Advanced Computational Methods in Statistics
Lecture 1

O. Deniz Akyildiz

LTCC Advanced Course

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Imperial College London

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

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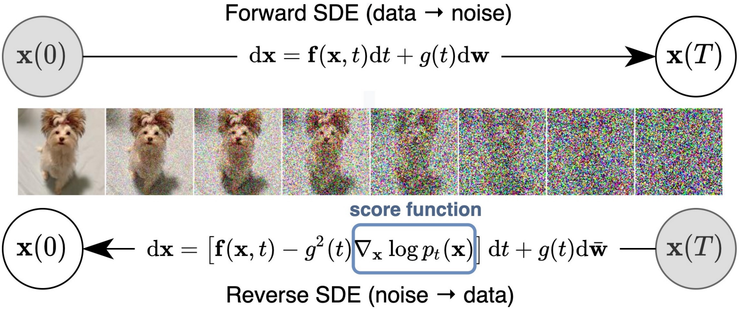
Goal: Sample from p_{data} by only accessing data $\{Y_i\}_{i=1}^n$.

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



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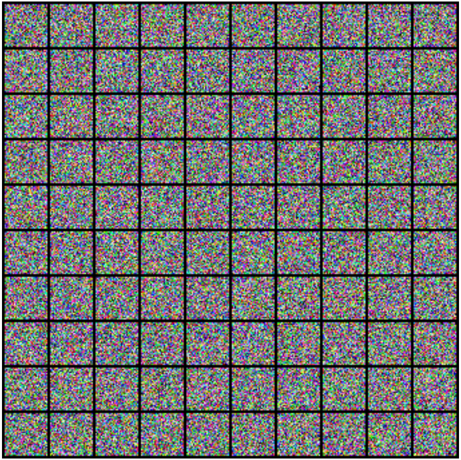

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Let's get to our first motivating example.

Estimating π

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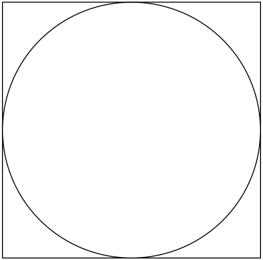
Can we estimate π using sampling? Any ideas?

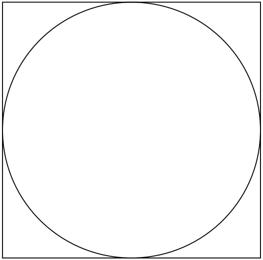
Estimating π



Given the knowledge that:

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

Estimating π



Given the knowledge that:

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Can we phrase this question probabilistically?

What does this mean?

- Write down the estimation problem as

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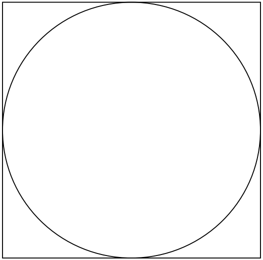
Most of the time, expectation is the most general way.

Estimating π



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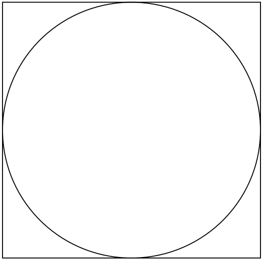
Estimating π



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Estimating π

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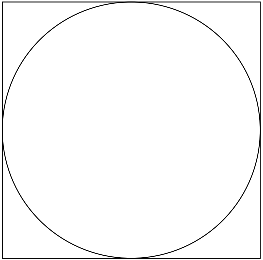

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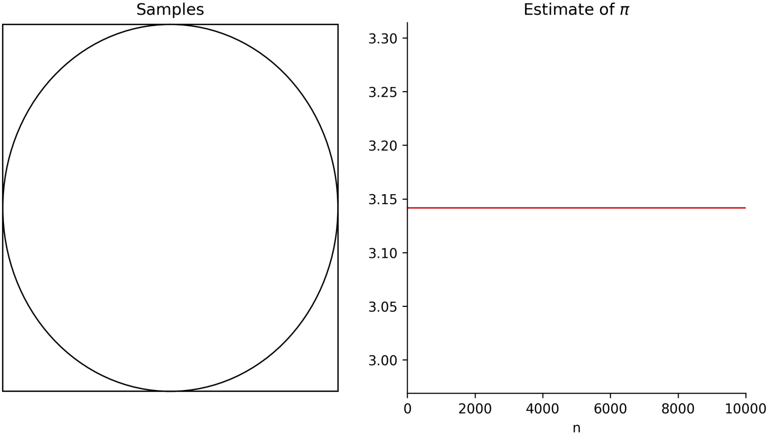
- The 'probability' of the square (whole space) is 1.
- The 'probability of the circle' (set) is precisely the ratio of areas.

