Monte Carlo Sampling Methods

Jasmina L. Vujic

Nuclear Engineering Department
University of California, Berkeley

Email:	vujic@nuc.berkeley.edu
phone:	(510) 643-8085
fax:	(510) 643-9685

Monte Carlo

Monte Carlo is a computational technique based on constructing a random process for a problem and carrying out a NUMERICAL EXPERIMENT by N-fold sampling from a random sequence of numbers with a PRESCRIBED probability distribution.

x - random variable

$$\hat{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$\hat{x}$ - the estimated or sample mean of x

$\bar{x}$ - the expectation or true mean value of x

If a problem can be given a PROBABILISTIC interpretation, then it can be modeled using RANDOM NUMBERS.

Monte Carlo

- Monte Carlo techniques came from the complicated diffusion problems that were encountered in the early work on atomic energy.
- 1772 Compte de Bufon - earliest documented use of random sampling to solve a mathematical problem.
- 1786 Laplace suggested that π could be evaluated by random sampling.
- Lord Kelvin used random sampling to aid in evaluating time integrals associated with the kinetic theory of gases.
- Enrico Fermi was among the first to apply random sampling methods to study neutron moderation in Rome.
- 1947 Fermi, John von Neuman, Stan Frankel, Nicholas Metropolis, Stan Ulam and others developed computer-oriented Monte Carlo methods at Los Alamos to trace neutrons through fissionable materials

Monte Carlo methods can be used to solve:

a) The problems that are stochastic (probabilistic) by nature:

- particle transport,
- telephone and other communication systems,
- population studies based on the statistics of survival and reproduction.

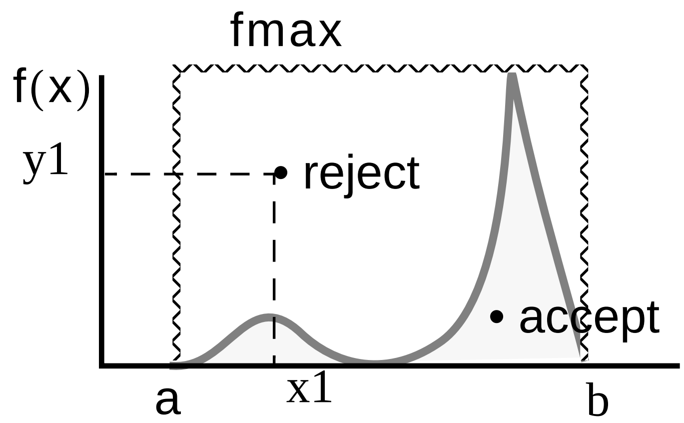
b) The problems that are deterministic by nature:

- the evaluation of integrals,
- solving the systems of algebraic equations,
- solving partial differential equations.

Monte Carlo methods are divided into:

a) ANALOG, where the natural laws are PRESERVED - the game played is the analog of the physical problem of interest
(i.e., the history of each particle is simulated exactly),

b) NON-ANALOG, where in order to reduce required computational time the strict analog simulation of particle histories is abounded (i.e., we CHEAT!)
Variance-reduction techniques:
- Absorption suppression
- History termination and Russian Roulette
- Splitting and Russian Roulette
- Forced Collisions
- Source Biasing



$I = \int_a^b f(x)dx$ - area uder the function f(x), $R = (b-a)f_{max}$ - area of rectangle

$P = \frac{I}{R}$ - is a probability that a random point lies under f(x), thus $I = RP$

Step 1: Choose a random point (x1,y1): $x1 = a + (b-a)\xi_1$ and $y1 = f_{max}\xi_2$

Step 2: Check if $y1 \le f(x1)$ - accept the point, if $y1 < f(x1)$ - reject the point

Step 3: Repeat this process N times, Ni - the number of accepted points

Step 4: Determine $P = \frac{Ni}{N}$ and the value of integral $I = R\frac{Ni}{N}$

Major Components of a Monte Carlo Algorithm

- **Probability distribution functions (pdf's) - the physical (or mathematical) system must be described by a set of pdf's.**
- **Random number generator - a source of random numbers uniformly distributed on the unit interval must be available.**
- **Sampling rule - a prescription for sampling from the specified pdf, assuming the availability of random numbers on the unit interval.**
- **Scoring (or tallying) - the outcomes must be accumulated into overall tallies or scores for the quantities of interest.**
- **Error estimation - an estimate of the statistical error (variance) as a function of the number of trials and other quantities must be determined.**
- **Variance reduction techniques - methods for reducing the varinace in the estimated solution to reduce the computational time for Monte Carlo simulation.**
- **Parallelization and vectorization - efficient use of advanced computer architectures.**

Probability Distribution Functions

Random Variable, x, - a variable that takes on particular values with a frequency that is determined by some underlying probability distribution.

