I3344
Numerical Simulation & Modeling

Ahmad Fadlallah

Tentative Syllabus

- ✓ Interpolation and extrapolation
  - ✓ Linear: linear regression y = ax + b; correlation, standard deviation, etc.
  - ✓ Non-linear: k nearest neighbors (KNN)
  - ✓ Validation of two models: k-fold cross validation method.
- ✓ Solving a linear equation
  - ✓ Direct methods: Gauss and LU
  - ✓ Iterative methods: Jacobi and Gauss-Seidel
- ✓ Derivation
  - ✓ Finite difference method (FDM): Euler and Runge-kutta
- **Integration: surface estimation**
  - **Finite Element Method (FEM).**
  - **Monte Carlo method.**
  - **Comparison of two methods.**
- ✓ Non-linear problems
  - ✓ Bisection method
- Introduction to the notion of parallel computing and underlying algorithms

Outline

- Introduction
- Finite Element Method
- Monte Carlo Method
- Comparison

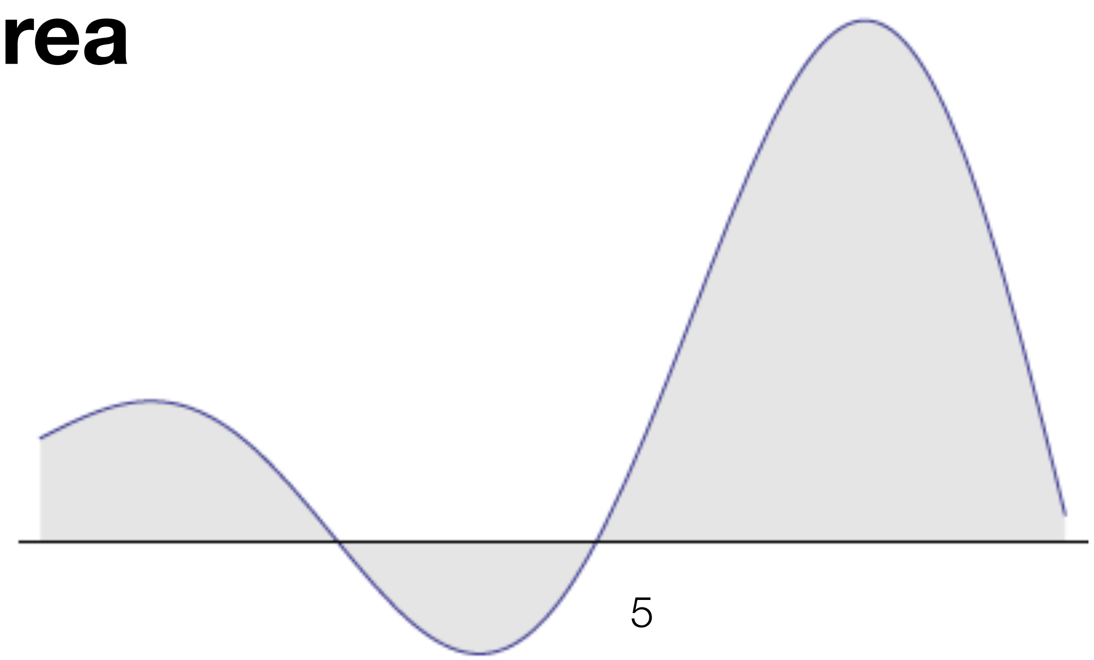
Integration using Finite Elements Methods

