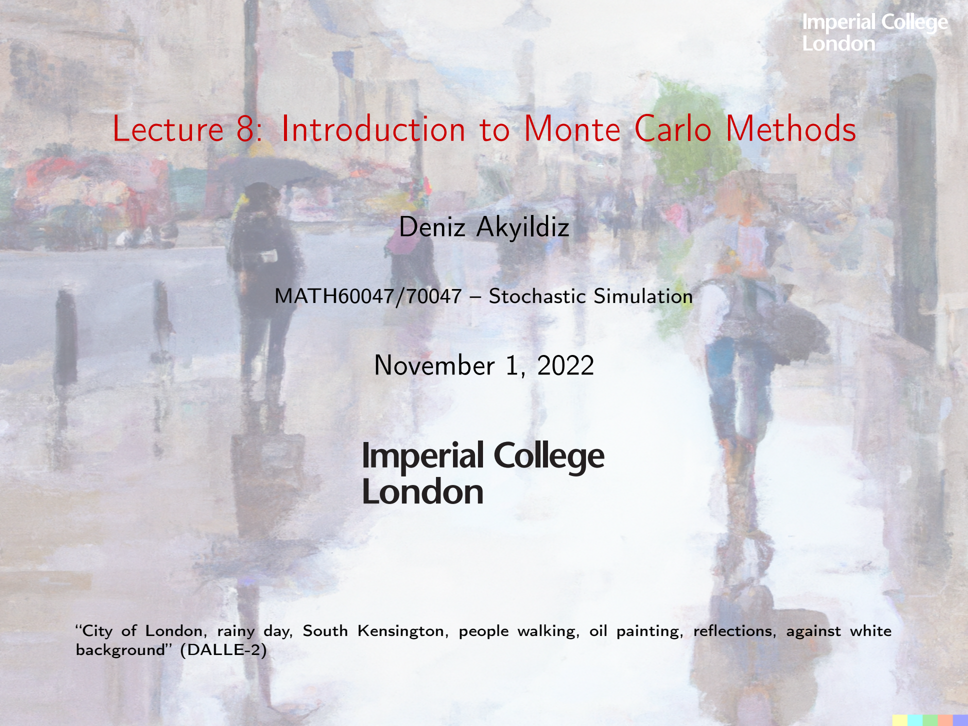

Imperial College London

Lecture 8: Introduction to Monte Carlo Methods

Deniz Akyildiz

MATH60047/70047 – Stochastic Simulation

November 1, 2022

Imperial College London

"City of London, rainy day, South Kensington, people walking, oil painting, reflections, against white background" (DALLE-2)

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- An introduction to Monte Carlo methods
  - A set of general methods for sampling from distributions, estimating expectations, computing integrals

Recall the posterior computation:

$$p(x|y) = \frac{p(y|x)p(x)}{p(y)} = \frac{p(y|x)p(x)}{\int p(y|x)p(x)dx}.$$

We did not discuss the denominator $p(y)$ in detail:

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It is an extremely important quantity for choosing models.

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A simple example: Choosing the right prior.

Consider two different models:

$$\begin{aligned} x &\sim p_0(x) = \mathcal{N}(x; \mu_0, \sigma_0^2) \\ y|x &\sim \mathcal{N}(y; x, \sigma_y^2) \end{aligned}$$

and

$$\begin{aligned} x &\sim p_1(x) = \mathcal{N}(x; \mu_1, \sigma_1^2) \\ y|x &\sim \mathcal{N}(y; x, \sigma_y^2) \end{aligned}$$

Consider observing y (a single data point). Which model is more likely?

Recall that, for these models, we have computed $p(y)$ analytically before. We can compute for both models:

$$\begin{aligned}
p_0(y) &= \int p(y|x)p_0(x)\mathrm{d}x \\
&= \int \mathcal{N}(y; x, \sigma_y^2)\mathcal{N}(x; \mu_0, \sigma_0^2)\mathrm{d}x \\
&= \mathcal{N}(y; \mu_0, \sigma_0^2 + \sigma_y^2)
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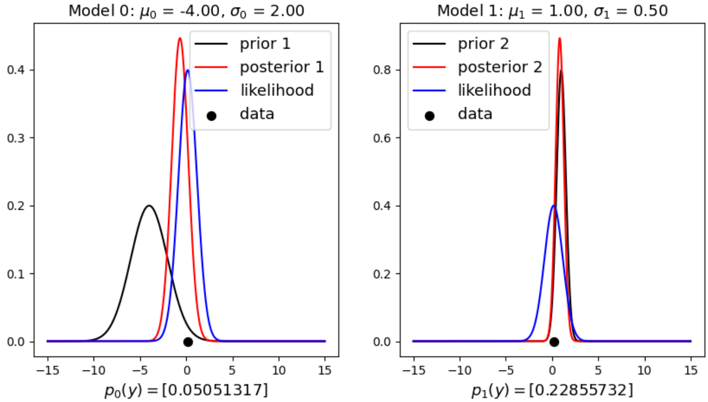
We will say Model 1 is better than Model 0 if $p_1(y) > p_0(y)$ for fixed y.


Model 0: μ_0 = -4.00, σ_0 = 2.00
prior 1
posterior 1
likelihood
data
0.0
0.1
0.2
0.3
0.4
−15
−10
−5
0
5
10
15
$p_0(y) = [0.05051317]$
Model 1: μ_1 = 1.00, σ_1 = 0.50
prior 2
posterior 2
likelihood
data
0.0
0.2
0.4
0.6
0.8
−15
−10
−5
0
5
10
15
$p_1(y) = [0.22855732]$

Bayesian no more...

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Monte Carlo methods are a set of general methods for solving these problems by generating random samples (rejection sampling counts as a Monte Carlo method).

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$$\bar{\varphi} = \mathbb{E}_p[\varphi(x)] = \int \varphi(x) p(x) \mathrm{d}x \tag{3}$$

can be estimated using $X_1, \ldots, X_N \sim p(x)$ as

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$$\bar{\varphi} = \mathbb{E}_p[\varphi(x)] \approx \frac{1}{N} \sum_{i=1}^{N} \varphi(X_i) = \hat{\varphi}^N \tag{4}$$

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Intuition: δ_y is a measure concentrated at y: It evaluates the integral at y and is zero everywhere else. An incorrect way to write it:

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Note that, the use of Dirac only makes sense with an integral!

Given samples $X_1, \ldots, X_N \sim p(x)$, a probability distribution is approximated as

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

The estimator is called the *empirical* distribution.

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by the definition of the Dirac measure.

The same idea can be used to estimate an integral. Consider the problem:

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This technique is sometimes called the Crude Monte Carlo estimator of the integral.

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&= \bar{\varphi}.
\end{aligned}
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&= \frac{1}{N}\mathsf{var}_p[\varphi(X)] = \frac{\sigma_\varphi^2}{N}
\end{aligned}
$$

Provided that $\mathsf{var}_p[\varphi(X)] < \infty$ and the estimator is consistent as $N \to \infty$.

Given

$$\begin{aligned}\mathsf{var}_p[\hat{\varphi}^N] &= \frac{1}{N}\mathsf{var}_p[\varphi(X)] \\ &= \frac{1}{N}\int(\varphi(x)-\bar{\varphi})^2 p(x)\mathrm{d}x\end{aligned}$$

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&= \sigma^2_{\varphi,N}.
\end{aligned}
$$

The variance can also be estimated using Monte Carlo method.

By the central limit theorem:

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Therefore, this can be used to build confidence intervals (however, not very trustable).

We can see that the standard deviation of the estimator is given by

$$\mathsf{std}_p(\hat{\varphi}^N) = \frac{\sigma_\varphi}{\sqrt{N}}.$$

This is one reason you may hear much about $\mathcal{O}(1/\sqrt{N})$ convergence rate (this is optimal).

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More on convergence later.

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Can we estimate probabilities?

