Lecture 2

Perturbative Calculations and Numerical Calculus

Bao-Jun Cai, 3/10/2026

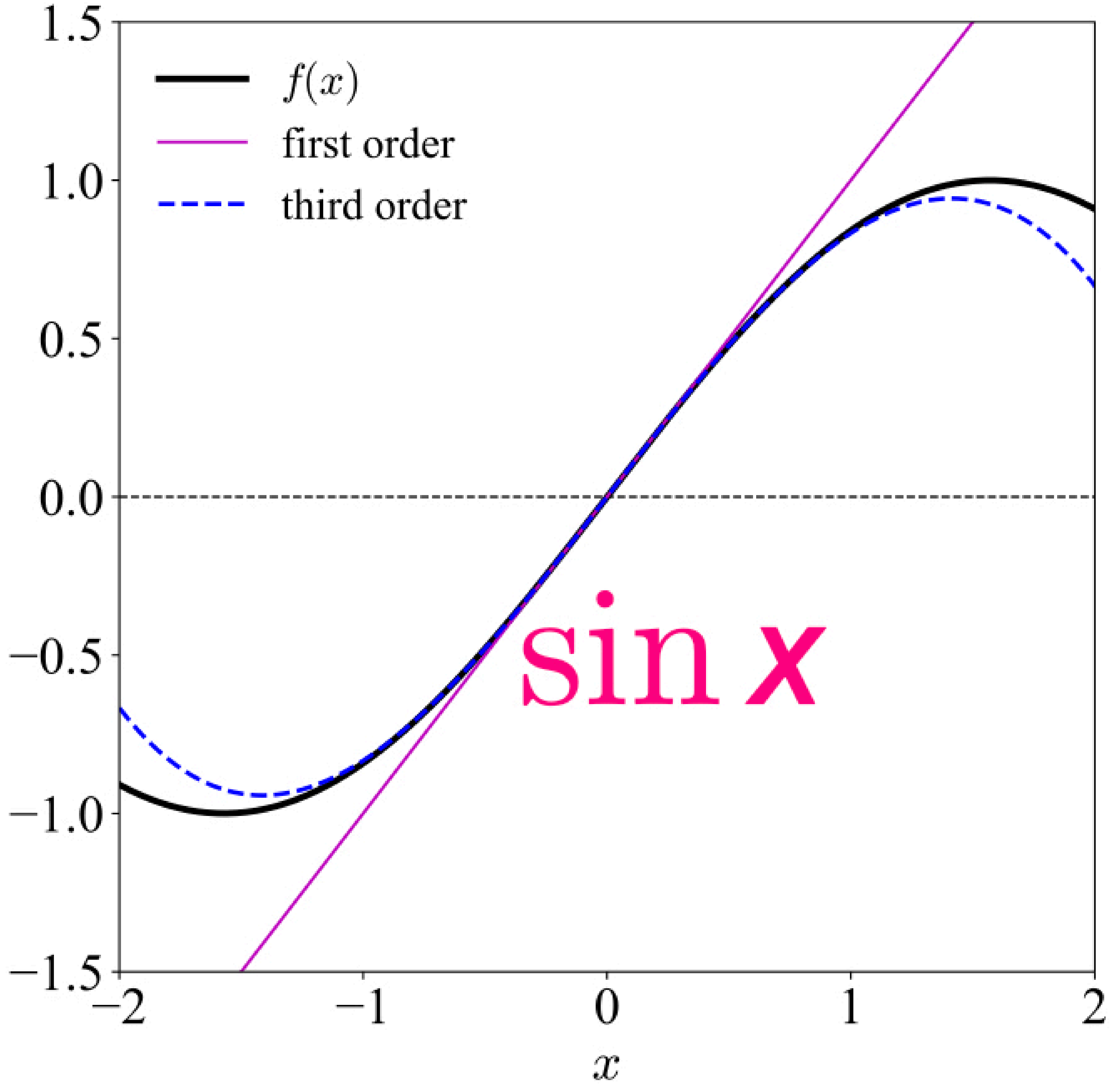
Introduction to Algorithms for Data Science and Physics IMP@Fudan, 2026

Topics of this lecture:

- Taylor's expansion of a function: polynomials $\to f(x)$
- numerical derivative and integration $\int \approx \sum$
- estimate pi: hitting and counting
- Buffon's needle experiment $\pi \sim$ certain probability
- random walk: first glimpse $R \sim \sqrt{N}$
- gradient and Hessian $\vec{g} = \partial f / \partial \vec{x}, \vec{H} = \partial^2 f / \partial \vec{x} \partial \vec{x}^\top$

Taylor's expansion of a function: simplicity of polynomial

$$f(x) \approx f(x_0) + f'(x_0)\delta x + \frac{1}{2}f''(x_0)\delta x^2 + \frac{1}{6}f'''(x_0)\delta x^3 + \cdots \leftrightarrow \boxed{\sum_{i=0}^{\infty}\frac{1}{i!}f^{(i)}(x_0)\delta x^i}, \quad \delta x = x - x_0$$



approximate the function $f(x)$ by polynomials:

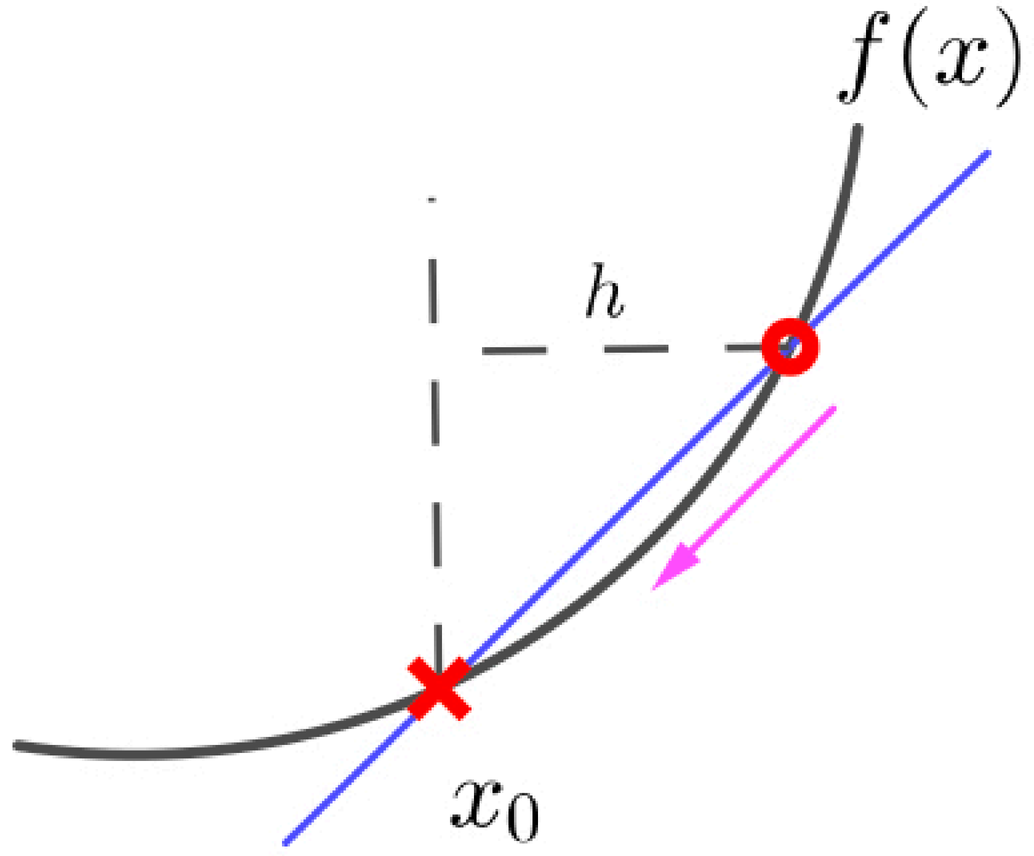
(1) (constant) zeroth-order $f(x_0)$

(2) (line) first-order $f(x_0) + f'(x_0)\delta x$

(3) (parabola) second-order $f(x_0) + f'(x_0)\delta x + 2^{-1}f''(x_0)\delta x^2$