Introduction

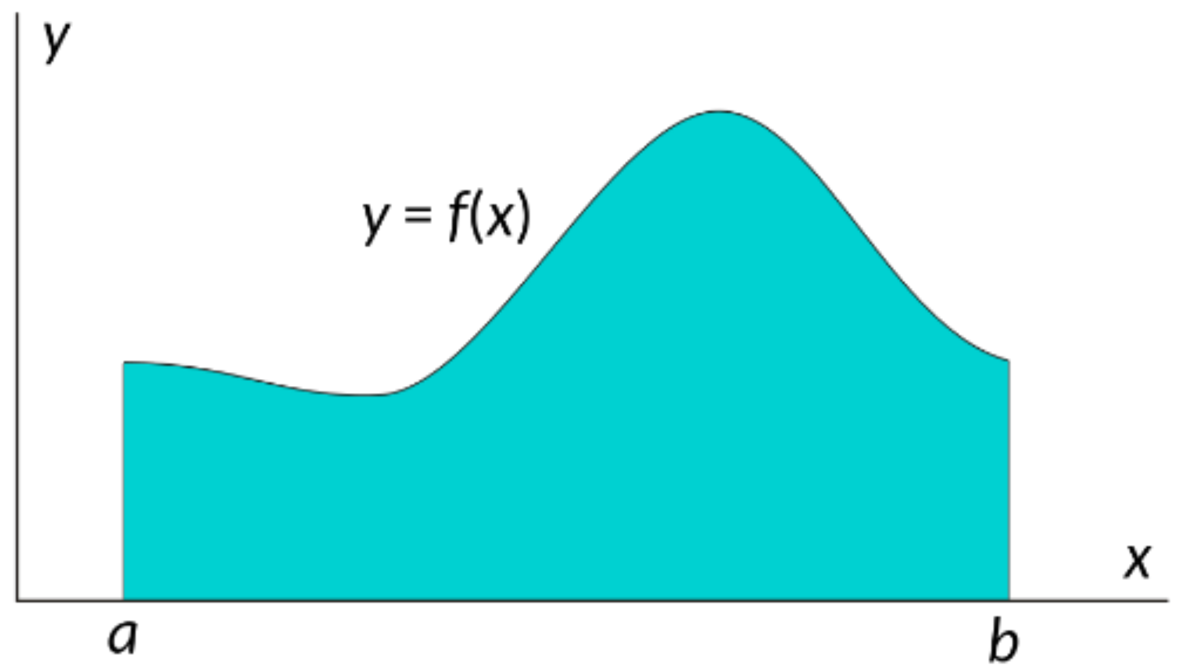
- Objective: compute numerical approximations to the integral of the function
- if f(x) is a function, then the integral of f from x=a to x=b is written

$$\int_a^b f(x)\,dx$$

- The integral gives the **area under the graph of f**, with the **area under the positive part** counting as **positive area**, and the **area under the negative part of f** counting as **negative area**



Integration - Exact Method



- A= $\int_a^b f(x)$ =F(b) – F(a) where F’= f

Introduction (cont'd)

- Let a and b be two real numbers with $a \leq b$.
- A **partition** of [a, b] is a finite sequence $\{x_i\}_{i=0...n}$ of increasing numbers in [a, b] with $x_0 = a$ and $x_n = b$

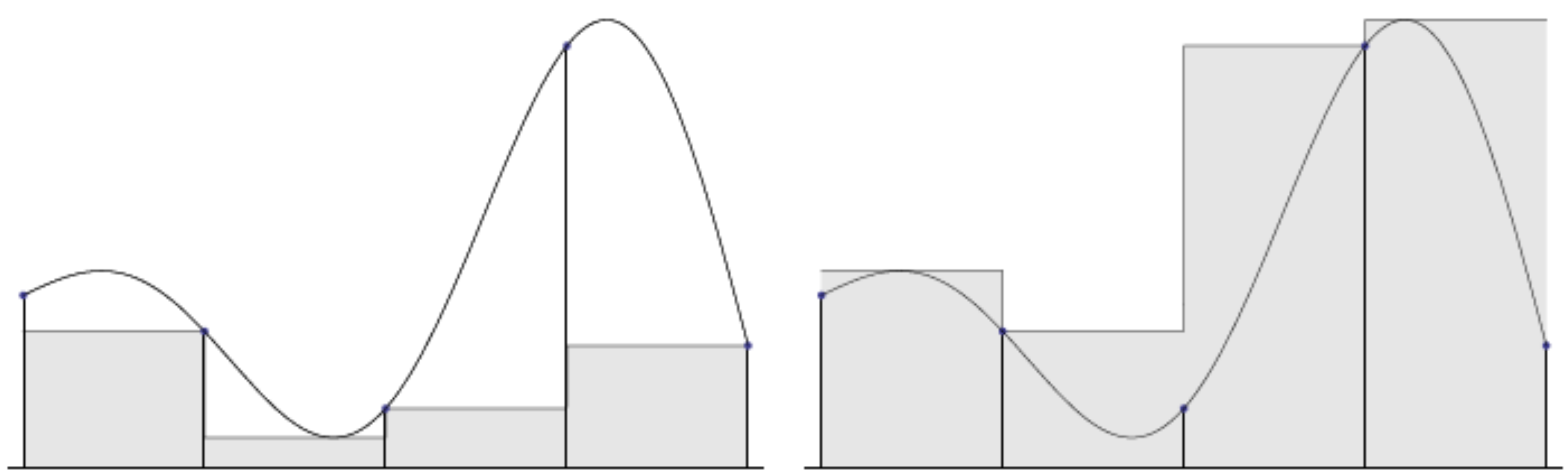
$$a = x_0 \leq x_1 \leq x_2 \ldots . \leq x_{n-1} \leq x_n = b.$$

- The partition is said to be uniform if ∃ a fixed number ***h***, called the step length , such that $\mathbf{x_i - x_{i-1} = h = (b - a)/n}$ for i=1 , . . . , n.

