## The Monte Carlo method

What it is: a numerical technique for calculating probabilities and related quantities using sequences of random numbers.
The usual steps:
(1) Generate sequence $r_{1}, r_{2}, \ldots, r_{m}$ uniform in $[0,1]$.
(2) Use this to produce another sequence $x_{1}, x_{2}, \ldots, x_{n}$
 distributed according to some $\operatorname{pdf} f(x)$ in which we're interested ( $x$ can be a vector).
(3) Use the $x$ values to estimate some property of $f(x)$, e.g., fraction of $x$ values with $a<x<b$ gives $\int_{a}^{b} f(x) d x$.
$\rightarrow$ MC calculation $=$ integration (at least formally)
MC generated values $=$ 'simulated data’
$\rightarrow$ use for testing statistical procedures

## Random number generators

Goal: generate uniformly distributed values in $[0,1]$. Toss coin for e.g. 32 bit number... (too tiring).
$\rightarrow$ 'random number generator'
$=$ computer algorithm to generate $r_{1}, r_{2}, \ldots, r_{n}$.
Example: multiplicative linear congruential generator (MLCG)

$$
\begin{aligned}
& n_{i+1}=\left(a n_{i}\right) \bmod m, \quad \text { where } \\
& n_{i}=\text { integer } \\
& a=\text { multiplier } \\
& m=\text { modulus } \\
& n_{0}=\text { seed (initial value) }
\end{aligned}
$$

N.B. $\bmod =$ modulus (remainder), e.g. $27 \bmod 5=2$.

This rule produces a sequence of numbers $n_{0}, n_{1}, \ldots$

## Random number generators (2)

The sequence is (unfortunately) periodic!

$$
\text { Example (see Brandt Ch 4): } a=3, m=7, n_{0}=1
$$

$$
\begin{aligned}
& n_{1}=(3 \cdot 1) \bmod 7=3 \\
& n_{2}=(3 \cdot 3) \bmod 7=2 \\
& n_{3}=(3 \cdot 2) \bmod 7=6 \\
& n_{4}=(3 \cdot 6) \bmod 7=4 \\
& n_{5}=(3 \cdot 4) \bmod 7=5 \\
& n_{6}=(3 \cdot 5) \bmod 7=1 \quad \leftarrow \text { sequence repeats }
\end{aligned}
$$

Choose $a, m$ to obtain long period (maximum $=m-1$ ); $m$ usually close to the largest integer that can represented in the computer.

Only use a subset of a single period of the sequence.

## Random number generators (3)

$r_{i}=n_{i} / m$ are in $[0,1]$ but are they 'random'?
Choose $a, m$ so that the $r_{i}$ pass various tests of randomness:
uniform distribution in $[0,1]$,
all values independent (no correlations between pairs),
e.g. L'Ecuyer, Commun. ACM 31 (1988) 742 suggests

$$
\begin{aligned}
& a=40692 \\
& m=2147483399
\end{aligned}
$$




Far better generators available, e.g. TRandom3, based on Mersenne twister algorithm, period $=2^{19937}-1$ (a "Mersenne prime").
See F. James, Comp. Phys. Comm. 60 (1990) 111; Brandt Ch. 4

## The transformation method

Given $r_{1}, r_{2}, \ldots, r_{n}$ uniform in [0, 1], find $x_{1}, x_{2}, \ldots, x_{n}$ that follow $f(x)$ by finding a suitable transformation $x(r)$.



Require: $P\left(r \leq r^{\prime}\right)=P\left(x \leq x\left(r^{\prime}\right)\right)$
i.e. $\int_{-\infty}^{r^{\prime}} g(r) d r=r^{\prime}=\int_{-\infty}^{x\left(r^{\prime}\right)} f\left(x^{\prime}\right) d x^{\prime}=F\left(x\left(r^{\prime}\right)\right)$

That is, $\quad$ set $F(x)=r$ and solve for $x(r)$.

