The Monte Carlo method

EUTEMPE-RX module 03

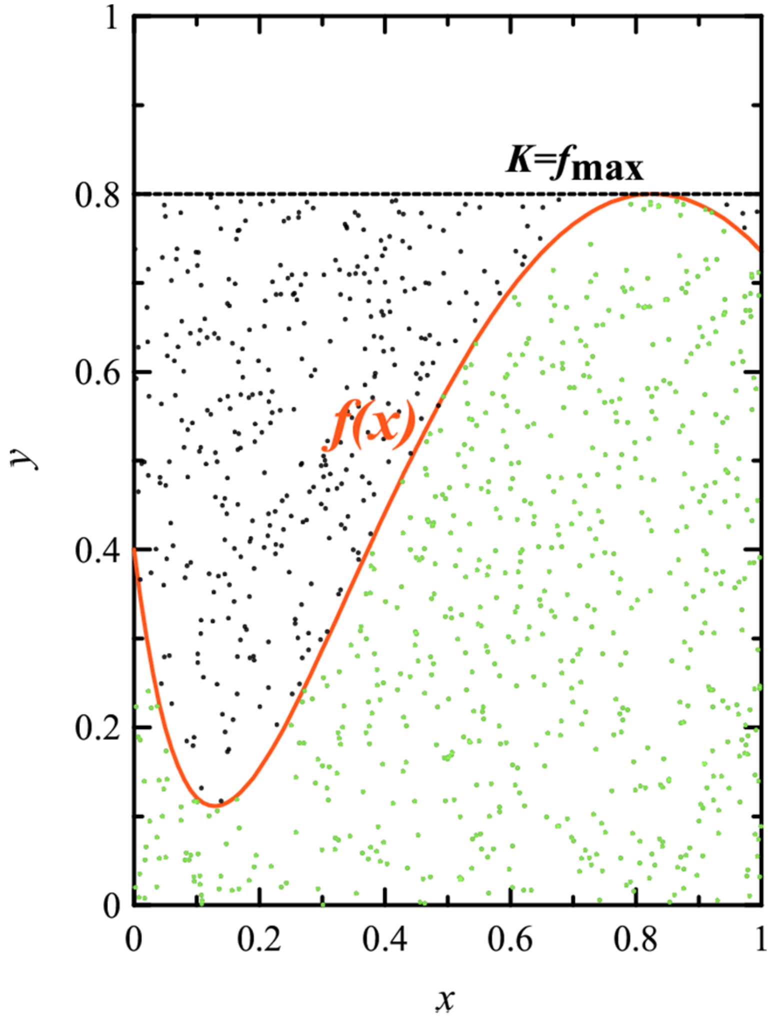
Monte Carlo simulation of x-ray imaging and dosimetry

Barcelona, June 2017

What is Monte Carlo?

- MC methods are a class of numerical techniques distinguished by the use of **stochastic** (i.e. non-deterministic) algorithms to simulate the behaviour of physical or mathematical systems.
- Based on the modelling of individual object-object relationships (conceptual **simplicity** and **flexibility**).
- It involves random sampling of many individual object-object interactions to find the average value of some quantity of interest (**repetitive** calculation). Computers are well suited for this task.
- There are applications in game theory, traffic flow, social science, mathematics, finance, quantum chemistry, **radiation physics**, etc.

An example: MC integration



$$I = A\frac{N_{\text{hits}}}{N} = A\frac{\sum_{i=1}^{N} q_i}{N}$$

q_i = 0 or 1

I is a random variable

$$\langle I \rangle = A\frac{\sum \langle q_i \rangle}{N} = A\langle q \rangle$$

$$\sigma^2(I) = A^2\frac{\sum \sigma^2(q_i)}{N^2} = A^2\frac{\sigma^2(q)}{N}$$

$$\text{uncertainty} \sim \frac{1}{\sqrt{N}}$$

A little bit of history

- The underlying concept of using random numbers can be traced back to the early pioneers of prob. theory (Buffon, Gosset).

Source: Wikipedia

Georges L Leclerc
(Comte de Buffon)
1707 (France) - 1788

William S Gosset
(a.k.a. Student)
1876 (UK) - 1937

Source: Wikipedia

- Fermi used random numbers in the 30s to evaluate some properties of the newly discovered neutron.

Source: Wikipedia

Enrico Fermi
1901 (Italy) - 1954

- Simulations during the Manhattan Project (WW2), limited by computing power.

- With the advent of electronic computers (1945) MC methods were taken seriously.