(4) higher order approximations

$$f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

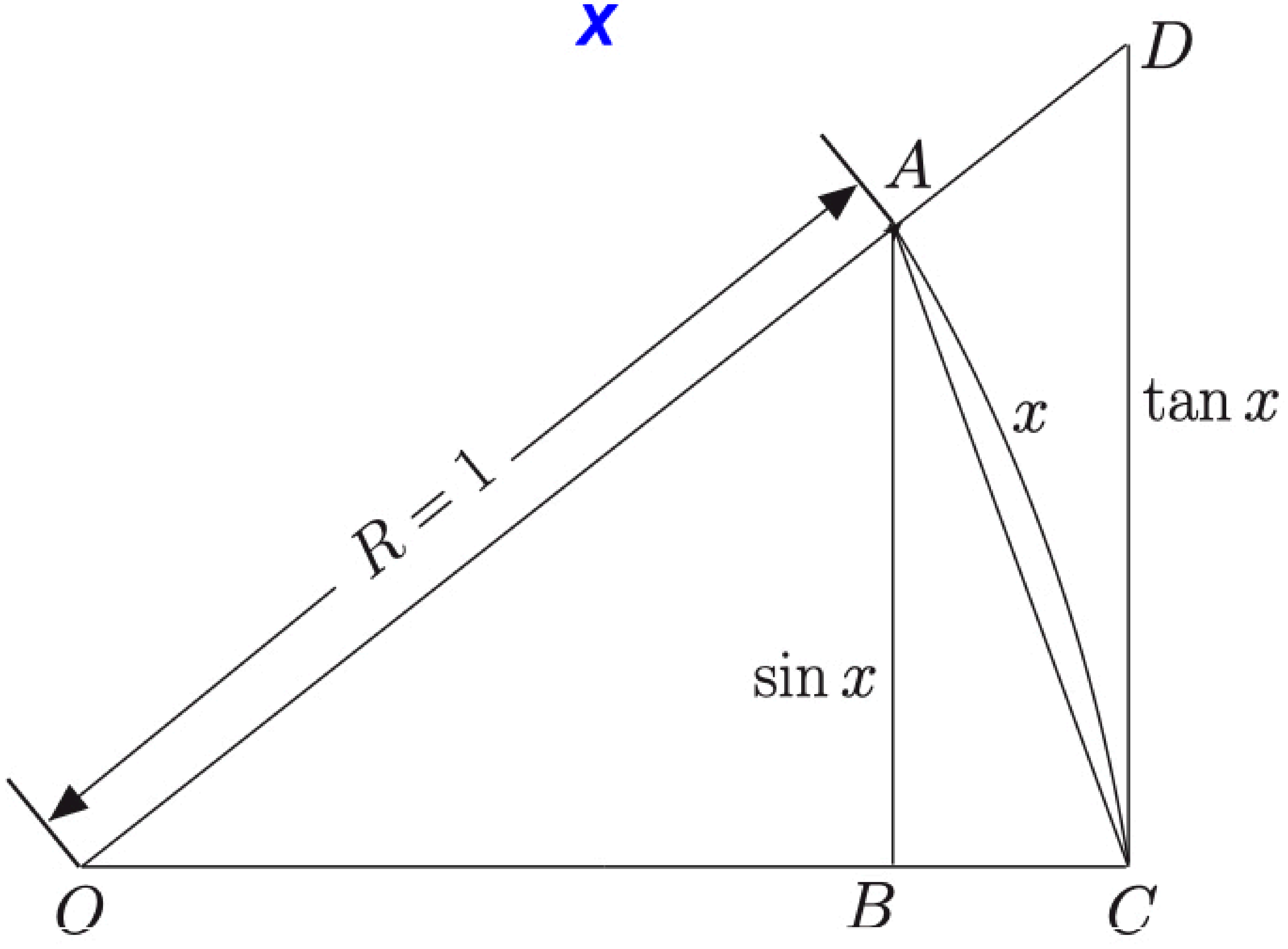


Warm up: derivative of the sine function

$$S_{\triangle OAC} < S_{\measuredangle OAC} < S_{\triangle ODC}$$

$$\leftrightarrow \sin x < x < \tan x = \frac{\sin x}{\cos x}$$

$$\leftrightarrow \cos x < \frac{\sin x}{x} < 1$$



$$\lim_{x \to 0} \frac{\sin x}{x} = 1$$

$$\sin \mu - \sin \nu = 2 \cos \frac{\mu + \nu}{2} \sin \frac{\mu - \nu}{2}$$

$$\frac{\delta y}{\delta x} = \frac{\sin(x + \delta x) - \sin x}{\delta x} = \cos\left(x + \frac{\delta x}{2}\right) \sin \frac{\delta x}{2} \Big/ \frac{\delta x}{2}$$

$$(\sin x)' = \frac{d \sin x}{dx} = \lim_{x \to 0} \frac{\delta y}{\delta x} = \cos x$$

Ex.: What is the first-order derivative of the cosine function? Do it by definition or use the relation: $\cos x = \sin(\pi/2 - x)$.

More examples around x=0

Ex.: What is the expansion of $e^{\sin x}$ around $x \approx 0$?

$$e^x \approx 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \cdots$$

$$\sin x \approx x - \frac{1}{6}x^3 + \frac{1}{120}x^5 - \frac{1}{5040}x^7 + \cdots$$

$$\cos x \approx 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 - \frac{1}{720}x^6 + \cdots$$

