Monte Carlo Methods

Spring Semester 2013/14, Department of Applied Mathematics, University of Crete

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Part II: Monte Carlo Integration, Random Numbers generators

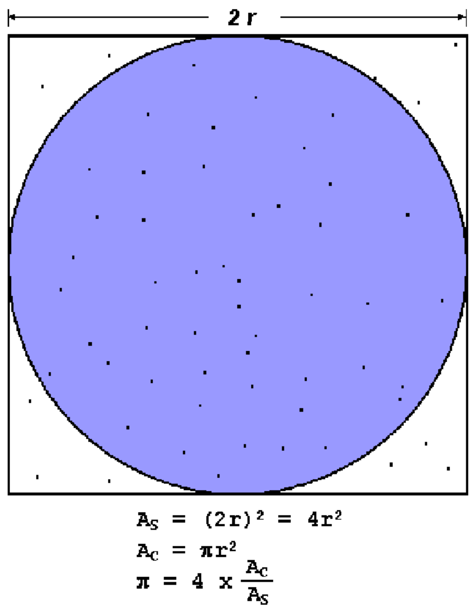
Introductory Examples: Calculate π

Calculation of number π with the following method:

- Περικλείουμε κύκλο με ένα τετράγωνο. Δημιουργούμε *m* τυχαία σημεία μέσα στο τετράγωνο.

- Βρίσκουμε τα σημεία που εμπεριέχονται και μέσα στον κύκλο, *n*.

- Αν $r = n/m$, τότε ο αριθμός π προσεγγίζεται ως $\pi \approx 4r$. Όσο περισσότερα τα σημεία *m* τόσο μεγαλύτερη ακρίβεια του υπολογισμού.



Introductory Examples: Calculate π

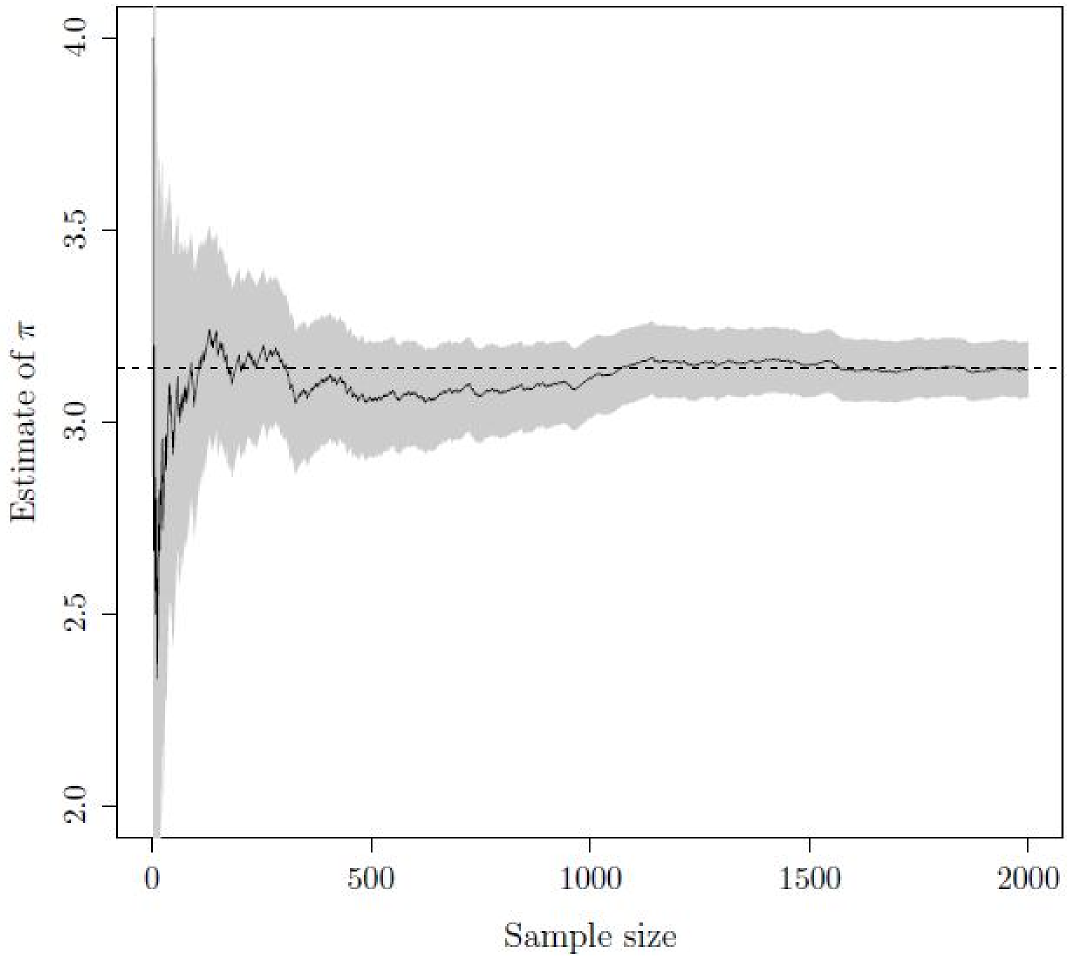
Algorithm:

```
npoints = 1000000
circle_count = 0
do j = 1, npoints
      generate 2 random numbers between 0 and 1
      xcoordinate = random1
      ycoordinate = random2
      if (xcoordinate, ycoordinate) inside circle then
        circle_count = circle_count + 1
 end do
 PI = 4.0*circle_count/npoints
```

