# Probabilistic Inference and Learning
# Lecture 04
# Sampling

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# A Computational Challenge

Integration is the core computation of probabilistic inference

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Probabilistic inference requires **integrals**:

- Evidences. Example from Lecture 3:

$$p(\pi|x_1,\dots,x_N) = \frac{\prod_i^N p(x_i \mid \pi)p(\pi)}{\int_0^1 \prod_i^N p(x_i \mid \pi)p(\pi)\,d\pi} = \frac{\prod_i^N \pi^n(1-\pi)^{N-n}}{\int_0^1 \prod_i^N \pi^n(1-\pi)^{N-n}\,d\pi}$$

- Expectations (actually, evidences are expectations, too)

| | |
|---|---|
| $\langle f \rangle_p := \mathbb{E}_p[f] := \int f(x)p(x)\,\mathrm{d}x$ | "Expectation of $f$ under $p$" |
| $f(x) = x$ | mean |
| $f(x) = (x - \mathbb{E}_p(x))^2$ | variance |
| $f(x) = x^p$ | $p$-th moment |
| $f(x) = -\log x$ | entropy |
| $\vdots$ | |

## The Toolbox

### Framework:

$$\int p(x_1, x_2)\, dx_2 = p(x_1) \qquad p(x_1, x_2) = p(x_1 \mid x_2)p(x_2) \qquad p(x \mid y) = \frac{p(y \mid x)p(x)}{p(y)}$$

### Modelling:

- Directed Graphical Models
-
-
-
-
-

### Computation:

- Monte Carlo
-
-
-
-

# Randomized Methods — Monte Carlo

the idea

- the “simplest thing to do”: replace integral with sum:

$$\int f(x)p(x)\,\mathrm{d}x \approx \frac{1}{S}\sum_{i=1}^{S} f(x_i); \qquad \int p(x,y)\,\mathrm{d}x \approx \sum_i p(y \mid x_i); \qquad \text{if } x_i \sim p(x)$$

- this requires being able to sample $x_i \sim p(x)$

**Definition (Monte Carlo method)**

*Algorithms that compute expectations in the above way, using samples $x_i \sim p(x)$ are called Monte Carlo methods (Stanisław Ulam, John von Neumann).*


