MFC CDT Probability and Statistics
Week 6

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Mathematics for our Future Climate: Theory, Data and Simulation (MFC CDT).

November 11, 2024

IMPERIAL

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

Timeline

- Week 6: Exact sampling methods, rejection samplers, importance samplers

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- Week 10: Parameter Estimation in State-Space Models: Maximum Likelihood and Bayesian Estimation

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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).

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One very effective way is to use Bayesian statistical methodology.

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

$$p(x|y) \propto p(y|x)\pi(x), \tag{1}$$

and estimating expectations w.r.t. them.

In this case, we have samples $\{Y_i\}_{i=1}^n$ from a dataset. Underlying data distribution $Y_i \sim p_{\text{data}}$ is not accessible in any way.

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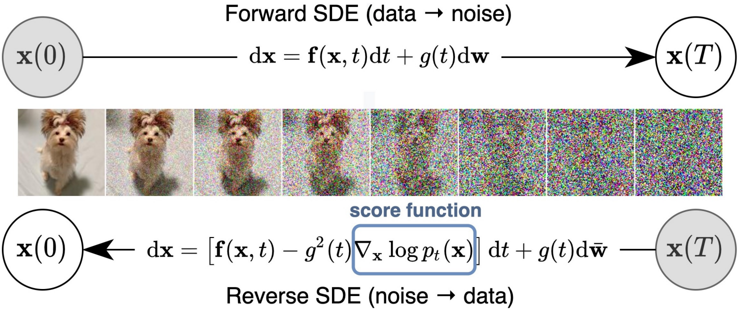
Goal: Sample from p_{data} by only accessing data $\{Y_i\}_{i=1}^n$.

The standard way to do it is to run forward and backward stochastic differential equations[1]



[1] Figure from: `https://yang-song.net/blog/2021/score/`

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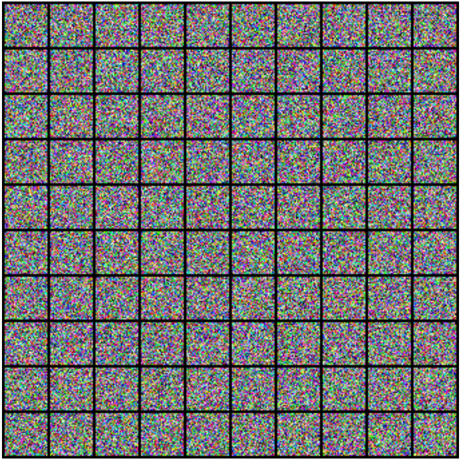

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Let's get to our first motivating example.

In this course, a core focus will be estimating certain quantities (probabilities, expectations, etc.) using *sampling*.

Estimating π

Without being too clever

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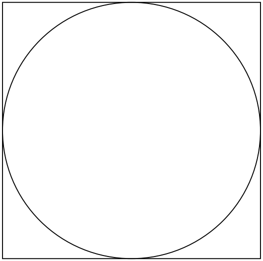
Can we estimate π using sampling? Any ideas?



Given the knowledge that:

$$\frac{\text{area of circle}}{\text{area of square}} = \frac{\pi r^2}{4r^2} = \frac{\pi}{4}.$$

Estimating π

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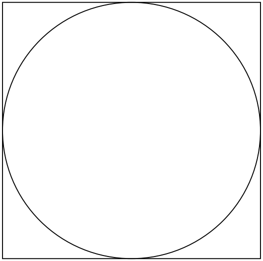

Given the knowledge that:

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Can we phrase this question probabilistically?

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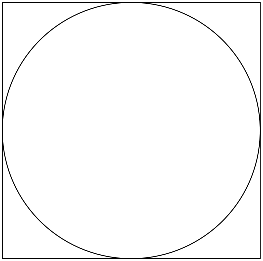
Most of the time, expectation is the most general way.