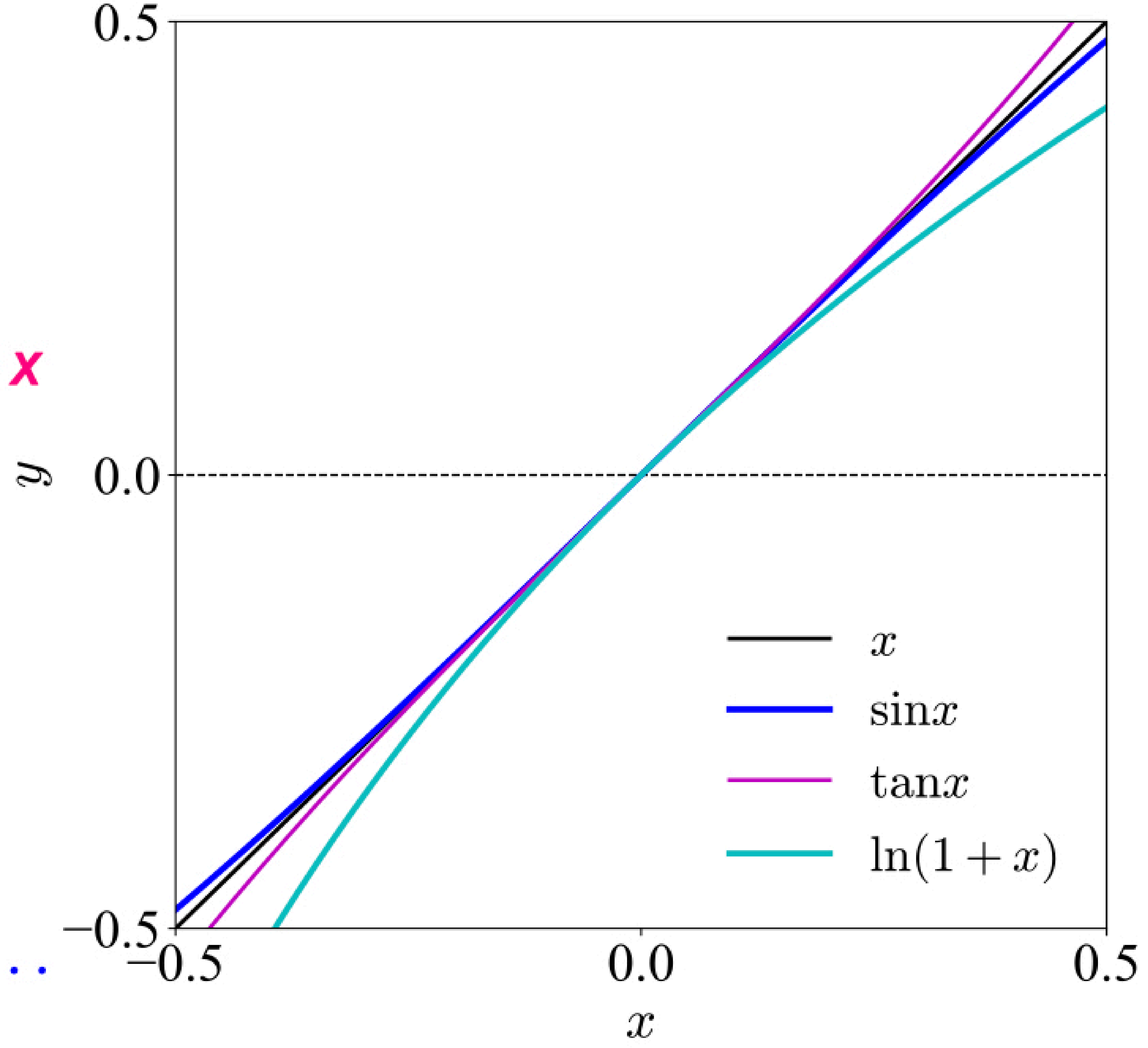
$$\tan x = \sin x / \cos x$$

$$\tan x \approx x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{17}{315}x^7 + \cdots$$

$$\ln(1+x) \approx x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \cdots$$

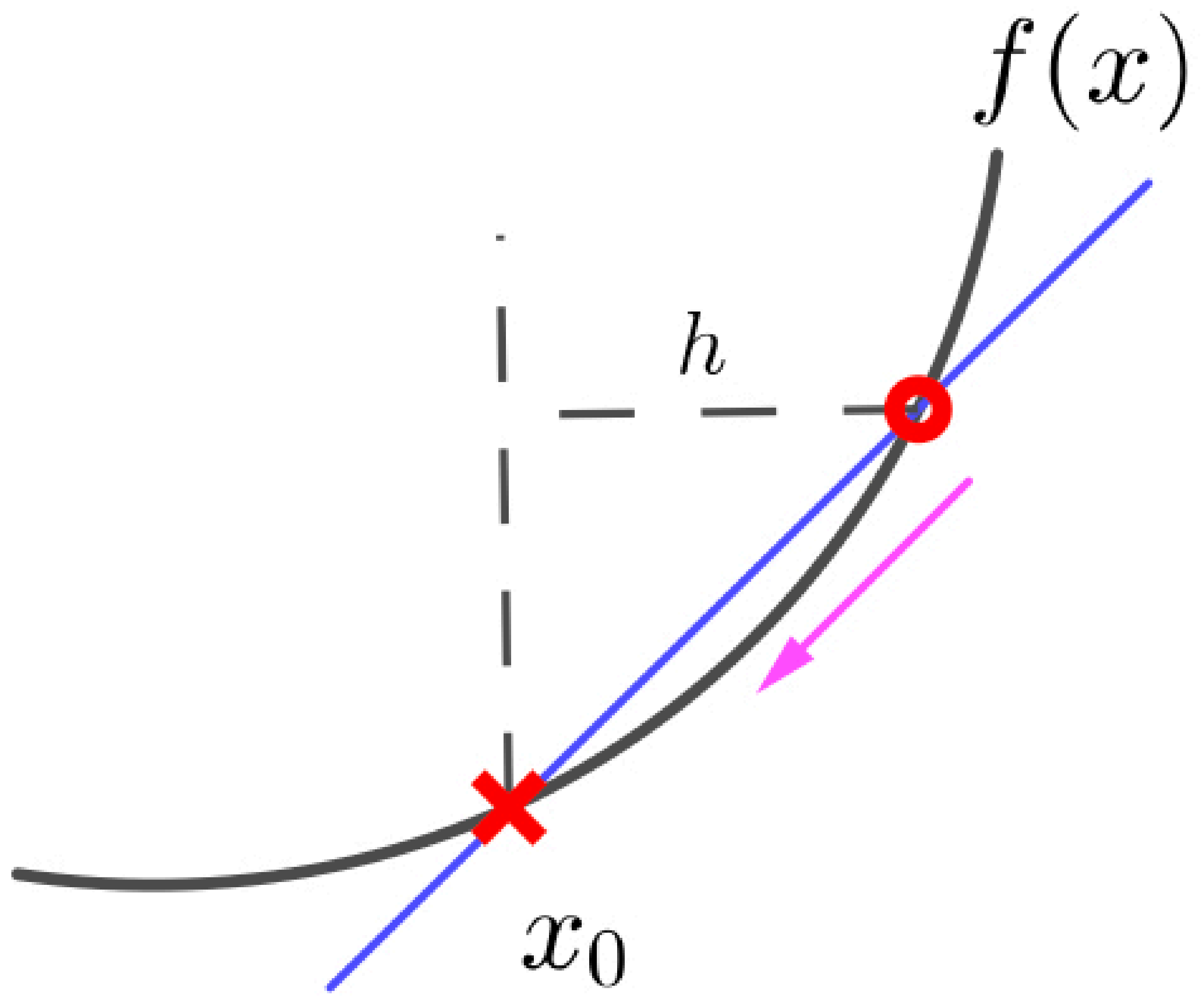
$$\frac{1}{1+x} \approx 1 - x + x^2 - x^3 + x^4 + \cdots$$

