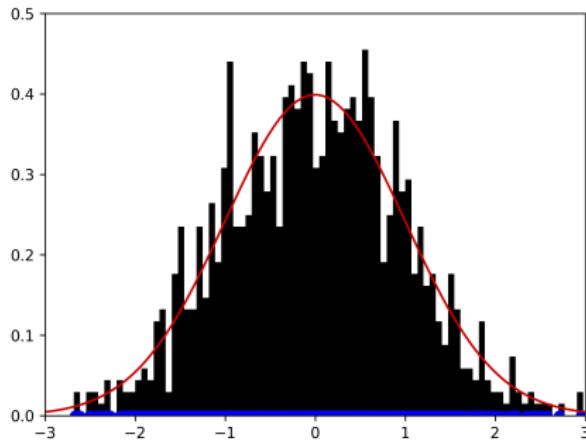
Next up: Pseudo uniform random number generation.

What are pseudo-random numbers?



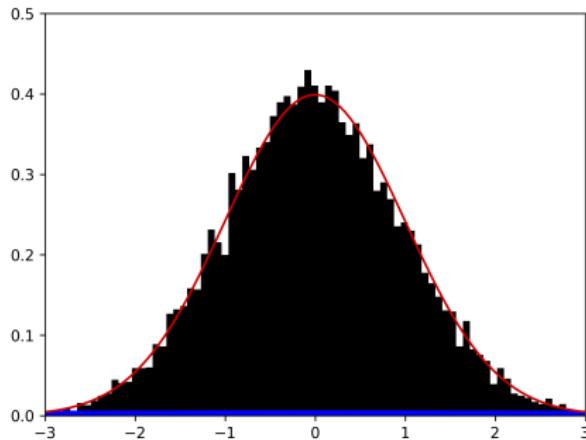
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- ▶ You can flip a coin every time you need a binary number
 - ▶ Is it really unbiased though?⁴
- ▶ Throw a die

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- ▶ On a computer
 - ▶ Try to measure some inner thermal noise (of circuits)
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As you can see, these are not very practical.

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It has become an entire research topic to design *deterministic* algorithms which gives samples that match the desired characteristics.

We will start from the simplest: The uniform distribution.

The key to simulate many (many) other random variables is to be able to simulate uniform random numbers.

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Uniform pseudo-random numbers

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We denote the task

$$U \sim \text{Unif}(u; 0, 1).$$

More precisely

$$U \sim p(u) = 1 \quad \text{for } 0 \leq u \leq 1.$$

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We will look into an old way of doing it:

- ▶ Linear congruential random number generators

These methods are based on generating a *deterministic linear recursion* with a careful design ⁵.

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Linear congruential generators (LCGs from now on) are based on simulating a recursion:

$$x_{n+1} \equiv ax_n + b \pmod{m}$$

where x_0 is the **seed**, m is the **modulus**, b is the **shift**, and a is the **multiplier**.

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where x_0 is the **seed**, m is the **modulus**, b is the **shift**, and a is the **multiplier**.

- ▶ m is an integer
- ▶ $x_0, a, b \in \{0, \dots, m-1\}$.

Given $x_n \in \{0, \dots, m-1\}$, we generate the uniform random numbers

$$u_n = \frac{x_n}{m} \in [0, 1) \quad \forall n.$$

Uniform pseudo-random numbers

Example code (try and make it work!)

