C. Monte Carlo methods

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The Monte Carlo method: a numerical technique for calculating probabilities and related quantities using sequences of random numbers (it is equivalent to integration in perhaps many dimensions).

1. Random number generation
2. Generators for general distributions
3. Simulation
4. Integration

Statistical accuracy proportional to $1/\sqrt{n}$.

1. Random number generation

Basis for Monte Carlo simulations are uniformly distributed random numbers in $[0,1]$.

$u_j \in U(0,1)$ uniform on (0,1) `u = ran()`

$$g(u) = \begin{cases} 1 & \text{if } 0 \le u < 1 \\ 0 & \text{else} \end{cases} \qquad G(u) = \begin{cases} 0 & \text{if } u < 0 \\ u & \text{if } 0 \le u < 1 \\ 1 & \text{if } u \le 1 \end{cases} .$$

Methods:

- toss coins for e.g. a 32 bit number $\rightarrow$ to tiring
- use computer algorithm to generate sequence of random numbers

Linear congruential generator

Based on the recurrence relation

$$I_j = (a \cdot I_{j-1} + c) \mod m \qquad j = 1, 2, \ldots$$

integer random numbers I_j between 0 and $m-1$ are generated.

Parameters: factor a increment c modulus m

Integer I_j is converted to a real number $u = I_j/m$.

Values $u = 0$ and $u = 1$ usually excluded.

The maximum value m of the period is reached under the following conditions:

1. increment $c \neq 0$;
2. the increment c and the modulus m do not have a common divisor;
3. $(a-1)$ is a multiple of the prime number p for each prime number p, which is a divisor of the modulus m;
4. $(a-1)$ is a multiple of 4, if modulus m is a multiple of 4.

Numerical example

factor $a = 3$ increment $c = 0$ modulus $m = 7$

$$\begin{aligned}
I_0 &= 1 \quad \text{(start value = seed)} \\
I_1 &= (3 \cdot 1 + 0) \mod 7 = 3 \\
I_2 &= (3 \cdot 3 + 0) \mod 7 = 2 \\
I_3 &= (3 \cdot 2 + 0) \mod 7 = 6 \\
I_4 &= (3 \cdot 6 + 0) \mod 7 = 4 \\
I_5 &= (3 \cdot 4 + 0) \mod 7 = 5 \\
I_6 &= (3 \cdot 5 + 0) \mod 7 = 1 \quad \text{sequence repeats}
\end{aligned}$$

- start with seed I_0, which determines the whole sequence
- use different seeds in continued or repeated calculation (e.g. seed derived from daytime)
- use same seed during program development

Title

Are these numbers really *random* numbers? $\rightarrow$ tests!

In a given calculation only a small fraction of the total period should be used ($\rightarrow$ large period required).

Deficiencies of the LCG:

- Low-order bits are less "random" than high-order bits.
- Sequential correlations exist: d subsequent random numbers in d-dimensional space lie on $(d-1)$-dimensional hyperplanes
- there are at most $m^{1/d}$ such planes
- maximum period reached only for certain parameter sets.

Good parameter sets:

a	205	281	1021	421
c	29573	28411	25673	54773
m	139968	134456	121500	259200

Some sets result in integer overflows (machine-dependence).

Improvements

How to improve random number generation? Use *good* random number generator and combine > 1 generator!

Combination of two generators:

- fill array with random numbers of one random generator;
- use second random generator to select from array.

Good random number generators:

- lagged-Fibonacci based generators efficient and long period;
- RANLUX, based on the method of Lüscher, has a solid theoretical basis in chaos theory;
- Gutbrods generator (used in examples)

Test for generators

Basic test is for uniform distribution (histogram).