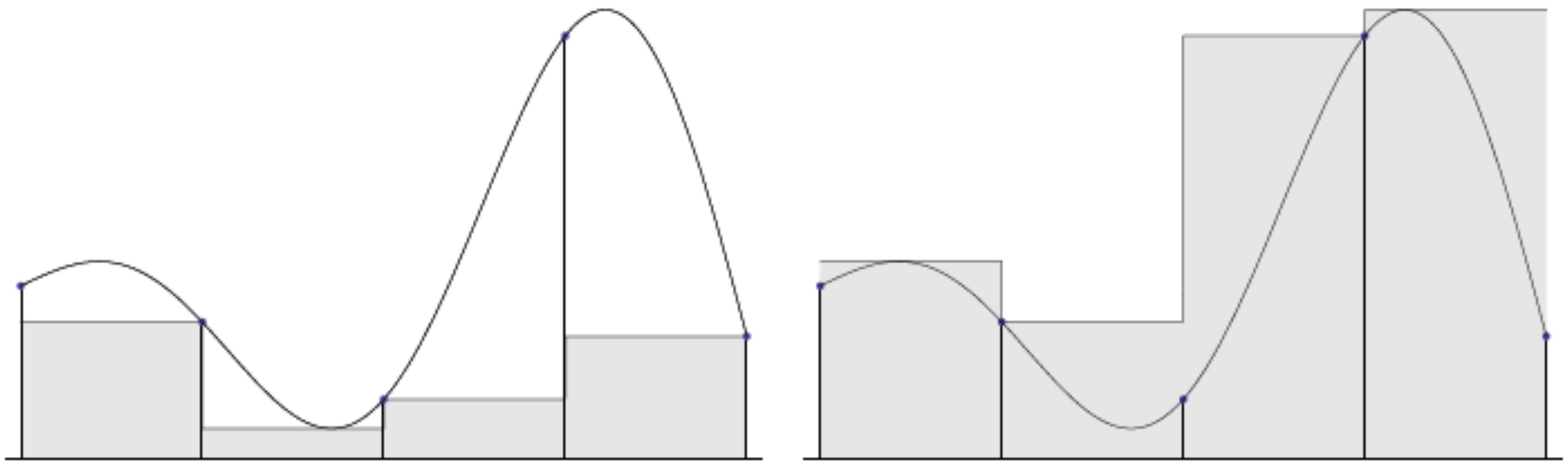
Integration

- The traditional definition of the integral is based on a numerical approximation to the area.
- Pick a partition $\{x_i\}_{i=0\ldots n}$ of $[a, b]$
- In each subinterval $[x_{i-1}, x_i]$, determine the maximum and minimum of f

$$m_i = \min_{x\in[x_{i-1},x_i]} f(x), \quad M_i = \max_{x\in[x_{i-1},x_i]} f(x)$$



Integration - Definition (cont'd)



- Compute two approximations for $\int_a^b f(x)$

$$\underline{I} = \sum_{i=1}^{n} m_i (x_i - x_{i-1}), \quad \overline{I} = \sum_{i=1}^{n} M_i (x_i - x_{i-1}),$$

$$I = \int_a^b f(x)\,dx = \sup \underline{I} = \inf \overline{I}$$ *(sup and inf over all possible partitions of [a, b]*

Numerical Integration

***Theorem**: Suppose that f is integrable on the interval [a, b], let $\{x_i\}_{i=0\ldots n}$ be a partition of [a, b], and let t_i be a number in $[x_{i-1}, x_i]$ for i = 1, . . . , n.*

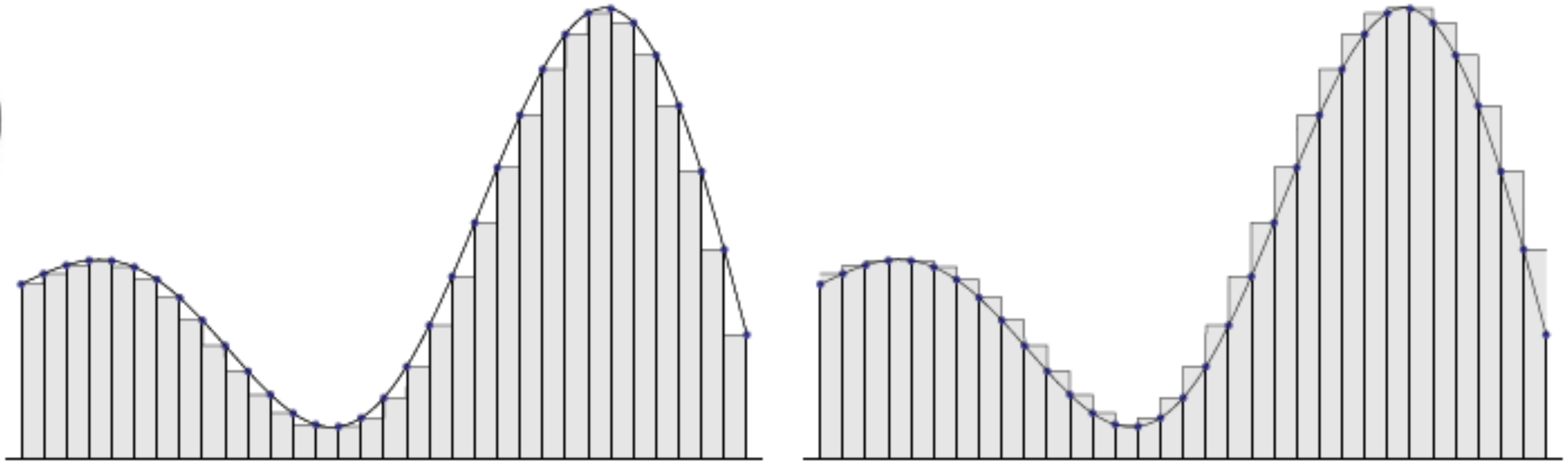
$$\tilde{I} = \sum_{i=1}^{n} f(t_i)(x_i - x_{i-1})$$