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Estimating π

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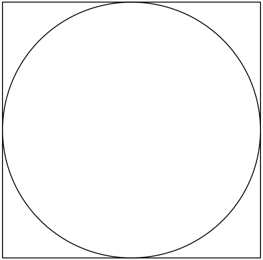

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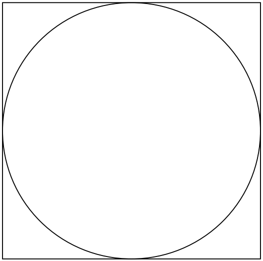


Consider a 2D uniform distribution on $[-1, 1] \times [-1, 1]$.

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

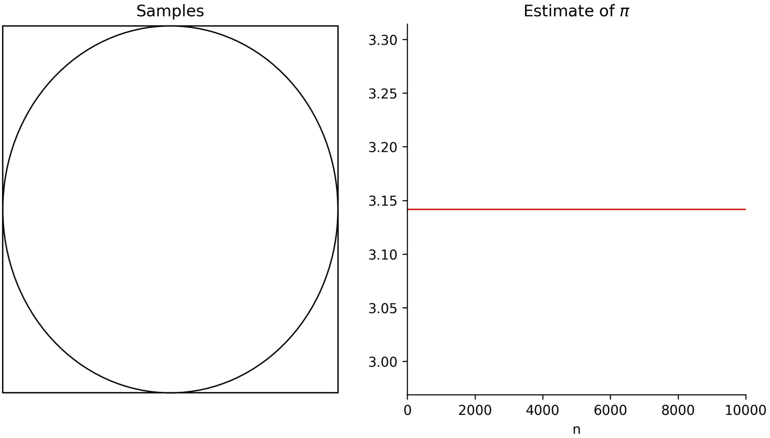
$$\mathbb{P}(\text{Circle}) = \frac{\pi}{4}.$$

Last question:

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

Estimating π

Without being too clever



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 $\pi(x)\mathrm{d}x$[3] and a function $\varphi(x)$. If we have access to i.i.d samples from $X_i \sim \pi(x)$, then

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

using a particle approximation

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

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Note by definition of the Dirac measure

$$\varphi(y) = \int \varphi(x)\delta_y(\mathrm{d}x).$$

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

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

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

Let A be the "circle" s.t. $A \subset \mathrm{X}$. Now, the probability of A is given

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

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 $Z = \int \gamma(x)\mathrm{d}x$ is the normalizing constant. Our general aim throughout this course is to compute

$$(\varphi, \pi) = \int \varphi(x)\pi(x)\mathrm{d}x,$$

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

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

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Perfect Monte Carlo

The general problem

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- CLT holds

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

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

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

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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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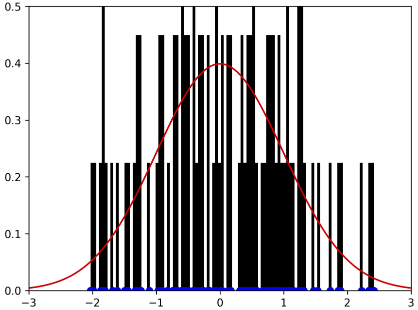
Next up: Pseudo uniform random number generation.

What are pseudo-random numbers?

Why do we need them?



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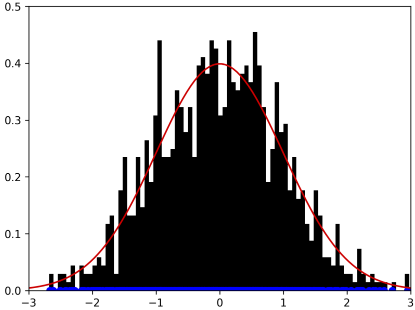

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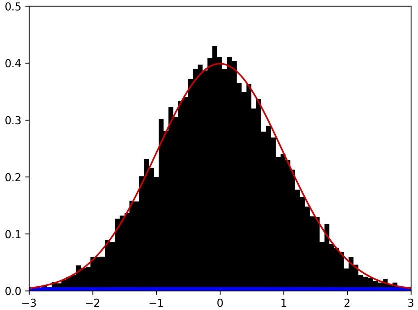

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- You can flip a coin every time you need a binary number
  - Is it really unbiased though?[4]
- Throw a die

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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.