Continuous Probability Distribution

$$P\{a \le x \le b\}$$

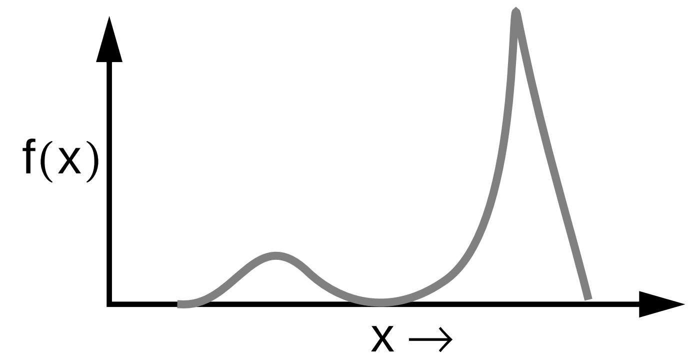
Discrete Probability Distribution

$$P\{x = x_i\} = p_i$$

PDFs and CDFs (continuous)

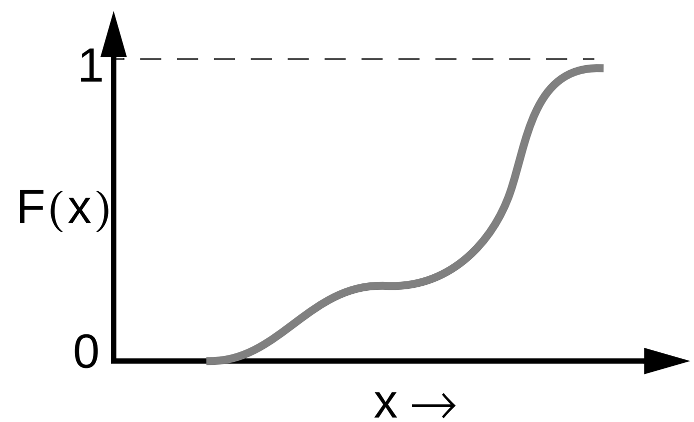
Probability Density Function (PDF) - continuous

- $f(x)$, $f(x)dx = P\{x \le x' \le x + dx\}$
- $0 \le f(x)$, $\int_{-\infty}^{\infty} f(x)dx = 1$
- $\text{Probability}\{ a \le x \le b \} = \int_a^b f(x)dx$



Cumulative Distribution Function (CDF) - continuous

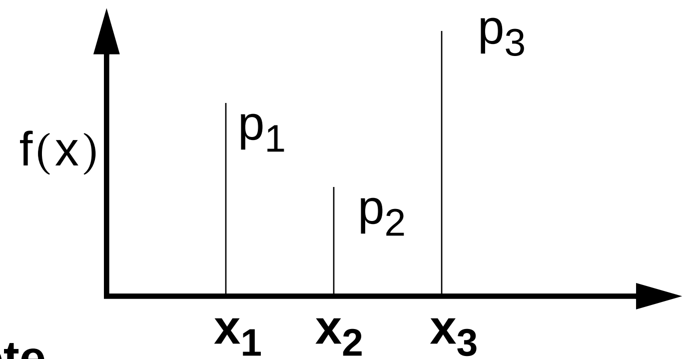
- $F(x) = \int_{-\infty}^{x} f(x')dx' = P\{x' \le x\}$
- $0 \le F(x) \le 1$
- $0 \le \frac{d}{dx}F(x) = f(x)$
- $\int_a^b f(x')dx' = P\{a \le x \le b\} = F(b) - F(a)$



PDFs and CDFs (discrete)