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$$\begin{aligned}\mathbb{P}(X \in A) &= \int_A p(x)\mathrm{d}x \\ &= \int \mathbf{1}_A(x)p(x)\mathrm{d}x,\end{aligned}$$

where $\mathbf{1}_A(x)$ is the indicator function of A.

$$
\begin{aligned}
\mathbb{P}(X \in A) &= \int \mathbf{1}_A(x) p(x) \mathrm{d}x, \\
&\approx \int \mathbf{1}_A(x) p^N(x) \mathrm{d}x, \\
&= \int \mathbf{1}_A(x) \frac{1}{N} \sum_{i=1}^N \delta_{X_i}(x) \mathrm{d}x, \\
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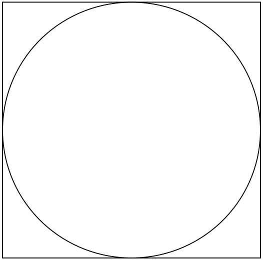
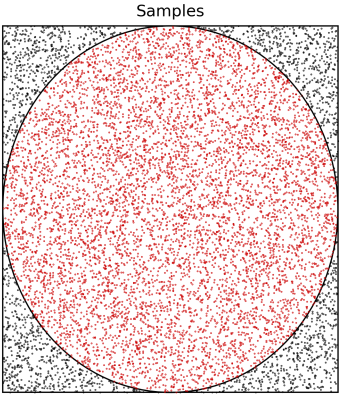
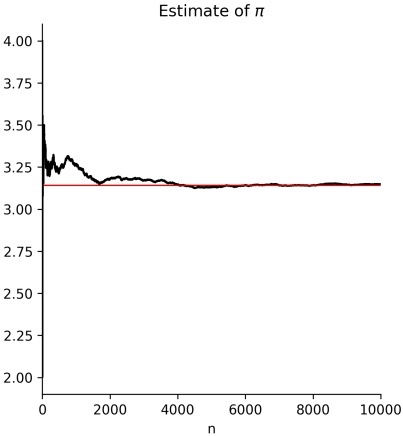
$\varphi(x) = \mathbf{1}_A(x)$ to estimate $\mathbb{P}(X \in A)$.

Our old problem:



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


Samples


Estimate of π
4.00
3.75
3.50
3.25
3.00
2.75
2.50
2.25
2.00
0
2000
4000
6000
8000
10000
n

For probabilists, 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 $x_i \sim \mathbb{P}$.

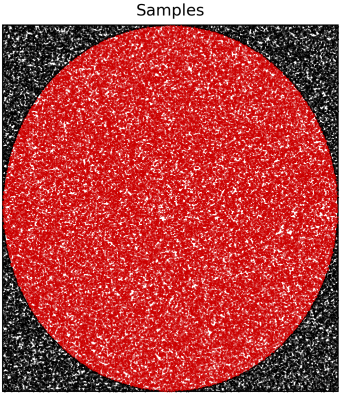
For probabilists, let $\mathsf{X} = [-1, 1] \times [-1, 1]$ and define the uniform measure such that $\mathbb{P}(\mathsf{X}) = 1$.

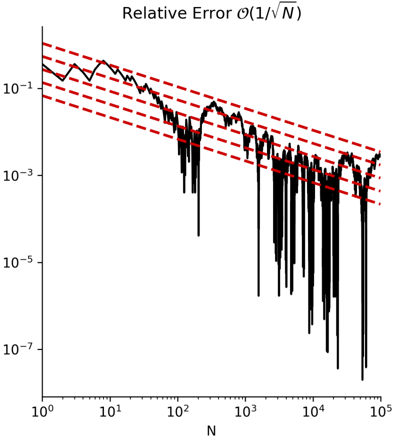
Let A be the "circle" s.t. $A \subset \mathsf{X}$. Now, the probability of A is given

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

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

What about the convergence rate?


Samples


Relative Error $\mathcal{O}(1/\sqrt{N})$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
N

Let us consider the integral (Example 3.4 from Robert and Casella, 2004)

$$\int_0^1 h(x)\mathrm{d}x = \int_0^1 [\cos(50x) + \sin(20x)]^2 \mathrm{d}x. \tag{11}$$

The exact value of this integral is 0.965 (yes, you can compute it).

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The exact value of this integral is 0.965 (yes, you can compute it).

We can use Monte Carlo integration to estimate this integral. Choose $p(x) = \mathsf{Unif}(0,1)$, then

$$\int_0^1 h(x)\mathrm{d}x = \int_0^1 h(x)p(x)\mathrm{d}x$$

so a uniform sample from $[0,1]$ is sufficient to estimate this integral.