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

def lcg(a, b, m, n, x0):
    x = np.zeros(n)
    u = np.zeros(n)
    x[0] = x0
    u[0] = x0 / m
    for k in range(1, n):
        x[k] = (a * x[k - 1] + b) % m
        u[k] = x[k] / m
    return u
```

Uniform pseudo-random numbers

A few things to know about LCGs:

- ▶ They generate *periodic* sequences.

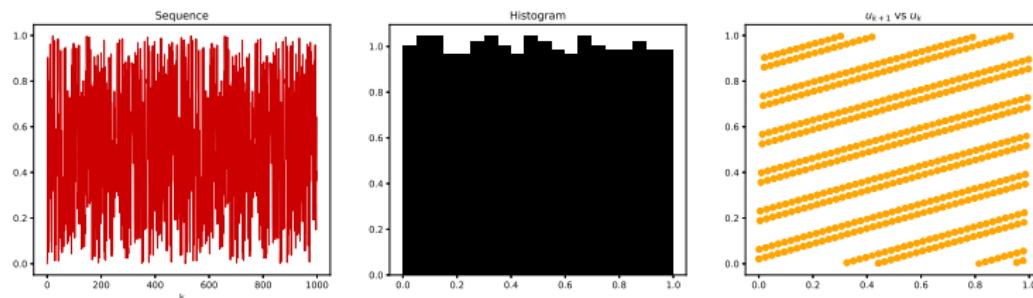


Figure: $m = 2048$, $a = 43$, $b = 0$, $x_0 = 1$.

period $T \leq m$ (m : the modulus).

- ▶ Full period: $T = m$

Choice of good parameters rely on some theory, some art.

Uniform pseudo-random numbers

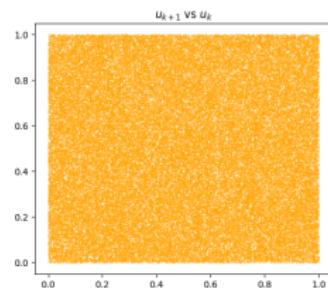
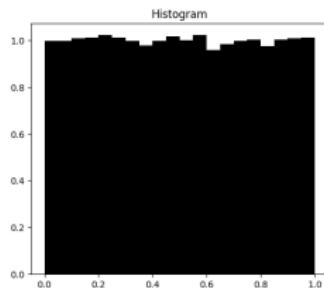
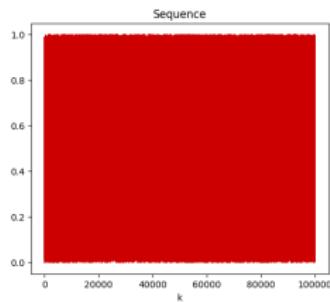
Wikipedia has a list of parameters for professional implementations:

Parameters in common use <small>[edit]</small>				
Source	modulus m	multiplier a	increment c	output bits of seed in <code>rand()</code> or <code>Random(L)</code>
ZX81	$2^{16} + 1$	75	74	
<i>Numerical Recipes</i> from the "quick and dirty generators" list, Chapter 7.1, Eq. 7.1.8 parameters from Knuth and H. W. Lewis	2^{32}	1664525	1013904223	
Borland C/C++	2^{32}	22695477	1	bits 30..16 in <code>rand()</code> , 30..0 in <code>lrand()</code>
glibc (used by GCC) ^[17]	2^{31}	1103515245	12345	bits 30..0
ANSI C; Watcom, Digital Mars, CodeWarrior, IBM VisualAge C/C++ ^[18] C99, C99, C11: Suggestion in the ISO/IEC 9899, ^[19] C17	2^{31}	1103515245	12345	bits 30..16
Borland Delphi, Virtual Pascal	2^{32}	134775813	1	bits 63..32 of (seed $\times L$)
Turbo Pascal	2^{32}	134775813 (8088405_{16})	1	
Microsoft Visual/Quick C/C++	2^{32}	214013 (343FD ₁₆)	2531011 (269EC3 ₁₆)	bits 30..16
Microsoft Visual Basic (6 and earlier) ^[20]	2^{34}	1140671485 (43FD43FD ₁₆)	12820163 (C39EC3 ₁₆)	
RanUniform from Native API ^[21]	$2^{31} - 1$	2147483629 (7FFFFFFD ₁₆)	2147483587 (7FFFFFFC3 ₁₆)	
Apple CarbonLib, C++11's				

from: https://en.wikipedia.org/wiki/Linear_congruential_generator

Uniform pseudo-random numbers

Better parameters:



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Next up: Exact sampling methods

We will cover methods to sample more general nonuniform $\pi(x)$:

- ▶ Inversion method

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Next up: Sampling via inversion.

Exact sampling of distributions

How to simulate from any $\pi(x)$?

Simulating from a given $\pi(x)$ is an endless research area (simulation, sampling, generative models) and still flourishing.

Exact sampling of distributions

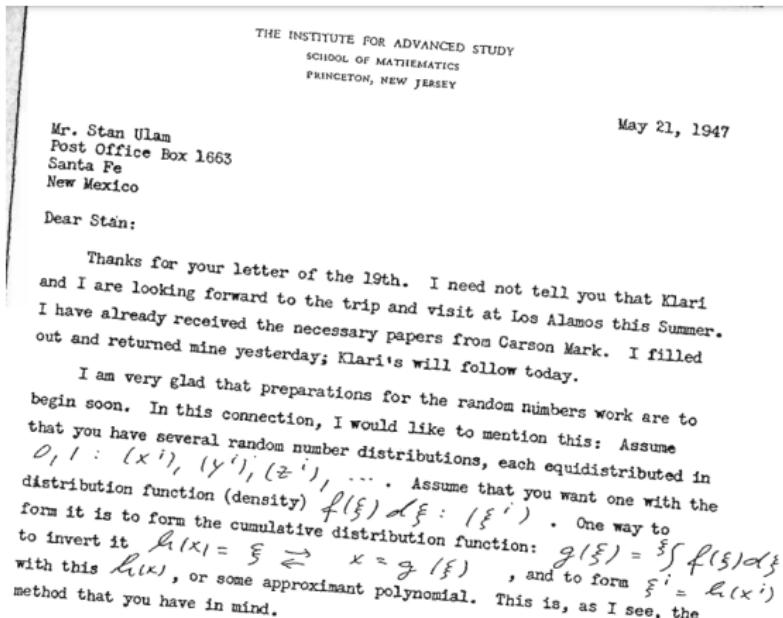