Up-down- or sequence test: generate $n+1$ random numbers and determine number of sequences $N(k)$ of increasing or decreasing random numbers, satisfying

$$\sum_{k=1}^{n} k \cdot N(k) = n \qquad \sum_{k=1}^{n} N(k) = \frac{(2n-1)}{3} .$$

For truely uncorrelated random numbers u_j the following values are expected:

$$N(1) = \frac{5n+1}{12} \qquad N(2) = \frac{11n-14}{60}$$

$$N(k) = \frac{2\left[\left(k^2+3k+1\right)n - \left(k^3+3k^2-k-4\right)\right]}{(k+3)!}$$

Especially the numbers $N(k)$ from larger values of k allow sensitive tests of the random number generator.

2. Generators for general distributions

MC simulation/integration requires random numbers from different distributions, e.g. normal (also many-dimensional), exponential, Poisson ...

Methods

- inverse transform for continuous variable
- examples and special methods
- inverse ransform for discrete variable
- acceptance/rejection method

Inverse transfrom for continuous variable

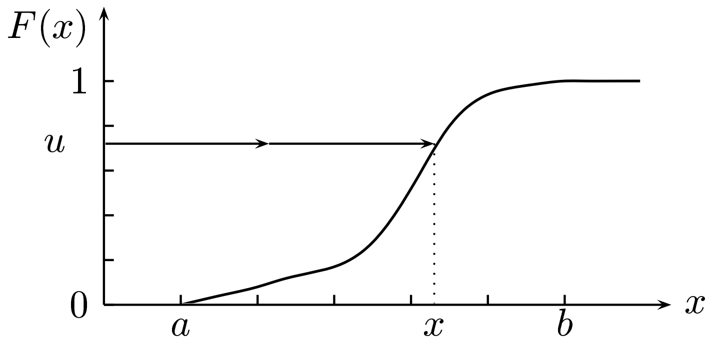
If x is chosen from density $f(x)$, then the cumulative probability $F(x)$ is itself a rn which will occur with uniform density $g(u)$ on $[0,1]$:

$$f(x)\mathrm{d}x = g(u)\,\mathrm{d}u \qquad \int_{-\infty}^{x} f(x')\,\mathrm{d}x' = F(x) = u.$$

The equation $u = F(x)$ is solved for the variable x by

$$x = F^{(-1)}(u)$$

with the inverse function $F^{(-1)}(u)$, provided the inverse function can be found.



Exponential distribution

$$f(x)\,\mathrm{d}x = \lambda e^{-\lambda x} \qquad \text{exponential distribution} \qquad x \in (0, +\infty)$$

Inverse transform method:

$$\int_0^x f(x')\,\mathrm{d}x' = -e^{-\lambda x'}\Big|_0^x = 1 - e^{-\lambda x} = u$$

$$e^{-\lambda x} = 1 - u \qquad x = -\frac{1}{\lambda}\ln(1-u) \quad \text{or} \quad x = -\frac{1}{\lambda}\ln u$$

Random angle and direction

Azimuthal angle ϕ: $\sin\phi$ and $\cos\phi$ of an uniformly distributed random angle ϕ is generated by the algorithm (with any function call)

1. Generate u_1 and u_2, then $v_1 = 2u_1 - 1$, $v_2 = u_2$;
2. calculate $r^2 = v_1^2 + v_2^2$; if $r^2 > 1$, goto step 1;
3. calculate

$$\sin\phi = 2\frac{v_1 v_2}{r^2} \qquad \cos\phi = \frac{v_1^2 - v_2^2}{r^2}$$

based on

$$\sin\phi = 2\cos\frac{\phi}{2}\cdot\sin\frac{\phi}{2} \qquad \cos\phi = \cos^2\frac{\phi}{2} - \sin^2\frac{\phi}{2}$$

Polar angle θ: $\cos\theta = 2u - 1$ corresponds to distribution uniform in $\cos\theta$.

Random unit vector: $(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ (note: all components follow the same distribution!)

Normal distribution

A simple approximate method based on Central limit theorem:

$$z = \sum_{i=1}^{12} u_i - 6 \qquad \text{add 12 random numbers } u_i \in U(0,1)$$

Box-Muller method: starts from χ^2 variable with 2 degrees of freedom, which has an exponential distribution.