- Ο χρόνος υπολογισμού είναι κυρίως ο χρόνος εκτέλεσης της επαναληπτικής διαδικασίας (loop).
- Αυτό οδηγεί σε (σχεδόν) ‘τέλειο παραλληλισμό’ (**embarrassingly parallelism**):
    - ➢Εντατικοί υπολογισμοί.
    - ➢Ελάχιστη επικοινωνία, ελάχιστο I/O.

Introductory Examples: Calculate π

❑ **Estimate π as a function of sample size:**



Monte Carlo Integration

- Two major classes of numerical problems that arise in statistical inference
  - *optimization* problems
  - *integration* problems
- Although optimization is generally associated with the likelihood approach, and integration with the Bayesian approach, these are not strict classifications

- Generic problem of evaluating the integral

$$\mathrm{E}_f[h(X)] = \int_{\mathcal{X}} h(x)\, f(x)\, dx\,.$$

- Based on previous developments, it is natural to propose using a sample $(X_1, \ldots, X_m)$ generated from the density f
- Approximate the integral by the empirical average
- This approach is often referred to as the *Monte Carlo method*

Monte Carlo Integration

Strong Law

- For a sample $(X_1, \ldots, X_m)$, the empirical average

$$\overline{h}_m = \frac{1}{m} \sum_{j=1}^{m} h(x_j) \;,$$

converges almost surely to

$$\mathrm{E}_f[h(X)]$$

- This is the Strong Law of Large Numbers

Monte Carlo Integration

Central Limit Theorem

- Estimate the variance with

$$\mathrm{var}(\overline{h}_m) = \frac{1}{m} \int_{\mathcal{X}} \left(h(x) - \mathrm{E}_f[h(X)]\right)^2 f(x)dx$$

- For m large,

$$\frac{\overline{h}_m - \mathrm{E}_f[h(X)]}{\sqrt{v_m}}$$

  is therefore approximately distributed as a $\mathcal{N}(0, 1)$ variable

- This leads to the construction of a convergence test and of confidence bounds on the approximation of $\mathrm{E}_f[h(X)]$.