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We will start by describing some general methods to sample from more general distributions.

Direct sampling of distributions

Inversion



Direct sampling of distributions

Inversion

The inversion technique is based on the following theorem (Theorem 2.1 of notes):

Theorem 1

Consider a random variable X with a CDF F_X . Then the random variable $F_X^{-1}(U)$ where $U \sim \text{Unif}(0, 1)$, has the same distribution as X .

Proof.

The proof is one line:

$$\mathbb{P}(F_X^{-1}(U) \leq x) = \mathbb{P}(U \leq F_X(x)) = F_X(x).$$

which is the CDF of the target distribution. ■

Exact sampling of distributions

Inversion

Note that above result is written for the case where F_X^{-1} exists, i.e., the CDF is continuous. If this is not the case, one can define the generalised inverse function,

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

Exact sampling of distributions

Inversion

Going back to statement: If $U \sim \text{Unif}(0, 1)$ then $X' = F_X^{-1}(U)$ has the desired distribution, i.e.,

$$X' \sim p_X(x).$$

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Of course, this is limited to the cases where we *can* invert the CDF.

Exact sampling of distributions

Inversion: Discrete (categorical) distribution

Let us consider some examples.

The most generic one is the **discrete (categorical) distribution**. For $K \geq 1$ (integer), define K states s_1, \dots, s_K where

$$p(s_k) \in [0, 1] \quad \text{where} \quad \sum_{k=1}^K p(s_k) = 1.$$

Simpler than it looks, consider the die:

$$s_k = k \text{ (the face of die)}$$

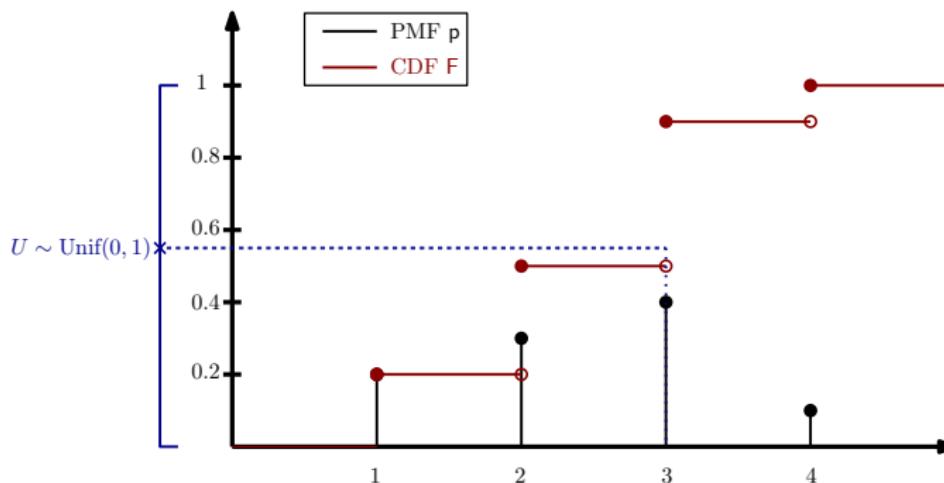
and their probabilities

$$p(s_k) = 1/6.$$

Exact sampling of distributions

Inversion: Discrete (categorical) distribution

How does the sampling work?

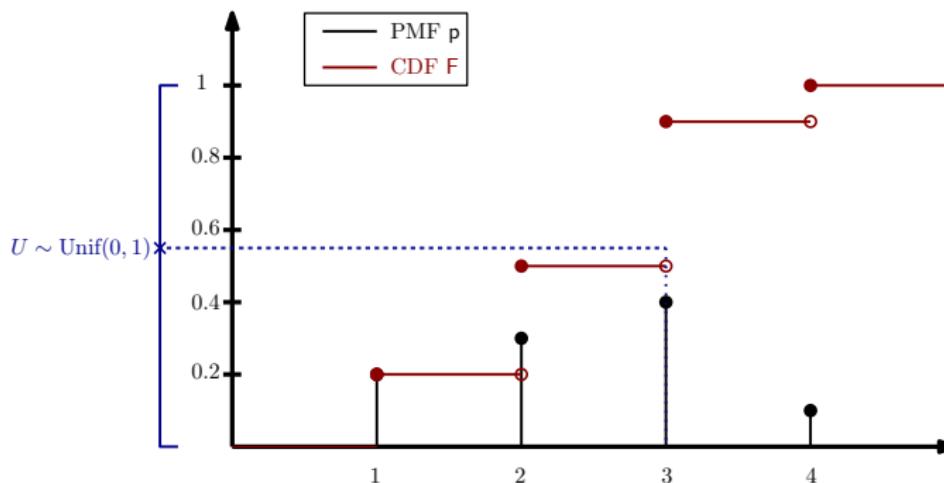


- ▶ Draw $U \sim \text{Unif}(0, 1)$
- ▶ Choose $F_X^{-1}(u) = \min\{x : F_X(x) \geq u\}$

Exact sampling of distributions

Inversion: Discrete (categorical) distribution

How does the sampling work?



- ▶ Draw $U \sim \text{Unif}(0, 1)$
- ▶ Choose $F_X^-(u) = \min\{x : F_X(x) \geq u\}$ generic for discrete dist.

Exact sampling of distributions

Inversion: Discrete (categorical) distribution

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

w = np.array([0.2, 0.3, 0.4, 0.1]) # pmf
s = np.array([1, 2, 3, 4])          # support (states)

def discrete_cdf(w):
    return np.cumsum(w)

cw = discrete_cdf(w)

def plot_discrete_cdf(w, cw):
    fig, ax = plt.subplots(1, 2, figsize=(20, 5))
    ax[0].stem(s, w)
    ax[1].plot(s, cw, 'o-', drawstyle='steps-post')
    plt.show()

plot_discrete_cdf(w, cw)
```