1. Generate two random numbers u_1 and u_2 and construct $v_1 := 2u_1 - 1$ and $v_2 := 2u_2 - 1$.
2. calculate $r^2 = v_1^2 + v_2^2$; if $r^2 > 1$, goto step 1;
3. calculate the two independent random numbers

$$z_1 = v_1\sqrt{\frac{-2\ln r^2}{r^2}} \qquad z_2 = v_2\sqrt{\frac{-2\ln r^2}{r^2}}$$

The random number z is transformed to a random number z' from the normal distribution with mean μ and standard deviation σ by $z' = \mu + \sigma z$.

Normal distribution in n dimensions

Density

$$f(\boldsymbol{x}) = \frac{|\boldsymbol{W}|^{1/2}}{(2\pi)^{n/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu_x})^T \boldsymbol{W} (\boldsymbol{x}-\boldsymbol{\mu_x}) \right)$$

with $\boldsymbol{W} = \boldsymbol{V}^{-1}$ and $|\boldsymbol{W}| = \det\ \boldsymbol{W} = |\boldsymbol{V}^{-1}|$.

Random number generation based on Cholesky decomposition of $\boldsymbol{V} = \boldsymbol{R}^T\boldsymbol{R}$ or $\boldsymbol{W} = \boldsymbol{R}^{-1}(\boldsymbol{R}^{-1})^T$.

$$\boldsymbol{x} = \boldsymbol{\mu} + \boldsymbol{R}^T\,\boldsymbol{z}$$

where $\boldsymbol{z}$ = vector of independent random numbers from the normal distribution $N(0,1)$.

Proof, assuming $\boldsymbol{\mu} = 0$: $\quad \boldsymbol{x}^T\boldsymbol{W}\boldsymbol{x} = \boldsymbol{x}^T\boldsymbol{R}^{-1}(\boldsymbol{R}^{-1})^T\boldsymbol{x} = \boldsymbol{z}^T\boldsymbol{1}\boldsymbol{z}$

$$\boldsymbol{z} = (\boldsymbol{R}^{-1})^T\boldsymbol{x} \quad \rightarrow \quad \boldsymbol{x} = \boldsymbol{R}^T\boldsymbol{z}$$

Normal distribution in 2 dimensions

Covariance matrix $\boldsymbol{V}$ and right triangular matrix $\boldsymbol{R}$:

$$\boldsymbol{V} = \begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} = \boldsymbol{R}^T\boldsymbol{R} \qquad \boldsymbol{R} = \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix}$$

Result of decomposition:

$$R_{11} = \sqrt{V_{11}} = \sigma_1 \qquad R_{12} = \frac{V_{11}}{\sqrt{V_{11}}} = \rho\sigma_2 \qquad R_{22} = \sqrt{V_{22} - R_{12}^2} = \sigma_2\sqrt{1-\rho^2}$$

Generate z_1, $z_2 \in N(0,1)$ (uncorrelated) and transform:

$$\begin{aligned} x_1 &= \mu_1 + \sigma_1 z_1 \\ x_2 &= \mu_2 + \sigma_2\left(\rho z_1 + \sqrt{1-\rho^2}z_2\right) \end{aligned}$$

resulting random values x_1 and x_2 are correlated.

Cholesky decomposition

The matrix $\boldsymbol{W}$ is transformed to the matrix $\boldsymbol{R}$ in steps. Starting with $\boldsymbol{W}^{(0)} = \boldsymbol{W}$ the transformation is

$$W_{ij}^{(k)} = W_{ij}^{(k-1)} - R_{ki} R_{kj} \qquad i,\, j = k+1,\, k+2,\, \ldots\, n\,.$$

for $k = 1,\, 2,\, \ldots\, (n-1)$. First $k = 1$ and the elements wih $i,\, j = 2,\, 3, \ldots\, n$ are transformed, the $k = 2$ and the elements with $i,\, j = 3,\, 4, \ldots\, n$ are transformed by

$$R_{ii} = \sqrt{W_{ii}^{(i-1)}} \qquad R_{ij} = \frac{W_{ij}^{(i-1)}}{R_{ii}} \quad \text{für} \quad j > i\,.$$