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

Last question:

Can we estimate the probability of this set, if we had access to samples from 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 $\pi(x)\mathrm{d}x$[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 $\mathsf{X} = [-1, 1] \times [-1, 1]$ and define the uniform measure such that $\mathbb{P}(\mathsf{X}) = 1$.

Let A be the "circle" s.t. $A \subset \mathsf{X}$. 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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- 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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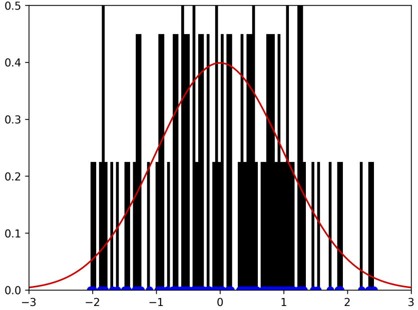
Next up: Pseudo uniform random number generation.

What are pseudo-random numbers?



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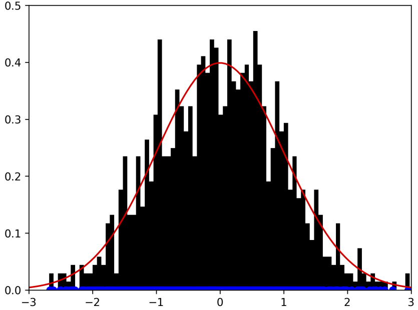

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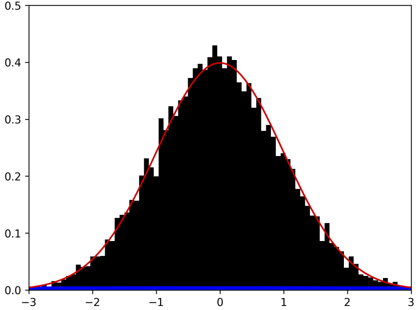

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- You can flip a coin every time you need a binary number
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- On a computer
  - Try to measure some inner thermal noise (of circuits)
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As you can 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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We denote the task

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

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:

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

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

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

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
```

A few things to know about LCGs:

- They generate *periodic* sequences.

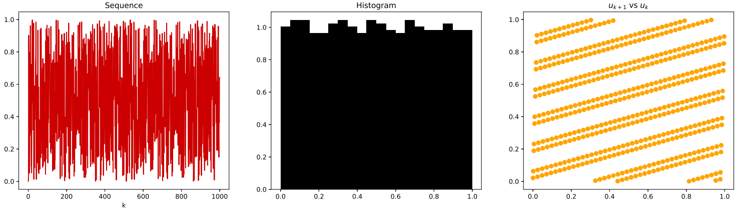


Figure: $m = 2048$, $a = 43$, $b = 0$, $x_0 = 1$.

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:

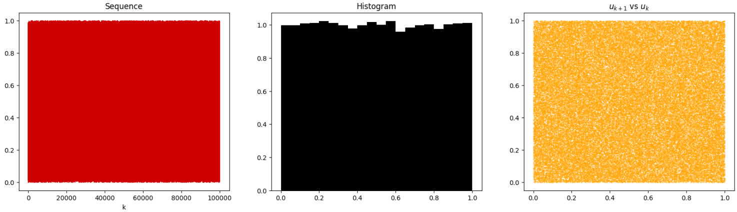
Parameters in common use [edit]

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`

Better parameters:



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  ```
  rng.uniform(0, 1, n)
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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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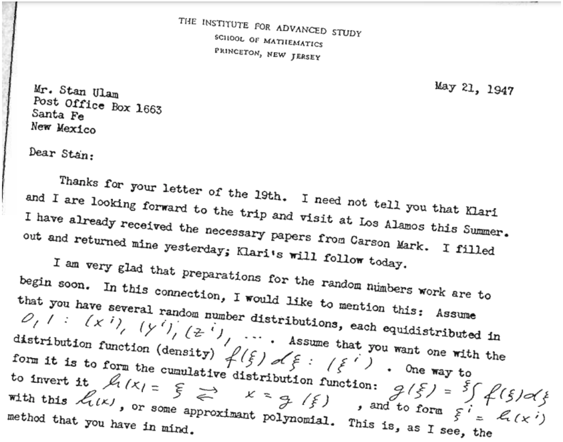
We will start by describing some general methods to sample from more general distributions.



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), ... Assume that you want one with the distribution function (density) $f(\xi)\,d\xi$: (ξ^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.,

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- Draw $X = F_X^{-1}(U)$.

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

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

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

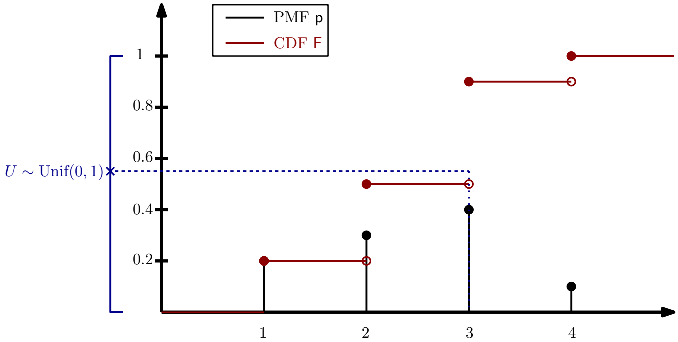
Simpler than it looks, consider the die:

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

and their probabilities

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

How does the sampling work?



- Draw $U \sim \text{Unif}(0, 1)$
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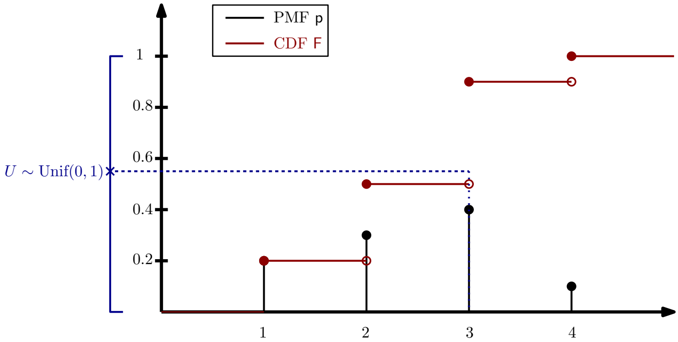


- Draw $U \sim \text{Unif}(0,1)$
- Choose $F_X^-(u) = \min\{x : F_X(x) \geq u\}$ generic for discrete dist.

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()

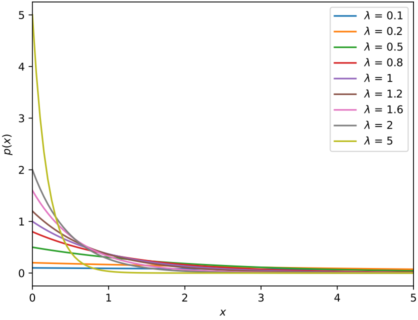
plot_discrete_cdf(w, cw)
```

see simulation.

The exponential density

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

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



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We calculate the CDF

$$\begin{aligned} F_X(x) &= \int_0^x \pi(x')\mathrm{d}x', \\ &= \lambda \int_0^x e^{-\lambda x'}\mathrm{d}x', \end{aligned}$$

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Deriving the inverse:

$$u = 1 - e^{-\lambda x}$$

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So what is the algorithm?

- Generate $u_i \sim$ Unif$([0,1])$
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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.

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

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Transformation method:

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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 $[0, 1]$.

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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?

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

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

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

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

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

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

The inverse transform is:

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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?

Finally, we provide the Box-Müller method for Gaussians: Let $U_1, U_2 \sim$ 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

... 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 $y^i \leqslant f(x^i)$ 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

Recap: We have seen

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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

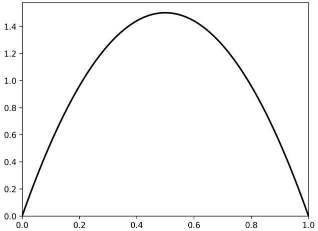
$$\mathsf{A} = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \gamma(x)\}. \tag{2}$$

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

Let

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

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



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

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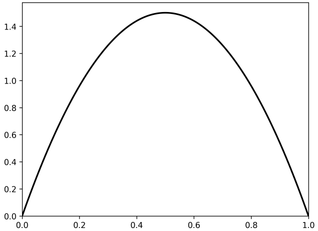

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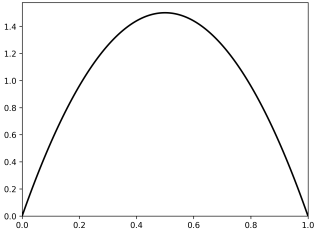
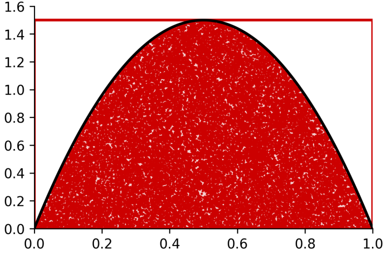


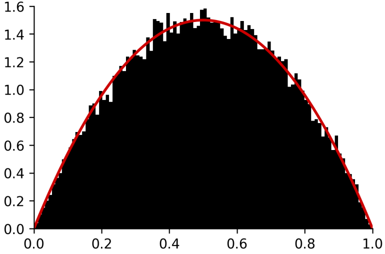
Its maximum is 1.5 in this specific case. Can we sample uniformly?