Monte Carlo Integration: Example

- **Example: Calculate the integral of a function h(x)**

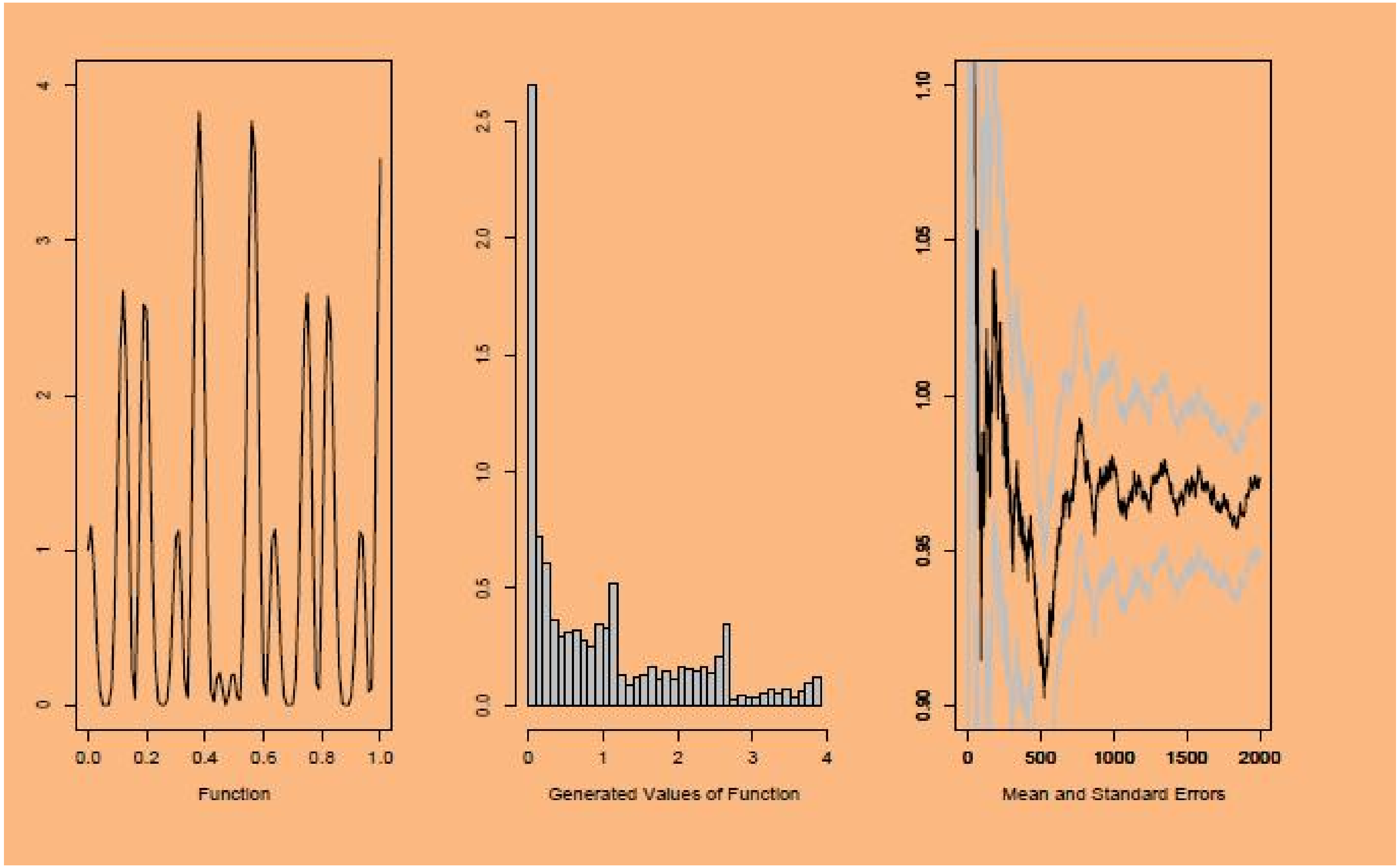
$$h(x) = [\cos(50x) + \sin(20x)]^2$$

.