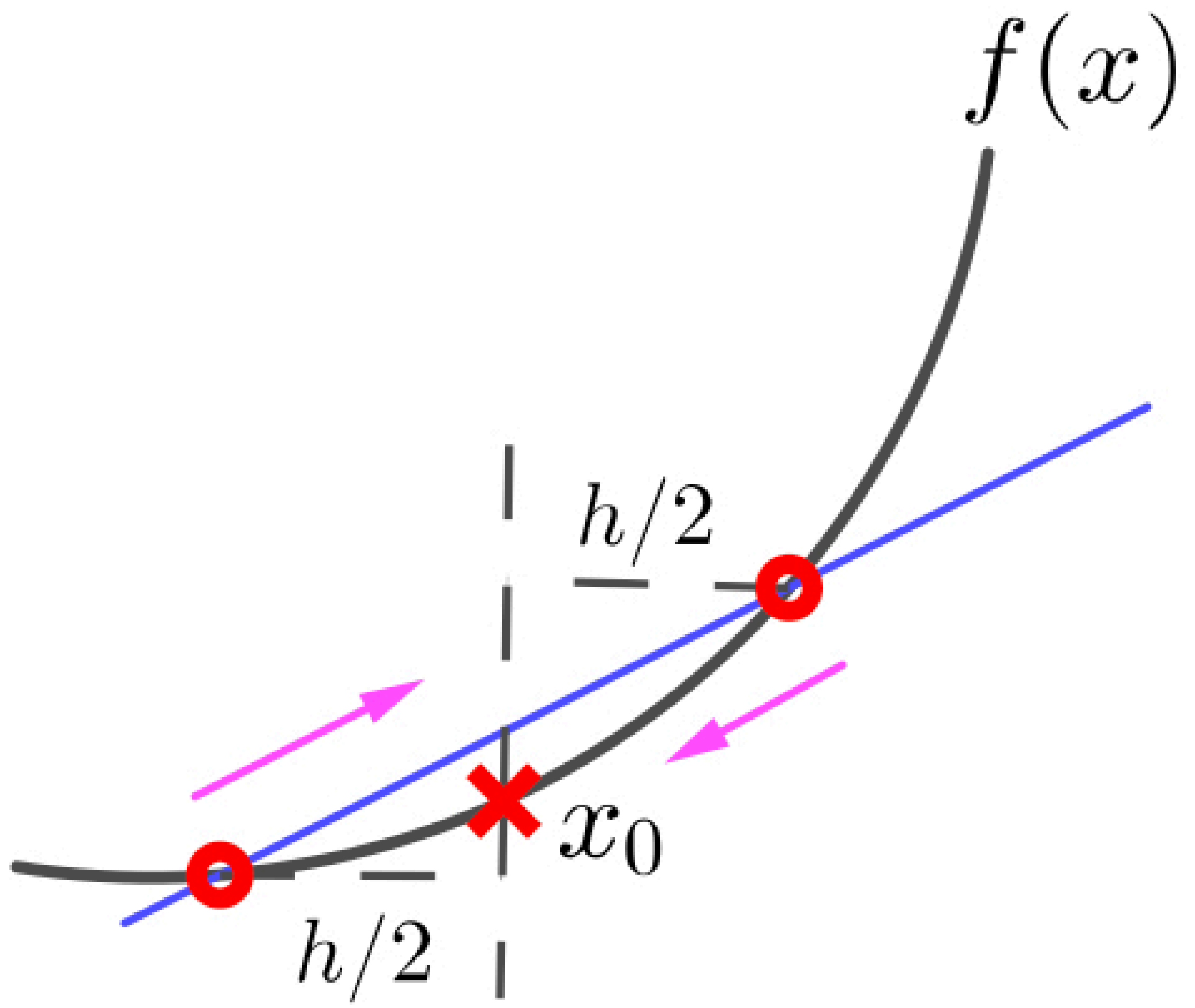
$$(1+x)^\beta \approx 1 + \beta x + \frac{1}{2}\beta(\beta-1)x^2 + \frac{1}{6}\beta(\beta-1)(\beta-2)x^3 + \cdots$$

