

Lecture 3 -Crude Monte Carlo, importance sampling

Monte Carlo method

Example of a multidimensional integral

$$\int_a^b dx_1 \int_a^b dx_2 \dots \int_a^b dx_n f(x_1, \dots, x_n)$$

Has to be evaluated.

A deterministic method: a uniform

bin each variable $\{x_i\}$ into 100 points

Question? Largest N which can be directly used?

A₁ Answer memory limit $16b \sim 10^9$ values

Total number of points

$$100 \cdot 100 \cdot \dots \cdot 100 = 100^N = 10^{2N}$$

Memory $10^9 \approx 10^{2N}$; $N \sim 4-5$

A₂ Whole capacity of internet $\sim 10^{24}$ bytes

$$10^{24} \sim 10^{2N}; N \approx 12$$

Size of the digital universe

- in 2020 44 zettabytes
- is doubled every two years
- 1 ZB = 10^{21} B

→ instead stochastic methods can be used

Crude Monte Carlo method (hit-or-miss meth.)

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$$\int_a^b f(x) dx = (b-a) \int_a^b f(x) p(x) dx$$

where $p(x) = \frac{1}{b-a}$ is the uniform distribution

CLT can be applied:

- expectation value of $f(x)$
- with respect to the uniform distribution on $[a; b]$

$$\langle f \rangle = \int_a^b f(x) dx = \lim_{N \rightarrow \infty} (b-a) \frac{1}{N} \sum_{i=1}^N f(x_i)$$

where x_i are taken from a uniform distribution

- expectation \rightarrow approximation for the integral
Statistical error:

$$\frac{\sigma^2}{N} = \lim_{N \rightarrow \infty} \frac{(b-a)^2}{N} \left[\frac{1}{N} \sum_{i=1}^N f^2(x_i) - \left(\frac{1}{N} \sum_{i=1}^N f(x_i) \right)^2 \right]$$

Monte Carlo method with importance sampling

- sample the important region
- another application of CLT in a form

$$\int f(x) p(x) dx$$

where $p(x)$ is a PDF

- any integral can be written in the form

$$\int f(x) dx = \int \left[\frac{f(x)}{p(x)} \right] p(x) dx$$

from MC interpretation:

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x in uniform distribution $\xrightarrow{\quad}$ x in distribution $p(x)$

$$\left. \frac{1}{N} \sum_{i=1}^N f(x_i) \right|_{x_i \text{ uniform}} \quad \left. \frac{1}{N} \sum_{i=1}^N \frac{f(x_i)}{p(x_i)} \right|_{x_i \text{ according to } p(x)}$$

Variance:

$$\int f^2(x) dx - \langle f \rangle^2 \quad \underbrace{\int \left[\frac{f(x)}{p(x)} \right]^2 p(x) dx - \langle f \rangle^2}$$

can be reduced
by a proper choice of $p(x)$

Choose $p(x)$ in such a way that it samples more important points, the ones which provide large contribution

Generating a non-uniform PDF

- random values u_i from uniform random distribution can be used to generate a PDF $p(x)$ for which its cumulative function $P(x)$ is known and can be inverted
- $x_i = P^{-1}(u_i)$ are distributed according to $p(x)$

Ex: generate distribution $p(x) = 2xe^{-x^2}, x \geq 0$
 $\int p(x) dx = 1$

Its cumulative function

$$P(x) = \int_0^x p(x') dx' = \int_0^x 2x' e^{-x'^2} dx = e^{-x'^2} \Big|_0^x \\ = -e^{-x^2} + 1$$

Inverse function: $x(u)$

$$u = 1 - e^{-x^2}$$

$$e^{-x^2} = 1 - u$$

$$-x^2 = \ln(1-u)$$

$$x^2 = -\ln(1-u)$$

$$x = \sqrt{-\ln(1-u)} \leftarrow \text{desired random variable}$$

where $0 < u < 1$ is a uniformly distributed random variable

Actually $1-u$ is also a uniform distribution

$\Rightarrow x = \sqrt{-\ln u}$ can be as well used

Normal Random generator

Goal: generate random variables corresponding to Normal PDF:

$$p(x) = \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\}$$

Box-Muller method, polar coordinates

- use uniform random generator to calculate two random values u_1, u_2 :
 $0 < u_1 < 1$
 $0 < u_2 < 1$
- calculate $r = \sqrt{-2 \ln u_1}$ - radius
 $\varphi = 2\pi u_2$ - angle
- calculate two independent random variables

$$z_0 = r \cdot \cos \varphi$$

$$z_1 = r \cdot \sin \varphi$$

distributed according PDF: $p(z) = \exp\left\{-\frac{z^2}{2}\right\}$

- adjust the mean value and the variance

$$x_0 = \mu + z_0 \cdot \sigma$$

$$x_1 = \mu + z_1 \cdot \sigma$$