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).

- Random number generation
- Generators for general distributions
- Simulation
- Integration

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

Random number generation

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

$$u_j \in U(0,1) \quad \text{uniform on } (0,1) \qquad \texttt{u = ran()}$$

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

Methods:

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

Required: truely uncorrelated random numbers with large period.

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:

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

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

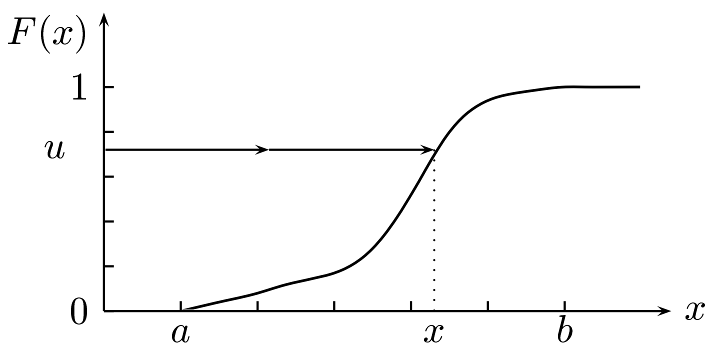
Especially the numbers $N(k)$ from larger values of k allow sensitive tests of the random number generator.

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 $F^{(-1)}(u)$, if possible.



Example: $f(x)\,\mathrm{d}x = \lambda e^{-\lambda x} \quad \rightarrow \quad x = -\frac{1}{\lambda}\ln u$

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

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

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:

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

Improvement by variance reducing methods.

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: $N^{-2/d} = N^{-1/2} \quad \to d > 4$

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

Variance reducing methods

- Importance sampling: change of the variable

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

- Stratified sampling: 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.

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

  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.
  Adaptive Monte Carlo methods: subregions and the number of points N_j in each subregion are optimized during the calculation.

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