- To calculate the integral, we generate $U_1, U_2, \ldots, U_n$ iid $\mathcal{U}(0,1)$ random variables, and approximate $\int h(x)dx$ with $\sum h(U_i)/n$.
- It is clear that the Monte Carlo average is converging, with value of 0.963 after $10,000$ iterations.

Monte Carlo Integration: Example

❑ **Example: Estimators**



Monte Carlo Integration

❑ **Generalization of Integration: Riemann sums vs MC method (see hand notes).**

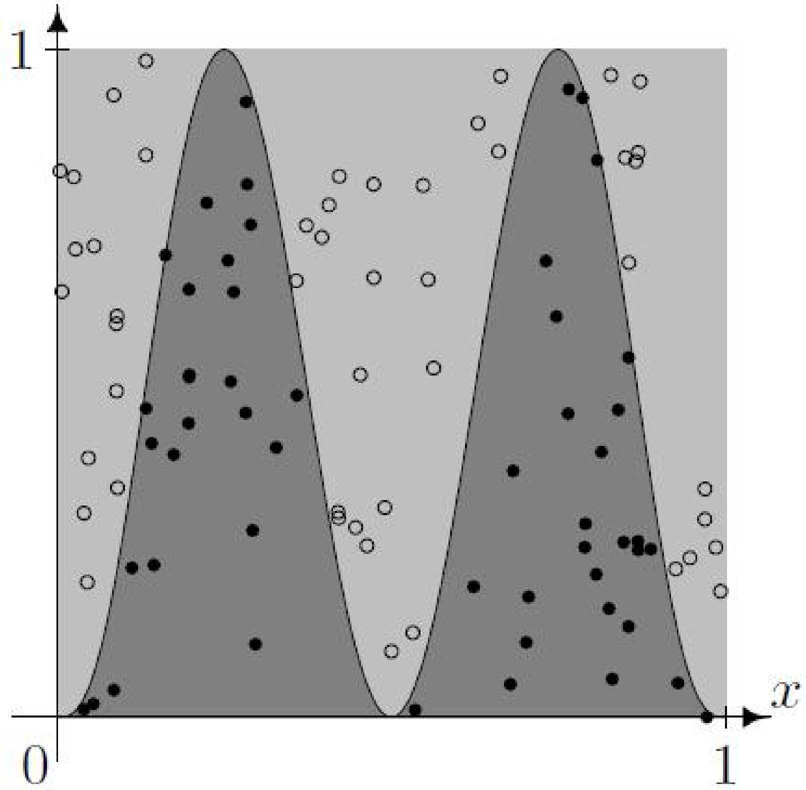
$$\int_0^1 f(x)\,dx$$

$$= \int_0^1 \int_0^{f(x)} 1\;dt\;dx$$

$$= \iint_{\{(x,t):t\le f(x)\}} 1 dt\;dx$$

$$= \frac{\iint_{\{(x,t):t\le f(x)\}} 1\;dt\;dx}{\iint_{\{0\le x,t\le 1\}} 1 dt\;dx}$$

$f:\ [0,1] \rightarrow [0,1]$



Monte Carlo Integration

❑ **Comparison – Speed of Convergence:**

- Speed of convergence of Monte Carlo integration is $O_{\mathbb{P}}(n^{-1/2})$.
- Speed of convergence of numerical integration of a *one-dimensional* function by Riemann sums is $O(n^{-1})$.
- Does not compare favourably for one-dimensional problems.
- However:
  - Order of convergence of Monte Carlo integration is *independent* of the dimension.
  - Order of convergence of numerical integration techniqes like Riemann sums deteriorates with the dimension increasing.

$\leadsto$ Monte Carlo methods can be a good choice for high-dimensional integrals.

Random Number Generators

- Philosophical paradox:
  - We need to reproduce randomness by a computer algorithm.
  - A computer algorithm is deterministic in nature.

$\rightsquigarrow$ "pseudo-random numbers"

- Pseudo-random number from U$[0,1]$ will be our only "source of randomness".
- Other distributions can be derived from U$[0,1]$ pseudo-random numbers using deterministic algorithms.