Then the sum will converge to the integral when the distance between all neighboring x_i tends to zero

***Practical Note:** $n \uparrow \Rightarrow$ **step** $\downarrow \Rightarrow$ **precision** $\uparrow$*

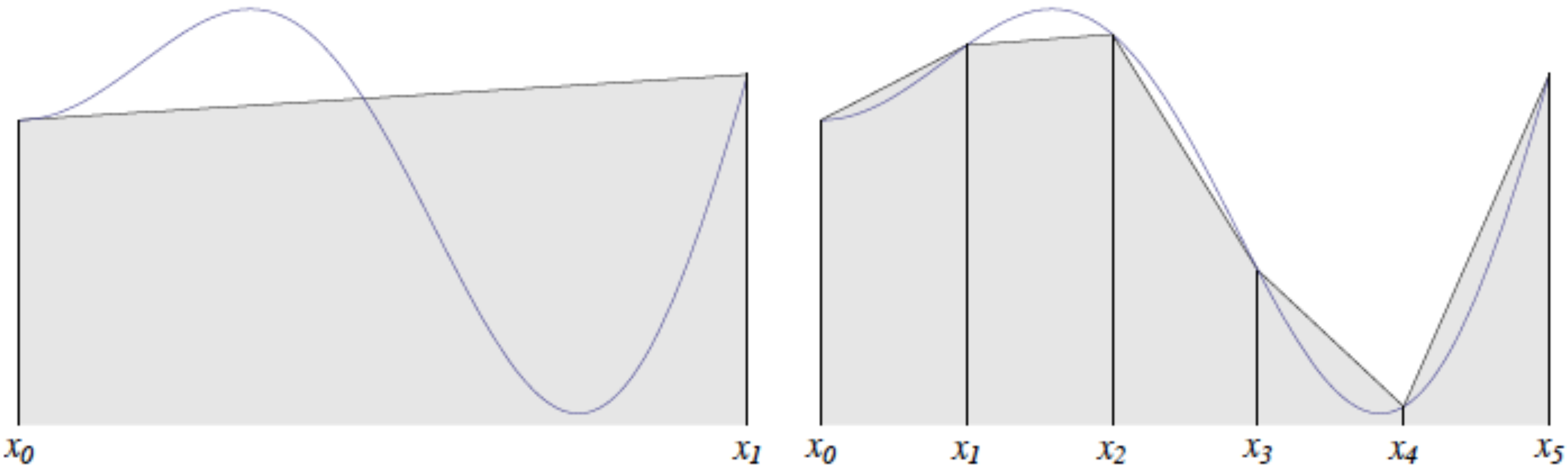
Numerical Integration (cont'd)

$$\tilde{I} = \sum_{i=1}^{n} f(t_i)(x_i - x_{i-1})$$



- Finite Element Methods (FEM)
  - $f(t_i) = f(x_{i-1})$
  - $f(t_i) = f(x_i)$
  - $f(t_i) = min\ (f(x_{i-1}), f(x_i))$
  - $f(t_i) = max\ (f(x_{i-1}), f(x_i))$
  - $f(t_i) = f((x_{i-1} + x_i)/2)$ *(Midpoint)*

Trapezoidal Rule



$$\int_a^b f(x)\,dx = \sum_{i=1}^{n} \int_{x_{i-1}}^{x_i} f(x)\,dx \approx \sum_{i=1}^{n} \frac{f(x_{i-1}) + f(x_i)}{2} h.$$

Exercises

- Use the six methods to calculate the integral of the $f(x)=x^2$ over [0,1] with two subintervals
- Calculate the error for each of the six methods