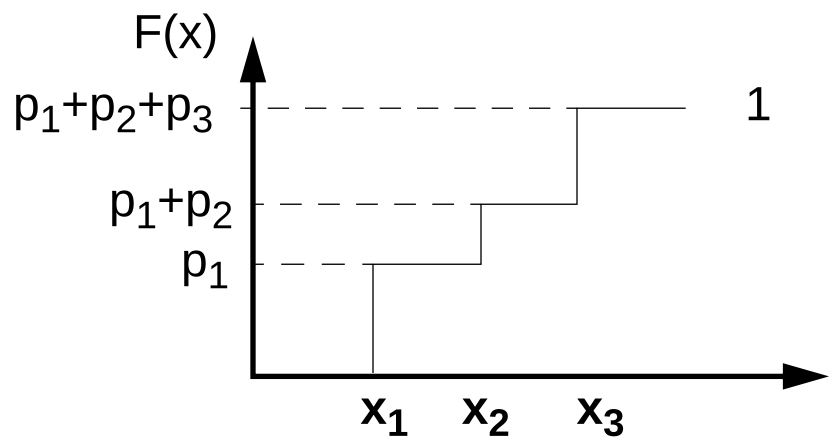
Probability Density Function (PDF) - discrete

- $f(x_i)$, $f(x_i) = p_i \delta(x - x_i)$
- $0 \le f(x_i)$
- $\sum_i f(x_i)(\Delta x_i) = 1$ or $\sum_i p_i = 1$



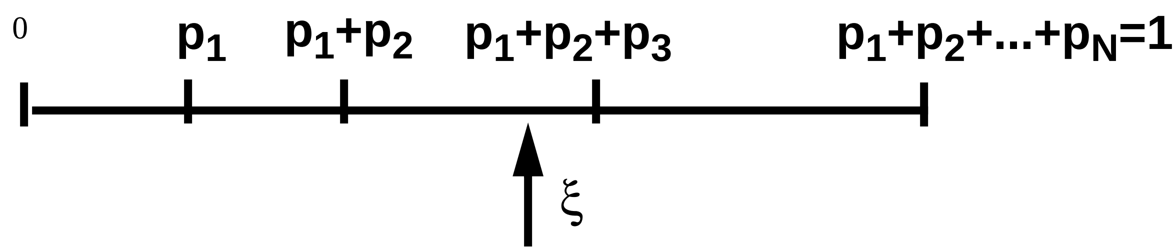
Cumulative Distribution Function (CDF) - discrete

- $F(x) = \sum_{x_i < x} p_i = \sum_{x_i < x} f(x_i)\Delta x_i$
- $0 \le F(x) \le 1$
-



Sampling from a given discrete distribution

Given $f(x_i) = p_i$ and $\sum_i p_i = 1$, i = 1, 2, ..., N



and $0 \le \xi \le 1$, then $P(x = x_k) = p_k = P(\xi \in d_k)$ or

$$\sum_{i=1}^{k-1} p_i \le \xi < \sum_{i=1}^{k} p_i$$

Sampling from a given continuous distribution

If f(x) and F(x) represent PDF and CDF od a random variable x, and if ξ is a random number distributed uniformly on [0,1] with PDF $g(\xi)=1$, and if x is such that

$$F(x) = \xi$$

than for each ξ there is a corresponding x, and the variable x is distribute according to the probability density function f(x).

Proof:

For each ξ in $(\xi,\xi+\Delta\xi)$, there is x in $(x,x+\Delta x)$. Assume that PDF for x is q(x). Show that q(x) = f(x):

$$q(x)\Delta x = g(\xi)\Delta\xi = \Delta\xi = (\xi+\Delta\xi)-\xi = F(x+\Delta x)- F(x)$$

$$q(x) = [F(x+\Delta x)- F(x)]/\Delta x = f(x)$$

Thus, if $x = F^{-1}(\xi)$, then x is distributed according to f(x).

Monte Carlo Codes

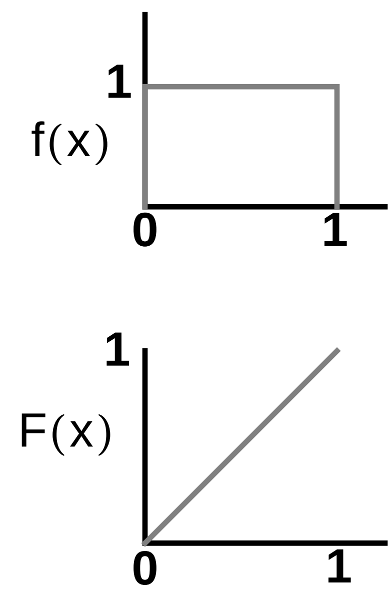
Categories of Random Sampling

- Random number generator — uniform PDF on [0,1]
- Sampling from analytic PDF's — normal, exponential, Maxwellian, ...
- Sampling from tabulated PDF's — angular PDF's, spectrum, cross sect

For Monte Carlo Codes...