Pseudo-Random Number Generators

- A pseudo-random number generator (RNG) should produce output for which the U$[0, 1]$ distribution is a suitable model.
- The pseudo-random numbers $X_1, X_2, \ldots$ should thus have the same *relevant* statistical properties as independent realisations of a U$[0, 1]$ random variable.
  - They should reproduce independence ("lack of predictability"): $X_1, \ldots, X_n$ should not contain any discernible information on the next value X_{n+1}.This property is often referred to as the lack of predictability.
  - The numbers generated should be spread out evenly across $[0, 1]$.

Pseudo-Random Number Generators

- **A simple example: Congruential pseudo-RNG.**

Algorithm 1.1: Congruential pseudo-random number generator

1. Choose $a, M \in \mathbb{N}$,$c \in \mathbb{N}_0$, and the initial value ("seed") $Z_0 \in \{1, \ldots M-1\}$.
2. For $i = 1, 2, \ldots$

   Set $Z_i = (aZ_{i-1} + c) \mod M$, and $X_i = Z_i/M$.

$Z_i \in \{0, 1, \ldots, M-1\}$, thus $X_i \in [0, 1)$.

Pseudo-Random Number Generators

Cosider the choice of $a = 81$, $c = 35$, $M = 256$, and seed $Z_0 = 4$.

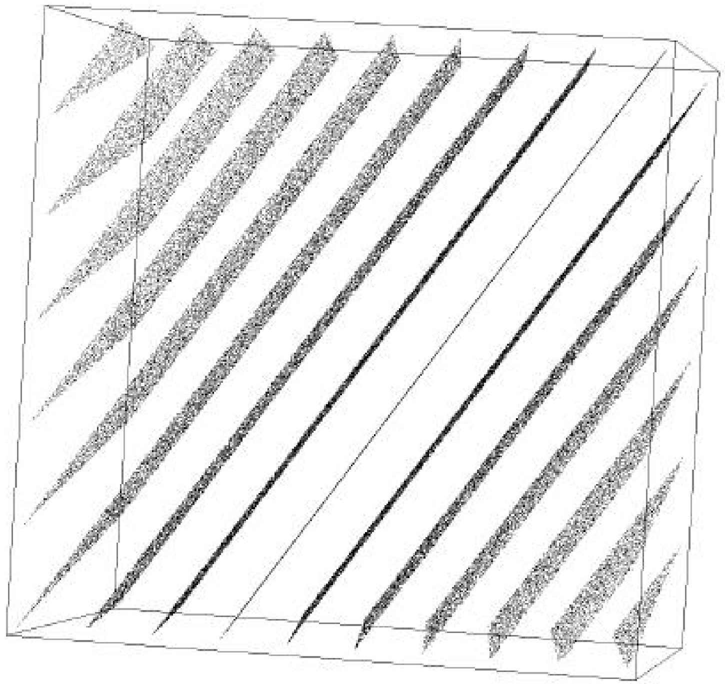
$$
\begin{aligned}
Z_1 &= (81 \cdot 4 + 35) \mod 256 = 359 \mod 256 = 103 \\
Z_2 &= (81 \cdot 103 + 35) \mod 256 = 8378 \mod 256 = 186 \\
Z_3 &= (81 \cdot 186 + 35) \mod 256 = 15101 \mod 256 = 253 \\
& \ldots
\end{aligned}
$$

The corresponding X_i are $X_1 = 103/256 = 0.4023438$,
$X_2 = 186/256 = 0.72656250$, $X_1 = 253/256 = 0.98828120$.

Pseudo-Random Number Generators

❑ RANDU: A typical poor choice of RNG.

- Very popular in the 1970s (e.g. System/360, PDP-11).
- Linear congruential generator with $a = 2^{16} + 3$, $c = 0$, and $M = 2^{31}$.
- The numbers generated by RANDU lie on only 15 hyperplanes in the 3-dimensional unit cube!