- In the 50's MC was used at Los Alamos for early work on the H-bomb.

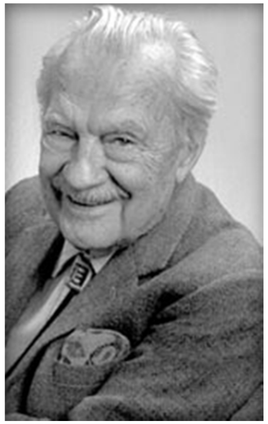
- The invention of the Monte Carlo method is attributed to Stanislaw Ulam, a Polish-born mathematician who worked for John von Neumann on the Manhattan Project (Ulam is primarily known, with Edward Teller, for the H-bomb design in 1951).

Source: Wikipedia

Stanislaw M. Ulam
1909 (Austria-Hungary)-1984

Source: Wikipedia

John von Neumann
1903 (Austria-Hungary)-1957



Source: Wikipedia

Nicholas C. Metropolis
1915 (USA) - 1999

Random number generators

- Truly RNGs can be based on random processes, like thermal noise, radioactive decay, coin flipping...

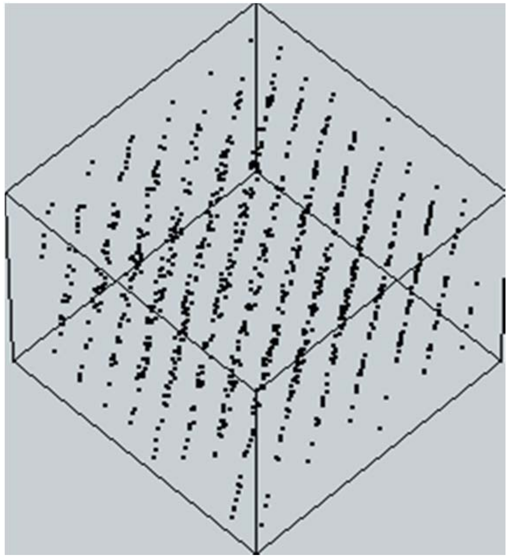
There are good reasons **not** to do it in this way: computing **speed** and **repeatability.**

- Or on arithmetic, and therefore deterministic, algorithms: pseudo-random.

Multiplicative Linear Congruential (MLCG)

An MLCG is defined by $S_{i+1} = (aS_i)\,\mathrm{MOD}\,m \;, \quad u_i = \frac{S_i}{m}$

- Cyclical, with a period $T \leq (m-1)$. For 32-bit-long signed integers, $T \sim 2 \times 10^9$ at most, insufficient for present-day applications.
- a and m must be chosen carefully to ensure good random properties.
- The **spectral test** (Marsaglia 1968) is of particular interest.



spectral test failure

A bad example: RANDU (SSP package):

$$S_{i+1} = (65539\, S_i)\,\mathrm{MOD}\,2^{31}$$

RANECU (l'Ecuyer)

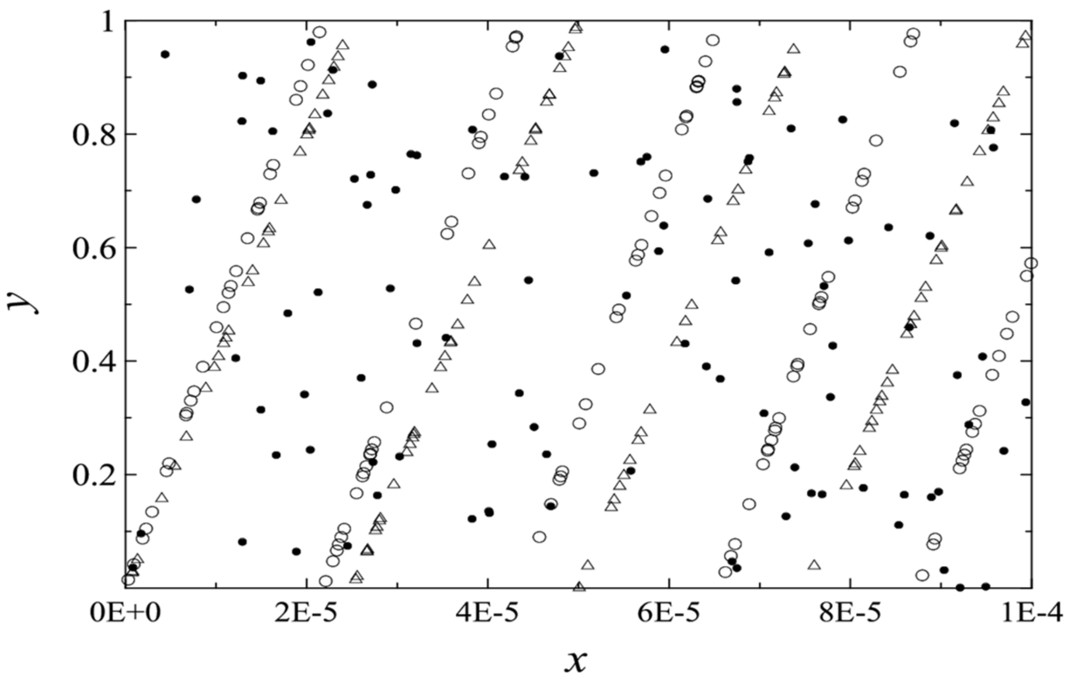
P. l'Ecuyer
Comm. ACM 31 (1988)

