

Geant 4

Basics of Monte Carlo Simulation

condensed from a presentation
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Geant4 Tutorial at Lund University

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- Historical review of Monte Carlo methods
- Basics of Monte Carlo method
 - probability density function
 - mean, variance and standard deviation
- Two Monte Carlo particle transport examples
 - decay in flight, Compton scattering
- Boosting simulation
 - variance reduction techniques
- A partial list of Monte Carlo codes

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Historical review of
Monte Carlo method

- A technique of numerical analysis that uses random sampling to simulate the real-world phenomena
- Applications:
 - Particle physics
 - Quantum field theory
 - Astrophysics
 - Molecular modeling
 - Semiconductor devices
 - Light transport calculations
 - Traffic flow simulations
 - Environmental sciences
 - Financial market simulations
 - Optimization problems
 - ...

- The Monte Carlo method is a stochastic method for numerical integration.

- Generate N random “points” \vec{x}_i in the problem space
- Calculate the “score” $f_i = f(\vec{x}_i)$ for the N “points”
- Calculate

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^N f_i, \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^N f_i^2$$

- According to the Central Limit Theorem, for large N $\langle f \rangle$ will approach the true value \bar{f} . More precisely,

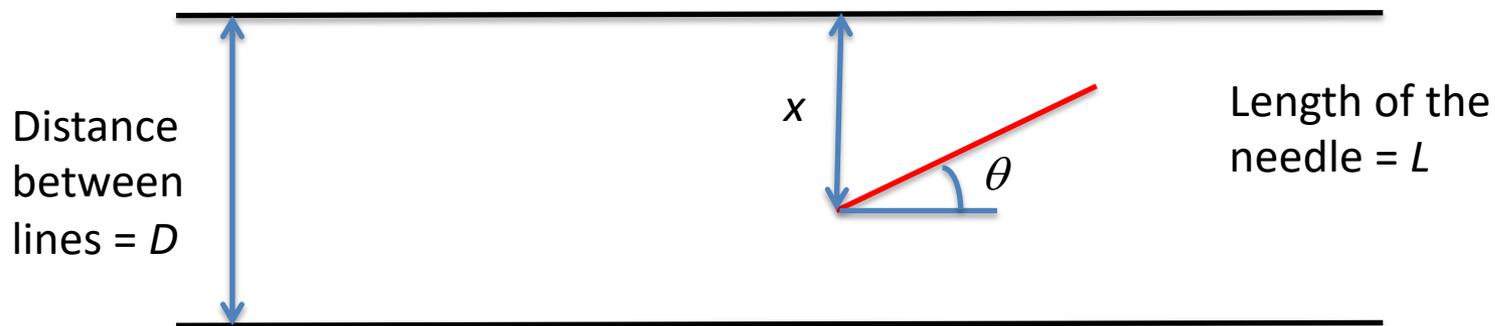
$$p(\langle f \rangle) = \frac{\exp \left[- (\langle f \rangle - \bar{f})^2 / 2\sigma^2 \right]}{\sqrt{2\pi}\sigma}, \quad \sigma^2 = \frac{\langle f^2 \rangle - \langle f \rangle^2}{N - 1}$$

Buffon's Needle

- One of the oldest problems in the field of geometrical probability, first stated in 1777.
- Drop a needle on a lined sheet of paper and determine the probability of the needle crossing one of the lines
- Remarkable result: probability is directly related to the value of π
- The needle will cross the line if $x \leq L \sin(\vartheta)$. Assuming $L \leq D$, how often will this occur?

$$P_{cut} = \int_0^\pi P_{cut}(\theta) \frac{d\theta}{\pi} = \int_0^\pi \frac{L \sin \theta}{D} \frac{d\theta}{\pi} = \frac{L}{\pi D} \int_0^\pi \sin \theta d\theta = \frac{2L}{\pi D}$$

- By sampling P_{cut} one can estimate π .

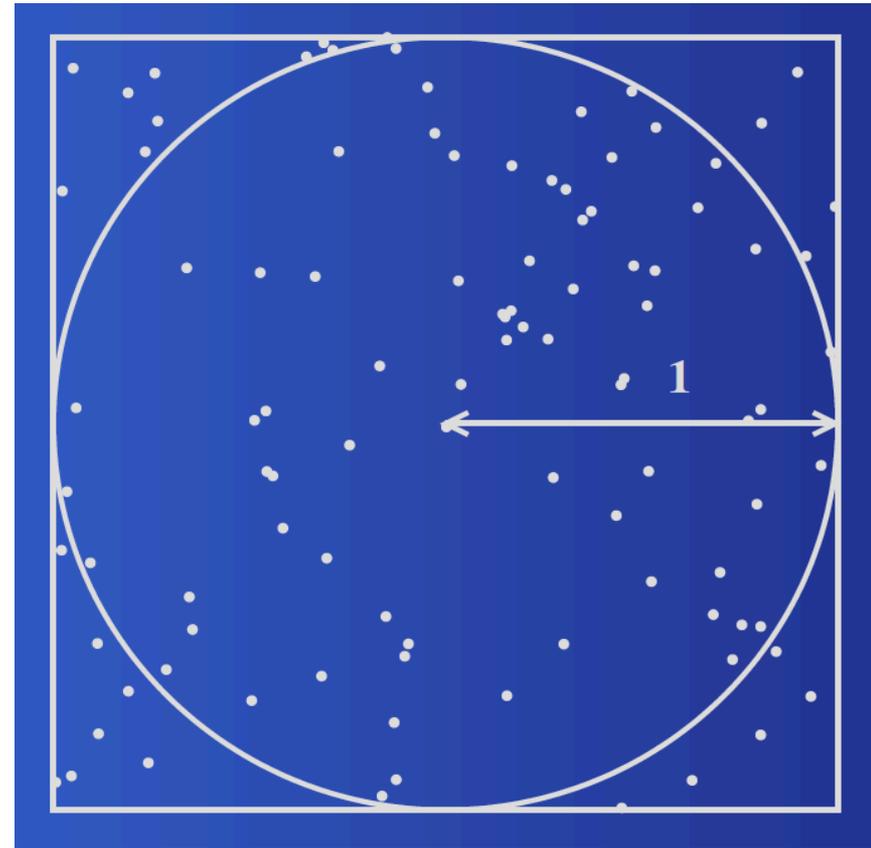


Laplace's method of calculating π (1886)

- Area of the square = 4
- Area of the circle = π
- Probability of random points inside the circle = $\pi / 4$

- Random points : N
- Random points inside circle : N_c

$$\pi \sim 4 N_c / N$$



- Fermi (1930): random method to calculate the properties of the newly discovered neutron
- Manhattan project (40's): simulations during the initial development of thermonuclear weapons. von Neumann and Ulam coined the term "Monte Carlo"
- Metropolis (1948) first actual Monte Carlo calculations using a computer (ENIAC)
- Berger (1963): first complete coupled electron-photon transport code that became known as ETRAN
- Exponential growth since the 1980's with the availability of digital computers

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Basics of Monte Carlo method

- Variable is **random** (also called **stochastic**) if its value cannot be specified in advance of observing it
 - let x be a single continuous random variable defined over some interval. Interval can be finite or infinite.
- Value of x for any observation cannot be specified in advance, but it is possible to talk in terms of probabilities
 - $\text{Prob}\{x_i \leq X\}$ represents the probability that an observed value x_i will be less than or equal to some specified value X . More generally, $\text{Prob}\{E\}$ is used to represent the probability of an event E
- **Probability Density Function** (PDF) of a single stochastic variable is a function that has three properties:
 - 1) defined on an interval $[a, b]$
 - 2) is non-negative on that interval
 - 3) is normalized such that $\int_a^b f(x) dx = 1$ with a and b real numbers, $a \rightarrow -\infty$ and/or $b \rightarrow \infty$

- A PDF $f(x)$ is a density function, i.e., it specifies the probability per unit of x , so that $f(x)$ has units that are the inverse of the units of x
- For given x , $f(x)$ is not the probability of obtaining x
 - infinitely many values that x can assume
 - probability of obtaining a single specific value is zero
- Rather, $f(x)dx$ is the probability that a random sample x_i will assume a value within x and $x+dx$
 - often, this is stated in the form
$$f(x) = \text{Prob}\{ x \leq x_i < x+dx \}$$

- The integral defined by

$$F(x) \equiv \int_a^x f(x') dx'$$

where $f(x)$ is a PDF over the interval $[a, b]$, is called the **Cumulative Distribution Function** (CDF) of f .