Lab Exercise

- In this exercise we are going to study the definition of the integral for the function $f(x) = e^x$ on the interval [0,1].
- Write the necessary java classes to implement the six different methods previously mentioned for a uniform partition consisting of n subintervals (n variable)
- Determine the absolute errors of each method compared to the exact value $e - 1 = 1.718281828$ of the integral.
- How many subintervals are needed for each method to achieve an absolute error less than ε ? test for different values of ε (e.g., 10^{-3}, 10^{-10})

Monte Carlo Integration

Introduction

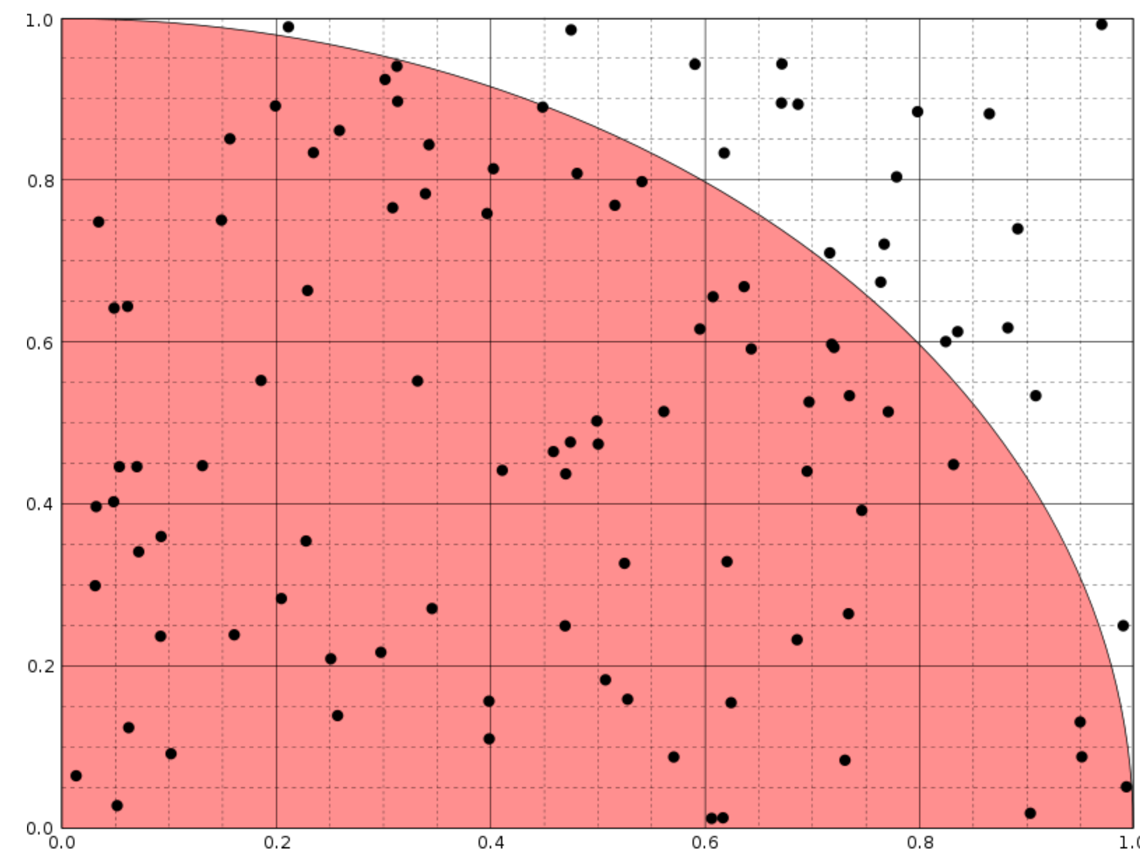
- Monte Carlo methods are numerical techniques which **rely on random sampling** to approximate their results.
  - **Essential idea**: using randomness to solve problems that might be deterministic in principle.
  - Often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other approaches
  - Mainly used in **optimization** and in **numerical integration**
- Monte Carlo integration applies this process to the numerical estimation of integrals
- Monte Carlo integration is a powerful method for **computing the value of complex integrals** using **probabilistic techniques**

Introduction (cont'd)

- While **other algorithms** usually evaluate the integrand at a regular grid, **Monte Carlo** **randomly** choose points at which the integrand is evaluated.
- This method is particularly useful for higher-dimensional integrals.

Monte Carlo Method - Example
Determining the value of π

- Let M be a point of coordinates (x, y), where 0 <x <1 and 0 <y <1.
- The values of x and y are **<u>randomly</u>** drawn between 0 and 1 according to a **<u>uniform law</u>**.
- The point M belongs to the **disk of center (0,0) and radius R = 1** if and only if $x^2 + y^2 \leq 1$.