Combines two MLCGs : $S_i \;=\; (S_i^{(1)} - S_i^{(2)})\ \mathrm{MOD}\ (m^{(1)} - 1)$

Parameters of the MLCGs that are used in RANECU

	Modulus (m)	Multiplier (a)
1st generator	2 147 483 563	40 014
2nd generator	2 147 483 399	40 692

$$T = \mathrm{lcm}(m^{(1)} - 1, m^{(2)} - 1) \sim 2 \times 10^{18}$$



good spectral properties

Some other good RNGs

- RANLUX (Lüscher 1994), based on a lagged Fibonacci algorithm called subtract-and-borrow (c_i is the carry bit, 1 or 0):

$$S_i = (S_{i-10} - S_{i-24} - c_{i-1}) \ \mathrm{MOD}\ 2^{24} \ , \quad i > 23$$

Some elements are discarded to eliminate short-ranged correlations

- High-quality, with a period $T \sim 10^{171}$ (!), but slow.

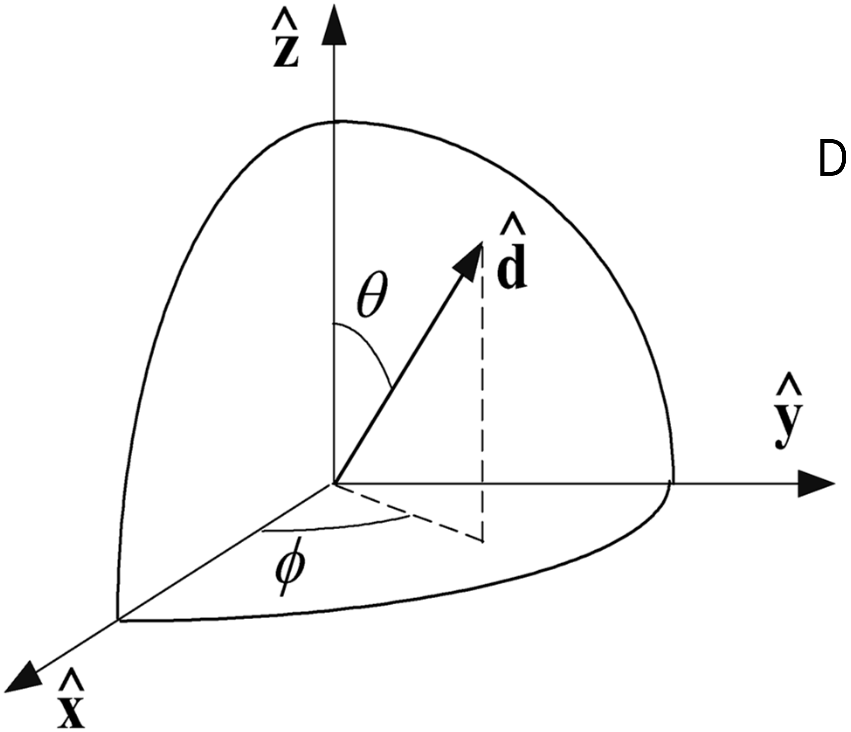
- Mersenne Twister (M Matsumoto et al 2000), based on a linear feedback shift register, which involves binary operations with the seed bits
  - considerably faster than RANLUX and RANECU.
  - has passed the most relevant random tests.
  - cycle period ~ 10^{6001} (!!!)
  - lack of a theoretical basis for its weaknesses.

All the previous RNGs can be “parallelized”.

Elements of probability theory

- Understand underlying concepts and simulation results.
- Prepare/adapt your own routines (*e.g.* radiation sources).