- 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).

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Rejection sampling

More than a box

Using a box wrapping the density is very inefficient:

- You need the maximum of the density

$$p^\star = \max \pi(x)$$

  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

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

$$\pi(x) \leq M q(x),$$

for $M \geq 1$.

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

For rejection sampling, we always choose a proposal such that

$$\pi(x) \leq M q(x),$$

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

But how to obtain a sample under the curve?

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We can do

Rejection sampling

The algorithm

Imperial College London

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

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. $\pi(x)$)

To implement the method:

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- Sample $x' \sim q(x)$,
- Sample $u \sim \text{Unif}(u; 0, 1)$

Rejection sampling

The algorithm: A closer look

To implement the method:

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- Accept if

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

The rejection sampler:

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

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

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$$\pi(x) = \frac{\gamma(x)}{Z}.$$

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Note the terminology and convention:

- $\gamma(x)$ 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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Rejection sampling

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

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

Rejection sampling

Examples: Acceptance matters

Rejection sampler:

- Sample $x' \sim q(x)$,
- Sample $u \sim \mathsf{Unif}(u; 0, 1)$
- Accept if

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

Rejection sampler:

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

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).

How to compute acceptance rate?

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Proposition 1

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

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

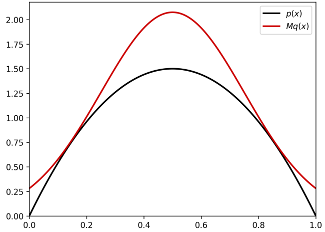
where $M > 1$ in order to satisfy the requirement that q covers π. For an unnormalised target density $\gamma(x)$ with the normalising constant $Z = \int \gamma(x)\mathrm{d}x$, the acceptance rate is given as

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

Choose

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

with $M = 1.3$.



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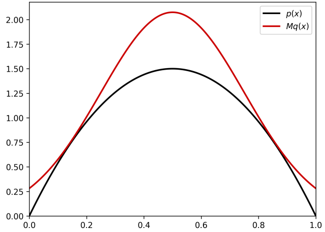
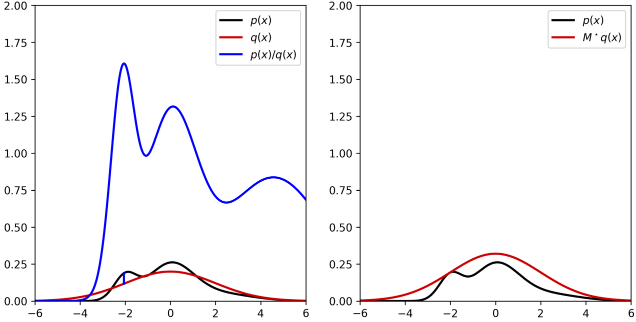


Simulation.

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

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- If $U \leq \gamma(X')/Mq(X')$,
  - Accept X'

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

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

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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 $\pi(x) = 0 \implies q(x) = 0$.

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

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

When π and q admit densities,

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

Given

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

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

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

where $\mathsf{w}_i = w(X_i)$. We will call this estimator the importance sampling (IS) estimator.

Mini-quiz: Is this estimator unbiased?

Mini-quiz: Is this estimator unbiased?

Yes.

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

What is the variance?

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

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.

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

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

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

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

We have

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

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

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

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

$$(\varphi, \tilde{\pi}^N) = \sum_{i=1}^{N}\mathsf{w}_i.\varphi(X_i)$$

Mini-quiz: Is this estimator unbiased?

Mini-quiz: Is this estimator unbiased?

No.

Mini-quiz: Is this estimator unbiased?

No.

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

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.

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Theorem 3

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

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

where

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

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

Proof. We first note the following inequalities,

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

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

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

We can now take the expectation of both sides,

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

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

Bounding the MSE of these integrals yields

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

Therefore, we can straightforwardly write,

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

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

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

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

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

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

■

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!

References I

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- Akyildiz, Ömer Deniz and Joaquín Míguez (2021). "Convergence rates for optimised adaptive importance samplers". In: *Statistics and Computing* 31.2, pp. 1–17.