- Random numbers, ξ, are produced by the R.N. generator on [0,1]
- Non-uniform random variates are produced from the ξ's by
  - — direct inversion of CDFs
  - — rejection methods
  - — transformations
  - — composition (mixtures)
  - — sums, products, ratios, ...
  - — table lookup + interpolation
  - — lots (!) of other tricks .....
- < 10% of total cpu time (typical)

Random Number Generator



Pseudo-Random Numbers

- Not strictly "random", but good enough
  - — pass statistical tests
  - — reproducible sequence
- Uniform PDF on [0,1]
- Must be easy to compute, must have a large period

Multiplicative congruential method

- Algorithm

S_0 = initial seed, odd integer, < M

$S_k = G \bullet S_{k-1} \mod M, \qquad k = 1, 2, ...$

$\xi_k = S_k / M$

- Typical (***vim, mcnp***):

$S_k = 5^{19} \bullet S_{k-1} \mod 2^{48}$

$\xi_k = S_k / 2^{48}$

period $= 2^{46} \approx 7.0 \times 10^{13}$

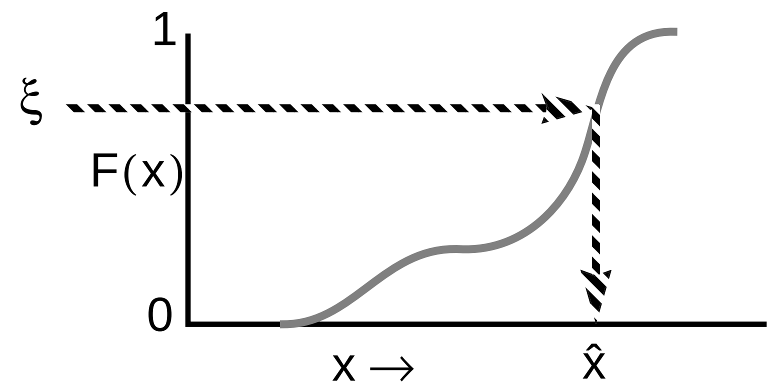
Direct Sampling (Direct Inversion of CDFs)

Direct Solution of

$$\hat{x} \leftarrow F^{-1}(\xi)$$

Sampling Procedure:

- Generate ξ
- Determine $\hat{x}$ such that $F(\hat{x}) = \xi$



Advantages

- Straightforward mathematics & coding
- "High-level" approach

Disadvantages

- Often involves complicated functions
- In some cases, F(x) cannot be inverted (e.g., Klein-Nishina)

Rejection Sampling

Used when the inverse of CDF is costly ot impossible to find.
Select a bounding function, g(x), such that

- $c \cdot g(x) \geq f(x)$ for all x
- g(x) is an easy-to-sample PDF

Sampling Procedure:

- sample $\hat{x}$ from g(x): $\hat{x} \leftarrow g^{-1}(\xi_1)$
- test: $\xi_2 \cdot cg(\hat{x}) \leq f(\hat{x})$

if ***true*** accept $\hat{x}$, done
if ***false*** reject $\hat{x}$, try again

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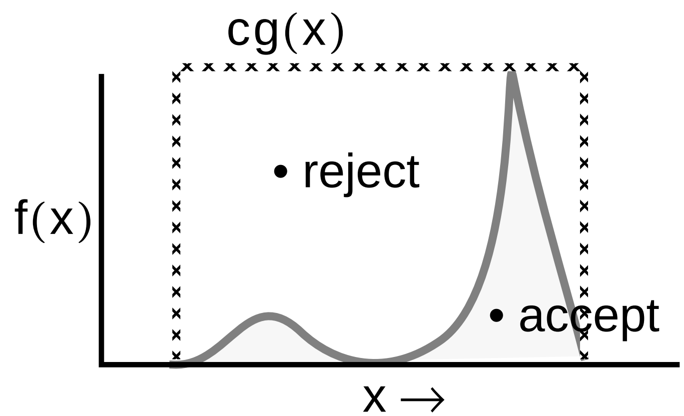