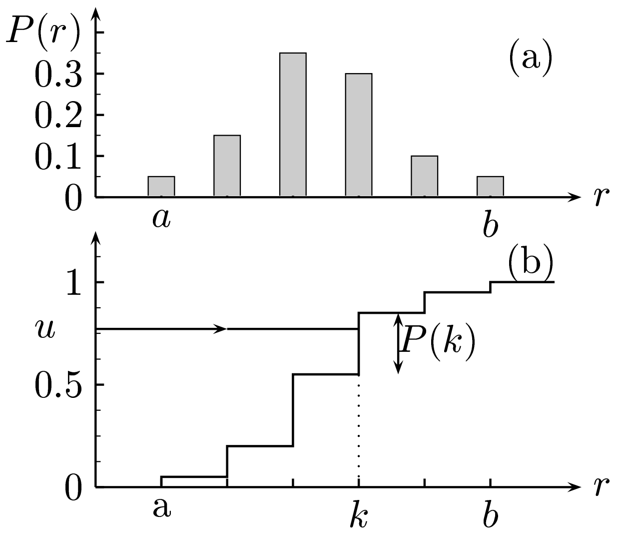
The relation

$$W_{jj} = \sum_{i=1}^{j} R_{ij}^2 \qquad j = 1,\, 2, \ldots\, n$$

shows that the elements of the Cholesky factors $\boldsymbol{R}$ are limited by the positive diagonal elements of the matrix $\boldsymbol{W}$.

Inverse transformation method for discrete variable

In a discrete distribution an index k is assigned to the discrete random values with $k = 1,\, 2, \ldots$. The discrete values x_k occurs with probability $P(x_k)$.



Chose random number $u \in U(0,1)$ and find index k with

$$P_{k-1} < u \le P_k$$

where $P_0 = 0$.

Poisson distribution

$$P_\mu(k) = \frac{\mu^k}{k!}\, e^{-\mu} \qquad k = 0, 1, \ldots \qquad \text{Poisson distribution, parameter} = \mu$$

Random number generation of integer k:

1. Set $k := 0$ and $A := 1.0$;
2. generate a random number u and replace A by $u\,A$: $A := u\,A$; if $A \le e^{-\mu}$, accept k and stop
3. increase k by 1: $k := k + 1$ and goto step 2

For larger values of μ like $\mu = 100$ the method makes no sense, because $e^{-\mu}$ may be already outside the floating point range of the computer.

Already for $\mu > 10 \ldots 20$ it is better to use the normal approximation of the Poisson distribution and to generate a random variable z from $N(0, 1)$; the real random number is then converted to the random integer k by $k = \max\left(0, \left[\mu + z\sqrt{\mu} + 0.5\right]\right)$.

Acceptance-rejection method

Obtaining the inverse function $F^{(-1)}(u)$ is often impossible, although the density function can be computed for any possible value of x. The method due to Neumann is based on the relation

$$f(x) \le C\, h(x) \qquad \text{for all } x$$

where $h(x)$ is a density, where the random values x are easily generated; the factor C is a (positive) constant. The algorithm is as follows:

1. Choose a random number x according to distribution $h(x)$;
2. generate u;
3. if the product $u\,C\,h(x) > f(x)$, reject x and repeat step 1; otherwise accept x.

Because both $f(x)$ and $h(x)$ are normalized, the factor $C > 1$; the acceptance probability in the last step is equal to the ratio of the areas, which is $1/C < 1$. The factor C will not be much larger than 1, if the shape of $h(x)$ is similar to the shape of $f(x)$; in this case the efficiency of the algorithm will be close to 100 %.

Acceptance-rejection method contnd.