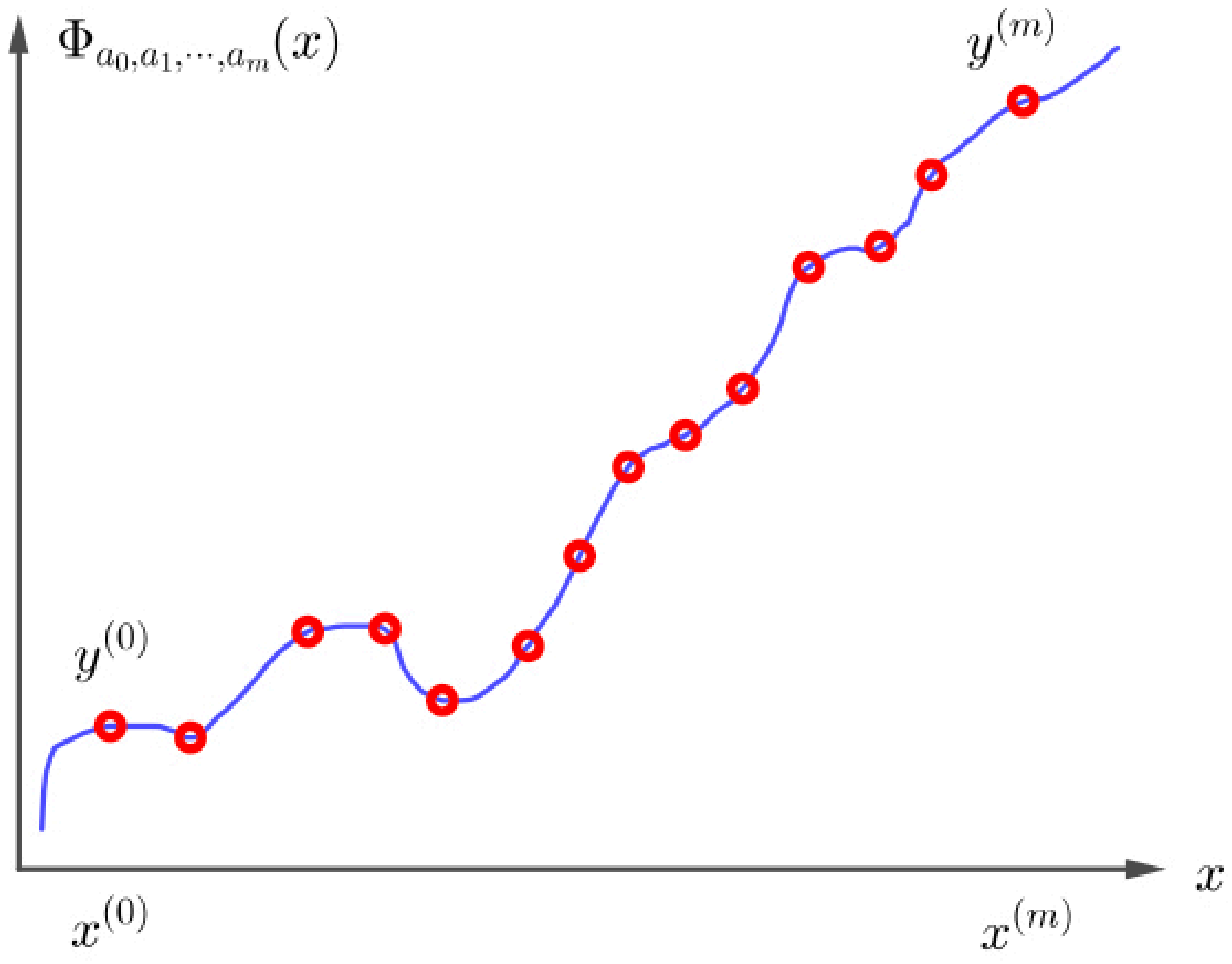


Definition as the basic algorithm for derivative

motivation/example: determine the velocity if the position of the motion of a robot is measured/observed







What's the difference of these two algorithms?

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

$$f'(x_0) \approx \frac{f(x_0 + h/2) - f(x_0 - h/2)}{h}$$

Taylor's expansion as a tool for error-analysis

one-side approximation:

$$f(x_0+h) \approx f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3, \quad x - x_0 = h$$

$$\text{approximation of the derivative} \approx \frac{f(x_0+h)-f(x_0)}{h} \approx f'(x_0) \underbrace{+\frac{1}{2}f''(x_0)h + \frac{1}{6}f'''(x_0)h^2 + \cdots}_{\text{error of the approximation}}$$

$\rightarrow$ leading-order error $\sim h$

Continued: central scheme

Algorithm design makes all the different!

central (two-side) approximation:

$$f\left(x_0+\frac{h}{2}\right)\approx f(x_0)+f'(x_0)\left(\frac{h}{2}\right)+\frac{1}{2}f''(x_0)\left(\frac{h}{2}\right)^2+\frac{1}{6}f'''(x_0)\left(\frac{h}{2}\right)^3+\cdots$$

$$f\left(x_0-\frac{h}{2}\right)\approx f(x_0)+f'(x_0)\left(-\frac{h}{2}\right)+\frac{1}{2}f''(x_0)\left(-\frac{h}{2}\right)^2+\frac{1}{6}f'''(x_0)\left(-\frac{h}{2}\right)^3+\cdots$$

