

Question: What is the most probable number for the sum of two dice?

| $\bullet$ |  | $\underline{2}$ | $\underline{2}$ | $\underline{3}$ | $\underline{4}$ | $\underline{5}$ | $\underline{6}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $1 \mid$ | 2 | 3 | 4 | 5 | 6 | 7 |
| 36 possibilities | $3 \mid$ | 4 | 5 | 5 | 6 | 7 | 8 |
|  | 5 | 7 | 7 | 8 | 9 | 10 |  |
| 6 times - for 7 | $5 \mid$ | 6 | 7 | 8 | 9 | 10 | 11 |
|  | $6 \mid$ | 7 | 8 | 9 | 10 | 11 | 12 |

## How do we do that?

- You let the computer to throw "the coin" and record the outcome
- You need a program that generates randomly a variable
... with relevant probability distribution


## Applications for MC simulation

- Stochastic processes
- Complex systems (science)
- Numerical integration
- Risk management
- Financial planning

■ ...

## Random Number Generators (RNG)

- There are no true random number generators but pseudo RNG!
- Reason: computers have only a limited number of bits to represent a number
- It means: the sequence of random numbers will repeat

\left.| How do we do that? |
| :--- |
| - You let the computer to throw "the coin" and record |
| the outcome |
| You need a program that generates randomly a |
| variable |
| ... with relevant probability distribution |$\right]$ itself (period of the generator)

## Good Random Number Generators

- equal probability for any number inside interval $[a, b]$
- yet independent of the previous number
- long period
- produce the same sequence if started with same initial conditions
- fast

Linear Congruent Method for RNG
Generates a random sequence of numbers
$\left\{x_{1}, x_{2}, \ldots x_{k}\right\}$ of length $M$ over the interval $[0, M-1]$

$$
x_{i}=\bmod \left(a x_{i-1}+c, M\right)
$$

- starting value $\mathrm{x}_{0}$ is called "seed"
- coefficients a and $c$ should be chosen very carefully
note:
$\bmod (b, M)=b-\operatorname{int}(b / M) * M$

Example: $\quad \begin{array}{ll}x_{i}=\bmod \left(a x_{i-1}+c, M\right) \\ \bmod (b, M)=b-\operatorname{int}(b / M) * M\end{array}$
$a=4, c=1, M=9, x_{1}=3$
$x_{2}=4$
$x_{3}=8$
$x_{4}=6$
$x_{5-10}=7,2,0,1,5,3$
interval: 0-8, i.e. [0,M-1]
period: 9 i.e. M numbers (then repeat)

## Random Numbers on interval $[A, B]$

- Scale results from $x_{i}$ on $[0, M-1]$ to $y_{i}$ on $[0,1]$
$y_{i}=x_{i} /(M-1)$
- Scale results from $x_{i}$ on $[0,1]$ to $y_{i}$ on $[A, B]$
$y_{i}=A+(B-A) x_{i}$

Magic numbers for Linear Congruent Method

- $M$ (length of the sequence) is quite large
- However there is no overflow (for 32 bit machines $\mathrm{M}=2^{31} \approx 2^{\star} 10^{9}$ )
- Good "magic" number for linear congruent method:
$x_{i}=\bmod \left(a x_{i-1}+c, M\right)$
$a=16,807, c=0, M=2,147,483,647$

How can we be check the RNG?
Plots:

- 2D figure, where $x_{i}$ and $y_{i}$ are from two random sequences (parking lot test)
- 3D figure $\left(\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}, \mathrm{z}_{\mathrm{i}}\right)$
- 2D figure for correlation ( $\mathrm{x}_{\mathrm{i}}, \mathrm{x}_{\mathrm{K}} .$. )



## How can we check the RNG?

Example of other assessments
Uniformity. A random number sequence should contain numbers distributed in the unit interval with equal probability. Use bins.
k-th momentum $\left\langle x^{k}\right\rangle=\frac{1}{N} \sum_{i=1}^{N} x_{i}^{k} \approx \frac{1}{k+1}$
near-neighbor correlation $\frac{1}{N} \sum_{i=1}^{N} x_{i} x_{i+k} \approx \frac{1}{4}$

## "Industrial" methods

- rand
- random
- drand48
- rn
- drand
- srand
- ...