- A CDF has the following properties:

- 1) $F(a) = 0.$, $F(b) = 1.$

- 2) $F(x)$ is monotonically increasing, as $f(x)$ is always non-negative

- CDF is a direct measure of probability. The value $F(x_i)$ represents the probability that a random sample of the stochastic variable x will assume a value between a and x_i , i.e., $\text{Prob}\{a \leq x \leq x_i\} = F(x_i)$.

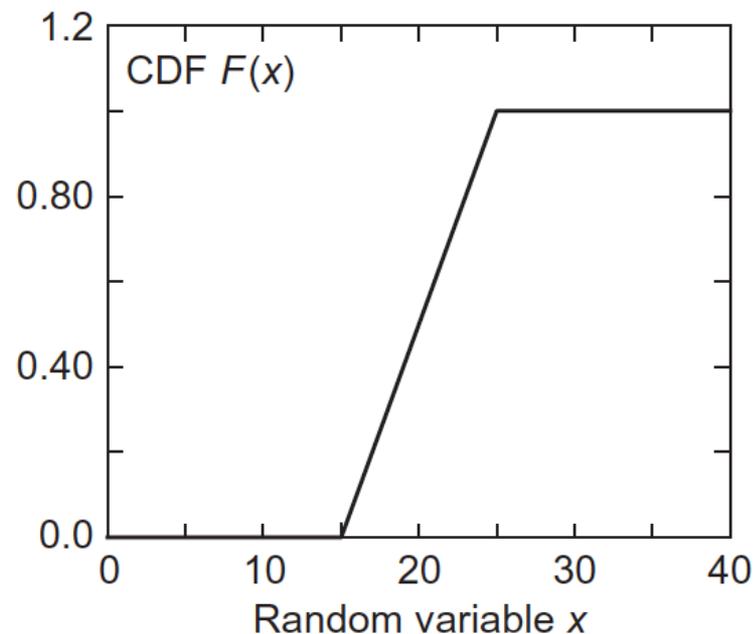
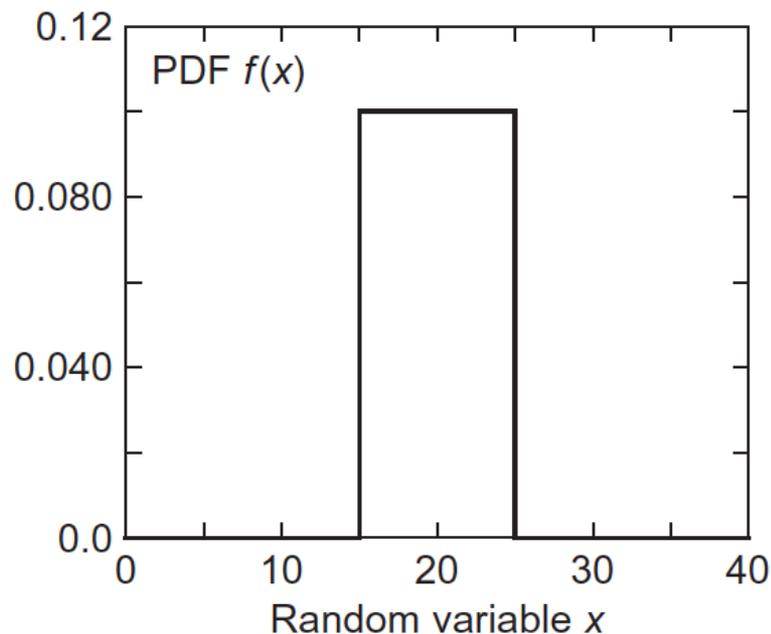
- More generally,

$$\text{Prob}\{x_1 \leq x \leq x_2\} = \int_{x_1}^{x_2} f(x) dx = F(x_2) - F(x_1).$$

Some example distributions – Uniform PDF

- The uniform (rectangular) PDF on the interval $[a, b]$ and its CDF are given by

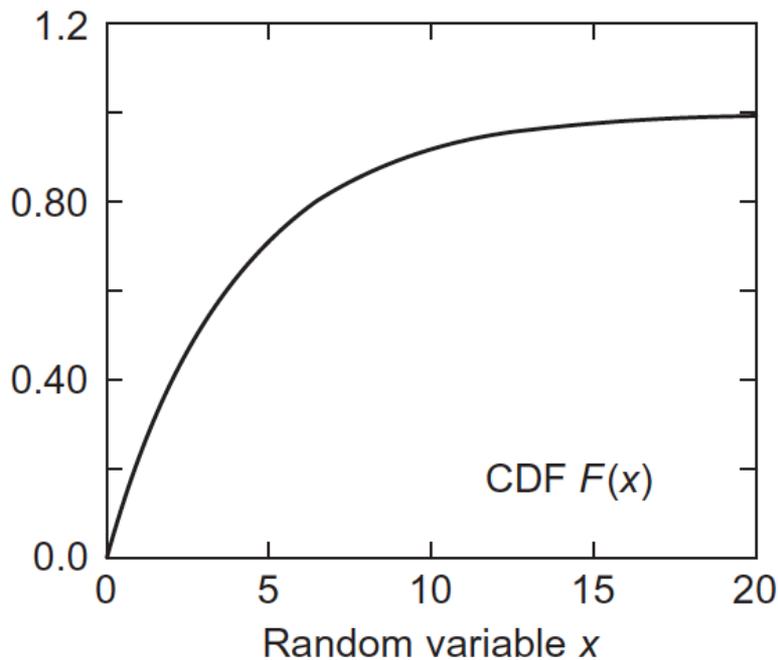
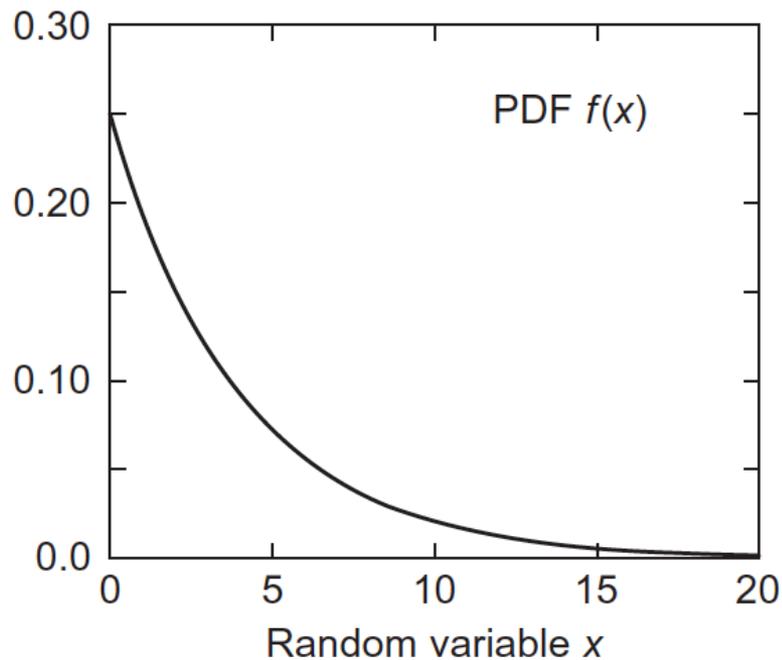
$$f(x) = \frac{1}{b-a}, \quad F(x) = \int_a^x \frac{1}{b-a} dx' = \frac{x-a}{b-a}.$$

