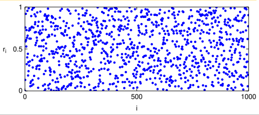
Random numbers in algorithms

- A **deterministic** algorithm is a sequence of operations giving the correct answer (or failing to do so in such a way that we know about the failure).
  Example: matrix inversion by the Gauss–Jordan elimination with full pivoting.
- A **Monte Carlo** algorithm as a procedure using (pseudo)random number to obtain a result, which is correct with certain probability; typically, a numerical result subject to a stochastic error.
  Example: Solving the traveling salesman problem by simulated annealing.
- A **Las Vegas** algorithm uses random numbers to obtain a deterministic result.
  Example: matrix inversion by the Gauss–Jordan elimination with the pivot element selected at random from several (large enough) pivot candidates.

Example of pseudo random number generator +

$$n_i = 7^5 n_{i-1} \bmod (2^{31}-1), \quad r_i = n_i/2^{31}$$



Monte Carlo integration (naive Monte Carlo)

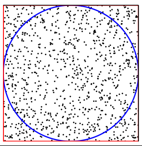
Example: Calculate π by MC integration

```
INTEGER n  total # of points
INTEGER i
INTEGER nu  # of points in a circle
REAL x,y  coordinates of a point in a sphere
REAL rnd(-1,1)  function returning a random number in interval [−1, 1)

nu := 0
FOR i := 1 TO n DO
   x := rnd(-1,1)
   y := rnd(-1,1)
   IF x*x+y*y < 1 THEN nu := nu + 1

PRINT "pi=", 4*nu/n  area of square = 4

PRINT "std. error=", 4*sqrt((1-nu/n)*(nu/n)/(n-1))
```



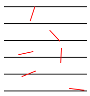
Also "random shooting". Generally

$$\int_\Omega f(x_1,\ldots,x_D)\,dx_1\ldots dx_D \approx \frac{|\Omega|}{K}\sum_{k=1}^{K} f(x_1^{(k)},\ldots,x_D^{(k)})$$

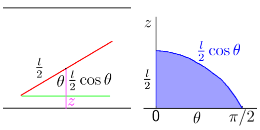
where $(x_1^{(k)},\ldots,x_D^{(k)})$ is a random vector from region Ω
($|\Omega|$ = area, volume, ...; calculation of π: $\Omega=(-1,1)^2$, $|\Omega|=4$)

Exercise – Buffon's needle

Let a needle of length l be tossed randomly on a plane with parallel lines d units apart, $l \le d$. The probability that the needle crosses a line is $p = 2l/\pi d$.
[Georges-Louis Leclerc, Comte de Buffon, 1707–1788]



Proof:



expression $(a < b)$ gives 1 if the inequality holds true, 0 otherwise (Iverson bracket)

$$p = \frac{1}{d/2}\int_0^{d/2}\frac{dz}{\pi/2}\int_0^{\pi/2} d\theta \left(z < \frac{l}{2}\cos\theta\right) = \frac{1}{d/2}\frac{1}{\pi/2}\int_0^{\pi/2}\frac{l}{2}\cos\theta\, d\theta = \frac{2l}{\pi d}$$

Usage (δp is the standard error of p)

$$\pi \approx \frac{2l}{pd}, \quad \text{where } p = \frac{n_{\text{crosses}}}{n_{\text{total}}}, \quad \delta p \approx \sqrt{\frac{p(1-p)}{n-1}}, \quad \delta\pi = \frac{2l}{pd}\frac{\delta p}{p}$$

(rel. error: $\delta p / p$)

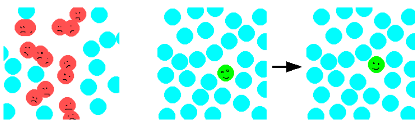
for me: grid: pic/buffon-grid.pdf and buffon.sh / https://www.youtube.com/watch?v=6jkXBqBOR6o

Importance sampling

$$\sum e^{-\beta U(\vec r^N)} f(\vec r^N) \to \frac{1}{K}\sum_{k=1}^{K} f(\vec r^{N,(k)})$$

where $\vec r^{N,(k)}$ is a random vector with a probability density $\propto e^{-\beta U(\vec r^N)}$.

Metropolis algorithm: $\vec r^{N,(k+1)}$ generated sequentially from $\vec r^{N,(k)}$



naive MC — importance sampling

Metropolis method (intuitively)

- Choose a particle, i (e.g., randomly)
- Try to move it, e.g.:

$$x_i^{tr} = x_i + u_{(-d,d)}, \quad y_i^{tr} = y_i + u_{(-d,d)}, \quad z_i^{tr} = z_i + u_{(-d,d)}$$

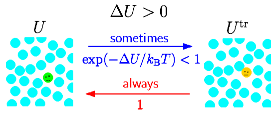
  or in/on sphere, Gaussian,...

  so that the **probability of the reversed move is the same**
- Calculate the change in the potential energy, $\Delta U = U^{tr} - U$
- **If** $\Delta U \le 0$, the change is accepted
  If $\Delta U \ge 0$, the change is accepted with probability $\exp(-\beta\Delta U)$, otherwise rejected

Because then it holds for the probability ratio:

$$\text{new} : \text{old} = p^{tr} : p = \exp(-\beta\Delta U)$$

(moves there and back are compared, always the probability the U-decreasing move = 1, and of the opposite move = Boltzmann)



Algorithm – details

- Choose a particle (lattice site, ...) to move
- $A^{tr} := A^{(k)}$ + random move (spin) of the chosen particle
- $\Delta U := U(A^{tr}) - U(A^{(k)}) \equiv U^{tr} - U^{(k)}$
- The configuration is accepted ($A^{(k+1)} := A^{tr}$) with probability $\min\{1, e^{-\beta\Delta U}\}$ otherwise rejected:

Version 1	Version 2	Version 3
$u := u_{(0,1)}$ IF $u < \min\{1, e^{-\beta\Delta U}\}$ THEN $A^{(k+1)} := A^{tr}$ ELSE $A^{(k+1)} := A^{(k)}$	$u := u_{(0,1)}$ IF $u < e^{-\beta\Delta U}$ THEN $A^{(k+1)} := A^{tr}$ ELSE $A^{(k+1)} := A^{(k)}$	IF $\Delta U < 0$ THEN $A^{(k+1)} := A^{tr}$ ELSE $u := u_{(0,1)}$ IF $u < e^{-\beta\Delta U}$ THEN $A^{(k+1)} := A^{tr}$ ELSE $A^{(k+1)} := A^{(k)}$

- $k := k + 1$ and again and again

How to choose a particle to move

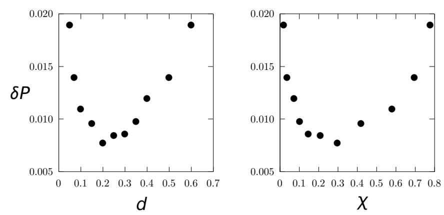
- In a cycle – check the reversibility!
  Deterring examples of microreversibility violation:
  Three species A, B, C in a ternary mixture moved sequentially in the order of A–B–C–A–B–C– ⋯
  Sequence: move molecule A – move molecule B – change volume – ⋯
- Randomly

Chaos is better than bad control

Acceptance ratio

$$\chi = \frac{\text{number of accepted configurations}}{\text{number of all configurations}}$$

χ depends on the displacment d. Optimal χ depends on the system, quantity, algorithm. Often **0.3 is a good choice**. Exception: diluted systems...



LJ (reduced units): $T = 1.2$, $\rho = 0.8$