## Example of the transformation method

Exponential pdf: $\quad f(x ; \xi)=\frac{1}{\xi} e^{-x / \xi} \quad(x \geq 0)$

$$
\begin{gathered}
\text { Set } \int_{0}^{x} \frac{1}{\xi} e^{-x^{\prime} / \xi} d x^{\prime}=r \quad \text { and solve for } x(r) . \\
\rightarrow \quad x(r)=-\xi \ln (1-r) \quad(x(r)=-\xi \ln r \text { works too. })
\end{gathered}
$$



1. Generation of random, Pseudo-random numbers
2. Random variable $r$ uniformly distributed between 0 and 1
3. Sampling of a discrete random variable

Example:
A discrete random variable x with 3 values, $\mathrm{x} 1, \mathrm{x} 2$, x 3 with probabilities P1, P2 and P3
respectively $(\Sigma \mathrm{Pi}=1)$.
Extract $y=r$
if $0<y<$ P1 $=>x=x 1$
if $\mathrm{P} 1<\mathrm{y}<(\mathrm{P} 1+\mathrm{P} 2)=>\mathrm{x}=\mathrm{x} 2$
if $(\mathrm{P} 2+\mathrm{P} 3)<\mathrm{y}<1=>\mathrm{x}=\mathrm{x} 3$
4. Sampling of a continuous random variable $x$ with arbitrary $\operatorname{pdf} f(x)$

Extract $y=r$
$\mathrm{x}=\mathrm{F}^{-1}(\mathrm{y})$ with $\mathrm{y}=\mathrm{F}(\mathrm{x})=\int_{0} \mathrm{x} f\left(\mathrm{x}^{\prime}\right) \mathrm{dx} \mathrm{x}^{\prime}$
Examples:
$f(x)=1 /(b-a) \quad=>x=a+(b-a) r$
$f(\theta)=\sin \theta / 2 \quad=>\cos \theta=1-2 r \quad=>\quad \theta=\operatorname{acos}(1-2 r)$
$\mathrm{f}(\mathrm{x})=\mu \exp (-\mu \mathrm{x})=>\mathrm{x}=-\ln (1-\mathrm{r}) / \mu=>\mathrm{x}=-\ln (\mathrm{r}) / \mu$

## The acceptance-rejection method

Enclose the pdf in a box:

(1) Generate a random number $x$, uniform in $\left[x_{\min }, x_{\max }\right]$, i.e. $x=x_{\text {min }}+r_{1}\left(x_{\max }-x_{\text {min }}\right), r_{1}$ is uniform in $[0,1]$.
(2) Generate a 2 nd independent random number $u$ uniformly distributed between 0 and $f_{\max }$, i.e. $u=r_{2} f_{\max }$.
(3) If $u<f(x)$, then accept $x$. If not, reject $x$ and repeat.

## Example with acceptance-rejection method

$$
\begin{aligned}
& f(x)=\frac{3}{8}\left(1+x^{2}\right) \\
& (-1 \leq x \leq 1)
\end{aligned}
$$

If dot below curve, use $x$ value in histogram.


## Improving efficiency of the acceptance-rejection method

The fraction of accepted points is equal to the fraction of the box's area under the curve.

For very peaked distributions, this may be very low and thus the algorithm may be slow.
Improve by enclosing the $\operatorname{pdf} f(x)$ in a curve $C h(x)$ that conforms to $f(x)$ more closely, where $h(x)$ is a pdf from which we can generate random values and $C$ is a constant.


Generate points uniformly over $C h(x)$.

If point is below $f(x)$, accept $x$.