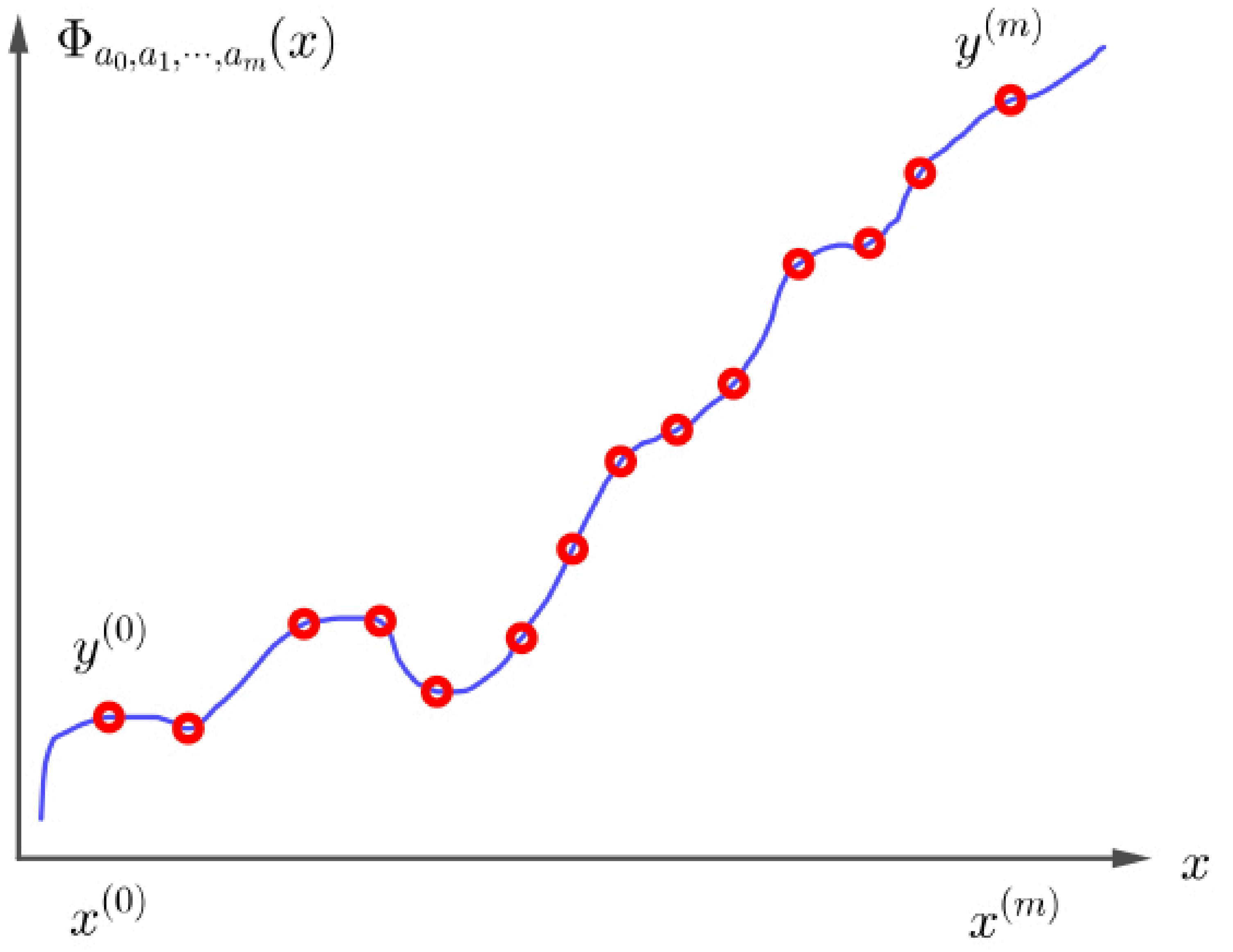
approximation of the derivative $\approx \dfrac{f(x_0+h/2)-f(x_0-h/2)}{h}\approx f'(x_0)\quad \underbrace{+\frac{1}{24}f'''(x_0)h^2+\cdots}_{\text{error of the approximation}}$

$\rightarrow$ leading-order error $\sim h^2$

Ex.: Work out the next-leading order in error proportional to h^4 in the central scheme.

Advanced method: interpolation using multiple-steps

$$p(h) = a + bh^2 = \text{diff}_0 \cdot \frac{h^2 - h_0^2/4}{h_0^2 - h_0^2/4} + \text{diff}_1 \cdot \frac{h^2 - h_0^2}{h_0^2/4 - h_0^2} \rightarrow p(0) = -\frac{1}{3}\text{diff}_0 + \frac{4}{3}\text{diff}_1$$



$$\text{diff}_i = \text{diff}(h_0/2^{i-1})$$

$$x^{(0)} \leftrightarrow h_0^2, \quad x^{(1)} \leftrightarrow h_1^2 = h_0^2/4, \; L_0(x) = \frac{x - x^{(1)}}{x^{(0)} - x^{(1)}}, \quad L_1(x) = \frac{x - x^{(0)}}{x^{(1)} - x^{(0)}}$$

$$\text{diff}(h) \equiv \frac{f(x+h) - f(x-h)}{2h} \approx f'(x) + \frac{h^2}{6}f'''(x) + \frac{h^4}{120}f^{(5)}(x) + \cdots$$

$$p(0) \approx -\frac{1}{3}\left(f'(x) + \frac{h_0^2}{6}f'''(x) + \frac{h_0^4}{120}f^{(5)}(x) + \cdots\right)$$
$$+\frac{4}{3}\left(f'(x) + \frac{h_0^2}{4\cdot 6}f'''(x) + \frac{h_0^4}{16\cdot 120}f^{(5)}(x) + \cdots\right)$$
$$\approx f'(x) - \frac{1}{4}\frac{h_0^4}{120}f^{(5)}(x)$$
$$\rightarrow f'(x) \approx -\frac{1}{3}\text{diff}(h_0) + \frac{4}{3}\text{diff}\left(\frac{h_0}{2}\right) + \frac{1}{4}\frac{h_0^4}{120}f^{(5)}(x)$$