Uniform pseudo-random numbers

The most important sampling task

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
- $x_0, a, b \in \{0, \ldots, m-1\}$.

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

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

Uniform pseudo-random numbers

The most important sampling task

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

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A few things to know about LCGs:

- They generate *periodic* sequences.

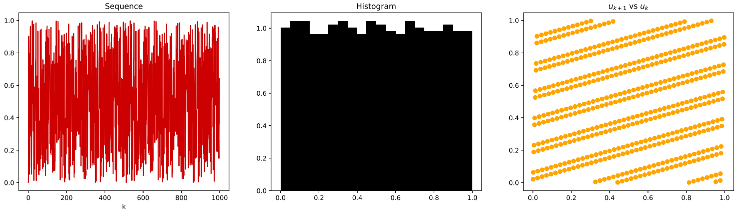


Figure: $m = 2048$, $a = 43$, $b = 0$, $x_0 = 1$.

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

- Full period: $T = m$

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

Wikipedia has a list of parameters for professional implementations:

Parameters in common use [edit]

The following table lists the parameters of LCGs in common use, including built-in *rand()* functions in runtime libraries of various compilers. This table is to show popularity, not examples to emulate; *many of these parameters are poor.* Tables of good parameters are available.[10][2]

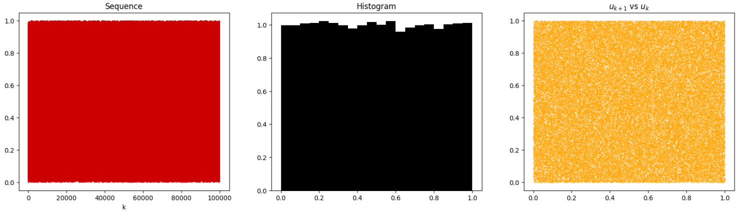
Source	modulus *m*	multiplier *a*	increment *c*	output bits of seed in *rand()* or *Random(L)*
ZX81	$2^{16}+1$	75	74	
Numerical Recipes from the "quick and dirty generators" list, Chapter 7.1, Eq. 7.1.6 parameters from Knuth and H. W. Lewis	2^{32}	1664525	1013904223	
Borland C/C++	2^{32}	22695477	1	bits 30..16 in *rand()*, 30..0 in *lrand()*
glibc (used by GCC)[17]	2^{31}	1103515245	12345	bits 30..0
ANSI C: Watcom, Digital Mars, CodeWarrior, IBM VisualAge C/C++[18] C90, 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 × 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^{24}	1140671485 ($43FD43FD_{16}$)	12820163 ($C39EC3_{16}$)	
RtlUniform from Native API[21]	$2^{31}-1$	2147483629 ($7FFFFFED_{16}$)	2147483587 ($7FFFFFC3_{16}$)	
Apple CarbonLib, C++11's				

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

Uniform pseudo-random numbers

The most important sampling task

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

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

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

THE INSTITUTE FOR ADVANCED STUDY
SCHOOL OF MATHEMATICS
PRINCETON, NEW JERSEY

May 21, 1947

Mr. Stan Ulam
Post Office Box 1663
Santa Fe
New Mexico

Dear Stan:

Thanks for your letter of the 19th. I need not tell you that Klari and I are looking forward to the trip and visit at Los Alamos this Summer. I have already received the necessary papers from Carson Mark. I filled out and returned mine yesterday; Klari's will follow today.

I am very glad that preparations for the random numbers work are to begin soon. In this connection, I would like to mention this: Assume that you have several random number distributions, each equidistributed in $0, 1$: $(x^i), (y^i), (z^i), \ldots$. Assume that you want one with the distribution function (density) $f(\xi)\,d\xi : (\xi^i)$. One way to form it is to form the cumulative distribution function: $g(\xi) = \int^{\xi} f(\xi)\,d\xi$ to invert it $h(x) = \xi \rightleftarrows x = g(\xi)$, and to form $\xi^i = h(x^i)$ with this $h(x)$, or some approximant polynomial. This is, as I see, the method that you have in mind.