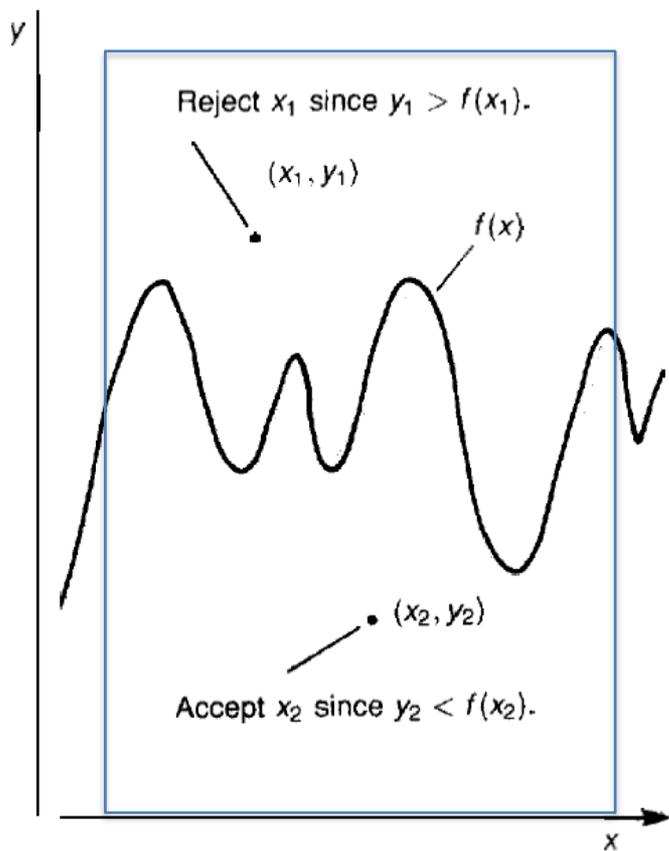


Some example distributions – Exponential PDF

- The exponential PDF on the interval $[0, \infty]$ and its CDF are given by

$$f(x) = f(x|\alpha) = \alpha e^{-\alpha x}, \quad F(x) = \int_0^x \alpha e^{-\alpha x'} dx' = 1 - e^{-\alpha x}$$





- If x_i and y_i are selected randomly from the range and domain, respectively, of the function f , then each pair of numbers represents a point in the function's coordinate plane (x, y)
- When $y_i > f(x_i)$ the point lies above the curve for $f(x)$, and x_i is rejected; when $y_i \leq f(x_i)$ the points lies on or below the curve, and x_i is accepted
- Thus, fraction of accepted points is equal to fraction of the area below curve
- This technique, first proposed by von Neumann, is also known as the **acceptance-rejection method** of generating random numbers for arbitrary Probability Density Function (PDF)

- Two important measures of PDF $f(x)$ are its **mean** μ and **variance** σ^2 .
- The mean μ is the expected or averaged value of x defined as

$$\langle x \rangle \equiv E(x) \equiv \mu(x) \equiv \int_a^b x f(x) dx.$$

- The variance σ^2 describes the spread of the random variable x from the mean and defined as

$$\begin{aligned}\sigma^2(x) &\equiv \langle [x - \langle x \rangle]^2 \rangle = \int_a^b [x - \langle x \rangle]^2 f(x) dx. \\ &= \int_a^b [x^2 - 2x\langle x \rangle + \langle x \rangle^2] f(x) dx \\ &= \int_a^b x^2 f(x) dx - 2\langle x \rangle \int_a^b x f(x) dx + \langle x \rangle^2 \int_a^b f(x) dx \\ &= \langle x^2 \rangle - \langle x \rangle^2\end{aligned}$$

Note: $\int_a^b x^2 f(x) dx = \langle x^2 \rangle$ $\int_a^b f(x) dx = 1$

- The square root of the variance is called the **standard deviation** σ .

- Consider a function $z(x)$, where x is a random variable described by a PDF $f(x)$.
- The function $z(x)$ itself is a random variable. Thus, the expected or mean value of $z(x)$ is defined as such.

$$\langle z \rangle \equiv \mu(z) \equiv \int_a^b z(x) f(x) dx.$$

- Then, variance of $z(x)$ is given as this.

$$\begin{aligned} \sigma^2(z) &= \langle [z(x) - \langle z \rangle]^2 \rangle = \int_a^b [z(x) - \langle z \rangle]^2 f(x) dx, \\ &= \langle z^2 \rangle - \langle z \rangle^2 \end{aligned}$$

- The heart of a Monte Carlo analysis is to obtain an estimate of a mean value (a.k.a. **expected value**). If one forms the estimate

$$\bar{z} = \frac{1}{N} \sum_{i=1}^N z(x_i)$$

where x_i are suitably sampled from PDF $f(x)$, one can expect

$$\lim_{N \rightarrow \infty} \bar{z} = \langle z \rangle$$

- The equation of the previous page can be written as

$$\text{Prob}\{\bar{z} - \lambda s(x)/\sqrt{N} \leq \langle z \rangle \leq \bar{z} + \lambda s(x)/\sqrt{N}\} \simeq \frac{1}{\sqrt{2\pi}} \int_{-\lambda}^{\lambda} e^{-u^2/2} du.$$

where $s(z)$ is the calculated sample standard deviation.

- Right-hand side can be evaluated numerically and called the **confidence coefficient**. The confidence coefficients expressed as percentages are called **confidence level**. For a given λ in unit of standard deviation, the Monte Carlo estimate of $\langle z \rangle$ is usually reported as $\bar{z} \pm \lambda s(z)/\sqrt{N}$.

λ	confidence coefficient	confidence level
0.25	0.1974	20%
0.50	0.3829	38%
1.00	0.6827	68%
1.50	0.8664	87%
2.00	0.9545	95%
3.00	0.9973	99%
4.00	0.9999	99.99%

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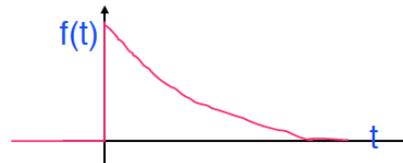
Two Monte Carlo Particle Transport Examples

Simplest case – decay in flight (1)

- Suppose an unstable particle of life time t has initial momentum p (\rightarrow velocity v).
 - Distance to travel before decay : $d = t v$
- The decay time t is a random value with probability density function

$$f(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right) \quad t \geq 0$$

τ is the mean life of the particle



- the probability that the particle decays at time t is given by the cumulative distribution function F which is itself is a random variable with uniform probability on $[0,1]$

$$r = F(t) = \int_{-\infty}^t f(u) du$$

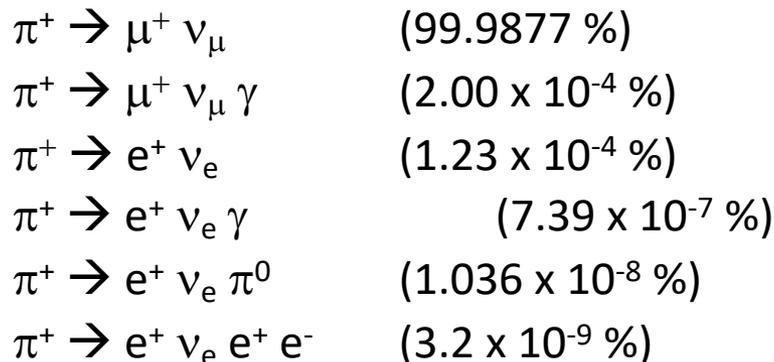
- Thus, having a uniformly distributed random variable r on $[0,1]$, one can sample the value t with the probability density function $f(t)$.