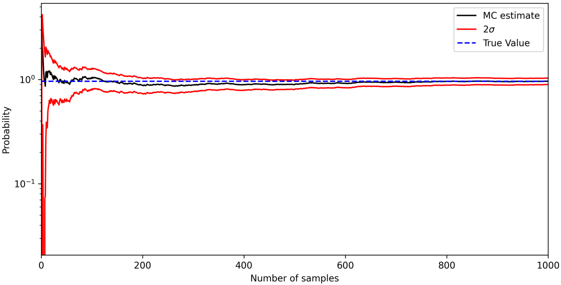

Figure: Monte Carlo integration of $h(x) = [\cos(50x) + \sin(20x)]^2$

Assume $X \sim \mathcal{N}(0, 1)$ and we are interested in

$$\mathbb{P}(X > 2) = \int_2^\infty \mathcal{N}(x; 0, 1)\mathrm{d}x. \tag{12}$$

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We can formulate this as a Monte Carlo problem by choosing

$$\varphi(x) = \mathbf{1}_{\{x>2\}}. \tag{13}$$

Our estimation task is then sample $X_1, \ldots, X_n \sim \mathcal{N}(0,1)$ then

$$
\begin{aligned}
\mathbb{P}(X > 2) &= \int_2^\infty \mathcal{N}(x; 0, 1)\mathrm{d}x \\
&= \int_{-\infty}^\infty \mathbf{1}_{\{x>2\}} \mathcal{N}(x; 0, 1)\mathrm{d}x \\
&\approx \frac{1}{n} \sum_{i=1}^n \mathbf{1}_{\{X_i > 2\}}.
\end{aligned}
$$

Let us investigate the mean and the variance of this estimate against a numerical integrator (ground truth).

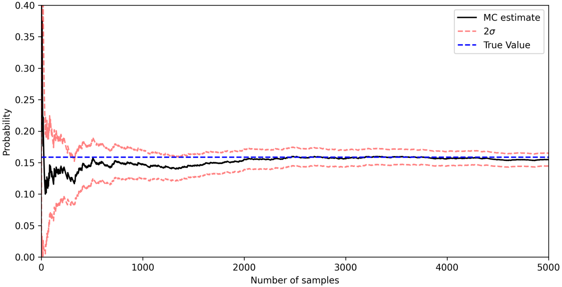

Figure: Monte Carlo estimation of the tail probability $X > 2$

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- Error metrics (bias, variance, MSE, etc.)
- Examples of estimating integrals, probabilities, and marginal likelihoods
- Explicit computations for variance

We will give a general review about how to compute the error of a generic estimator.

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We will then apply these ideas to the Monte Carlo estimators.

Consider

- the target quantity: $\bar{\varphi}$
- the estimator: $\hat{\varphi}^N$

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We define the bias:

$$\text{bias}_p(\hat{\varphi}^N) = \mathbb{E}[\hat{\varphi}^N] - \bar{\varphi}. \tag{14}$$

In the perfect Monte Carlo case (samples exactly from p), the bias is zero.

Consider

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We define the variance

$$\mathsf{var}_p(\hat{\varphi}^N) = \mathbb{E}_p\left[\left(\hat{\varphi}^N - \mathbb{E}_p[\hat{\varphi}^N]\right)^2\right],$$
$$= \mathbb{E}_p\left[\left(\hat{\varphi}^N\right)^2\right] - \mathbb{E}_p\left[\hat{\varphi}^N\right]^2.$$

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$$\mathsf{MSE}(\hat{\varphi}^N) = \mathbb{E}[\big(\hat{\varphi}^N - \bar{\varphi}\big)^2].$$

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Prove that (in-class exercise) this is also

$$\mathsf{MSE}(\hat{\varphi}^N) = \mathsf{var}_p(\hat{\varphi}^N) + \mathsf{bias}_p(\hat{\varphi}^N)^2.$$

Proof.

$$\mathsf{MSE}(\hat{\varphi}^N) \quad = \quad \mathbb{E}[\big(\hat{\varphi}^N - \bar{\varphi}\big)^2]$$

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$$\begin{aligned}\mathsf{MSE}(\hat{\varphi}^N) &= \mathbb{E}[\big(\hat{\varphi}^N - \bar{\varphi}\big)^2] \\ &= \mathbb{E}[\big(\hat{\varphi}^N\big)^2] - 2\bar{\varphi}\mathbb{E}[\hat{\varphi}^N] + \bar{\varphi}^2\end{aligned}$$