Advantages

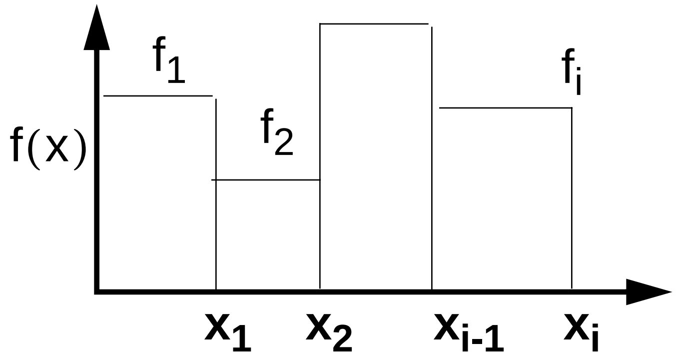
- Simple computer operations

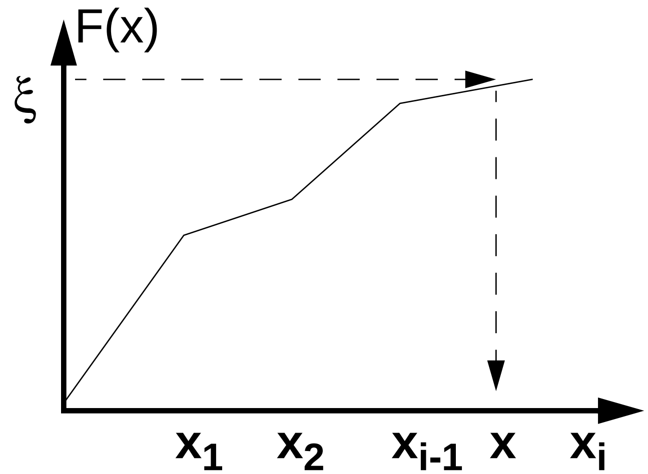
Disadvantages

- "Low-level" approach, sometimes hard to understand

Table Look-Up

Used when f(x) is given in a form of a histogram





Then by linear interpolation

$$F(x) = \frac{(x - x_{i-1})F_i + (x_i - x)F_{i-1}}{x_i - x_{i-1}} , \qquad x = \frac{[(x_i - x_{i-1})\xi - x_i F_{i-1} + x_{i-1} F_i]}{F_i - F_{i-1}}$$

Sampling Multidimensional Random Variables

If the random quantity is a function of two or more random variables that are independent, the joint PDF and CDF can be written as

$$f(x, y) = f_1(x)f_2(y)$$

$$F(x, y) = F_1(x)F_2(y)$$

EXAMPLE: Sampling the direction of isotropically scattered particle in 3D

$$\underline{\Omega} = \underline{\Omega}(\theta, \varphi) = \Omega_x \underline{i} + \Omega_y \underline{j} + \Omega_z \underline{k} = \underline{v} + \underline{w} + \underline{u} ,$$

$$\frac{d\underline{\Omega}}{4\pi} = \frac{\sin\theta d\theta d\varphi}{4\pi} = \frac{-d(\cos\theta)d\varphi}{4\pi} = \frac{-d\mu d\varphi}{4\pi}$$

$$f(\underline{\Omega}) = f_1(\mu)f_2(\varphi) = \frac{1}{2}\frac{1}{2\pi}$$

$$F_1(\mu) = \int_{-1}^{\mu} f_1(\mu')d\mu' = \frac{1}{2}(\mu + 1) = \xi_1 \quad \text{or } \mu = 2\xi_1 - 1$$

$$F_1(\varphi) = \int_0^{\varphi} f_2(\varphi')d\varphi' = \frac{\varphi}{2\pi} = \xi_2 \text{ , or } \varphi = 2\pi\xi_2$$

