Lecture October 22

Monte Carlo methods

— MC integration.

$$\mathbb{E}[f] = \langle f \rangle = \int_{x \in D} f(x)\, p(x)\, dx = \mu_f$$

$$\sigma_f^2 = \int_{x \in D} (f(x) - \mu_f)^2 p(x)\, dx$$

$$\left[\begin{array}{l} \mu_f = \sum_{i \in D} f(x_i)\, p(x_i) \\ \sigma_f^2 = \sum_{i \in D} (f(x_i) - \mu_f)^2 p(x_i) \end{array} \right.$$

Sample mean and other sample expectation values

$$\mu_f \neq \bar{\mu}_f = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

$$\bar{\sigma}_f^2 = \frac{1}{N} \sum_{i=1}^{N} (f(x_i) - \bar{\mu}_f)^2$$

standard deviation

$$\sigma_f \sim \frac{1}{\sqrt{N}}$$

Central limit theorem (later)

MC - integration (smarter)

- change of variables
- importance sampling

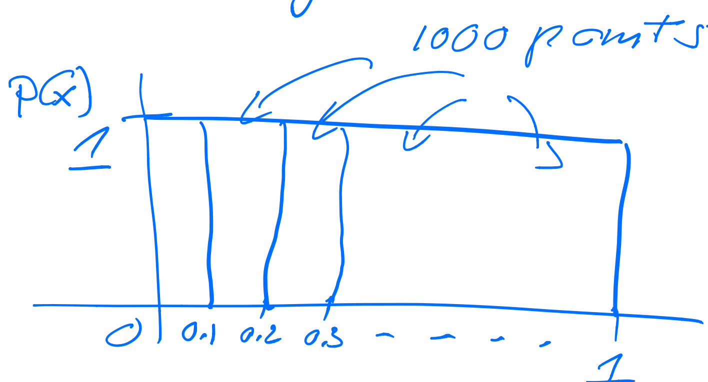
$$I = \int_a^b f(x)\,dx \simeq \frac{1}{N}\sum f(x_i)$$

$$x_i \in [a,b]$$

RNG, uniform distribution

RN = random numbers

RN $\tilde{x}_i \in [0,1]$ with uniform PDF $p(x)\,dx$



$N = 10^4$

can map $\tilde{x}_i \in [0,1] \to x_i \in [a,b]$

$$\boxed{x_i = a + (b-a)\tilde{x}_i}$$

$$\int_0^\infty e^{-x} x^2\, dx$$

changes of variables;

$$p(x)\,dx = \begin{cases} dx & 0 \le x \le 1 \\ 0 & \text{else} \end{cases}$$

$$\int_{x \in D} p(x)\,dx = 1$$

Probability is conserved

$$p(y)\,dy = p(x)\,dx$$

uniform distrib.

$$p(y)\,dy = dx$$

$$x(y) = \int_0^y p(y')\,dy' =$$

CDF or cumulative distribution function.

$$p(y)\,dy = \begin{cases} \frac{dy}{b-a} & a \le y \le b \\ 0 & \text{else} \end{cases}$$

$$p(y)\,dy = \frac{dy}{b-a} = dx$$

$$x(y) = \int_0^y \frac{dy}{b-a} \Rightarrow$$

$$y = a + (b-a)\,x$$

$y \in [0, 2\pi]$ $\qquad$ $x \in [0, 1]$

RNG

$y = 2\pi \cdot x$

Example: $\quad p(y)\,dy = e^{-y}\,dy$

$\qquad y \in [0, \infty)$

$$p(y)\,dy = dx$$

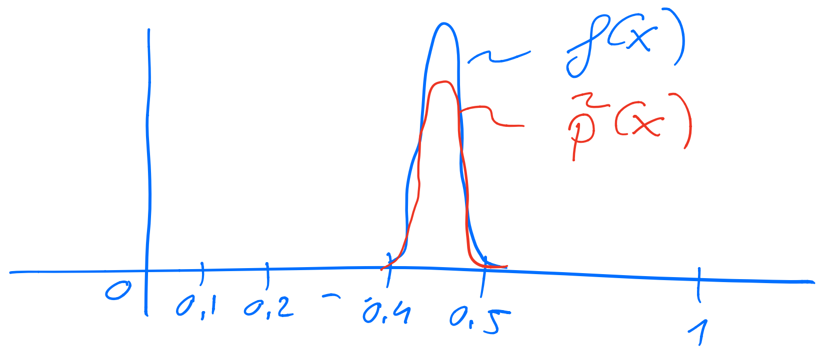
$$x(y) = \int_0^y e^{-y'}\,dy' = 1 - e^{-y}$$

$$\Rightarrow \quad y(x) = -\ln(1-x)$$

$x \in [0, 1]$

Analytically integrable CDF.

$$I = \int_0^1 f(x)\,dx$$



RNG given by uniform distribution $x \in [0, 1]$

$N = 10^6$

$$\left.\begin{matrix}\tilde{p}(x)\\ f(x)\end{matrix}\right\} \; x \in [0{,}4;\, 0{,}5]$$

$$\frac{f(x)}{\tilde{p}(x)} = \underline{\text{constant}},$$

change of variables + importance sampling

$$I = \int_0^1 f(x)\,dx = \int_0^1 \underline{\tilde{p}(x)}\, \frac{f(x)}{\tilde{p}(x)}\, \underline{dx}$$

$$= \int_0^1 \tilde{p}(x)\, F(x)\, dx$$

$x \in [0,1]$

$$\sigma_F^2 = \frac{1}{N} \sum_{x \in D} \left(F(x_i) - \mu_F \right)^2$$

$$= \frac{1}{N} \sum_{x \in D} \left(F(x_i) \right)^2 - \mu_F^2$$

$$\mu_F = \text{constant}$$

$$= 0\ ?$$

Example

$$I = \int_0^1 \frac{1}{1+x^2}\, dx = \frac{\pi}{4}$$

New $p(x)\,dx = \frac{1}{3}(4-2x)\,dx$

$$\int_0^1 p(x)\,dx = 1 \qquad x \in [0,1]$$

$$f(x) = \frac{1}{1+x^2}$$

$$\frac{f(0)}{p(0)} = \frac{f(1)}{p(1)} = 3/4$$

$$y(x) = \int_0^x p(x')\,dx' = \frac{1}{3}x(4-x)$$

$$x = 2 - (4-3y)^{3/2}$$

$y=0 \quad x=0 \qquad 1 \quad y=1 \quad x=1$

$$\int_0^1 f(x)\,dx = \int_0^1 p(x)\frac{f(x)}{p(x)}\,dx$$

$$= \int_0^1 \frac{f(x(y))}{p(x(y))}\,dy$$

$$p(x)\,dx = \underbrace{p(y)\,dy}_{\text{uniform dist}} = dy$$

$$\frac{f(x(y))}{p(x(y))} = \text{constant}$$

$I = \text{constant} \Rightarrow$

$$\sigma_f^2 = 0$$

$$\int_a^b f(x)\,dx = \int_a^b p(x)\,\frac{f(x)}{p(x)}\,dx$$

$$\int_{\tilde{a}}^{\tilde{b}} \frac{f(x(y))}{p(x(y))}\,dy$$

$$\sigma_F^2 = \frac{1}{N}\sum_{i=1}^{N}\left(F(x_i) - \mu_F\right)^2$$

$$= \frac{1}{N}\sum F^2(x_i) + \mu_F^2$$

$$- 2\mu_F \underbrace{\frac{1}{N}\sum F(x_i)}_{\mu_F}$$

$$= \frac{1}{N}\sum F^2(x_i) - \mu_F^2$$