The distribution $h(x)$ may be even a uniform distribution between the limits a and b of x and in this case one has to choose the constant C such that $f(x) \leq C$ for all x. Then the algorithm is:

1. Choose x_i uniformly distributed between a und b:
   $x = a + u_1 \cdot (b - a)$ with $u_1 \in U(0, 1)$;
2. choose another random number $u_2 \in U(0, 1)$.
3. if the product $u_2 \cdot C > f(x)$, goto step 1, otherwise accept x.

3. Integration

One-dimensional integration:

many excellent methods exist for numerical integration

- trapezoidal rule
-
- Gauss quadrature

Numerical integration in space of high dimension, often difficult because of complicated integration region.

Monte Carlo methods become relatively efficient and allow to work with complicated integration regions.

Integral by trapezoidal rule and by MC

Approximation of the integral of the function $g(x)$

$$\mathrm{I} = \int_a^b g(x)\,\mathrm{d}x$$

- Numerical integration: trapezoidal rule

$$I_{TR} = \frac{b-a}{n}\sum_{j=0}^{n} w_j g(x_j) + R_n \qquad R_n = -\frac{1}{12}\frac{(b-a)^3}{n^2}\tilde{g}''$$

- Monte Carlo method: random $x \in U(a,b)$

$$I = (b-a)\int_a^b g(x)\cdot\frac{1}{(b-a)}\,\mathrm{d}x = (b-a)\,E[g(x)]$$

Monte-Carlo estimate I_{MC}

$$I_{\mathrm{MC}} = \frac{b-a}{n}\sum_{i=1}^{n} g(x_i) \qquad x_i \in U(a,b)$$

Accuracy of Monte Carlo estimate

Variance of MC estimate by standard statistical methods:

$$V[I_{MC}] = V\left[\frac{b-a}{n}\sum_{i=1}^{n} g_i\right] = \left(\frac{b-a}{n}\right)^2 V\left[\sum_{i=1}^{n} g_i\right] = \frac{(b-a)^2}{n} V\left[g_i\right] \propto 1/n$$

The standard deviation has, in agreement with the law of large numbers, a dependence $\propto 1/\sqrt{n}$.

Factor $V\left[g_i\right]$ may be large:

$$V\left[g_i\right] = E\left[(g_i - \bar{g})^2\right] \approx \left[\frac{\sum g_i^2}{n} - \left(\frac{\sum g_i}{n}\right)^2\right]$$

Variance reducing methods discussed later.

Numerical integration in d dimensions

- Numerical integration on unit hypercube $(0,1)^d$ with trapezoidal rule in d dimensions, applying trapezoidal rule with $n+1$ points in each dimension:

$$I_{TR} = \frac{1}{n^d} \sum_{j_1=0}^{n} \sum_{j_2=0}^{n} \cdots \sum_{j_d=0}^{n} w_{j_1} w_{j_2} \cdots w_{j_d} \cdot g\left(\frac{j_1}{n}, \frac{j_2}{n}, \ldots \frac{j_d}{n}\right) + \mathcal{O}\left(\frac{1}{n^2}\right)$$

  where the function $g(x_1, x_2, \ldots x_d)$ has to be evaluated $N = (n+1)^d \approx n^d$ times. Although the deviation is still proportional to $1/n^2$, the dependence on the number N of function evaluations is $N^{-2/d}$.
- Monte Carlo method: $\sigma \propto 1/\sqrt{n}$

Cross-over point: $N^{-2/d} = N^{-1/2} \quad \rightarrow d > 4$

complicated integration boundaries are simpler for the Monte Carlo method than for numerical methods.

Variance reducing methods

However, the convergence of the Monte Carlo estimate I_{MC} by a rate of $1/\sqrt{N}$ is slow; it depends on the variance of the function and techniques to reduce the variance are important.