## Monte Carlo event generators

Simple example: $\mathrm{e}^{+} \mathrm{e}^{-} \rightarrow \mu^{+} \mu^{-}$
Generate $\cos \theta$ and $\phi$ :


$$
\begin{aligned}
& f\left(\cos \theta ; A_{\mathrm{FB}}\right) \propto\left(1+\frac{8}{3} A_{\mathrm{FB}} \cos \theta+\cos ^{2} \theta\right), \\
& g(\phi)=\frac{1}{2 \pi} \quad(0 \leq \phi \leq 2 \pi)
\end{aligned}
$$

Less simple: 'event generators' for a variety of reactions:

$$
\begin{aligned}
& \mathrm{e}^{+} \mathrm{e}^{-} \rightarrow \mu^{+} \mu^{-}, \text {hadrons, } . . \\
& \mathrm{pp} \rightarrow \text { hadrons, D-Y, SUSY,... }
\end{aligned}
$$

e.g. PYTHIA, HERWIG, ISAJET...

Output $=$ 'events', i.e., for each event we get a list of generated particles and their momentum vectors, types, etc.


## Monte Carlo detector simulation

Takes as input the particle list and momenta from generator.
Simulates detector response:
multiple Coulomb scattering (generate scattering angle), particle decays (generate lifetime), ionization energy loss (generate $\Delta$ ), electromagnetic, hadronic showers, production of signals, electronics response, ...

Output $=$ simulated raw data $\rightarrow$ input to reconstruction software: track finding, fitting, etc.

Predict what you should see at 'detector level' given a certain hypothesis for 'generator level'. Compare with the real data.

Estimate 'efficiencies' = \#events found / \# events generated.
Programming package: GEANT

## Monte Carlo integration method

- x uniform random variable in $[\mathrm{a}, \mathrm{b}]$ :

$$
\lim _{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^{n} f\left(x_{i}\right)=\frac{1}{b-a} \int_{a}^{b} f(x) d x
$$

- Hit or miss method, $x, y$ u.r.v., $x$ in [a.b], $y$ in [0, c]:

$$
\int_{a}^{b} f(x) d x=\frac{N_{h i t}}{N_{\text {TOT }}} c(b-a)
$$

Differential pair production cross section from circularly polarized photons


$$
\begin{aligned}
& d \sigma=\left|\sum_{\overrightarrow{\mathbf{L}}} e^{i \overrightarrow{\mathbf{q}} \cdot \overrightarrow{\mathbf{L}}}\right|^{2} d \sigma(\overrightarrow{\mathbf{q}}) \\
& \left|\sum_{\overrightarrow{\mathbf{L}}} e^{i \overrightarrow{\mathbf{q}} \cdot \overrightarrow{\mathbf{L}}}\right|^{2} \propto \sum_{\overrightarrow{\mathbf{g}}} \delta(\overrightarrow{\mathbf{q}}-\overrightarrow{\mathbf{g}}) \\
& \overrightarrow{\mathbf{q}}=\overrightarrow{\mathbf{g}} \\
& \text { [110] } \\
& \xrightarrow[0]{2} \\
& d^{5} \sigma(\overrightarrow{\mathbf{q}})=\frac{d^{5} \sigma}{d E_{+} d \Omega_{+} d \Omega_{-}}|J| d q d \Omega_{r} d E_{-} d \phi_{-} \\
& d \sigma_{c}^{5}=\left|\sum_{\overrightarrow{\mathbf{L}}} \exp (i \overrightarrow{\mathbf{q}} \cdot \overrightarrow{\mathbf{L}})\right|^{2} \exp \left(-A_{T} q^{2}\right) d \sigma^{5}(\overrightarrow{\mathbf{q}}) \\
& \left|\sum_{\text {diam }} \exp (i \overrightarrow{\mathbf{q}} \cdot \overrightarrow{\mathbf{L}})\right|^{2}=\frac{1}{8} N \frac{(2 \pi)^{3}}{\Delta} \sum_{\overrightarrow{\mathbf{B}}} D(\overrightarrow{\mathbf{g}}) \delta(\overrightarrow{\mathbf{q}}-\overrightarrow{\mathbf{g}})
\end{aligned}
$$



(germanium crystal $-Z=32-\mathrm{E}^{+} / K=0.5$ )