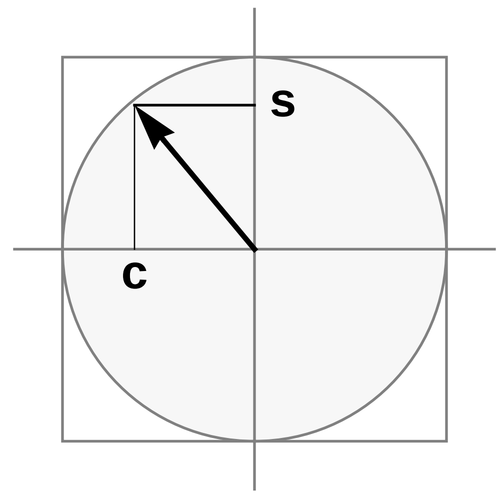
Probability Density Function		*Direct Sampling Method*
Linear: **(L1, L2)**	$f(x) = 2x, \quad 0 < x < 1$	$x \leftarrow \sqrt{\xi}$
Exponential: **(E)**	$f(x) = e^{-x}, \quad 0 < x$	$x \leftarrow -\log \xi$
2D Isotropic: **(C)**	$f(\vec{\rho}) = \frac{1}{2\pi}, \quad \vec{\rho} = (u, v)$	$u \leftarrow \cos 2\pi\xi_1$ $v \leftarrow \sin 2\pi\xi_1$
3D Isotropic: **(I1, I2)**	$f(\vec{\Omega}) = \frac{1}{4\pi}, \quad \vec{\Omega} = (u, v, w)$	$u \leftarrow 2\xi_1 - 1$ $v \leftarrow \sqrt{1-u^2} \cos 2\pi\xi_2$ $w \leftarrow \sqrt{1-u^2} \sin 2\pi\xi_2$
Maxwellian: **(M1, M2, M3)**	$f(x) = \frac{2}{T\sqrt{\pi}}\sqrt{\frac{x}{T}}\, e^{-x/T}, \quad 0 < x$	$x \leftarrow T(-\log\xi_1 - \log\xi_2 \cos^2 \frac{\pi}{2}\xi_3)$
Watt Spectrum: **(W1, W2, W3)**	$f(x) = \frac{2e^{-ab/4}}{\sqrt{\pi a^3 b}}\, e^{-x/a} \sinh\sqrt{bx}, \quad 0 < x$	$w \leftarrow a(-\log\xi_1 - \log\xi_2 \cos^2 \frac{\pi}{2}\xi_3)$ $x \leftarrow w + \frac{a^2 b}{4} + (2\xi_4 - 1)\sqrt{a^2 bw}$
Normal: **(N1, N2)**	$f(x) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$	$x \leftarrow \mu + \sigma\sqrt{-2\log\xi_1}\, \cos 2\pi\xi_2$

Example — 2D Isotropic

$$f(\vec{\rho}) = \frac{1}{2\pi}, \qquad \vec{\rho} = (u, v)$$

Rejection (*old vim*)

```
      SUBROUTINE AZIRN_VIM( S, C )
     IMPLICIT DOUBLE PRECISION  (A-H, O-Z)
  100 R1=2.*RANF() - 1.
      R1SQ=R1*R1
      R2=RANF()
      R2SQ=R2*R2
      RSQ=R1SQ+R2SQ
      IF(1.-RSQ)100,105,105
  105 S=2.*R1*R2/RSQ
      C=(R2SQ-R1SQ)/RSQ
      RETURN
      END
```



Direct (*racer, new vim*)

```
      subroutine azirn_new( s, c )
     implicit double precision  (a-h,o-z)
      parameter ( twopi = 2.*3.14159265 )
      phi = twopi*ranf()
      c = cos(phi)
      s = sin(phi)
      return
      end
```

Example — Watt Spectrum

$$(x) = \frac{2e^{-ab/4}}{\sqrt{\pi a^3 b}} e^{-x/a} \sinh\sqrt{bx}\ , \qquad 0 < x$$

Rejection (***mcnp***)

- Based on Algorithm **R12** from 3rd Monte Carlo Sampler, Everett & Cashwell
- Define $K = 1 + ab/8$, $L = a\{K + (K^2 - 1)_{1/2}\}$, $M = L/a - 1$
- Set $x \leftarrow -\log\xi_1$, $y \leftarrow -\log\xi_2$
- If $\{y - M(x+1)\}^2 \leq bLx$, accept: return (Lx)
  otherwise, reject

Direct (***new vim***)