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. ∎

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,

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

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

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

Exact sampling of distributions

Inversion

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Then this suggests an algorithm:

- Sample $U \sim \mathrm{Unif}([0, 1])$,
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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 $s_1, \ldots, s_K$ where

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

Simpler than it looks, consider the die:

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

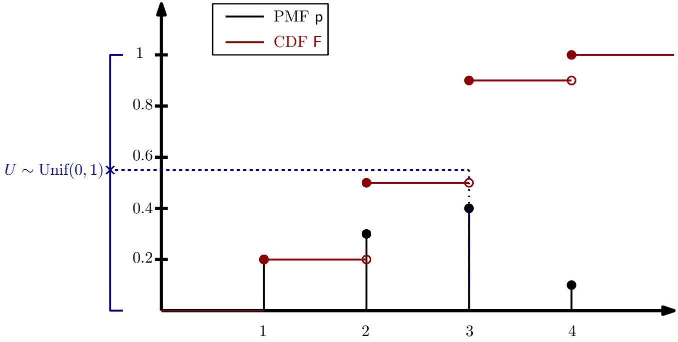
and their probabilities

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

Exact sampling of distributions

Inversion: Discrete (categorical) distribution

How does the sampling work?



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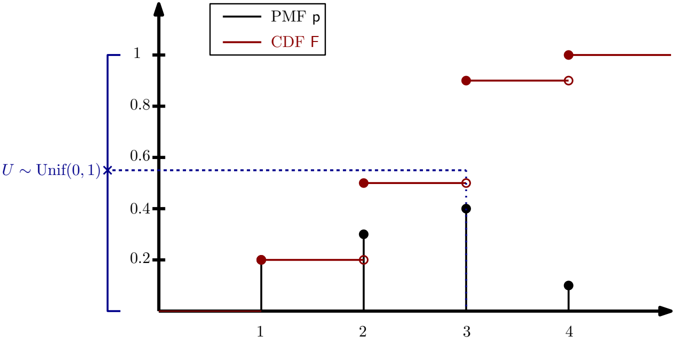

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- Choose $F_X^-(u) = \min\{x : F_X(x) \geq u\}$ generic for discrete dist.

Exact sampling of distributions

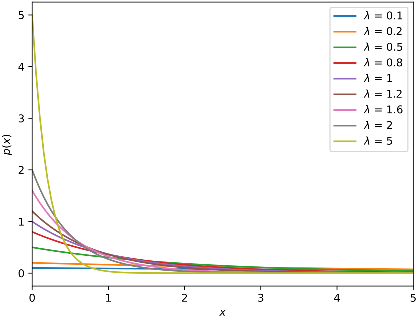
Inversion: Discrete (categorical) distribution

```
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)
```

The exponential density

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

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



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Exact sampling of distributions

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Deriving the inverse:

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- Generate $u_i \sim \text{Unif}([0,1])$
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Exact sampling of distributions

Inversion: Is Gaussian possible?

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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.

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

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- 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 $p_Y(y)$?

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

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

Exact sampling of distributions

Transformation method: An exercise

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

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

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which is

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

How to sample Gaussians from uniforms?

Box-Müller method

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

$$
\begin{aligned}
Z_1 &= \sqrt{-2\log U_1}\cos(2\pi U_2), \\
Z_2 &= \sqrt{-2\log U_1}\sin(2\pi U_2),
\end{aligned}
$$

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

Next step?

Follow von Neumann

… polynomial. This is, as I see, the method that you have in mind.

An alternative, which works if ξ and all values of $f(\xi)$ lie in 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 $\xi^j = x^i$ in the second case form no ξ^j at that step.