see simulation.

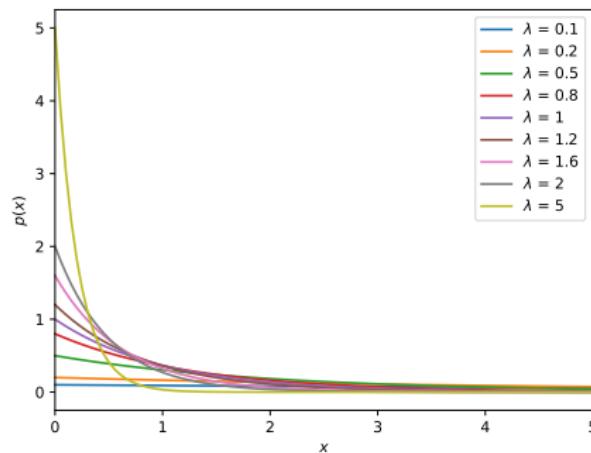
Exact sampling of distributions

Inversion: Exponential distribution

The exponential density

$$\pi(x) = \text{Exp}(x; \lambda) = \lambda e^{-\lambda x}.$$

for $x \geq 0$. Otherwise $\pi(x) = 0$.



Exact sampling of distributions

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Deriving the inverse:

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Simulation.

Exact sampling of distributions

Inversion: Is Gaussian possible?

Let $\pi(x) = \mathcal{N}(x; \mu, \sigma^2)$. Can we use inversion?

Exact sampling of distributions

Inversion: Is Gaussian possible?

Let $\pi(x) = \mathcal{N}(x; \mu, \sigma^2)$. Can we use inversion?

No. F_X^{-1} is impossible to compute and hard to approximate.

Exact sampling of distributions

Transformation method

Inversion is a special case of a general method called *transformation method*.

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Inversion is a special case of a general method called *transformation method*.

Transformation method:

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- ▶ Transform: $X_i = g(U_i)$.

Inversion is just setting $g = F_X^{-1}$.

Exact sampling of distributions

Transformation method: Sampling a custom uniform

The simplest example can be seen from sampling a uniform on $[a, b]$ using a uniform on $[0, 1]$.

Exact sampling of distributions

Transformation method: Sampling a custom uniform

The simplest example can be seen from sampling a uniform on $[a, b]$ using a uniform on $[0, 1]$.

- ▶ Draw $U_i \sim \text{Unif}(u; 0, 1)$
- ▶ Set $X_i = g(U_i) = (b - a)U_i + a$
then $X_i \sim \text{Unif}(x; a, b)$.

For general g , how do we compute the density?

Exact sampling of distributions

Transformation method

If $X \sim p_X(x)$ and $Y = g(X)$, what is $p_Y(y)$?

Exact sampling of distributions

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If $X \sim p_X(x)$ and $Y = g(X)$, what is $p_Y(y)$?

$$p_Y(y) = p_X(g^{-1}(y)) |\det J_{g^{-1}}(y)|$$

Exact sampling of distributions

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If $X \sim p_X(x)$ and $Y = g(X)$, what is $p_Y(y)$?

$$p_Y(y) = p_X(g^{-1}(y)) |\det J_{g^{-1}}(y)|$$

where J is the Jacobian of the inverse mapping g^{-1} , evaluated at y :

$$J_{g^{-1}} = \begin{bmatrix} \partial g_1^{-1}/\partial y_1 & \partial g_1^{-1}/\partial y_2 & \cdots & \partial g_1^{-1}/\partial y_n \\ \vdots & \ddots & \cdots & \vdots \\ \partial g_n^{-1}/\partial y_1 & \partial g_n^{-1}/\partial y_2 & \cdots & \partial g_n^{-1}/\partial y_n \end{bmatrix}.$$

Exact sampling of distributions

Transformation method: An exercise

If $X \sim \mathcal{N}(0, 1)$, derive the distribution of

$$Y = \sigma X + \mu.$$

Exact sampling of distributions

Transformation method: An exercise

The inverse transform is:

$$g^{-1}(y) = \frac{y - \mu}{\sigma}.$$

Exact sampling of distributions

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Therefore,

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The inverse transform is:

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Therefore,

$$p_Y(y) = p_X(g^{-1}(y)) \left| \frac{dg^{-1}}{dy} \right|,$$

which is

$$p_Y(y) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y - \mu)^2}{2\sigma^2}\right) \frac{1}{\sigma} = \mathcal{N}(\mu, \sigma^2)$$

How to sample Gaussians from uniforms?

Finally, we provide the Box-Müller method for Gaussians: Let $U_1, U_2 \sim \text{Unif}(0, 1)$ be independent. Then

$$Z_1 = \sqrt{-2 \log U_1} \cos(2\pi U_2),$$

$$Z_2 = \sqrt{-2 \log U_1} \sin(2\pi U_2),$$

are independent $\mathcal{N}(0, 1)$ -distributed random variables.

Next step?

Follow von Neumann

method that you have in mind.

An alternative, which works if f is a polynomial. This is, as I see, the 0, 1, is this: Scan pairs x^i, y^i and use or reject x^i, y^i according to whether $y^i \leq f(x^i)$ or not. In the first case, put $x^d = x^i$ in the second case form no x^d at that step.

The second method may occasionally be better.