Example: isotropic source



Direction of motion: $\hat{\mathbf{d}} = (u, v, w)$

- Prob. of *u*, *v* and *w* ?
- Sampling algorithm?

Probability distribution function (PDF)

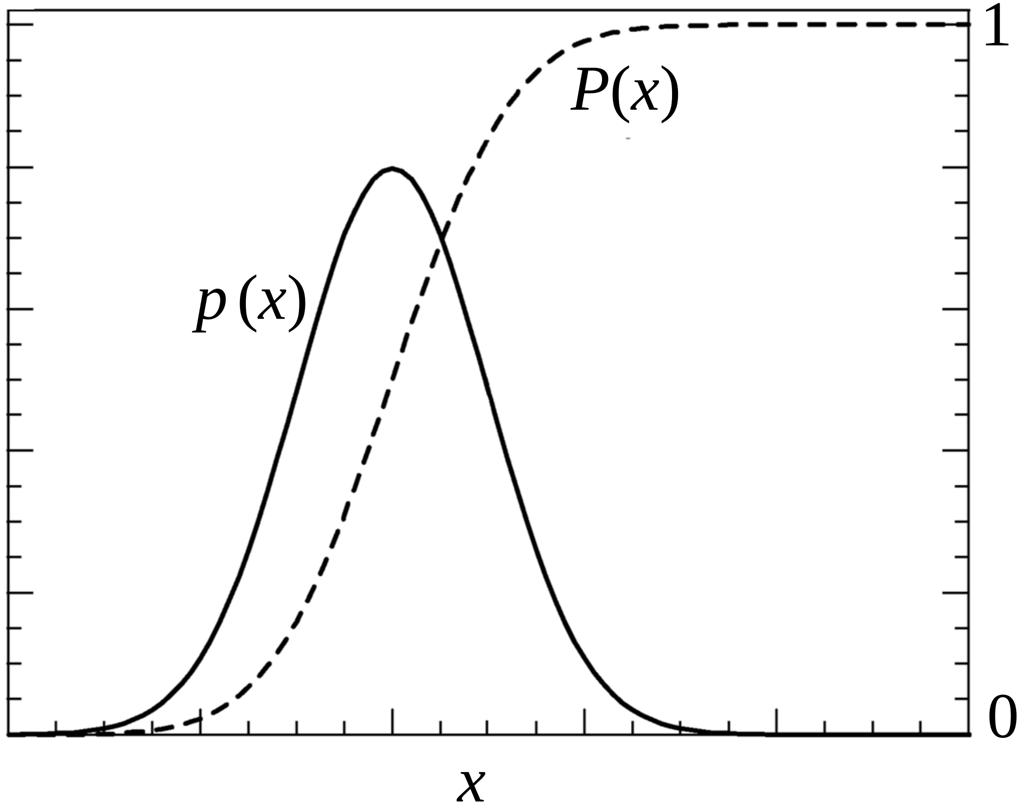
$$p_\eta(x) = \frac{\mathcal{P}(x < \eta < x + \mathrm{d}x)}{\mathrm{d}x}$$

$$p(x) \geq 0$$

$$\int_{-\infty}^{+\infty} \mathrm{d}x \; p(x) = 1$$

$$P(x) \equiv \int_{-\infty}^{x} \mathrm{d}x' \; p(x')$$

From PENELOPE's manual



For discrete variables $p(x) = \sum_i p_i \, \delta(x - x_i)$

Moments of a random variable

Expected value
‹·› is a linear operator

$$\langle x \rangle = \int \mathrm{d}x \; p(x) x$$

PDF of a dependent r.v.

$$p(y) = p(x) \; \left| \frac{\mathrm{d}x}{\mathrm{d}y} \right|$$

Expected value
of a derived r.v.

$$\langle y(x) \rangle = \int \mathrm{d}y \; p(y) y = \int \mathrm{d}x \; p(x) y(x)$$

Variance

$$\sigma^2(x) \equiv \left\langle (x - \langle x \rangle)^2 \right\rangle = \langle x^2 \rangle - \langle x \rangle^2$$