$$t = F^{-1}(r) = -\tau \ln(1 - r) \quad 0 \leq r < 1$$

Simplest case – decay in flight (2)

- When the particle has traveled the $d = t v$, it decays.
- Decay of an unstable particle itself is a random process → Branching ratio

– For example:

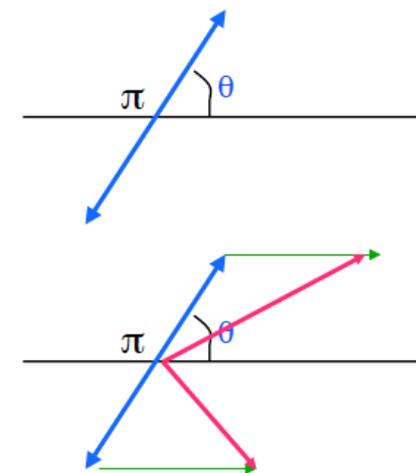


- Select a decay channel by shooting a random number
- In the rest frame of the parent particle, rotate decay products in $\theta [0, \pi)$ and $\phi [0, 2\pi)$ by shooting a pair of random numbers

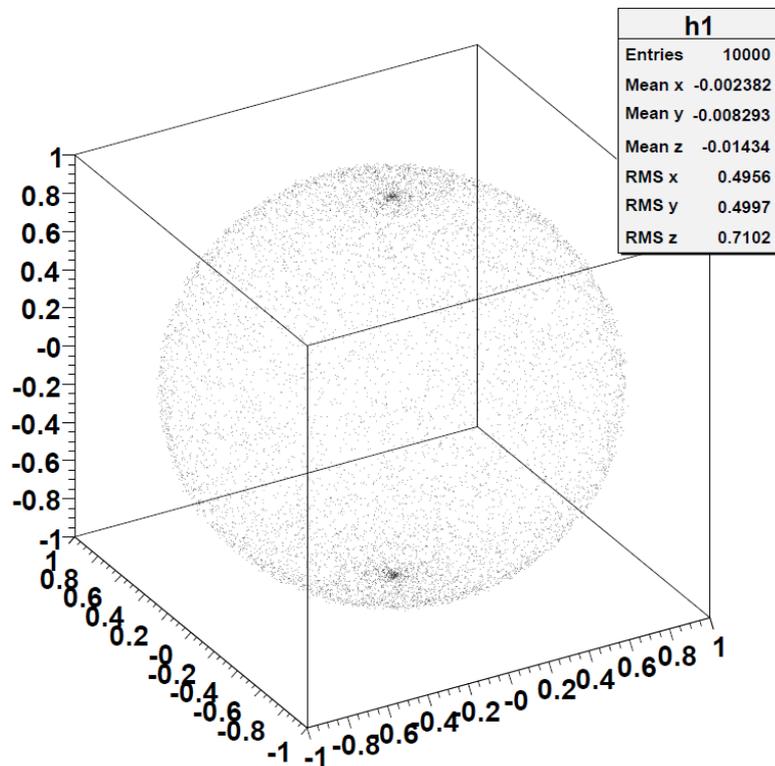
$$d\Omega = \sin\theta d\theta d\phi$$

$$\theta = \cos^{-1}(r_1), \quad \phi = 2\pi \times r_2 \quad 0 \leq r_1, r_2 < 1$$

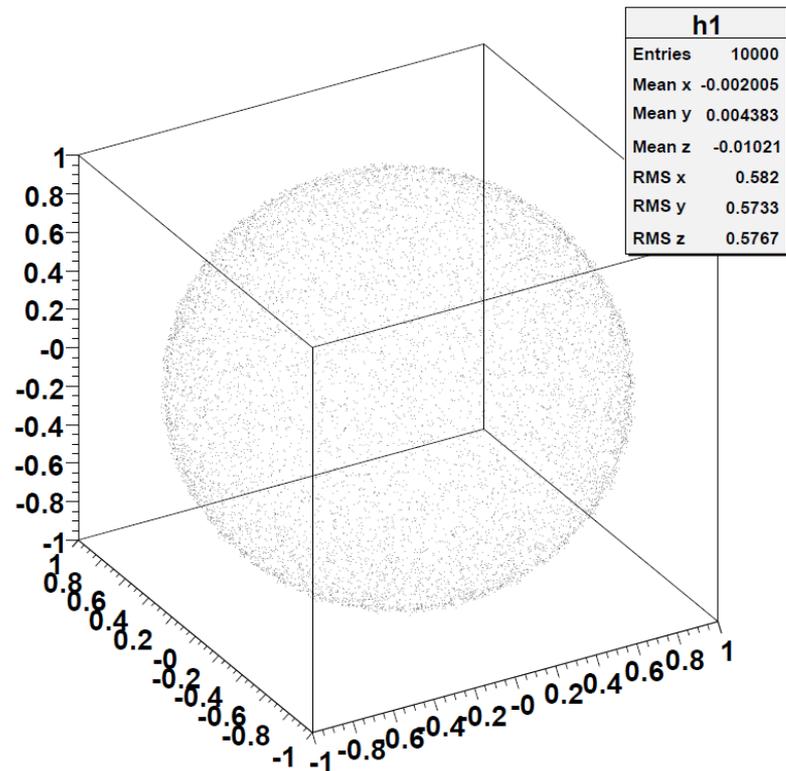
- Finally, Lorentz-boost the decay products
- You need at least 4 random numbers to simulate one decay in flight



$$\theta = \pi \times r_1, \phi = 2\pi \times r_2$$
$$0 \leq r_1, r_2 < 1$$



$$\theta = \cos^{-1}(r_1), \phi = 2\pi \times r_2$$
$$0 \leq r_1, r_2 < 1$$



$$d\Omega = \sin\theta d\theta d\phi$$

Compton scattering (1)

- Compton scattering

$$e^- \gamma \rightarrow e^- \gamma$$

- Distance traveled before Compton scattering, l , is a random value

$$\text{Cross section per atom : } \sigma(E, z)$$

$$\text{Number of atoms per volume : } n = \rho N_A / A$$

ρ : density, N_A : Avogadro number, A : atomic mass

$$\text{Cross section per volume : } \eta(E, \rho) = n \sigma$$

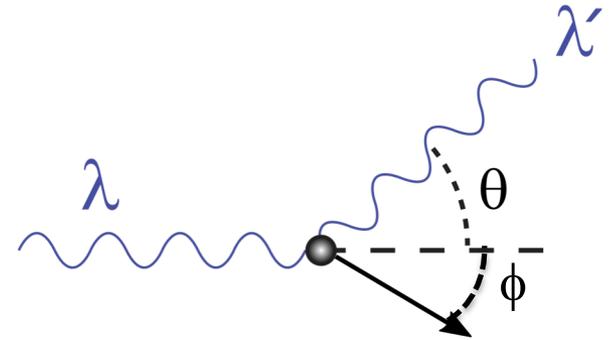
- η is the probability of Compton interaction per unit length. $\lambda(E, \rho) = \eta^{-1}$ is the **mean free path** associated with the Compton scattering process.

- The probability density function $f(l)$

$$f(l) = \eta \exp(-\eta l) = \frac{1}{\lambda} \exp\left(-\frac{l}{\lambda}\right)$$

- With a uniformly distributing random number r on $[0,1)$, One can sample the distance l .