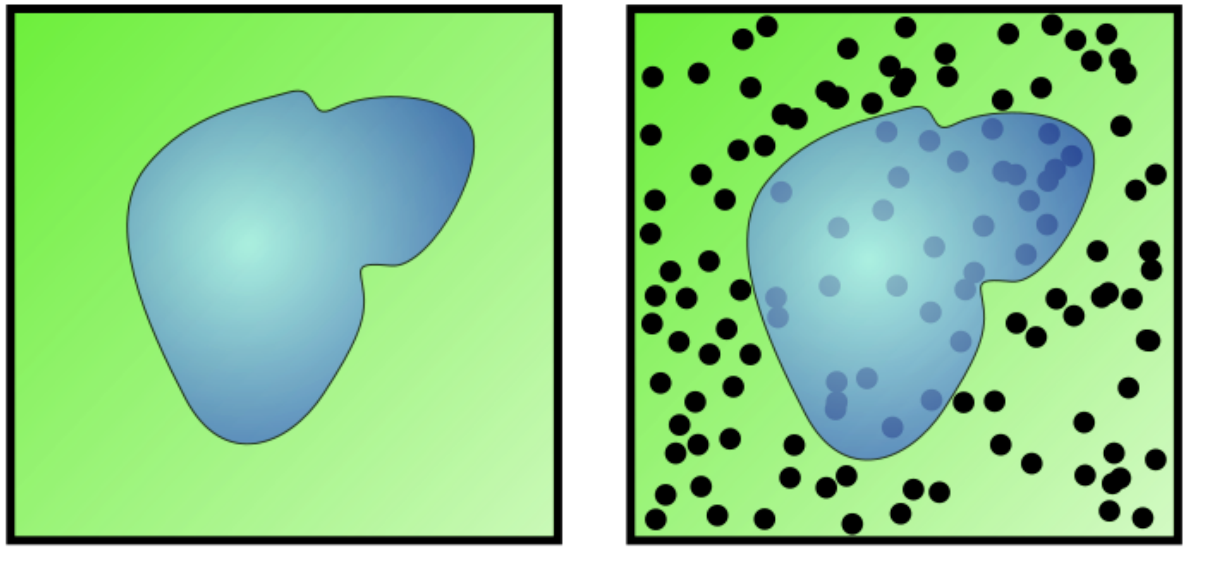


- The probability that the point M belongs to the disk is $\pi/4$ (surface of the quarter disk)
- Approximation of $\pi/4$ = **ratio of** the number of points in the disk to the number of draws (if the number of draws is large)

Monte Carlo Method - Example
Determining the area of a lake

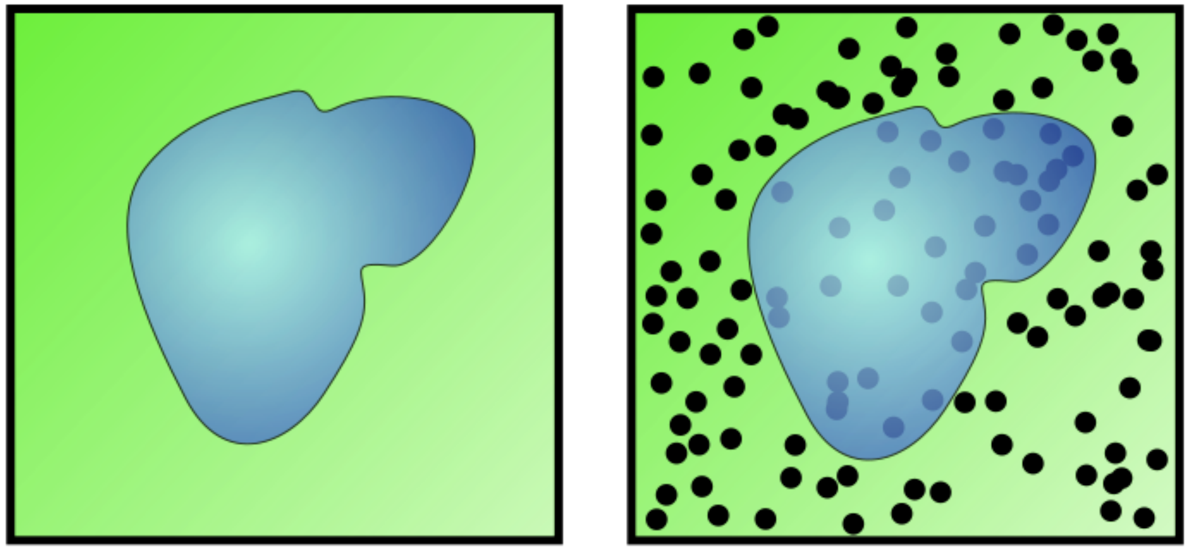
- Given a rectangular or square zone whose sides are of known length => Known area
- Within this area is a lake whose area is unknown.
- To find the area of the lake, an army is asked to fire X random shots on this area.
- **N: the number of balls which remained on the ground;**
- **The number of balls which fell in the lake = X**