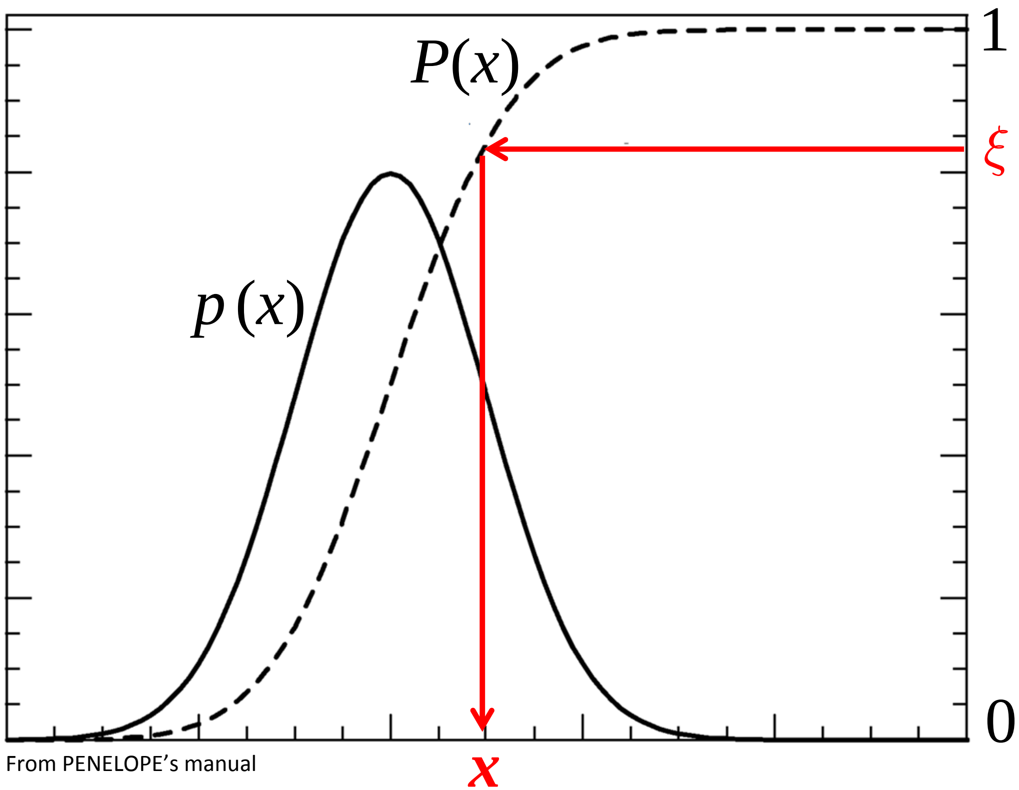
Can be readily extended to multiple r.v.'s using marginal PDFs

$$p(x_i) = \int \left(\prod_{j \neq i} \mathrm{d}x_j \right) \; p(x_1, \ldots, x_n)$$

Random sampling

Inverse transform

Define $\xi(x) = \int^{x} \mathrm{d}x' \; p(x')$ then $p(\xi) = p(x) \left| \frac{\mathrm{d}x}{\mathrm{d}\xi} \right| = p(x) \frac{1}{p(x)} = 1$



Examples

Uniform PDF $$p(\phi) = \frac{1}{2\pi} \qquad \phi \in (0, 2\pi)$$

Solution: $$\xi = \int_0^{\phi} \mathrm{d}\phi' \, \frac{1}{2\pi} = \frac{\phi}{2\pi} \quad \Rightarrow \quad \phi = 2\pi\xi$$

Exponential PDF $$p(s) = \frac{1}{\lambda} \exp(-s/\lambda) \qquad s \in (0, +\infty)$$