- Importance sampling
- Control variates
- Stratified sampling

Importance sampling

The method corresponds to a change of the variable. The integral of the function $g(x)$ in the intervall (a, b) is written in the form

$$I = \int_a^b g(x)\,\mathrm{d}x = \int_a^b \left[\frac{g(x)}{f(x)}\right] f(x)\,\mathrm{d}x = E\left[\frac{g(x)}{f(x)}\right],$$

with a probability density $f(x)$, normalized in the interval (a, b). Assuming that the density $f(x)$ can be integrated $(F(x))$ and the inverse $F^{(-1)}(u)$ can be found, the expectation value of the function $r(x) = g(x)/f(x)$ for probability density $f(x)$ can easily be determined with Monte Carlo methods.

$$I_{\mathrm{MC}} = \frac{1}{n}\sum_{i=1}^{n}\frac{g(x_i)}{f(x_i)} \quad \text{with} \quad x_i \in (a,\, b) \quad \text{from density } f(x)\,.$$

Importance sampling improves the accuracy of a Monte Carlo integration, if a density $f(x)$ can be found with a small variance of $r(x) = g(x)/f(x)$

$$V[r] = E\left[\left(r(x) - \overline{r}\right)^2\right]$$

Control variates

In this method for variance reduction a function $h(x)$ is subtracted from the function $g(x)$, which can be integrated analytically:

$$\int_a^b g(x)\,\mathrm{d}x = \int_a^b h(x)\,\mathrm{d}x + \int_a^b \left[g(x) - h(x)\right]\,\mathrm{d}x\,,$$

The first integral is calculated analytically, the second one by Monte Carlo methods. The function $h(x)$ should be chosen to reduce the variance of the second integral.

Stratified sampling

The full integration space is divided into subspaces and a Monte Carlo integration is performed in each subspace; the partial results are added up in the end. The method is based on the property

$$\int_a^b g(x)\,\mathrm{d}x = \int_a^c g(x)\,\mathrm{d}x + \int_c^b g(x)\,\mathrm{d}x \qquad\qquad a < c < b$$

for the Riemann-Integral.

For a d-dimensional integral the integration region is divided into k subregions M_j with $j = 1, 2, \ldots k$. A subregion has a volume $V(M_j)$ and in each subregion the Monte Carlo integration is done with N_j points. The Monte Carlo estimate of the complete integral is

$$I_{\mathrm{MC}} = \sum_{j=1}^{k} \frac{V(M_j)}{N_j} \sum_{i=1}^{N_j} g(\boldsymbol{x}_{ji}) \; .$$

Stratified sampling contnd.

The variance of the integral is, instead of $\sigma^2(g)/N$, given by the expression

$$V[I_{\mathrm{MC}}] = \sum_{j=1}^{k} \frac{V^2(M_j)}{N_j} \; \sigma^2(g)\big|_{M_j} \; ,$$

where the $\sigma^2(g)\big|_{M_j}$ are the variances in the subregions.

If the subregions and the numbers N_j are carefully chosen, the variance can be reduced compared to the simple Monte Carlo integral. The variances in the subregions should be small, and the number of points in each subregion should be proportional to the product of volume $V(M_j)$ and standard deviation $\sigma(g)|_{M_j}$ in each subregion.

In adaptive Monte Carlo methods the subregions are optimized during the calculation, and the number of points N_j in each subregion is optimized.

4. Simulation

Simulation of physical processes by Monte Carlo methods

Example from High Energy Physics: Generators for *ep*-interactions

Results are "events", i.e. list of final state particles and their momentum vectors.

ARIADNE A program for simulation of QCD cascades implementing the color dipole model.

AROMA Heavy quark production in boson-gluon fusion using full electroweak LO cross-sections (with quark masses) in ep collisions, DIS and photoproduction. Parton showers and Lund hadronization gives full events.

COMPTON Event generator of quasi-real QED Compton events in ep collisions.

Monte Carlo detector simulation

Aim:

- design and optimize the detectors
- develop and test the reconstruction and analysis programs, and
- interpret the experimental data

Takes as input the list of particles and their momenta from event generators.

Simulate the detector response

- description of geometry and material of the detector elements
- tracking of particles through the detector
- simulate their physical interactions in matter and the effects of fields and boundaries on their trajectory
- reproduce the electronic response of the sensitive detectors

Output is simulated "raw data" = input to reconstruction and analysis programs