According to a salesperson at the time: "We guarantee that each number is random individually, but we don't guarantee that more than one of them is random."

Pseudo-Random Number Generators

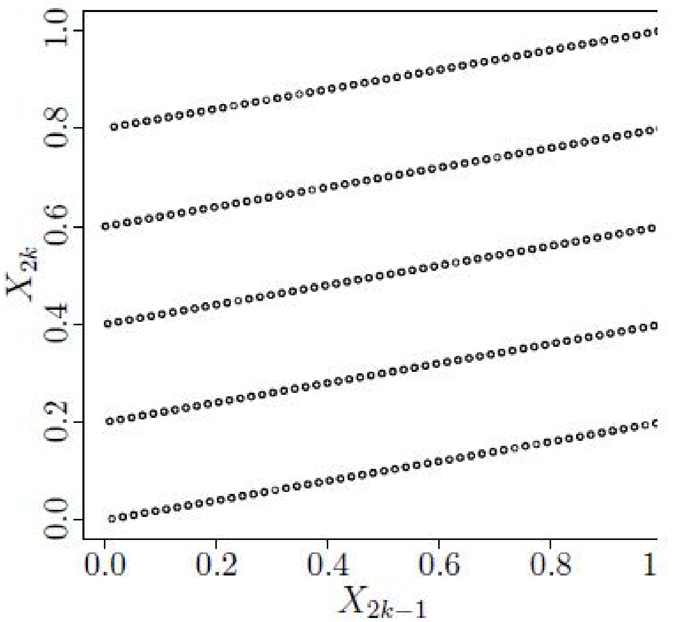
❑ Flaw of the linear congruential RNG.

- "Crystalline" nature is a problem for every linear congurentrial generator.
- Sequence of generated values $X_1, X_2, \ldots$ viewed as points in an n-dimension cube lies on a finite, and often very small number of parallel hyperplanes.
- Marsaglia (1968): "the points [generated by a congruential generator] are about as randomly spaced in the unit n-cube as the atoms in a perfect crystal at absolute zero."
- The number of hyperplanes depends on the choice of a, c, and M.
- For these reasons do not use the linear congurential generator! Use more powerful generators (like e.g. the *Mersenne twister*, available in GNU R).

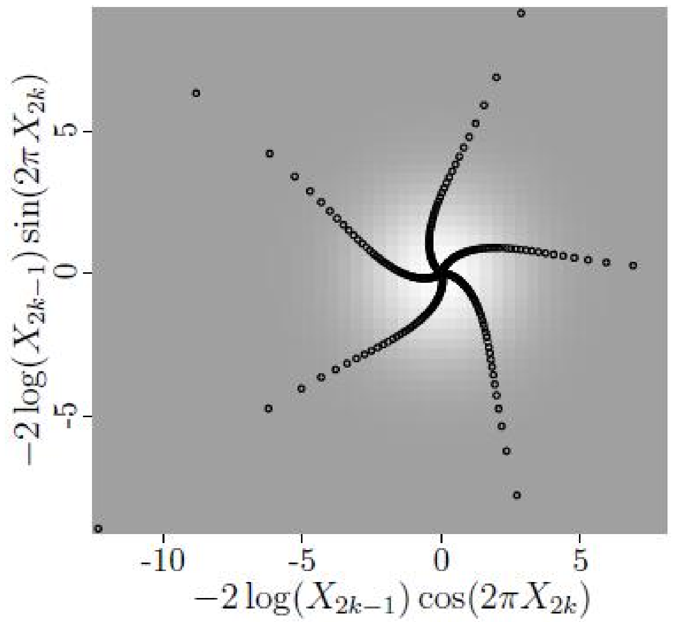
Pseudo-Random Number Generators

- Another problematic example:

Linear congruential generator with $a = 1229$, $c = 1$, and $M = 2^{11}$.



ʾairs of generated values (X_{2k-1}, X_{2k})



Transformed by Box-Muller method

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