Rejection sampling

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However, those methods required a quite specific structure for us to be able to sample.

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Can we still do *exact* sampling?

The Fundamental Theorem of Simulation

Is there a more general structure?

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

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

$$A = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \gamma(x)\}. \quad (2)$$

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

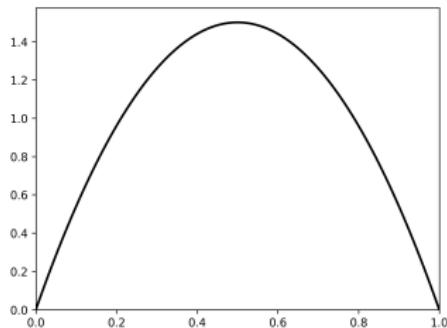
Sampling Beta density

Testing the theorem

Let

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

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



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

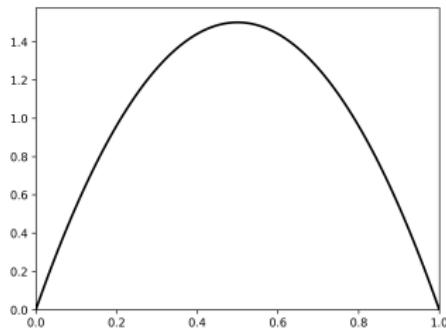
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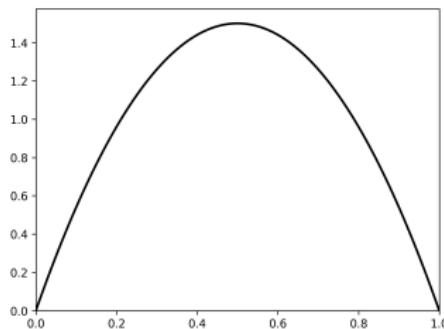
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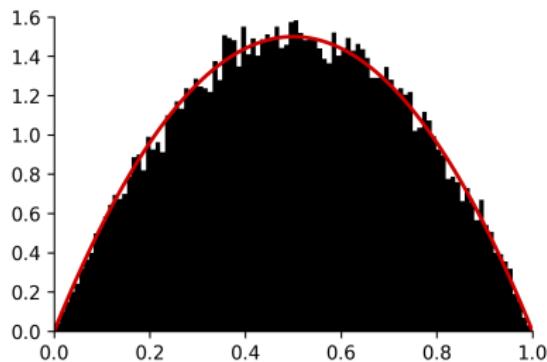
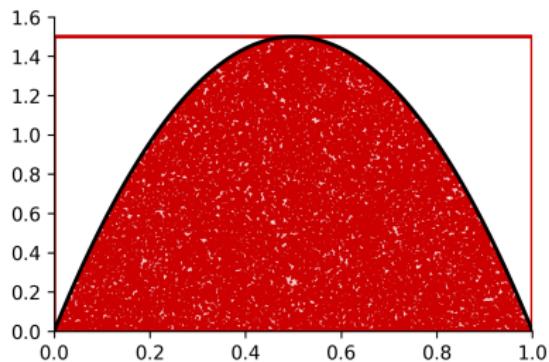


Its maximum is 1.5 in this specific case. Can we sample uniformly?

- ▶ 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

Testing the theorem



See simulation.

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We can get away with an unnormalised density $\gamma(x)$ (as FTS suggests).

Rejection sampling

More than a box

Using a box wrapping the density is very inefficient:

Rejection sampling

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- ▶ 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 $\pi(x)$ and a *proposal* density $q(x)$.

Rejection sampling

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

For rejection sampling, we always choose a proposal such that

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

for $M \geq 1$.

Rejection sampling

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

For rejection sampling, we always choose a proposal such that

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

Rejection sampling

The algorithm

But how to obtain a sample under the curve?

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Rejection sampling

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- ▶ Sample $x' \sim q(x)$
- ▶ Sample $u' \sim \text{Unif}(u'; 0, Mq(x'))$

Rejection sampling

The algorithm

But how to obtain a sample under the curve?

We can do

- ▶ Sample $x' \sim q(x)$
- ▶ Sample $u' \sim \text{Unif}(u'; 0, Mq(x'))$
- ▶ Accept if

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

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

Rejection sampling

The algorithm: A closer look

To implement the method:

- ▶ Sample $x' \sim q(x)$,

Rejection sampling

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To implement the method:

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$$u \leq \frac{\pi(x')}{Mq(x')}.$$

Rejection sampling

The algorithm

The rejection sampler:

Rejection sampling

The algorithm

The rejection sampler:

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Rejection sampling

The algorithm

The rejection sampler:

- ▶ $X' \sim q(x)$,
- ▶ Accept the sample X' with probability

$$a(X') = \frac{\pi(X')}{Mq(X')} \leq 1.$$

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- ▶ $\gamma(x)$ is called the *unnormalised* density
- ▶ Z is called the normalising constant
 - ▶ It is a super important quantity for many other purposes
- ▶ We write $\pi(x) \propto \gamma(x)$ to say p is proportional to $\gamma(x)$ but normalised to integrate (or sum) to one.

Rejection sampling

The algorithm: A closer look

To implement, choose M and q such that $\gamma(x) \leq Mq(x)$

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Exactly same – γ used instead of p provided that $\gamma(x) \leq Mq(x)$

Rejection sampling

Examples: Acceptance matters

Rejection sampler:

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In order for this algorithm to be implemented, we do not want many rejections (as we want many accepted samples to build our distribution).