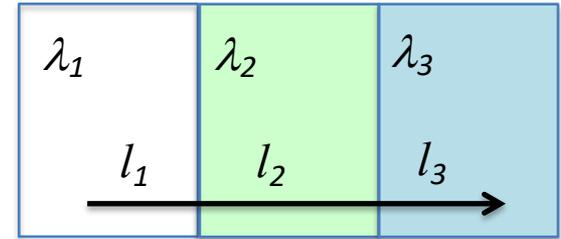
$$l = -\lambda \ln(r) \quad 0 \leq r < 1$$



Compton scattering (2)

- $\lambda(E, \rho)$ and l are material dependent. Distance measured by the unit of mean free path (n_λ) is independent.

$$n_\lambda = \frac{l_1}{\lambda_1} + \frac{l_2}{\lambda_2} + \frac{l_3}{\lambda_3} = \int_0^{end} \frac{dl}{\lambda(l)}$$



- n_λ is independent of the material and a random value with probability density function $f(n_\lambda) = \exp(-n_\lambda)$
 - sample n_λ at the origin of the particle

$$n_\lambda = -\ln(r) \quad 0 \leq r < 1$$

- update elapsed n_λ along the passage of the particle

$$n_\lambda = n_\lambda - l_i / \lambda_i$$

- Compton scattering happens at $n_\lambda = 0$

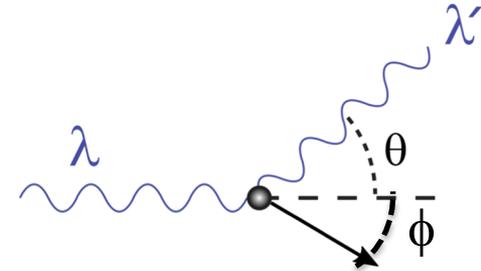
Compton scattering (3)

- The relation between photon deflection (θ) and energy loss for Compton scattering is determined by the conservation of momentum and energy between the photon and recoiled electron.

$$h\nu = \frac{h\nu_0}{1 + \left(\frac{h\nu_0}{m_e c^2}\right) (1 - \cos \theta)},$$

$$E = h\nu_0 - h\nu = m_e c^2 \frac{2(h\nu_0)^2 \cos^2 \phi}{(h\nu_0 + m_e c^2)^2 - (h\nu_0)^2 \cos^2 \phi},$$

$$\tan \phi = \frac{1}{1 + \left(\frac{h\nu_0}{m_e c^2}\right)} \cot \frac{\theta}{2},$$



$h\nu$: energy of incident photon
 $h\nu_0$: energy of scattered photon
 E : energy of recoil electron
 m_e : rest mass of electron
 c : speed of light

- For unpolarized photon, the Klein-Nishina angular distribution function per steradian of solid angle Ω

$$\frac{d\sigma_c^{KN}}{d\Omega}(\theta) = r_0^2 \frac{1 + \cos^2 \theta}{2} \frac{1}{[1 + h\nu(1 - \cos \theta)]^2} \left\{ 1 + \frac{h\nu^2(1 - \cos \theta)^2}{(1 + \cos^2 \theta)[1 + h\nu(1 - \cos \theta)]} \right\}$$

$$= \frac{1}{2} r_0^2 \left(\frac{k}{k_0}\right)^2 \left(\frac{k}{k_0} + \frac{k_0}{k} - \sin^2 \theta\right) \quad (cm^2 sr^{-1} electron^{-1}),$$

- One can use acceptance-rejection method to sample the distribution.

$$k_0 = \frac{h\nu_0}{m_e c^2}, \quad k = \frac{h\nu}{m_e c^2}$$

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Boosting simulation

- Variance reduction techniques

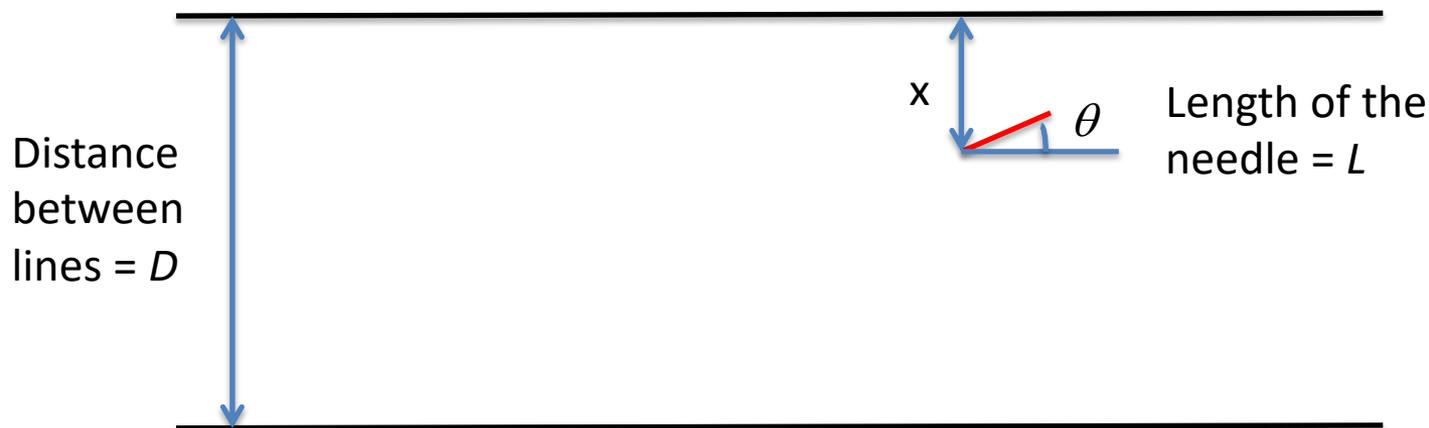
Buffon's needle – once again

- Suppose the distance between lines (D) is much larger than the length of the needle (L). In naïve simulation, the needle's location (x) is sampled uniformly over $[0, D)$.

$$\pi \sim (2 L / D) * (h / n)$$

- However, the needle has little chance to hit lines for $L < x < D - L$. Also, symmetry shows the probability of hitting lines for $[0, D/2)$ is equal to $[D/2, D)$.
- One can estimate π by sampling x over $[0, L]$, and because the probability of $0 \leq x < L$ is $L/(D/2)$, each successful count should be multiplied by the weight $D/2L$.

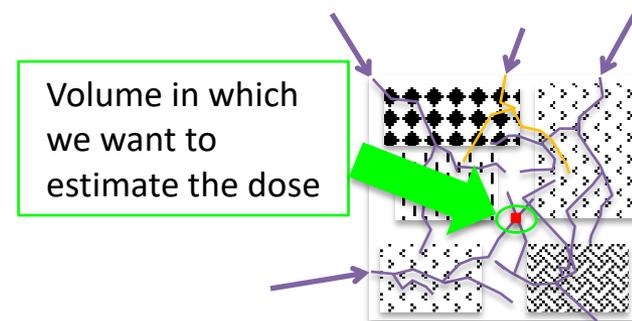
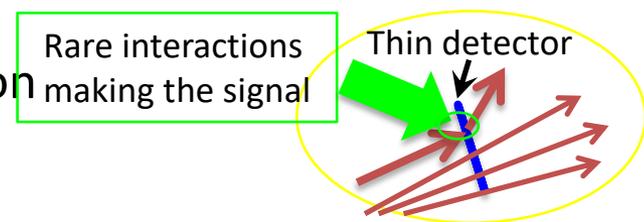
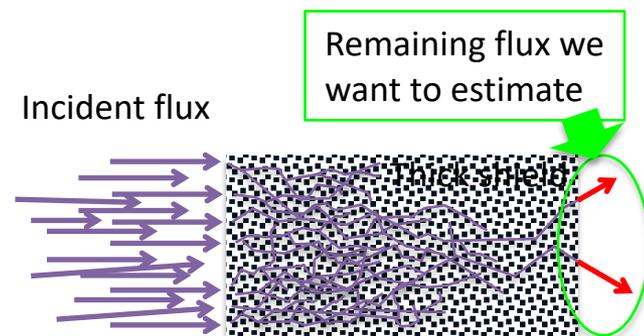
$$\pi \sim (2 L / D) * (h * (D / 2 L) / n)$$



- There are simulation problems where the event we are interested in is very rare due to physics and/or geometry.
- Over the years, many clever variance reduction techniques have been developed for performing biased Monte Carlo calculations
- The introduction of variance reduction methods into Monte Carlo calculations can make otherwise impossible Monte Carlo problems solvable. However, use of these variance reduction techniques requires skill and experience.
 - non-analog Monte Carlo, despite having a rigorous statistical basis, is, in many ways, an “art” form and cannot be used blindly.