Solution: $$s = -\lambda \ln(1 - \xi) = -\lambda \ln \xi$$

Rejection

Consider a PDF $p(x)$

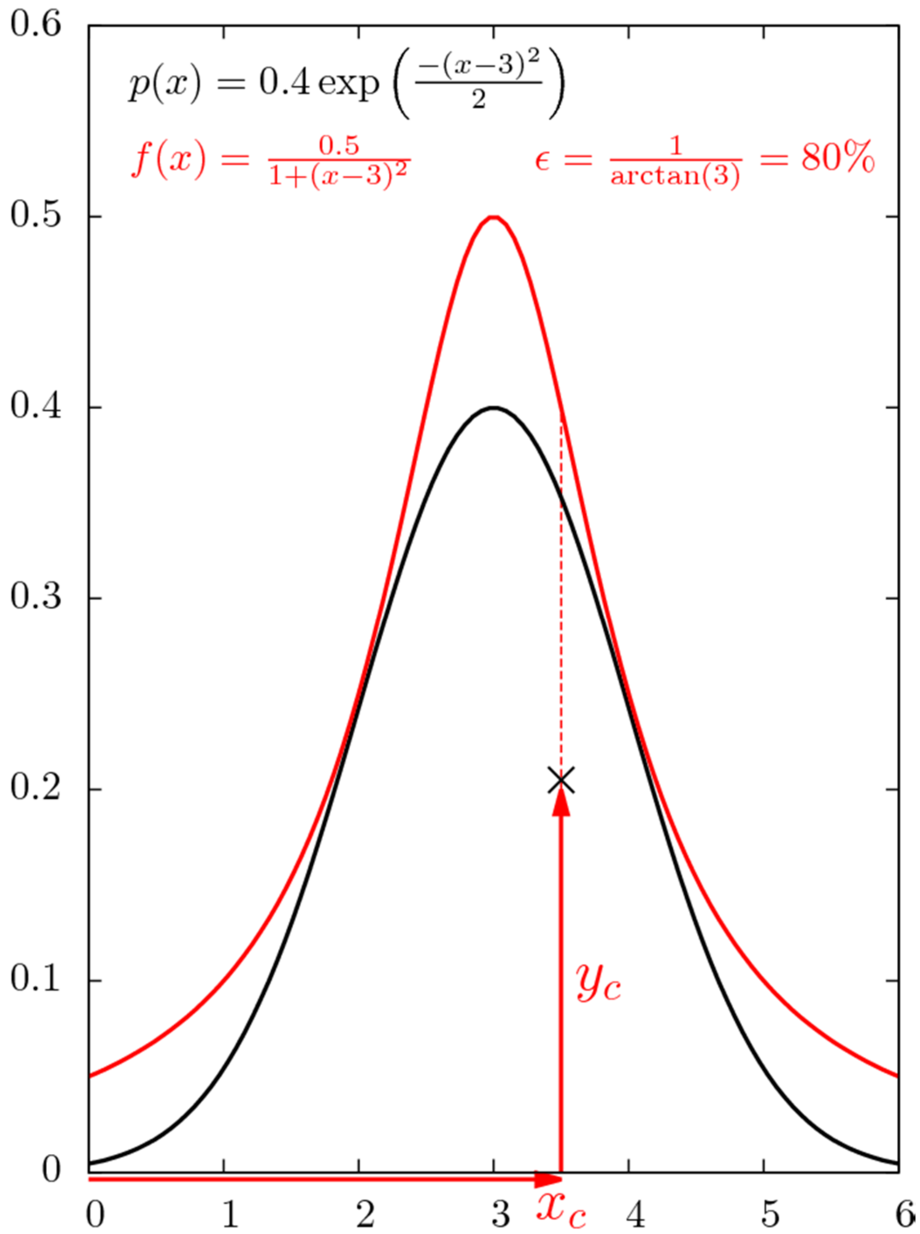
Define an arbitrary function $f(x) \geq p(x)$ that can be sampled easily (*e.g.*, inversion).

To sample $p(x)$ perform these steps:

1. Generate $x_c = \text{sample}\{f(x)\}$
2. Sample $y_c = \xi \cdot f(x_c)$
3. If $y_c > p(x_c)$ go to 1 (x_c rejected)
4. Deliver x_c

The ratio of success ("efficiency") of the process is

$$\epsilon = \frac{\text{area}\{p(x)\}}{\text{area}\{f(x)\}} = \frac{1}{\text{area}\{f(x)\}} \leq 1$$



Gaussian: Box-Müller method

G. E. P. Box and M. E. Muller
Ann. Math. Statist. 29 (1958)

Of particular interest is the sampling of a Gaussian PDF,

$$G(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right)$$

$$G(x,y) = \frac{1}{2\pi} \exp\left(-\frac{x^2+y^2}{2}\right)$$ (originally proposed by Laplace)

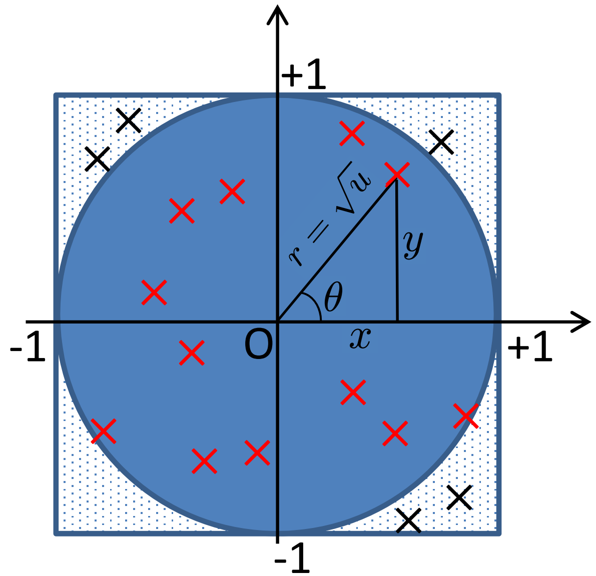
$$G(r,\theta) = rG(x,y) = \frac{r}{2\pi} \exp\left(-\frac{r^2}{2}\right) = \left[\frac{1}{2\pi}\right] \left[r \exp\left(-\frac{r^2}{2}\right)\right]$$