1. call SEED

Changes the starting point of the pseudorandom number generator.
2. call RANDOM

Returns a pseudorandom number greater than or equal to zero and less than one from the uniform distribution.

For real applications use "industrial" random number generators

## Practice 1 (homework)

1. Write a program to generate random numbers using the linear congruent method
2. Plot 2D distribution for two random sequences $x_{i}$ and $y_{i}$
3. Plot 2D distribution for correlation $\left(x_{i}, x_{i+4}\right)$
4. Evaluate 5 -th moment of the random number distribution
5. Use some built-in RNG for problems 2-4.

## Random Walk simulates:

- Brownian motion
(answer the question - how many collisions, on average, a particle must take to travel a distance R).
- Electron transport in metals, ...
- 

...

## Practice 2 (random walk)

1. Write a program that simulate a random 2D walk with the same step size . Four directions are possible (N, E, S, W). Your program will involve two large integers, $M=$ the number of random walks to be taken and $N=$ the maximum number of steps in a single walk.
2. Find the average distance to be from the origin point after $N$ steps
3. Is there any finite bound on the expected number of steps before the first return to the origin?


- There are very many methods for numerical integration
- Can MC approach compete with sophisticated methods?
- Can we gain anything from integration by "gambling"?


## Problem: High-Dimensional Integration

Example: Integration for a system with 12 electrons.

- $3 * 12=36$ dimensional integral
- If 64 points for each integration then $=643^{36}$ points to evaluate
- For 1 Tera Flop computer $=10^{53}$ seconds
- That is ... 3 times more then the age of the universe!

One more example


Compute $N$ pairs of random numbers $x_{i}$ and $y_{i}$ with $0.0 \leq x \leq 2.0$ and $-1.5 \leq y \leq 1.5$.

$$
F_{n}=A\left(\frac{n_{+}-n_{-}}{N}\right)
$$

Integration by mean value

$$
\begin{gathered}
I=\int_{a}^{b} f(x) d x=(b-a)\langle f\rangle \quad \text { and } \quad\langle f\rangle=\frac{1}{N} \sum_{i=1}^{N} f\left(x_{i}\right) \\
I=\int_{a}^{b} f(x) d x=(b-a) \frac{1}{N} \sum_{i=1}^{N} f\left(x_{i}\right)
\end{gathered}
$$

Traditional methods (Simpson, ...) - the N points are chosen with equal spacing

Monte Carlo method - random spacing

## Error in Monte Carlo integration

- error in Monte Carlo 1D integration

$$
\frac{1}{\sqrt{N}}
$$

- error in "common" 1D integration
- error in "common nD integration $\frac{1}{N}$
in
- error in Monte Carlo nD integration

$$
\frac{n}{N / n}
$$

$$
\frac{1}{\sqrt{N}}
$$

at $\mathrm{n}=4$ the error in Monte Carlo integration is similar to that of conventional scheme

## Practice: Integration

- Use Monte Carlo integration (both rejection and mean value methods) to evaluate
$\int_{0}^{3} \exp (-x) d x$ and $\int_{0}^{5} \sin \left(2 x^{2}\right) d x$
- Evaluate 7-D integral

$$
\int_{0}^{1} d x_{1} \int_{0}^{1} d x_{2} \int_{0}^{1} d x_{3} \int_{0}^{1} d x_{4} \int_{0}^{1} d x_{5} \int_{0}^{1} d x_{6} \int_{0}^{1}\left(x_{1}+x_{2}+\ldots+x_{7}\right)^{2} d x_{7}
$$

## Non-uniform distributions

Most situation in physics - random numbers with nonuniform distribution

- radioactive decay
- experiments with different types of distributions
- ...

Principal idea: Generating non-uniform random number distributions with a uniform random number generators

## Method 2: Inversion method

- Works if the function you are trying to use for a distribution has an inverse


## Practice: non-uniform distribution

Use the von Neumann rejection technique to generate a normal distribution of standard deviation 1.0

## Method 1: von Neumann rejection

Generating non-uniform distribution with a probability distribution $\mathrm{w}(\mathrm{x})$

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

- Example: exponential distribution
$w(x)=\exp (-x)$
$x=-\ln (1-y)$
very many program libraries have most common non-uniform distributions 29