Example use-cases of variance reduction

- Efficiency of a radiation shielding
 - E.g. large flux entering to a thick shield
 - Lots of interactions : compute intensive
 - Very few particles escape
- Response of thin detector
 - e.g. compact neutron detector
 - most particles pass through without interaction
 - signal is made by the interaction
- Dose in a very small component in a large setup
 - e.g. an IC chip in a large satellite in cosmic radiation environment
 - most of the incident radiation does not reach the IC chip



- EM physics
 - ETRAN (Berger & Seltzer; NIST)
 - EGS4 (Nelson, Hirayama, Rogers; SLAC)
 - EGS5 (Hirayama *et al.*; KEK/SLAC)
 - EGSnrc (Kawrakow & Rogers; NRCC)
 - Penelope (Salvat *et al.*; U. Barcelona)
- Hadronic physics / general purpose
 - Fluka (Ferrari *et al.*, CERN/INFN)
 - **Geant4** (Geant4 Collaboration)
 - MARS (James & Mokhov; FNAL)
 - MCNPX / MCNP5 (LANL)
 - PHITS (Niita *et al.*; JAEA)

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Backup



- One of the important features of Monte Carlo is that not only can one obtain an estimate of an expected value but also one can obtain an estimate of the **uncertainty** in the estimate.
- The **Central Limit Theorem** (CLT) is a very general and powerful theorem.
- For \bar{z} obtained by samples from a distribution with mean $\langle z \rangle$ and standard deviation $\sigma(z)$, CLT provides

$$\lim_{N \rightarrow \infty} \text{Prob} \left\{ \frac{|\bar{z} - \langle z \rangle|}{\sigma(z)/\sqrt{N}} \leq \lambda \right\} = \frac{1}{\sqrt{2\pi}} \int_{-\lambda}^{\lambda} e^{-u^2/2} du.$$

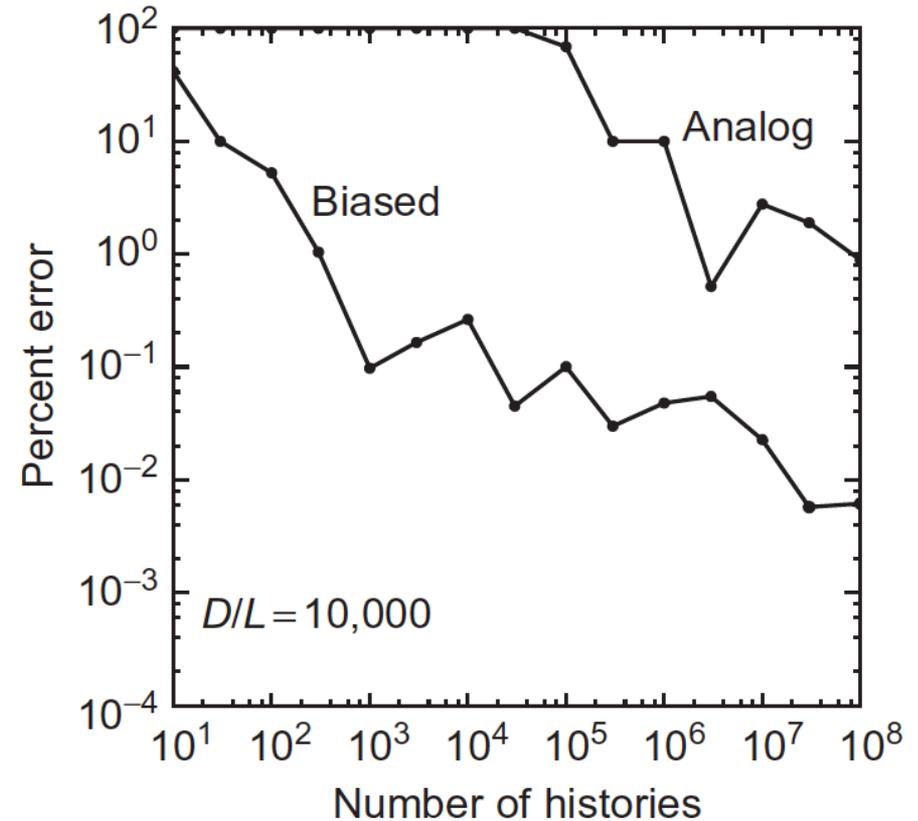
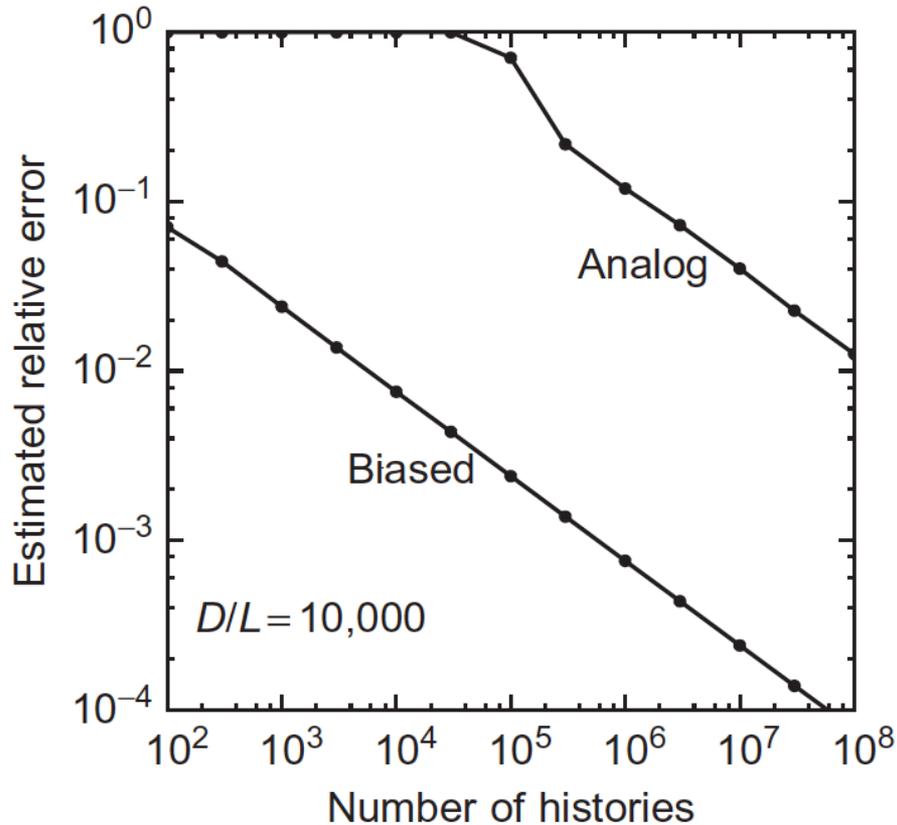
- Stated in words:

The CLT tells us that the asymptotic distribution of $\frac{|\bar{z} - \langle z \rangle|}{\sigma(z)/\sqrt{N}}$ is a unit

normal distribution or, equivalently, \bar{z} is asymptotically distributed as a normal distribution with mean $\mu = \langle z \rangle$ and standard deviation $\sigma(z)/\sqrt{N}$.

- Most importantly, it states that the uncertainty in the estimated expected value is proportional to $1/\sqrt{N}$, where N is the number of samples of $f(x)$.