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How to compute acceptance rate?

Rejection sampling

Examples: Acceptance matters

Proposition 1

When the target density $\pi(x)$ is normalised and M is prechosen, the acceptance rate is given by

$$\hat{a} = \frac{1}{M},$$

where $M > 1$ in order to satisfy the requirement that q covers π . For an unnormalised target density $\gamma(x)$ with the normalising constant $Z = \int \gamma(x)dx$, the acceptance rate is given as

$$\hat{a} = \frac{Z}{M}.$$

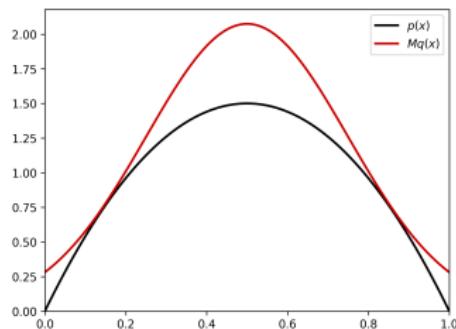
Rejection sampling

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

Choose

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

with $M = 1.3$.



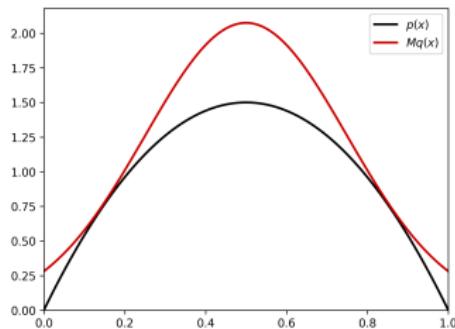
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$$q(x) = \mathcal{N}(0.5, 0.25),$$

with $M = 1.3$.



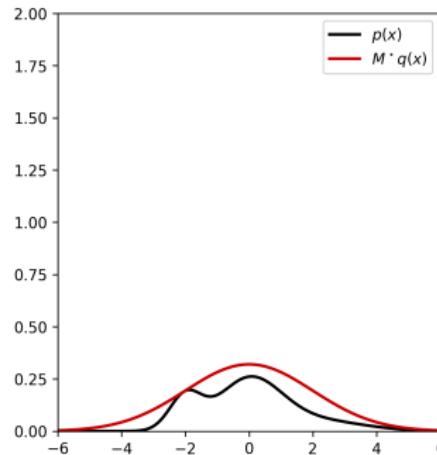
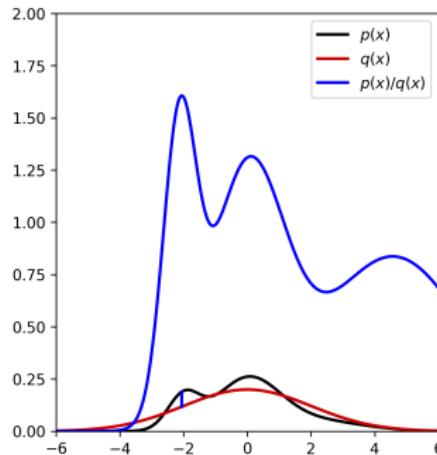
Simulation.

Rejection sampling

Choice of M

A standard choice for M is

$$M^* = \sup_x \frac{\pi(x)}{q(x)}.$$



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

$$\pi(x) = \frac{\gamma(x)}{Z} = \frac{\mathcal{N}(x; 0, 1)\mathbf{1}_{\{x:|x|\leq a\}}(x)}{\int_{-a}^a \mathcal{N}(y; 0, 1)dy}.$$

We can choose $q(x) = \mathcal{N}(x; 0, 1)$ anyway, and we have $\gamma(x) \leq q(x)$ (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 $[-a, a]$.

We have covered the rejection sampler:

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

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While very popular in 90s, it is extremely hard to compute M for modern large scale problems.

Importance Sampling

Monte Carlo integration

Another popular approach to compute expectations (φ, π) is called *importance sampling*.

Importance Sampling

Monte Carlo integration

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Assume, as in the rejection sampling case, π is absolutely continuous w.r.t. q , denoted as $\pi \ll q$, meaning $\pi(x) = 0 \implies q(x) = 0$.

Importance Sampling

Monte Carlo integration

Another popular approach to compute expectations (φ, π) is called *importance sampling*.

Assume, as in the rejection sampling case, π is absolutely continuous w.r.t. q , denoted as $\pi \ll q$, meaning $\pi(x) = 0 \implies q(x) = 0$.

Then, we can write

$$(\varphi, \pi) = \int \varphi(x)\pi(dx) = \int \varphi(x)\frac{d\pi}{dq}(x)q(x)dx.$$

When π and q admit densities,

$$(\varphi, \pi) = \int \varphi(x)\pi(x)dx = \int \varphi(x)\frac{\pi(x)}{q(x)}q(x)dx.$$

Importance Sampling

Monte Carlo integration

Given

$$(\varphi, \pi) = \int \varphi(x) \frac{\pi(x)}{q(x)} q(x) dx,$$

we can employ standard Monte Carlo by sampling $X_i \sim q$ and then constructing (by setting $w = p/q$)

$$\begin{aligned} (\varphi, \tilde{\pi}^N) &= \frac{1}{N} \sum_{i=1}^N \varphi(X_i) w(X_i), \\ &= \frac{1}{N} \sum_{i=1}^N w_i \varphi(X_i). \end{aligned}$$

where $w_i = w(X_i)$. We will call this estimator the importance sampling (IS) estimator.