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$$

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$$
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&= \mathsf{var}_p(\hat{\varphi}^N) + \big(\mathbb{E}[\hat{\varphi}^N] - \bar{\varphi}\big)^2,
\end{aligned}
$$

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\begin{aligned}
\mathsf{MSE}(\hat{\varphi}^N) &= \mathbb{E}[\left(\hat{\varphi}^N - \bar{\varphi}\right)^2] \\
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&= \mathsf{var}_p(\hat{\varphi}^N) + \left(\mathbb{E}[\hat{\varphi}^N] - \bar{\varphi}\right)^2, \\
&= \mathsf{var}_p(\hat{\varphi}^N) + \mathsf{bias}_p(\hat{\varphi}^N)^2.
\end{aligned}
$$

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Note though we will have biased cases.

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Note though we will have biased cases. Do not use them interchangeably.

Consider

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We generally plot

$$\mathsf{RAE}(\hat{\varphi}^N) = \frac{|\hat{\varphi}^N - \bar{\varphi}|}{|\bar{\varphi}|}.$$

Note that this is *random*, as no expectations are taken.

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- the estimator: $\hat{\varphi}^N$

We generally plot

$$\mathsf{RAE}(\hat{\varphi}^N) = \frac{|\hat{\varphi}^N - \bar{\varphi}|}{|\bar{\varphi}|}.$$

Note that this is *random*, as no expectations are taken.

It can be proven that the random error has

$$|\hat{\varphi}^N - \bar{\varphi}| \leq \mathcal{O}(U/\sqrt{N}),$$

see, e.g., Akyildiz, 2019, Corollary 2.1 for a proof.

Consider the following model:

$$
\begin{aligned}
p(x) &= \mathcal{N}(x; \mu_0, \sigma_0^2), \\
p(y|x) &= \mathcal{N}(y; x, \sigma^2).
\end{aligned}
$$

Assume that we have observed $y = 4$ and want to estimate the marginal likelihood $p(y)$.

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$$p(x) = \mathcal{N}(x; \mu_0, \sigma_0^2),$$
$$p(y|x) = \mathcal{N}(y; x, \sigma^2).$$

Assume that we have observed $y = 4$ and want to estimate the marginal likelihood $p(y)$.

From our past experience, we have access to this density:

$$\begin{aligned} p(y) &= \int p(y|x)p(x)\mathrm{d}x, \\ &= \mathcal{N}(y; \mu_0, \sigma_0^2 + \sigma^2). \end{aligned}$$

Therefore, we know exactly the value of $p(4)$ (i.e. $p(y = 4)$).

Given that the problem is an integral w.r.t. $p(x)$,

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

we could use our Monte Carlo estimator to get unbiased estimates of $p(y)$.

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Write down the estimator (in-class exercise).

Given that the problem is an integral w.r.t. $p(x)$,

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

we could use our Monte Carlo estimator to get unbiased estimates of $p(y)$.

Note here that $\varphi(x) = p(y|x)$ is a deterministic function of x for fixed y. Therefore, given $X_1, \ldots, X_N \sim p(x)$

$$\int \varphi(x)p(x)\mathrm{d}x \approx \frac{1}{N}\sum_{i=1}^{N}\varphi(X_i) = \frac{1}{N}\sum_{i=1}^{N}p(y|X_i).$$

For $y = 4$, we can compute this (given μ_0, σ_0, σ).