$$\frac{Area_{lake}}{Total\ Area} = \frac{X}{X+N}$$



Monte Carlo Method - Example
Determining the area of a lake

$$\frac{Area_{lake}}{Total\ Area} = \frac{X}{X+N}$$

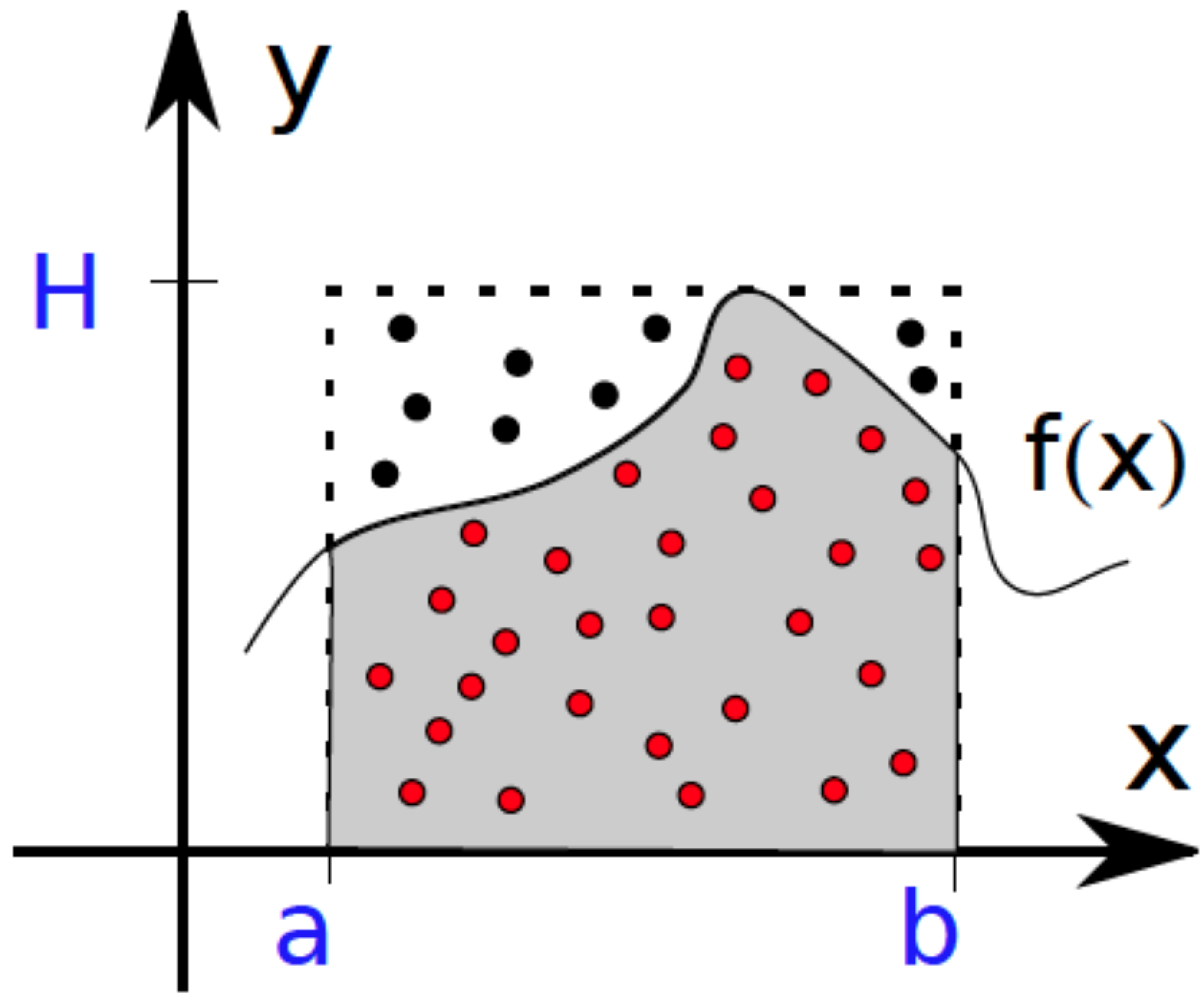


- Example: if the land is 1000 m², the army fires 500 cannonballs and 100 projectiles fell into the lake => an estimate of the area of the lake is: 1000 × 100 ÷ 500 = 200.

