Lecture October 16

$$I = \int d\vec{r}_1 \int d\vec{r}_2 \; |\psi(\vec{r}_1, \vec{r}_2)|^2 \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

$$d\vec{r}_1 = dx_1\, dy_1\, dz_1$$

$$d\vec{r}_2 = dx_2\, dy_2\, dz_2$$

$$r_i = \sqrt{x_i^2 + y_i^2 + z_i^2}$$

$$|\vec{r}_1 - \vec{r}_2| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$$

$x_1, x_2 \in [-\lambda, +\lambda]$ $((-\infty, +\infty))$

Legendre polynomial

$$\tilde{x}_i \in [-1, 1]$$

Repeat for y and z

$$I \simeq \int_{-\lambda}^{\lambda} dx_1 \int_{-\lambda}^{\lambda} dx_2 \cdots \int_{-\lambda}^{\lambda} dz_2 \; e^{-2\alpha(r_1 + r_2)} \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

Neon ; 10 electrons in 3d

$\Rightarrow$ 30 dim integral,

$$\int dx_1 \dots dx_{10} \int dy_1 \dots dy_{10} \int dz_1 \dots dz_{10} \; f(x_1 \dots z_{10})$$

$\sim 10^{30}$ Flops

10^{10} FLOPS $\Rightarrow 10^{20}$ s

> lifetime of universe

Monte Carlo Methods

- PDF (Discrete or continuous)
- RNG (Random number generator)
- sampling rule

- calculate expectation value
- Techniques for error improvements.

$\rightarrow$ moments

$$\mathbb{E}[X^k] = \langle x^k \rangle = \int_a^b p(x)\, x^k\, dx$$

or

$$\sum_{i \in D} p(x_i)\, x_i^k$$

Function $f = f(x)$

$$\mathbb{E}[f^k] = \int_a^b p(x)\, f^k(x)\, dx$$

or

$$\sum_{i \in D} p(x_i)\, f^k(x_i)$$

μ = mean value

$$\mu = \mathbb{E}[x] = \int x\, p(x)\, dx$$

or

$$\sum_{i \in D} x_i \underbrace{p(x_i)}_{\frac{1}{n}}$$

variance σ^2

$$\text{var}[x] = \sigma^2 = \int (x-\mu)^2\, p(x)\, dx$$

$$= \mathbb{E}[x^2] - \mu^2$$

σ = standard deviation

$$\left(\sigma^2 = \sum_{i \in D} (x_i - \mu)^2 p(x_i) \right)$$

sample mean $\bar{\mu}$

$$= \frac{1}{n} \sum_{i=1}^{n} x_i \qquad p(x_i) = \frac{1}{n}$$

finite n $\quad \bar{\mu} \neq \mu$ (true)

sample variance $\bar{\sigma}^2$

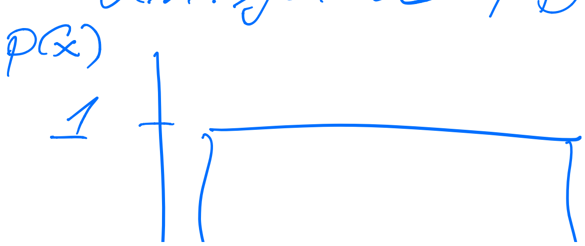
$$\bar{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{\mu})^2$$

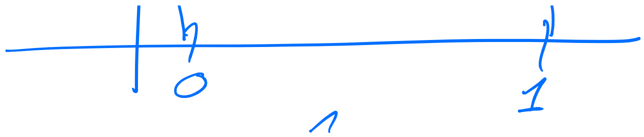
$$\bar{\sigma}^2 \neq \sigma^2$$

Our first MC calculation:

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

Uniform PDF





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

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

$$= \mathbb{E}[f] = \mu_f$$

$$\simeq \frac{1}{n} \sum_{i \in D} f(x_i)$$

Algo

Define n

— " — $f(x_i)$

initialize μ and $\sigma^2 = 0$

initialize RNG by a seed

FOR $i = 1 : n$

$x_i =$ RNG(uniform)

$f_i = f(x_i)$ ← accept all new x_i = sampling rule

$\overline{\mu} = \overline{\mu} + f_i$

$\overline{\sigma_2} = \overline{\sigma_2} + f_i^2$

END FOR

$\overline{\mu} = \overline{\mu} / n$

$$\overline{\sigma}^2 = \overline{\sigma^2}/n - \bar{\mu}^2$$