Set

$$\mu_0 = 0, \quad \sigma_0 = 1, \quad \sigma = 2, \quad y = 1$$

and generate $N = 100000$ samples from $p(x)$. We estimate

$$p^N(y) = \frac{1}{N} \sum_{i=1}^{N} p(y|X_i).$$

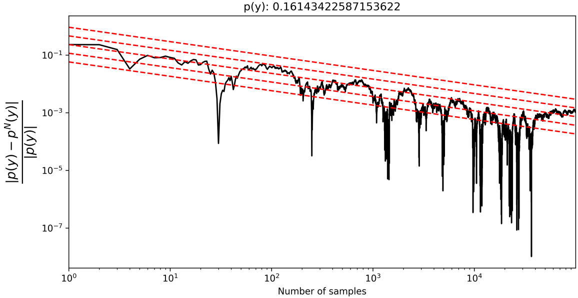

Figure: Estimating the marginal likelihood $p(y)$ for $y = 1$

Let

$$p(x) = \frac{1}{\pi(1+x^2)},$$

and let

$$\varphi(x) = \mathbf{1}_{\{x \geq 2\}}.$$

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and let

$$\varphi(x) = \mathbf{1}_{\{x \geq 2\}}.$$

We would like to compute

$$\begin{aligned}
\mathbb{P}(X > 2) &= \int_2^\infty p(x) \mathrm{d}x \\
&= \int \mathbf{1}_{\{x > 2\}}(x) p(x) \mathrm{d}x \\
&= \int \varphi(x) p(x) \mathrm{d}x.
\end{aligned}$$

We can compute the real value of this integral:

$$I = \bar{\varphi} = \int_2^{\infty} p(x)\mathrm{d}x = F(\infty) - F(2) = \frac{1}{2} - \frac{1}{\pi}\tan^{-1}(2) = 0.1476$$

Compute the variance of the Monte Carlo estimator for $N = 10$ samples.

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Compute the variance of the Monte Carlo estimator for $N = 10$ samples.

$$\mathsf{var}(\hat{\varphi}^N) = \frac{\mathsf{var}_p(\varphi)}{N}$$

So we need to compute:

$$\mathsf{var}_p(\varphi)$$

Now, we compute

$$\begin{aligned}
\mathsf{var}_p(\varphi) &= \int \varphi(x)^2 p(x)\mathrm{d}x - \left(\int \varphi(x)p(x)\mathrm{d}x\right)^2 \\
&= \int \mathbf{1}_{\{x>2\}}(x)^2 p(x)\mathrm{d}x - \left(\int \mathbf{1}_{\{x>2\}}(x)p(x)\mathrm{d}x\right)^2 \\
&= \int \mathbf{1}_{\{x>2\}}(x) p(x)\mathrm{d}x - \left(\int \mathbf{1}_{\{x>2\}}(x)p(x)\mathrm{d}x\right)^2 \\
&= 0.1476 - 0.1476^2 = 0.125.
\end{aligned}$$

Now, we compute

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\mathsf{var}_p(\varphi) &= \int \varphi(x)^2 p(x)\mathrm{d}x - \left(\int \varphi(x)p(x)\mathrm{d}x\right)^2 \\
&= \int \mathbf{1}_{\{x>2\}}(x)^2 p(x)\mathrm{d}x - \left(\int \mathbf{1}_{\{x>2\}}(x)p(x)\mathrm{d}x\right)^2 \\
&= \int \mathbf{1}_{\{x>2\}}(x) p(x)\mathrm{d}x - \left(\int \mathbf{1}_{\{x>2\}}(x)p(x)\mathrm{d}x\right)^2 \\
&= 0.1476 - 0.1476^2 = 0.125.
\end{aligned}$$

The variance of the estimator then

$$\mathsf{var}(\hat{\varphi}^N) = \frac{0.125}{10} = 0.0125.$$

Could we do better? An idea, the density is symmetric around zero

- This means $P(X > 2) = P(X < -2)$.

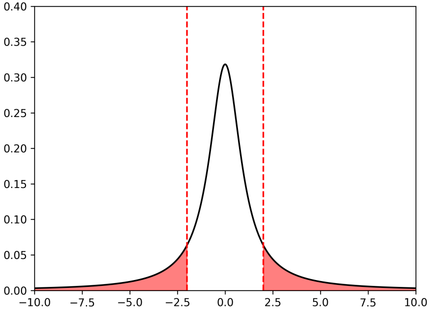

Figure: Cauchy density

We could compute:

$$\mathbb{P}(|X| > 2) = \mathbb{P}(X > 2) + \mathbb{P}(X < -2) = 2I.$$

Therefore, our new problem is $I = \frac{1}{2}\mathbb{P}(|X| > 2)$.

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Therefore, our new problem is $I = \frac{1}{2}\mathbb{P}(|X| > 2)$.

