Wed July 3 2019

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Go back to simple initial examples:

(i): LCG $0 \le J_i \le m-1$

(ii): Normalization $0 \le r_i \le 1$; $r_i = \frac{J_i}{(m-1)}$

Probability Density Function $p(x) = 1$

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

(iii) Normalization on other interval

$0 \le x_i \le a$; $x_i = a\, r_i$

Equal Probability Density Function $p(x) = \frac{1}{a}$

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

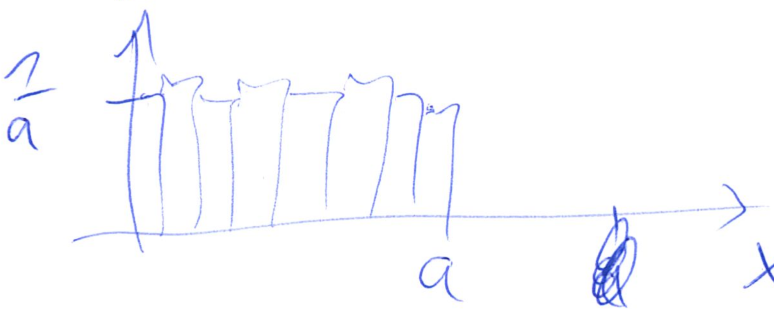
(iv) Generalized to volume: $\vec{x} = (x_1, \dots x_n) \in \mathbb{R}^n$

Volume $V \in \mathbb{R}^n$

Equal Probability DF $p(\vec{x}) = \frac{1}{V}$

$$\int_V p(\vec{x})\,d\vec{x} = 1$$

Approximation of integral: $J_N = \int_0^a p(x)\,dx = \sum_{i=1}^{N} p(x_i)\,\Delta x_i =$



$$= \frac{1}{a} \sum_{i=1}^{N} \Delta x_i$$

$$\lim_{N \to \infty} J_N \stackrel{!}{=} 1$$

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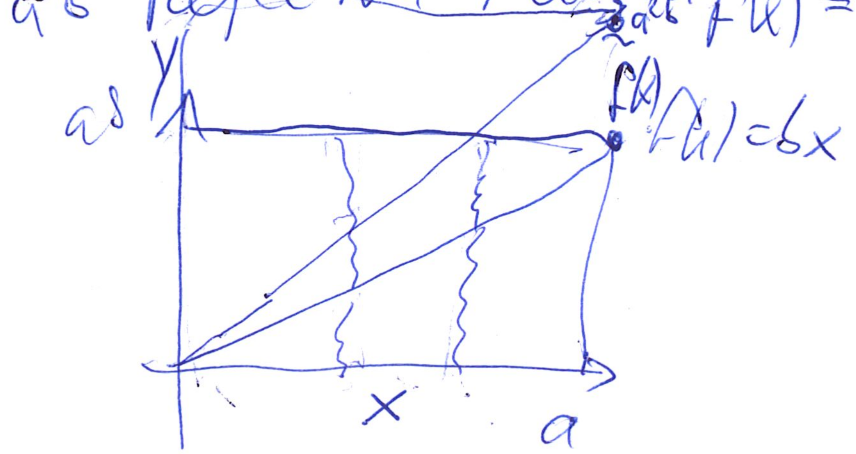
Rejection Method



Majorant: $\tilde{f}(x) = ab = \text{const.}$

$$y(x) = \tilde{F}(x) = \int_0^x \tilde{f}(x')dx' = abx + C$$

$$\tilde{F}(0) = 0 \quad \Rightarrow \quad C = 0$$

$$\tilde{F}(a) = a^2 b$$

$$x = \tilde{F}^{-1}(y) = \frac{y}{ab}$$

$0 \leq y_i \leq a^2 b$ equally distributed

$0 \leq x_i \leq a$ equally distributed

Now $0 \leq y_i' \leq \tilde{f}(x) = ab$

If $y_i' \leq f(x_i) = bx_i$ accept

$y_i' \geq f(x_i)$ reject

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9.1. Monte Carlo Integration

$p(\vec{x})$ PDF for random vectors $\vec{x} \in \mathbb{R}^n$
$V \subseteq$

(some average)

$\langle f \rangle_p$ expectation value of f over p

$$\langle f \rangle_p = \int_V f(\vec{x}) p(\vec{x}) d\vec{x} \; ; \quad V = \int_V d\vec{x}$$

In case of equally distributed PDF:

$$p(\vec{x}) = \frac{1}{V} = \text{const.} \quad \int_V p(\vec{x}) d\vec{x} = 1$$

In the following keep to 1D case:

$$\langle f \rangle_p = \int_a^b f(x) p(x) dx$$

$\left[\text{if const. PDF } p(\vec{x}) = \frac{1}{b-a}\right]$
$= \frac{1}{b-a} \int_a^b f(x) dx$

Squared Expectation value (mean square)
(second moment)

$$\langle f^2 \rangle_p = \int_a^b f^2(x) p(x) dx$$

Note: $\langle (f - \langle f \rangle_p)^2 \rangle = \int_a^b (f - \langle f \rangle_p)^2 p(x) dx$

$$= \langle f^2 \rangle_p + \langle f \rangle_p^2$$

Variance of f over p:

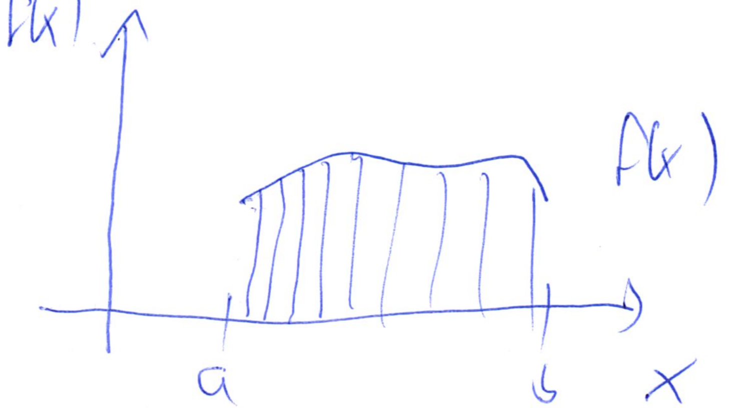
$\sigma^2 = Var(f) = \int (f - \langle f \rangle_p)^2 p(x) dx$

Empirical approximation of exp. value by finite set of random numbers:

$$\overline{f_N} = \frac{1}{N}\sum_{i=1}^{N} f(x_i) \qquad \overline{f_N^2} = \frac{1}{N}\sum_{i=1}^{N} f(x_i)^2$$

$\lim_{N\to\infty} \overline{f_N} = \langle f\rangle_p$ $\lim_{N\to\infty} \overline{f_N^2} = \langle f^2\rangle_p$

using x_i distributed according to $p(x)$



$\overline{f_N}$: average of f over interval

$\overline{f_N^2}$: average of f^2

They are called empirical mean and second moment.

By law of large numbers (central limit theorem) many $\overline{f_N}$ samples have a Gaussian distribution around the expectation value $\langle f\rangle_p$ with variance

$$\langle f\rangle_p = \overline{f_N} \pm \sigma_N(f) \qquad \lim_{N\to\infty} \overline{f_N} = \langle f\rangle$$

$$\sigma_N^2 = \frac{1}{N-1}\left[\overline{f_N^2} - \overline{f_N}^2\right] \sim \frac{1}{N}\left(\langle f^2\rangle - \langle f\rangle^2\right)$$

Conclusion:

- Determine $\langle f \rangle_p = \int f(x) p(x) dx$ in this way error decreases with $N^{-1/2}$ only! MC worse than other num. integrators!
- But robust and easy to use, esp. in multi-dimensional case.

Simple Demonstration of Central Limit Theorem:

Rolling Dice: $\overline{f_N} = \frac{1}{N} \sum x_i \quad 1 \leq x_i \leq 6$

One "Sweep": N times rolling dice

Expectation value for average: $\langle f \rangle = 3.5$

Many "Sweeps": Distribution of averages

Gaussian Distribution around $\langle f \rangle$ with $\sigma_N^2 \propto \frac{1}{N-1}$

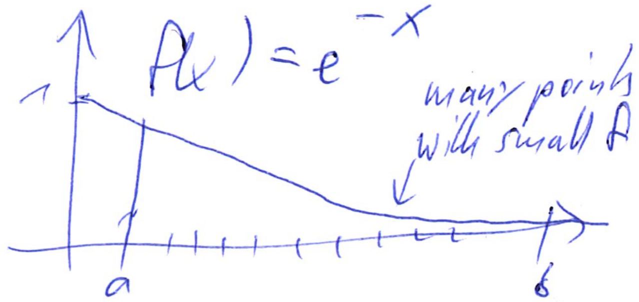
Importance Sampling

$$\langle f \rangle_p = \int_a^b f(x)\, p(x)\, dx \quad ; \quad \text{with } p(x) = \text{const.} = \frac{1}{b-a}$$

$$= \frac{1}{b-a} \int_a^b f(x)\, dx =: \frac{1}{(b-a)}\, I$$

(*) With $\overline{f_N} = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$ we can approximate $\langle f \rangle_p = I / (b-a)$

But if $f(x)$ is small in large parts of definition set, equally ~~spaced~~ distributed RV's are inefficient for sampling f



Choose $g(x)$ „near" $f(x)$:

$$I = \int_a^b \frac{f(x)}{g(x)}\, g(x)\, dx \quad ; \quad \text{choose RV's with PDF } g(x) : 1 = \int_a^b g(x)\, dx$$

Then

(**) $\overline{f_N} = \frac{1}{N} \sum \frac{f(x_i)}{g(x_i)}$ approximates I with RN distr. as $g(x_i)$

Note: in (*) we approx. $\langle f \rangle_p = I / b-a$; in (**) I directly approx.!!

Example: Method 1: $\overline{f_N} = \frac{1}{N} \sum e^{-x_i}$ x_i equally distr.

Method 2: $\overline{f_N} = \frac{1}{N} \sum e^{-x_i/2}$ x_i with PDF $c \cdot e^{-x_i/2}$!

(get with transformation)! c by normalization cond.!