Sampling algorithm (**Box-Müller method**):

$$x = r\cos\theta = \sqrt{-2\ln\xi_1}\;\cos(2\pi\xi_2)$$

$$y = r\sin\theta = \sqrt{-2\ln\xi_1}\;\sin(2\pi\xi_2)$$

Polar method



1. Sample (x, y) in a unit circle using a rejection method:

$$x = 1 - 2\xi_1 \quad , \quad y = 1 - 2\xi_2$$

$$\text{if } u \equiv x^2 + y^2 > 1 \ \Rightarrow \ \text{reject}; \ \left(\epsilon = \frac{\pi}{4} = 78.5\%\right)$$

2. In the (r, θ) and (u, θ) spaces the PDFs are

$$p(r,\theta) = p(x,y)\left|\det\frac{\partial(x,y)}{\partial(r,\theta)}\right| = \frac{r}{\pi} = \left(\frac{1}{2\pi}\right)(2r) = p(\theta)\,p(r)$$

$$p(u,\theta) = p(r,\theta)\left|\frac{\mathrm{d}r}{\mathrm{d}u}\right| = \frac{p(r,\theta)}{2r} = \left(\frac{1}{2\pi}\right)(1) = p(\theta)\,p(u)$$

Note that: (i) u and θ are independent; and (ii) u is uniformly distributed in (0,1).
The polar method takes advantage of these two facts.

G. Marsaglia and T. A. Bray
SIAM Review 6 (1964)

Marsaglia & Bray's polar method avoids (expensive) computations of trigonometric functions.

Box-Müller:

$$v_1 = r\cos\theta = \sqrt{-2\ln\xi_1}\,\cos(2\pi\xi_2)$$

$$v_2 = r\sin\theta = \sqrt{-2\ln\xi_1}\,\sin(2\pi\xi_2)$$

Polar method: (Recall that $u \equiv x^2 + y^2$ for (x, y) inside the unit circle.)

$$v_1 = \sqrt{-2\ln u}\,\frac{x}{\sqrt{u}} = x\sqrt{\frac{-2\ln u}{u}}$$

(we have used $\cos\theta = \dfrac{x}{\sqrt{u}}$)

$$v_2 = \sqrt{-2\ln u}\,\frac{y}{\sqrt{u}} = y\sqrt{\frac{-2\ln u}{u}}$$

Timings

- Intel Core i7 @ 2GHz running OSX v.10.10.2
- gfortran 4.9.0 with optimization -O
- RNGs are RANECU or simpleRNG (T=1e9)
- Speed is in ns per RNG call

Method	RANECU	sRNG	
Polar	2.93	1.92	(ns per RNG)
Polar-single	5.53	3.46	
BoxMuller	3.40	2.53	
BoxMuller-single	6.22	4.32	
LorentzReject	11.75	10.08	
CentralLimit	11.92	3.51	

Estimators, uncertainties and efficiency

- MC estimate of $\langle E \rangle$ after N independent histories :

$$\bar{E} = \frac{1}{N} \sum_{i=1}^{N} e_i$$

- $\bar{E}$ is a random variable:
  - Gaussian distributed (central limit theorem)
  - Unbiased: $\langle \bar{E} \rangle = \langle E \rangle$
  - Consistent: tends to $\langle E \rangle$ in probability (law of large numbers)
  - Efficient: lowest possible variance

- Statistical uncertainty:

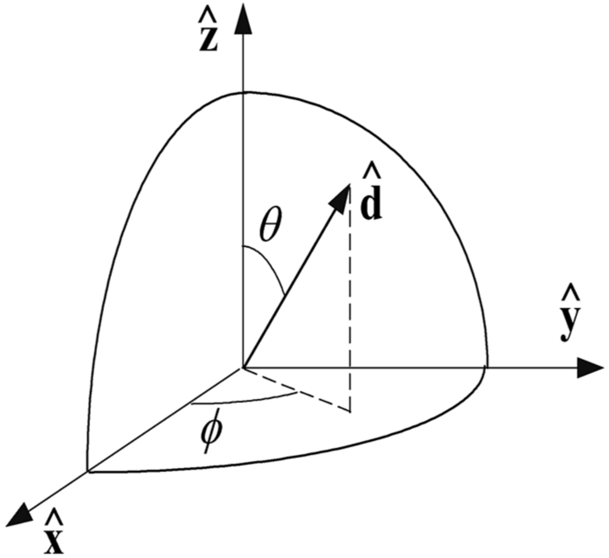
$$\sigma^2(\bar{E}) = \frac{\sigma^2(E)}{N} \simeq \frac{1}{N} \left[\frac{\sum e_i^2}{N} - \bar{E}^2 \right]$$

$$\sigma(\bar{E}) \sim N^{-1/2}$$

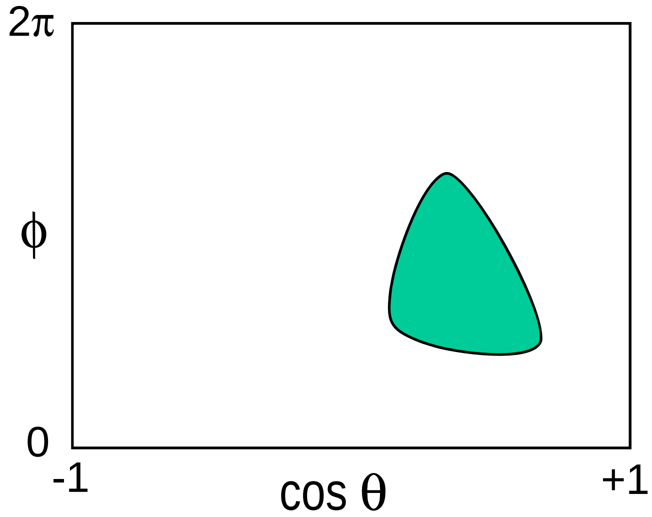
- Simulation efficiency :

$$\epsilon = \frac{1}{t\sigma^2}$$

Isotropic source — the solution



$$dS = r^2 \, d\phi \, d\cos\theta \quad \Rightarrow \quad d\Omega = d\phi \, d\cos\theta$$



Therefore, the problem can be readily solved in polar coordinates.

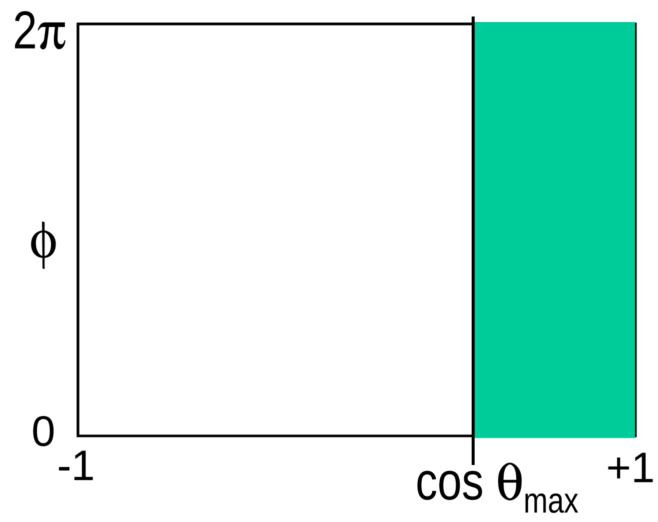
$$p(\phi, \cos\theta) = \left[\frac{1}{2\pi}\right] \left[\frac{1}{2}\right] = p(\phi) \; p(\cos\theta)$$

$$\phi = 2\pi\xi_1 \quad , \quad \cos\theta = -1 + 2\xi_2$$

$$\hat{\mathbf{d}} = (u, v, w) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$

Other useful exercises

- Initial direction uniformly distributed in a cone



Sol: $\phi = 2\pi\xi_1$

$$\cos\theta = \cos\theta_{\max} + \xi_2(1 - \cos\theta_{\max})$$

- Homogeneous radioactive source on a circle

Sol: $r = R\sqrt{\xi_1}$, $\phi = 2\pi\xi_2$

- Homogeneous radioactive source in a sphere

Sol: $r = R\xi_1^{1/3}$, $\phi = 2\pi\xi_2$, $\cos\theta = -1 + 2\xi_3$

Thank you.