Write it as

$$\begin{aligned} I &= \frac{1}{2}\int_{|x|>2} p(x)\mathrm{d}x, \\ &= \int \frac{1}{2}\mathbf{1}_{\{|x|>2\}}(x)p(x)\mathrm{d}x, \end{aligned}$$

Now define the test function

$$\varphi(x) = \frac{1}{2}\mathbf{1}_{\{|x|>2\}}(x).$$

We need to compute $\mathrm{var}_p(\varphi)$.

We need to compute $\mathsf{var}_p(\varphi)$.

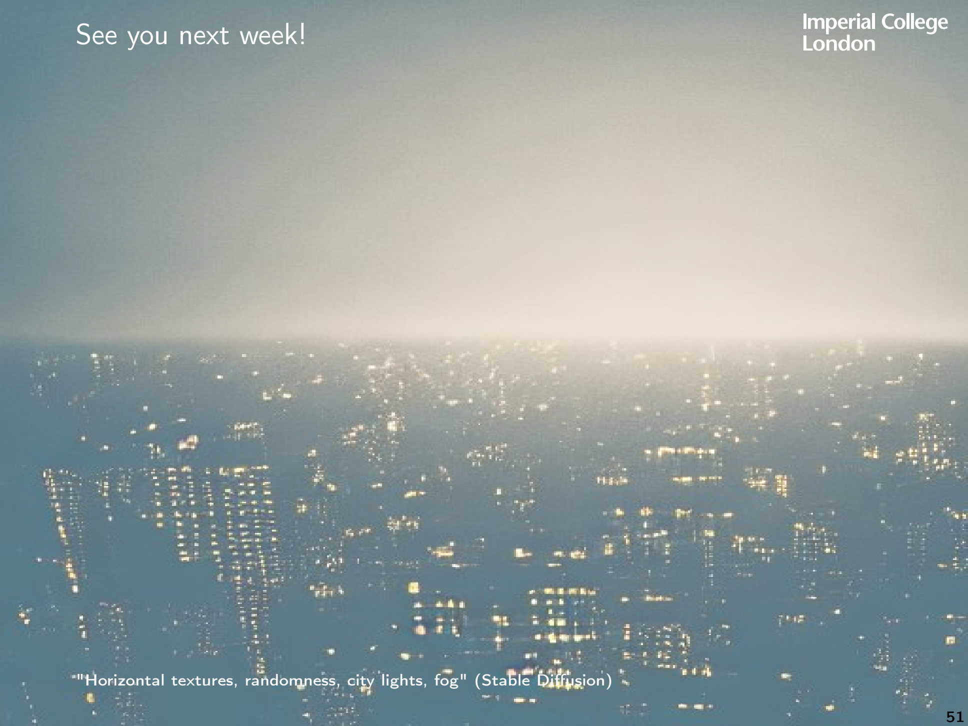
$$\begin{aligned}
\mathsf{var}_p(\varphi) &= \int \varphi(x)^2 p(x)\mathrm{d}x - \left(\int \varphi(x)p(x)\mathrm{d}x\right)^2 \\
&= \int \frac{1}{4}\mathbf{1}^2_{\{|x|>2\}}p(x)\mathrm{d}x - \left(\int \frac{1}{2}\mathbf{1}_{\{|x|>2\}}p(x)\mathrm{d}x\right)^2 \\
&= \int \frac{1}{4}\mathbf{1}_{\{|x|>2\}}p(x)\mathrm{d}x - \left(\int \frac{1}{2}\mathbf{1}_{\{|x|>2\}}p(x)\mathrm{d}x\right)^2 \\
&= \frac{1}{4} \times 2 \times 0.1476 - \frac{1}{4} \times (2 \times 0.1476)^2, \\
&= 0.052.
\end{aligned}$$

Therefore, the variance of the estimator for $N = 10$ samples is

$$\mathsf{var}(\hat{\varphi}^N) = \frac{0.052}{10} = 0.0052.$$

Improvement over the previous estimator! That was 0.0125.

See you next week!



"Horizontal textures, randomness, city lights, fog" (Stable Diffusion)

References I

- Robert, Christian P and George Casella (2004). *Monte Carlo statistical methods*. Springer.
- Akyildiz, Omer Deniz (2019). "Sequential and adaptive Bayesian computation for inference and optimization". Can be accessed from: http://akyildiz.me/works/thesis.pdf. PhD thesis. Universidad Carlos III de Madrid.