- Sample from Maxwellian in C-of-M, transform to lab

$$w \leftarrow a(-\log\xi_1 - \log\xi_2 \cos^2 \tfrac{\pi}{2}\xi_3)$$

$$x \leftarrow w + \frac{a^2 b}{4} + (2\xi_4 - 1)\sqrt{a^2 bw}$$

(assume isotropic emission from fission fragment moving with constant velocity in C-of-M)

- Unpublished sampling scheme, based on original Watt spectrum derivation

Example — Linear PDF

$$f(x) = 2x, \qquad 0 \le x \le 1$$

Rejection

(strictly — this is not "rejection", but has the same flavor)

$$\text{if} \quad \xi_1 \ge \xi_2, \quad \text{then} \quad \hat{x} \leftarrow \xi_1$$
$$\text{else} \quad \hat{x} \leftarrow \xi_2$$

or

$$\hat{x} \leftarrow \max(\xi_1, \xi_2)$$

or

$$\hat{x} \leftarrow |\xi_1 - \xi_2|$$

Direct Inversion

$$F(x) = x^2, \qquad 0 \le x \le 1$$

$$\leftarrow \sqrt{\xi}$$

Example — Collision Type Sampling

Assume (for photon interactions):

$$\mu_{tot} = \mu_{cs} + \mu_{fe} + \mu_{pp}$$

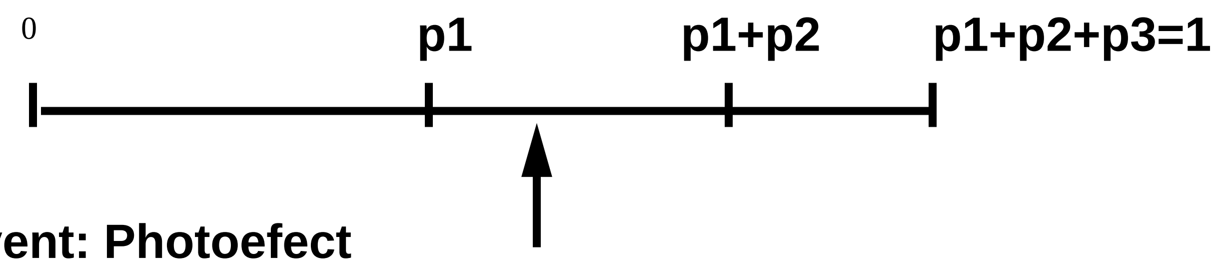
Define

$$p_1 = \frac{\mu_{cs}}{\mu_{tot}}, \quad p_2 = \frac{\mu_{fe}}{\mu_{tot}}, \text{ and } p_3 = \frac{\mu_{pp}}{\mu_{tot}}$$

with

$$\sum_{i=1}^{3} p_i = 1.$$

Then



Collision event: Photoefect

$$p_1 < \xi < p_1 + p_2$$

How Do We Model A Complicated Physical System?

a) Need to know the physics of the system
b) Need to derive equations describing physical processes
c) Need to generate material specific data bases (cross sections for particle interactions, kerma-factors, Q-factors)
d) Need to “translate” equations into a computer program (code)
e) Need to "describe" geometrical configuration of the system to computer
f) Need an adequate computer system

g) Need a physicist smart enough to do the job and dumb enough to want to do it.

Time-Dependent Particle Transport Equation (Boltzmann Transport Equation):

$$\frac{1}{v}\frac{\partial}{\partial t}\psi(\underline{r}, E, \underline{\Omega}, t) + \underline{\Omega} \bullet \nabla\psi(\underline{r}, E, \underline{\Omega}, t) + \Sigma_t(E)\psi(\underline{r}, E, \underline{\Omega}, t) =$$

$$\left(\int_0^\infty dE' \int_{4\pi} \Sigma_s(E' \rightarrow E, \underline{\Omega}' \rightarrow \underline{\Omega})\Psi(\underline{r}, E', \underline{\Omega}', t)d\underline{\Omega}'\right) +$$

$$\frac{\chi(E)}{4\pi}\left(\int_0^\infty dE' \int_{4\pi} \upsilon\Sigma_f(E')\Psi(\underline{r}, E', \underline{\Omega}', t)d\underline{\Omega}'\right) +$$

$$\frac{1}{4\pi}Q(\underline{r}, E, t)$$