CASINO
MONTE-CARLO
image source: wikipedia u:fruitpunchline

# A method from a different age

Monte Carlo Methods and the Manhattan Project

images: Los Alamos National Laboratory / wikipedia

Stanisław Ulam
1909–1984

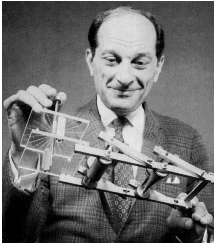
Nicholas Metropolis
1915–1999

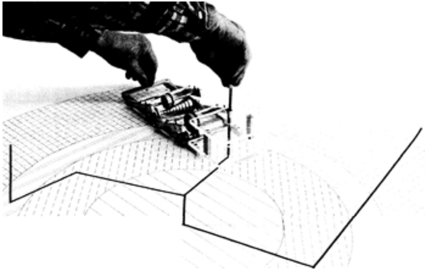
John von Neumann
1903–1957

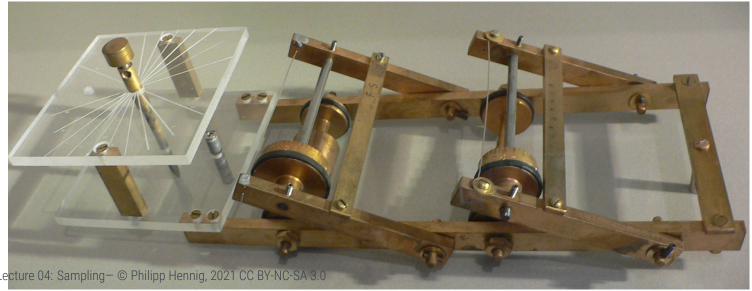
# The FERMIAC

analog Monte Carlo computer

images: wikipedia







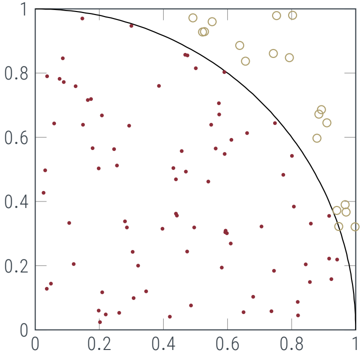
# Example

## a dumb way to compute $\pi$

- ratio of quarter-circle to square: $\dfrac{\pi/4}{1}$
- $\pi = 4 \int \mathbb{I}(x^\intercal x < 1) u(x) \, dx$
- draw $x \sim u(x)$, check $x^\intercal x < 1$, count

```python
from numpy.random import rand
S = 100000
sum((rand(S,2)**2).sum(axis=1) < 1) / S * 4
```

```
> 3.13708
> 3.14276
```



# Monte Carlo works on **every** Integrable Function

is this a good thing?



$$\phi := \int f(x)p(x)\,dx = \mathbb{E}_p(f)$$

- Let $x_s \sim p, s = 1, \dots, S$ iid. (i.e. $p(x_s = x) = p(x)$ and $p(x_s, x_t) = p(x_s)p(x_t)\ \forall s, t$)

$$\hat{\phi} := \frac{1}{S}\sum_{s=1}^{S} f(x_s) \qquad \leftarrow \text{the **Monte Carlo estimator** is ...}$$

$$\mathbb{E}(\hat{\phi}) =: \int \frac{1}{S}\sum_{s=1}^{S} f(x_s)p(x_s)\,dx_s = \frac{1}{S}\sum_{s=1}^{S}\int f(x_s)p(x_s)\,dx_s$$

$$= \frac{1}{S}\sum_{s=1}^{S}\mathbb{E}(f(x_s)) = \phi \qquad \leftarrow \text{... an **unbiased** estimator!}$$

- the only requirement for this is that $\int f(x)p(x)\,dx$ **exists** (i.e. $f$ must be Lebesgue-integrable relative to $p$). Monte Carlo integration can even work on discontinuous functions.

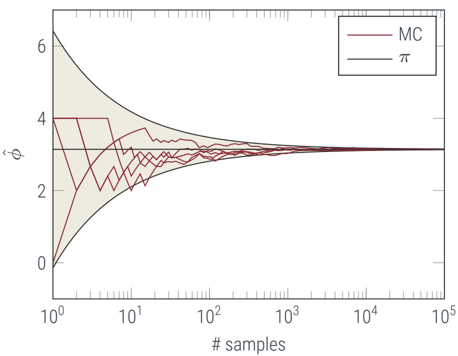
- The expected square error (variance) drops as $\mathcal{O}(S^{-1})$

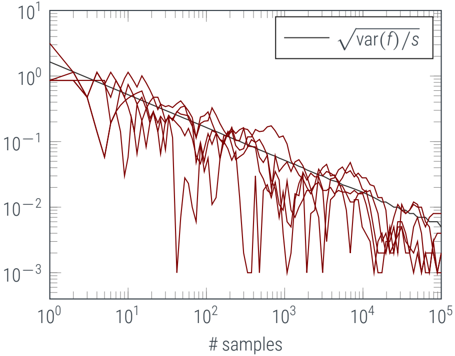
$$
\begin{aligned}
\mathbb{E}(\hat{\phi} - \mathbb{E}(\hat{\phi}))^2 &= \mathbb{E}\left[\frac{1}{S}\sum_{s=1}^{S}(f(x_s) - \phi)\right]^2 \\
&= \frac{1}{S^2}\sum_{s=1}^{S}\sum_{r=1}^{S}\mathbb{E}(f(x_s)f(x_r)) - \phi\mathbb{E}(f(x_s)) - \mathbb{E}(f(x_r))\phi + \phi^2 \\
&= \frac{1}{S^2}\sum_{s=1}^{S}\left(\left(\sum_{r\neq s}\underbrace{\phi^2 - 2\phi^2 + \phi^2}_{=0}\right) + \underbrace{\mathbb{E}(f^2) - \phi^2}_{=:\mathrm{var}(f)}\right) \\
&= \frac{1}{S}\mathrm{var}(f) = \mathcal{O}(S^{-1})
\end{aligned}
$$