Importance Sampling

Monte Carlo integration

Mini-quiz: Is this estimator unbiased?

Importance Sampling

Monte Carlo integration

Mini-quiz: Is this estimator unbiased?

Yes.

$$\begin{aligned}\mathbb{E}_q[(\varphi, \tilde{\pi}^N)] &= \mathbb{E}_q \left[\frac{1}{N} \sum_{i=1}^N \mathbf{w}_i \varphi(X_i) \right], \\ &= \frac{1}{N} \sum_{i=1}^N \mathbb{E}_q \left[\frac{p(X_i)}{q(X_i)} \varphi(X_i) \right] \\ &= \frac{1}{N} \sum_{i=1}^N \int \frac{p(x)}{q(x)} \varphi(x) q(x) dx \\ &= \int \varphi(x) p(x) dx = (\varphi, \pi).\end{aligned}$$

Importance Sampling

Monte Carlo integration

What is the variance?

$$\begin{aligned}\text{var}_q[(\varphi, \tilde{\pi}^N)] &= \text{var}_q \left[\frac{1}{N} \sum_{i=1}^N w_i \varphi(X_i) \right] \\ &= \frac{1}{N^2} \text{var}_q \left[\sum_{i=1}^N w(X_i) \varphi(X_i) \right] \\ &= \frac{1}{N} \text{var}_q [w(X) \varphi(X)] \quad \text{where } X \sim q(x) \\ &= \frac{1}{N} \left(\mathbb{E}_q [w^2(X) \varphi^2(X)] - \mathbb{E}_q [w(X) \varphi(X)]^2 \right) \\ &= \frac{1}{N} (\mathbb{E}_q [w^2(X) \varphi^2(X)] - \bar{\varphi}^2).\end{aligned}$$

Importance Sampling

Monte Carlo integration

Finally, the basic IS estimator satisfies the following L_p bound just like the perfect Monte Carlo

$$\|(\varphi, \pi) - (\varphi, \tilde{\pi}^N)\|_p \leq \frac{\tilde{c}_p \|\varphi\|_\infty}{\sqrt{N}},$$

where \tilde{c}_p is a constant depending on p and q .

Importance Sampling

Self-normalised IS

What if we only have access to $\gamma(x) \propto \pi(x)$?

Importance Sampling

Self-normalised IS

What if we only have access to $\gamma(x) \propto \pi(x)$?

Assume $\gamma \ll q$ and both abs. cont w.r.t. to the Lebesgue measure.
Then we can write

$$\begin{aligned}(\varphi, \pi) &= \int \varphi(x) \pi(x) dx \\&= \frac{\int \varphi(x) \frac{\gamma(x)}{q(x)} q(x) dx}{\int \frac{\gamma(x)}{q(x)} q(x) dx}.\end{aligned}$$

We can then perform the same Monte Carlo integration idea but now both for the numerator and denominator.

Importance Sampling

Self-normalised IS (SNIS)

We have

$$\begin{aligned} (\varphi, \pi) &= \int \varphi(x) \pi(x) dx \\ &= \frac{\int \varphi(x) \frac{\gamma(x)}{q(x)} q(x) dx}{\int \frac{\gamma(x)}{q(x)} q(x) dx}. \end{aligned}$$

Define $W(x) = \gamma(x)/q(x)$ and the SNIS approximation is given as

$$(\varphi, \pi) = \frac{\int \varphi(x) W(x) q(x) dx}{\int W(x) q(x) dx} \approx \frac{\frac{1}{N} \sum_{i=1}^N \varphi(X_i) W(X_i)}{\frac{1}{N} \sum_{j=1}^N W(X_j)}.$$

where $X_i \sim q(x)$. Let us write $W_i = W(X_i)$ and $w_i = W_i / \sum_{j=1}^N W_j$. Then the final estimator is

$$(\varphi, \tilde{\pi}^N) = \sum_{i=1}^N w_i \cdot \varphi(X_i)$$

Importance Sampling

Self-normalised IS (SNIS)

Mini-quiz: Is this estimator unbiased?

Importance Sampling

Self-normalised IS (SNIS)

Mini-quiz: Is this estimator unbiased?

No.

Importance Sampling

Self-normalised IS (SNIS)

Mini-quiz: Is this estimator unbiased?

No.

The estimator is a ratio of two unbiased estimators. However, this ratio is *not* unbiased.

Importance Sampling

Self-normalised IS (SNIS)

However, one can prove that

$$\|(\varphi, \pi) - (\varphi, \tilde{\pi}^N)\|_p \leq \frac{\tilde{c}_p \|\varphi\|_\infty}{\sqrt{N}},$$

where \tilde{c}_p is a constant depending on p and q and φ is bounded.