Buffon's needle – case of $D / L = 10,000$



- The real power of Monte Carlo is that the sampling procedure can be intentionally biased toward the region where the integrand is large or to produce simulated histories that have a better chance of creating a rare event, such as Buffon's needle falling on widely spaced lines.
 - “Analogue simulation” : follows the natural PDF
 - “Non-analogue (a.k.a. biased) simulation” : biased sampling
- Of course, with such biasing, the scoring then must be corrected by assigning weights to each history in order to produce a corrected, unbiased estimate of the expected value.
- In such non-analog Monte Carlo analyses, the sample variance $\sigma^2(z)$ of the estimated expectation value z is reduced compared to that obtained by an unbiased or analog analysis.
 - In the Buffon's needle example, biasing a simulation problem with widely spaced lines to force all dropped needles to have one end within a needle's length of a grid line was seen to reduce the relative error by two orders of magnitude over that of a purely analog simulation.

- Consider a function $z(x)$, where x is a random variable described by a PDF $f(x)$.
- The function $z(x)$ itself is a random variable. Thus, the expected or mean value of $z(x)$ is defined as such.

$$\langle z \rangle \equiv \mu(z) \equiv \int_a^b z(x) f(x) dx.$$

- Then, variance of $z(x)$ is given as such.

$$\begin{aligned} \sigma^2(z) &= \langle [z(x) - \langle z \rangle]^2 \rangle = \int_a^b [z(x) - \langle z \rangle]^2 f(x) dx, \\ &= \langle z^2 \rangle - \langle z \rangle^2 \end{aligned}$$

- The heart of a Monte Carlo analysis is to obtain an estimate of a mean value (a.k.a. **expected value**). If one forms the estimate

$$\bar{z} = \frac{1}{N} \sum_{i=1}^N z(x_i)$$

where x_i are suitably sampled from PDF $f(x)$, one can expect

$$\lim_{N \rightarrow \infty} \bar{z} = \langle z \rangle$$

- The aim of Monte Carlo calculation is to seek an estimate \bar{z} to an expected value $\langle z \rangle$. The goal of **variance reduction technique** is to produce a more precise estimate than could be obtained in a purely analogue calculation with the same computational effort.

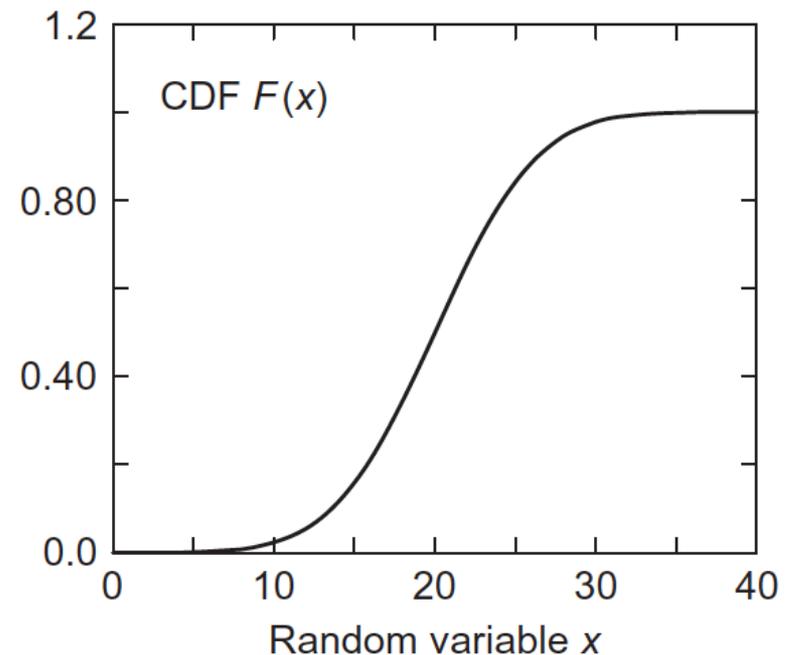
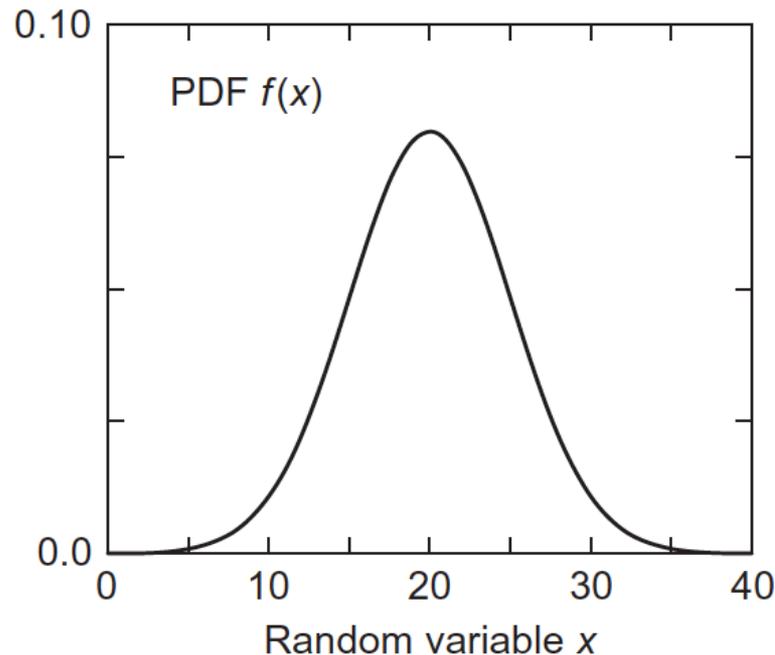
$$\langle z \rangle \equiv \int_V z(\mathbf{x})f(\mathbf{x}) d\mathbf{x} \simeq \bar{z} = \frac{1}{N} \sum_{i=1}^N z(\mathbf{x}_i) \quad s(\bar{z}) = \frac{1}{\sqrt{N-1}} \sqrt{\overline{z^2} - \bar{z}^2}.$$

- Because both $\overline{z^2}$ and \bar{z}^2 must always be positive, the sample variance s^2 can be reduced by reducing their difference.
- Thus, the various variance reduction techniques are directed, ultimately, to minimizing the quantity $\overline{z^2} - \bar{z}^2$
 - Note that, in principle, it is possible to attain zero variance, if $\overline{z^2} = \bar{z}^2$, which occurs if every history yields the sample mean. But this is not very likely. However, it is possible to reduce substantially the variance among histories by introducing various biases into a Monte Carlo calculation.