The second method may occasionally be better th…

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 $\pi(x) \propto \gamma(x)$ is equivalent to sampling uniformly on the two dimensional region defined by

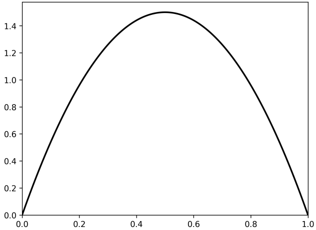
$$\mathrm{A} = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \gamma(x)\}. \tag{2}$$

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

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 $\text{Beta}(2, 2)$:



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

Sampling Beta density

Testing the theorem

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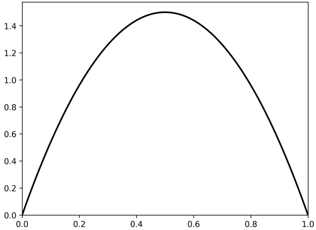

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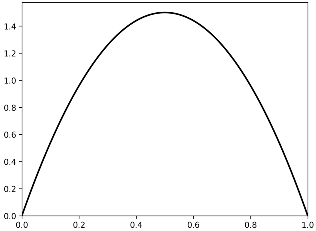
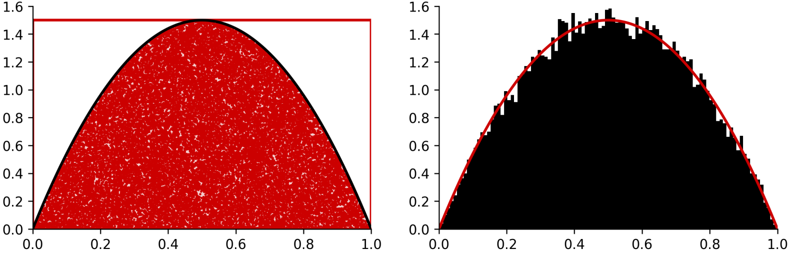


Its maximum is 1.5 in this specific case. Can we sample uniformly?

- 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



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

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Rejection sampling

More than a box

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  which could be as hard as the sampling problem!
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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 $q(x)$.

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For rejection sampling, we always choose a proposal such that

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

for $M \geq 1$.

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For rejection sampling, we always choose a proposal such that

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

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

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Rejection sampling

The algorithm

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

Rejection sampling

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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

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

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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- 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

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

Rejection sampler:

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How to compute acceptance rate?

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 $Z = \int \gamma(x)\mathrm{d}x$, the acceptance rate is given as

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

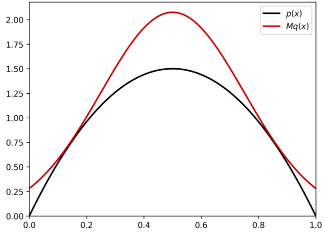
Rejection sampling

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

Choose

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

with $M = 1.3$.



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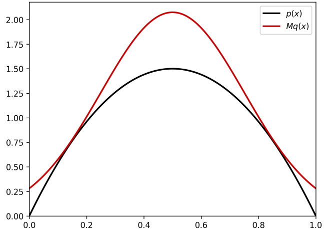
$$q(x) = \mathcal{N}(0.5, 0.25),$$

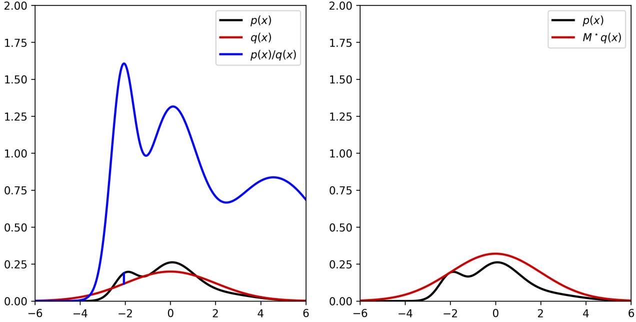
with $M = 1.3$.



Simulation.

A standard choice for M is

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



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

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

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 $X' \sim q(x)$
- 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.

See you next week!

Thanks!

References I

Martino, Luca, David Luengo, and Joaquín Míguez (2018). *Independent random sampling methods*. Springer.