Importance Sampling

Self-normalised IS (SNIS)

Theorem 3

The MSE (i.e., set $p = 2$ and square both sides) is bounded by

$$\mathbb{E} \left[((\varphi, \pi) - (\varphi, \tilde{\pi}^N))^2 \right] \leq \frac{4\|\varphi\|_\infty \rho}{N},$$

where

$$\rho = \chi^2(\pi || q) + 1.$$

Suggests that the discrepancy between π and q controls the MSE.

Importance Sampling

Self-normalised IS (SNIS), MSE bound

Proof. We first note the following inequalities,

$$\begin{aligned}
 |(\varphi, \pi) - (\varphi, \tilde{\pi}^N)| &= \left| \frac{(\varphi W, q)}{(W, q)} - \frac{(\varphi W, q^N)}{(W, q^N)} \right| \\
 &\leq \frac{|(\varphi W, q) - (\varphi W, q^N)|}{|(W, q)|} + |(\varphi W, q^N)| \left| \frac{1}{(W, q)} - \frac{1}{(W, q^N)} \right| \\
 &= \frac{|(\varphi W, q) - (\varphi W, q^N)|}{|(W, q)|} + \|\varphi\|_\infty |(W, q^N)| \left| \frac{(W, q^N) - (W, q)}{(W, q)(W, q^N)} \right| \\
 &= \frac{|(\varphi W, q) - (\varphi W, q^N)|}{(W, q)} + \frac{\|\varphi\|_\infty |(W, q^N) - (W, q)|}{(W, q)}.
 \end{aligned}$$

We take squares of both sides and apply the inequality $(a + b)^2 \leq 2(a^2 + b^2)$ to further bound the rhs,

$$\dots \leq 2 \frac{|(\varphi W, q) - (\varphi W, q^N)|^2}{(W, q)^2} + 2 \frac{\|\varphi\|_\infty^2 |(W, q^N) - (W, q)|^2}{(W, q)^2}$$

We can now take the expectation of both sides,

$$\begin{aligned} \mathbb{E} \left[((\varphi, \pi) - (\varphi, \tilde{\pi}^N))^2 \right] &\leq \frac{2\mathbb{E} \left[((\varphi W, q) - (\varphi W, q^N))^2 \right]}{(W, q)^2} + \\ &\quad \frac{2\|\varphi\|_\infty^2 \mathbb{E} \left[((W, q^N) - (W, q))^2 \right]}{(W, q)^2}. \end{aligned}$$

Note that, both terms in the right hand side are perfect Monte Carlo estimates of the integrals.

Bounding the MSE of these integrals yields

$$\begin{aligned} \dots &\leq \frac{2}{N} \frac{(\varphi^2 W^2, q) - (\varphi W, q)^2}{(W, q)^2} + \frac{2\|\varphi\|_\infty^2}{N} \frac{(W^2, q) - (W, q)^2}{(W, q)^2}, \\ &\leq \frac{2\|\varphi\|_\infty^2}{N} \frac{(W^2, q)}{(W, q)^2} + \frac{2\|\varphi\|_\infty^2}{N} \frac{(W^2, q) - (W, q)^2}{(W, q)^2}. \end{aligned}$$

Therefore, we can straightforwardly write,

$$\mathbb{E} \left[((\varphi, \pi) - (\varphi, \tilde{\pi}^N))^2 \right] \leq \frac{4\|\varphi\|_\infty^2}{(W, q)^2} \frac{(W^2, q)}{N}.$$

$$\mathbb{E} \left[\left((\varphi, \pi) - (\varphi, \tilde{\pi}^N) \right)^2 \right] \leq \frac{4\|\varphi\|_\infty^2}{(W, q)^2} \frac{(W^2, q)}{N}.$$

Now it remains to show the relation of the bound to χ^2 divergence.
Note that,

$$\begin{aligned} \frac{(W^2, q)}{(W, q)^2} &= \frac{\int \frac{\Pi^2(x)}{q^2(x)} q(x) dx}{\left(\int \frac{\Pi(x)}{q(x)} q(x) dx \right)^2} \\ &= \frac{Z^2 \int \frac{\pi^2(x)}{q^2(x)} q(x) dx}{Z^2 \left(\int \pi dx \right)^2} \\ &= \mathbb{E}_q \left[\frac{\pi^2(X)}{q^2(X)} \right] := \rho. \end{aligned}$$

Note that ρ is not exactly χ^2 divergence, which is defined as $\rho - 1$.
Plugging everything into our bound, we have the result,

$$\mathbb{E} \left[\left((\varphi, \pi) - (\varphi, \pi^N) \right)^2 \right] \leq \frac{4\|\varphi\|_\infty^2 \rho}{N}.$$



Importance Sampling

Optimised Adaptive IS

Moreover, if q is an exponential family, then ρ is convex (Akyildiz and Míguez, 2021). This suggests that we can optimise q to minimise ρ and hence the MSE. See Akyildiz and Míguez, 2021 for utilisation of stochastic convex optimisation techniques to obtain uniform-in-time bounds for adaptive SNIS.

See you next week!

- ⌚ Martino, Luca, David Luengo, and Joaquín Míguez (2018). *Independent random sampling methods*. Springer.
- ⌚ Akyildiz, Ömer Deniz and Joaquín Míguez (2021). “Convergence rates for optimised adaptive importance samplers”. In: *Statistics and Computing* 31.2, pp. 1–17.