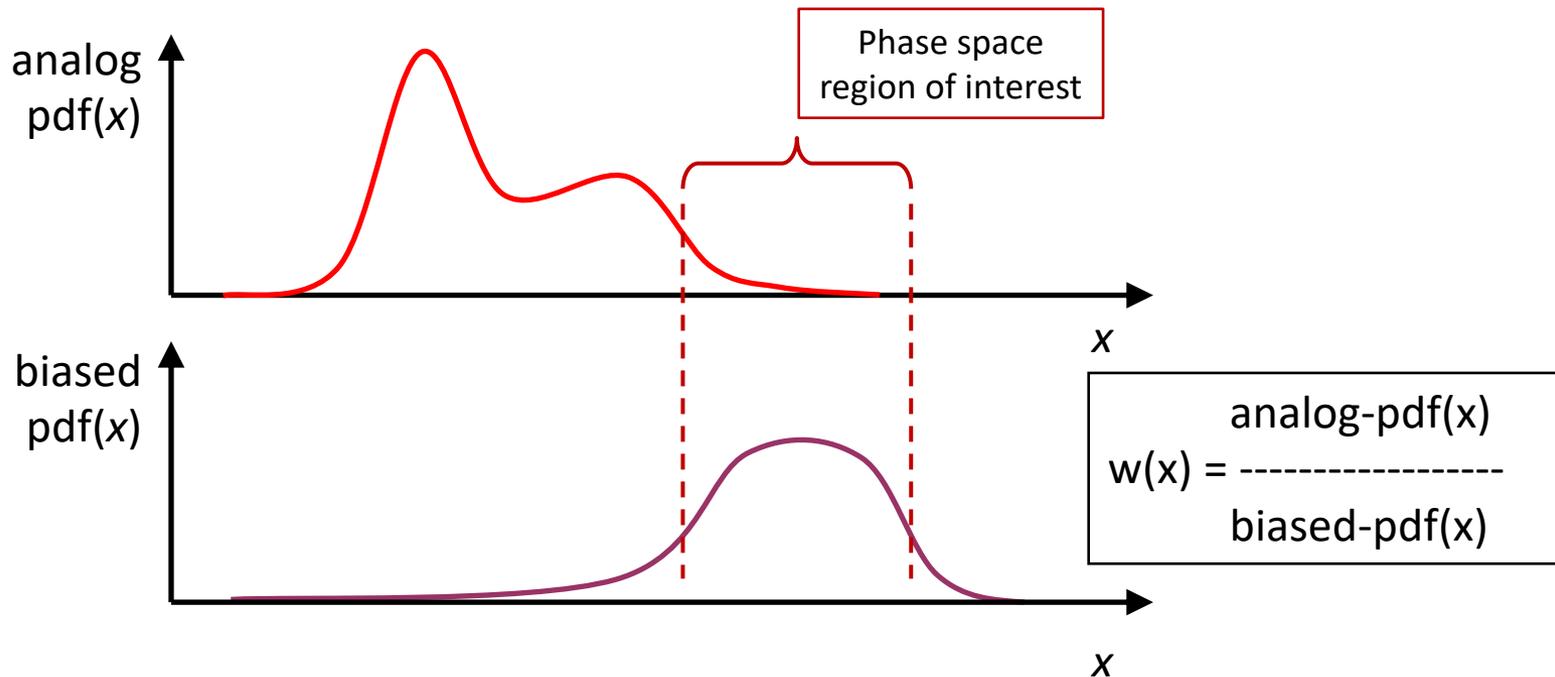
- The Gaussian PDF on the interval $[-\infty, \infty]$ and its CDF are given by

$$f(x) = f(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right],$$

$$F(x) = \frac{1}{\sigma\sqrt{2\pi}} \int_{-\infty}^x \exp\left[-\frac{(x'-\mu)^2}{2\sigma^2}\right] dx'$$

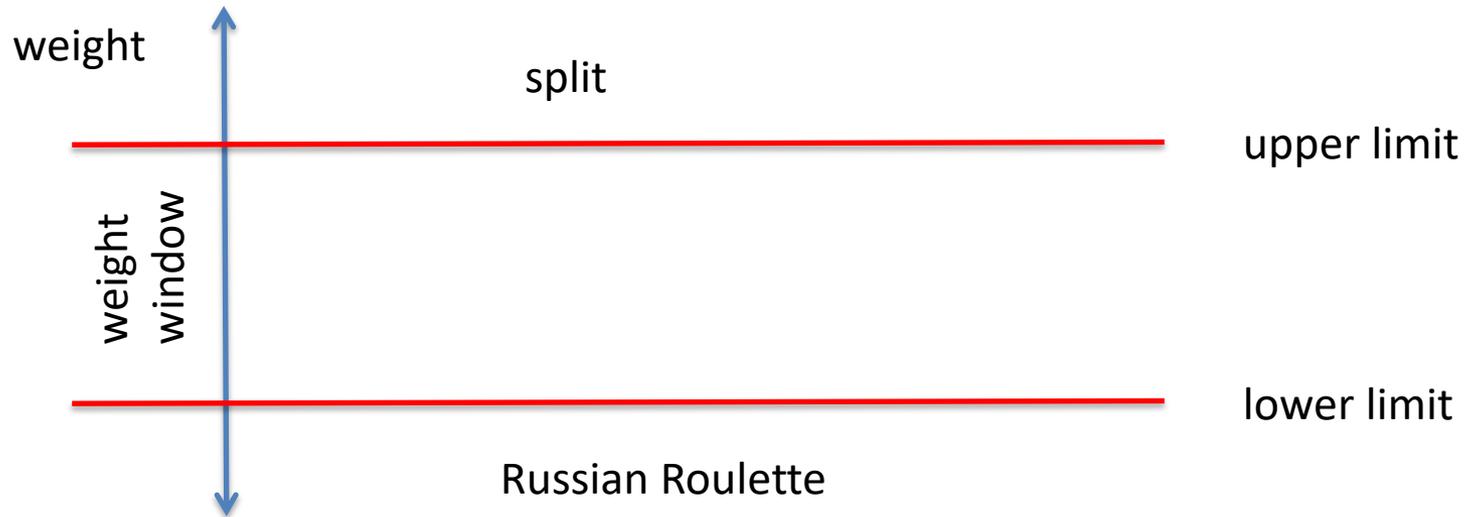


- In an **importance sampling** technique, the analog PDF is replaced by a biased PDF:

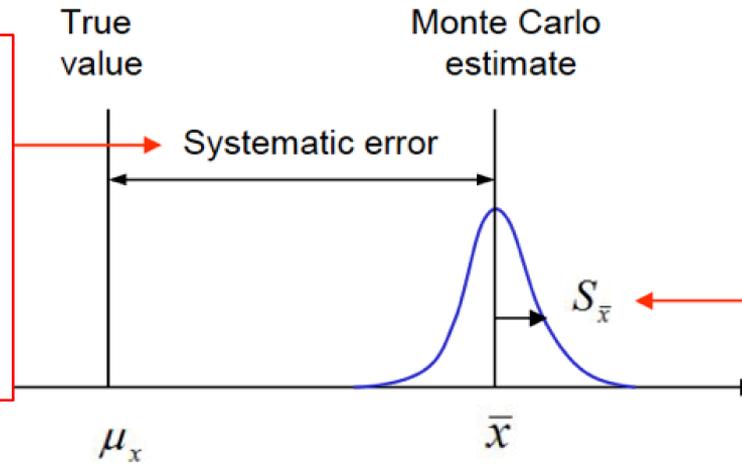


- The weight for a given value x , is the ratio of the analog over the biased distribution values at x .

- Monitor the weight of each particle
- If the weight becomes too high:
 - it makes too large a contribution to the estimate and slows the convergence → **make two particles with half the weight**
- If the weight becomes too low:
 - it does not contribute much to the estimate and thus wastes CPU → **kill the particle with 50% probability, the rest of the time double its weight**



Accuracy $\mu_x - \bar{x}$
 (a.k.a. systematic error)
 measure of how close is
 the expected $\langle x \rangle$ to the
 true value, which is
 seldom known.



Precision

$$S_{\bar{x}} = \sqrt{\frac{\overline{x^2} - \bar{x}^2}{N}} \propto \frac{1}{\sqrt{N}}$$

uncertainty of Monte Carlo estimate. It is possible to get a highly precise result that is far from the true value, if the model is not faithful.

Relative error

$$R = \frac{S_{\bar{x}}}{\bar{x}} \propto \frac{1}{\sqrt{N}}$$

measure of calculation
 (statistical) precision.

$R > 0.5$: not trustable

$0.1 < R < 0.5$: questionable

$R < 0.1$: reasonable

Figure of Merit

$$FOM = \frac{1}{R^2 T} \approx const$$

(T : time spent for the simulation)

usually constant except for very small statistics

Good measure of the efficiency of Monte Carlo method
 (the higher FOM is the better)

- In the Buffon's needle case, FOM for $z \ll 1$ is 1000 times better than FOM for $z > 1$.