- Thus, the expected error (the square-root of the expected square error) drops as $\mathcal{O}(S^{-1/2})$

# sampling is for rough guesses

recall example computation for $\pi$




- need only $\sim 9$ samples to get *order of magnitude* right ($\mathrm{std}(\phi)/3$)
- need $10^{14}$ samples for single-precision ($\sim 10^{-7}$) calculations!
- sampling is good for rough estimates, not for precise calculations
- **Always think of other options before trying to sample!**

- **samples** from a probability distribution can be used to **estimate** expectations, **roughly**, without having to design an elaborate integration algorithm
- The error of the estimate is **independent** of the dimensionality of the input domain!

How do we generate random samples from $p(x)$?

# Reminder: Change of Measure

## The transformation law

### Theorem (Change of Variable for Probability Density Functions)

*Let $X$ be a continuous random variable with PDF $p_X(x)$ over $c_1 < x < c_2$. And, let $Y = u(X)$ be a monotonic differentiable function with inverse $X = v(Y)$. Then the PDF of $Y$ is*

$$p_Y(y) = p_X(v(y)) \cdot \left| \frac{dv(y)}{dy} \right| = p_X(v(y)) \cdot \left| \frac{du(x)}{dx} \right|^{-1}.$$

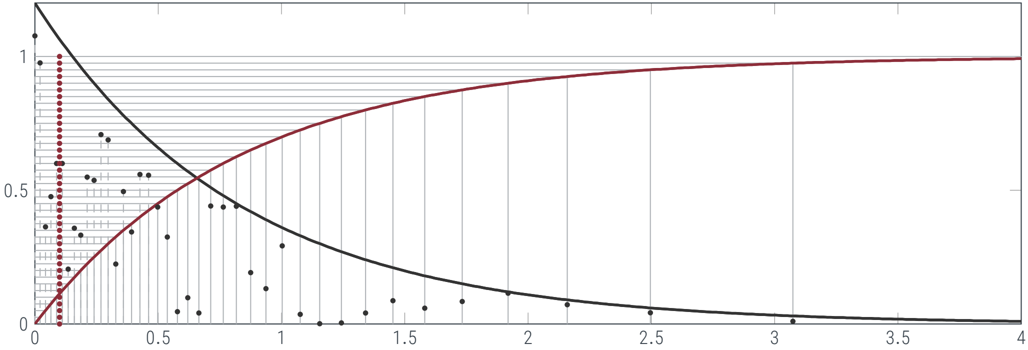
*Let $X = (X_1, \dots, X_d)$ have a joint density $p_X$. Let $g : \mathbb{R}^d \to \mathbb{R}^d$ be continously differentiable and injective, with non-vanishing Jacobian $J_g$. Then $Y = g(X)$ has density*

$$p_Y(y) = \begin{cases} p_X(g^{-1}(y)) \cdot |J_{g^{-1}}(y)| & \textit{if } y \textit{ is in the range of } g, \\ 0 & \textit{otherwise.} \end{cases}$$

*The Jacobian $J_g$ is the $d \times d$ matrix with $[J_g(x)]_{ij} = \frac{\partial g_i(x)}{\partial x_j}$.*

# Some special cases

sampling from an exponential distribution is analytic




$$p(x) = \frac{1}{\lambda} e^{-x/\lambda}$$

$$\int p(x)\, dx = 1 - e^{-x/\lambda}$$

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

$$x = -\lambda \log(u)$$

# Example: Sampling from a Beta Distribution

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## uniform variables

Consider $u \sim U[0,1]$ (i.e. $u \in [0,1]$, and $p(u) = 1$). The variable $x = u^{1/\alpha}$ has the Beta density

$$p_x(x) = p_u(u(x)) \cdot \left| \frac{\partial u(x)}{\partial x} \right| = \alpha \cdot x^{\alpha-1} = \mathcal{B}(x; \alpha, 1).$$

# Example: Sampling from a Beta Distribution



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## Homework:

Consider two *independent* variables

$$X \sim \mathcal{G}(\alpha, \theta) \qquad Y \sim \mathcal{G}(\beta, \theta)$$

where $\Gamma(\xi; \alpha, \theta) = \frac{1}{\Gamma(\alpha)\theta^k} \xi^{\alpha-1} e^{-\xi/\theta}$ is the *Gamma distribution*. Show that the random variable $Z = \frac{X}{X+Y}$ is Beta distributed, with the density

$$p(Z = z) = \mathcal{B}(z; \alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} z^{\alpha-1}(1-z)^{\beta-1}.$$

- **samples** from a probability distribution can be used to **estimate** expectations, **roughly**
- **‘random numbers’** don’t really need to be **unpredictable**, as long as they have as little **structure** as possible
- **uniformly distributed random numbers** can be **transformed** into other distributions. This can be done numerically efficiently in some cases, and it is worth thinking about doing so

What do we do if we don’t know a good transformation?

# Why is sampling hard?

Sampling is harder than global optimization

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To produce exact samples:

- need to know cumulative density everywhere
- need to know regions of high density (not just local maxima!)
- a global description of the entire function

Practical Monte Carlo Methods aim to construct samples from

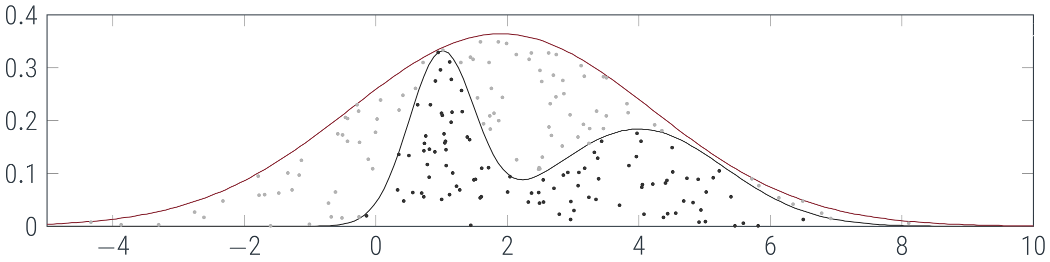
$$p(x) = \frac{\tilde{p}(x)}{Z}$$

assuming that it is possible to *evaluate* the *unnormalized* density $\tilde{p}$ (but not $p$) at arbitrary points.
Typical example: Compute moments of a posterior

$$p(x \mid D) = \frac{p(D \mid x)p(x)}{\int p(D, x)\, dx} \quad \text{as} \quad \mathbb{E}_{p(x|D)}(x^n) \approx \frac{1}{S}\sum_s x_i^n \quad \text{with } x_i \sim p(x \mid D)$$

# Rejection Sampling

a simple method [Georges-Louis Leclerc, Comte de Buffon, 1707–1788]

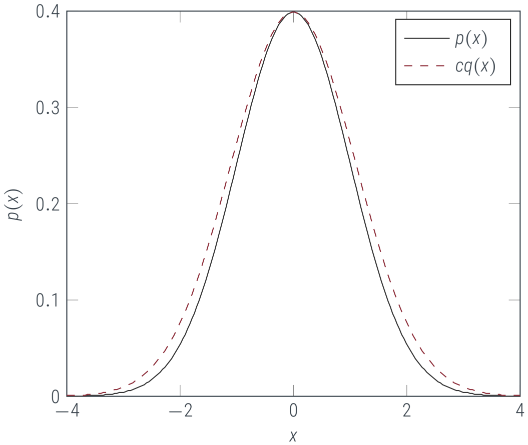



- for any $p(x) = \tilde{p}(x)/Z$ (normalizer $Z$ not required)
- choose $q(x)$ s.t. $cq(x) \geq \tilde{p}(x)$
- draw $s \sim q(x), u \sim \text{Uniform}[0, cq(s)]$
- reject if $u > \tilde{p}(s)$

# The Problem with Rejection Sampling

the curse of dimensionality [MacKay, §29.3]






Example:

- $p(x) = \mathcal{N}(x; 0, \sigma_p^2)$
- $q(x) = \mathcal{N}(x; 0, \sigma_q^2)$
- $\sigma_q > \sigma_p$
- optimal $c$ is given by

$$c = \frac{(2\pi\sigma_q^2)^{D/2}}{(2\pi\sigma_p^2)^{D/2}} = \left(\frac{\sigma_q}{\sigma_p}\right)^D = \exp\left(D \ln \frac{\sigma_q}{\sigma_p}\right)$$