- The quality of the estimate improves (slowly) by **increasing the number of shots** and ensuring that **gunners do not always aim for the same spot** but cover the area evenly => the quality of the random generator which is essential to have good results in the Monte Carlo method.
  - A biased generator is like a gun that always fires in the same place: the information it brings is reduced.

Integration using Monte Carlo Method (Hit-Miss Method)

$$\int_{a_x}^{b_x} f(x)dx = \frac{N_{inside}}{N_{total}} A_{box}$$

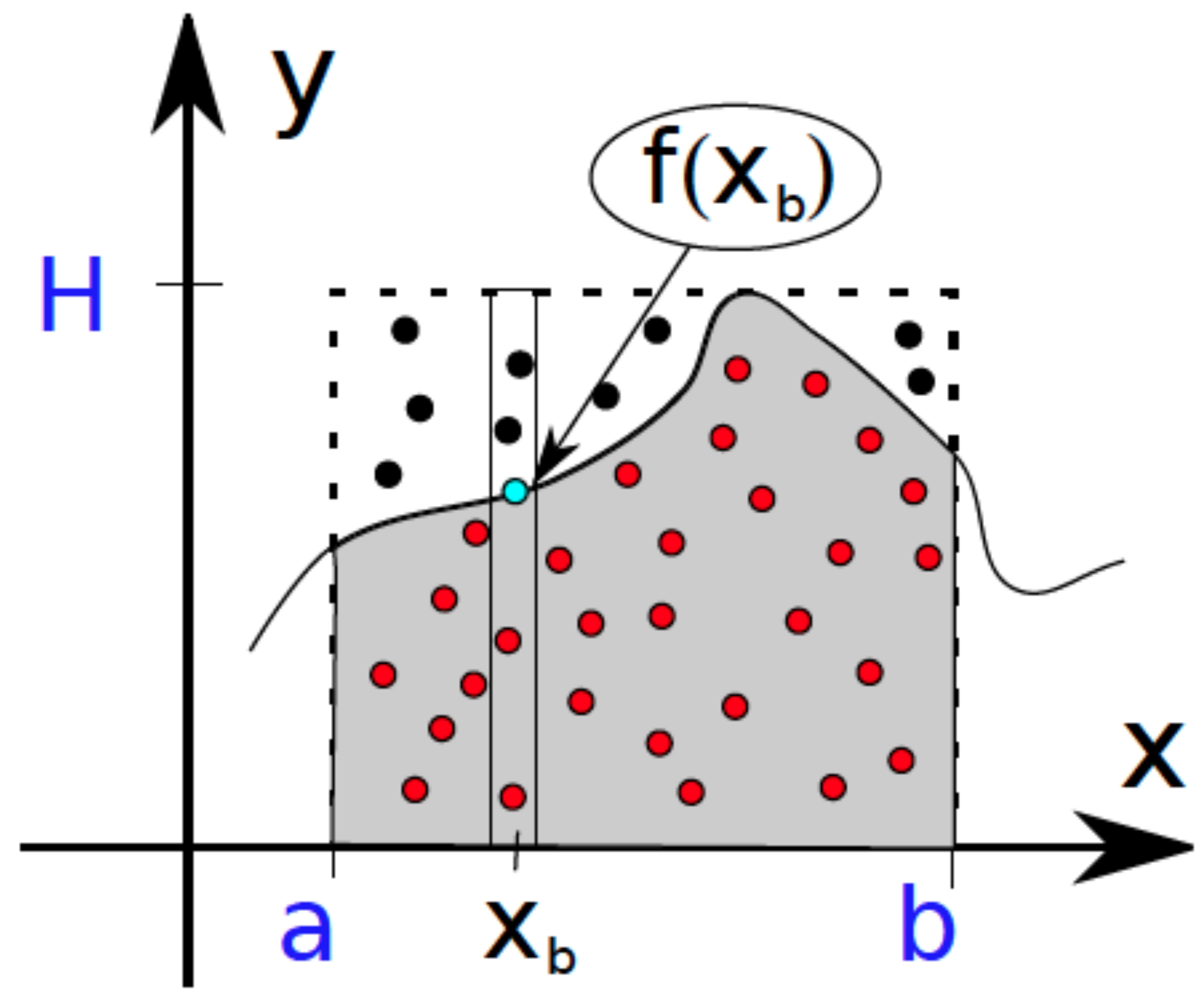


Not Optimal

Integration using Monte Carlo Method (Mean Value Method)

- Choose N uniformly and randomly distributed points x_i inside [a; b]

$$\int_a^b f(x)dx \approx \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$



Exercise

- Use the Mean Value Monte Carlo method to calculate the integral of the $f(x)=x^2$ over [0,1] with the following random numbers drawn from [0, 1]
- 0.0252 0.1620 0.9136 0.8292 0.5231 0.9583 0.0590 0.2855 0.5895 0.4813