- acceptance rate is ratio of volumes: $1/c$
- rejection rate rises **exponentially** in $D$
- for $\sigma_q/\sigma_p = 1.1, D = 100, 1/c < 10^{-4}$

# Importance Sampling

a slightly less simple method

- computing $\tilde{p}(x), q(x)$, then throwing them away seems wasteful
- instead, rewrite (assume $q(x) > 0$ if $p(x) > 0$)

$$\phi = \int f(x)p(x)\,\mathrm{d}x = \int f(x)\frac{p(x)}{q(x)}q(x)\,\mathrm{d}x$$
$$\approx \frac{1}{S}\sum_s f(x_s)\frac{p(x_s)}{q(x_s)} =: \frac{1}{S}\sum_s f(x_s)w_s \qquad \text{if } x_s \sim q(x)$$

- this is just using a new function $g(x) = f(x)p(x)/q(x)$, so it is an unbiased estimator
- $w_s$ is known as the **importance (weight)** of sample $s$
- if normalization unknown, can also use $\tilde{p}(x) = Zp(x)$

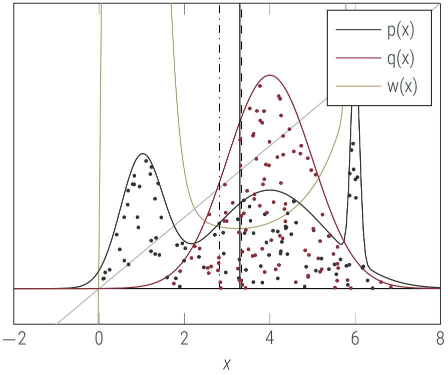
$$\int f(x)p(x)\,\mathrm{d}x = \frac{1}{Z}\frac{1}{S}\sum_s f(x_s)\frac{\tilde{p}(x_s)}{q(x_s)}$$
$$= \frac{1}{S}\sum_s f(x_s)\frac{\tilde{p}(x_s)/q(x_s)}{\frac{1}{S}\sum_t 1\tilde{p}(x_t)/q(x_t)} =: \sum_s f(x_s)\tilde{w}_s$$

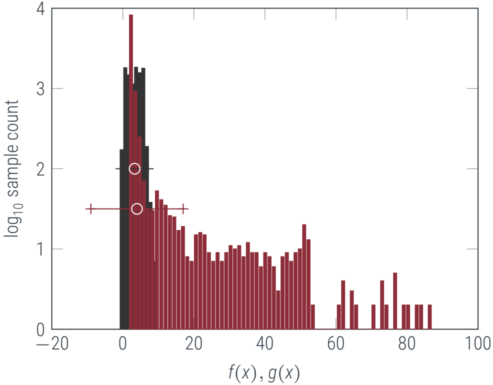
- this is consistent, but biased

# What's wrong with Importance Sampling?

the curse of dimensionality, revisited

- recall that $\operatorname{var}\hat{\phi} = \operatorname{var}(f)/S$ – importance sampling replaces $\operatorname{var}(f)$ with $\operatorname{var}(g) = \operatorname{var}\left(f\frac{p}{q}\right)$
- $\operatorname{var}\left(f\frac{p}{q}\right)$ can be very large if $q \ll p$ somewhere. In many dimensions, usually all but everywhere!
- if $p$ has "undiscovered islands", some samples have $p(x)/q(x) \to \infty$



## Sampling (Monte Carlo) Methods

Sampling is a way of performing rough probabilistic computations, in particular for expectations (including **marginalization**).

- samples from a probability distribution can be used to estimate expectations, roughly
- uniformly distributed random numbers can be **transformed** into other distributions. This can be done numerically efficiently in some cases, and it is worth thinking about doing so
- Rejection sampling is a primitive but **exact** method that works with **intractable** models
- Importance sampling makes more efficient use of samples, but can have high variance (and this may not be obvious)

### Next Lecture:

- **Markov Chain Monte Carlo** methods are more elaborate ways of getting approximate answers to intractable problems.