Lagrange polynomial interpolation:

$$\Phi_{a_0,a_1,\cdots,a_m}(x) \equiv p(x) = \sum_{i=0}^{m} y^{(i)} L_i(x) = \sum_{i=0}^{m} y^{(i)} \prod_{j=0, j\neq i}^{m} \frac{x - x^{(j)}}{x^{(i)} - x^{(k)}}$$

$$L_i(x) = \frac{(x - x^{(0)})\cdots(x - x^{(i-1)})(x - x^{(i+1)})\cdots(x - x^{(m)})}{(x^{(i)} - x^{(0)})\cdots(x^{(i)} - x^{(i-1)})(x^{(i)} - x^{(i+1)})\cdots(x^{(i)} - x^{(m)})}$$

Opposite: integration $\sum \rightarrow \int$

motivation/example: determine the velocity or the position of a robot from the measured acceleration

$$\vec{v} = \sum \vec{a}(t \rightarrow t + \delta t)\delta t$$

work $W = \sum \vec{F}(\vec{x} \rightarrow \vec{x} + \delta\vec{x}) \cdot \delta\vec{x}$

force $F = \mu x^2, \; 0 \leq x \leq D$

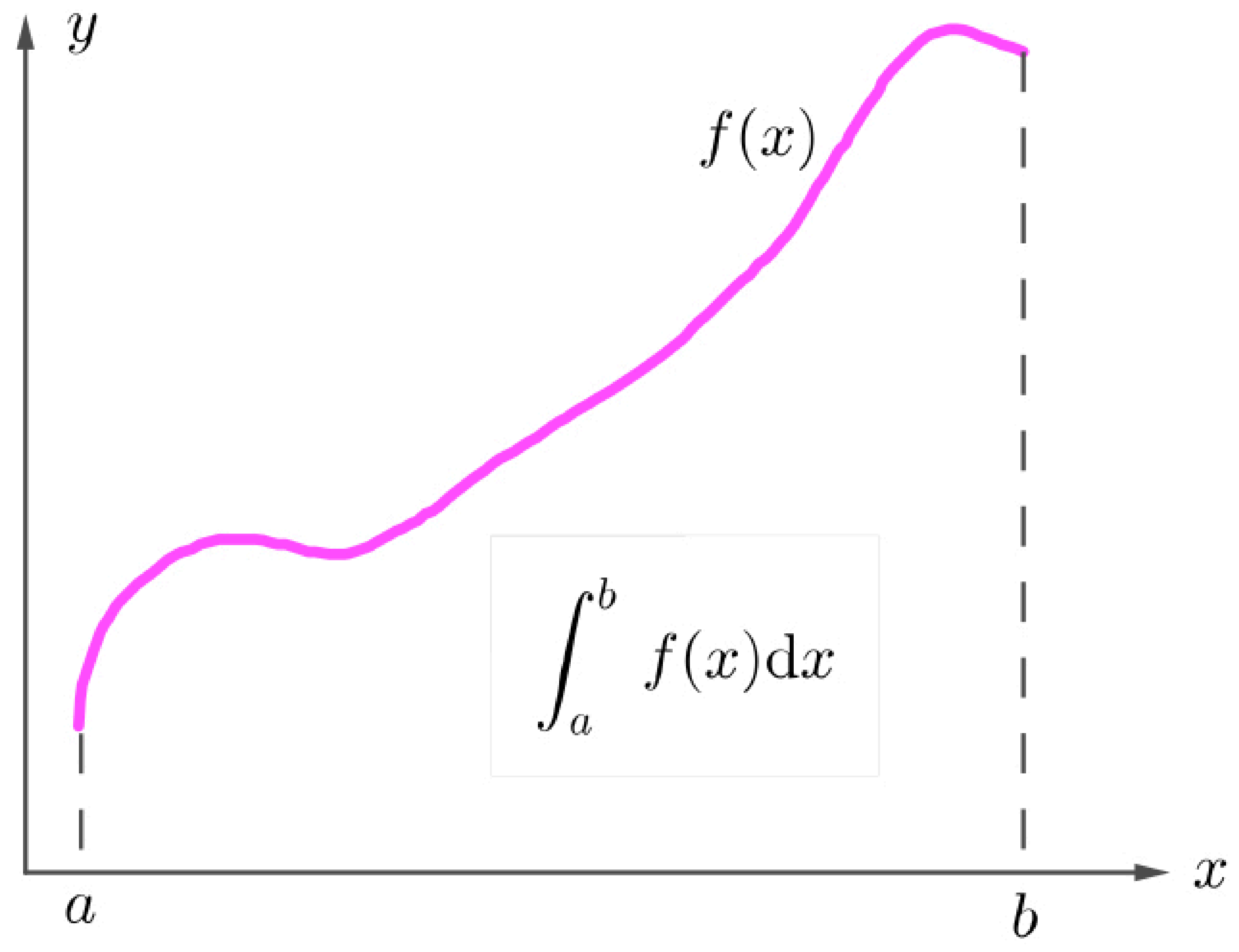
discretization $x^{(i)} = ih, h = D/m$

$$W \approx \sum_{i=0}^{m} \mu x^{(i),2} h = h^3 \sum_{i=1}^{m} i^2$$

Ex.: How to calculate $\sum i^2$?

$$\rightarrow W \approx \frac{1}{3}\mu D^3 \left(1 + \frac{3}{2}\frac{1}{m} + \frac{1}{2}\frac{1}{m^2}\right) \rightarrow \frac{1}{3}\mu D^3 = \int_0^D \mu x^2 dx$$

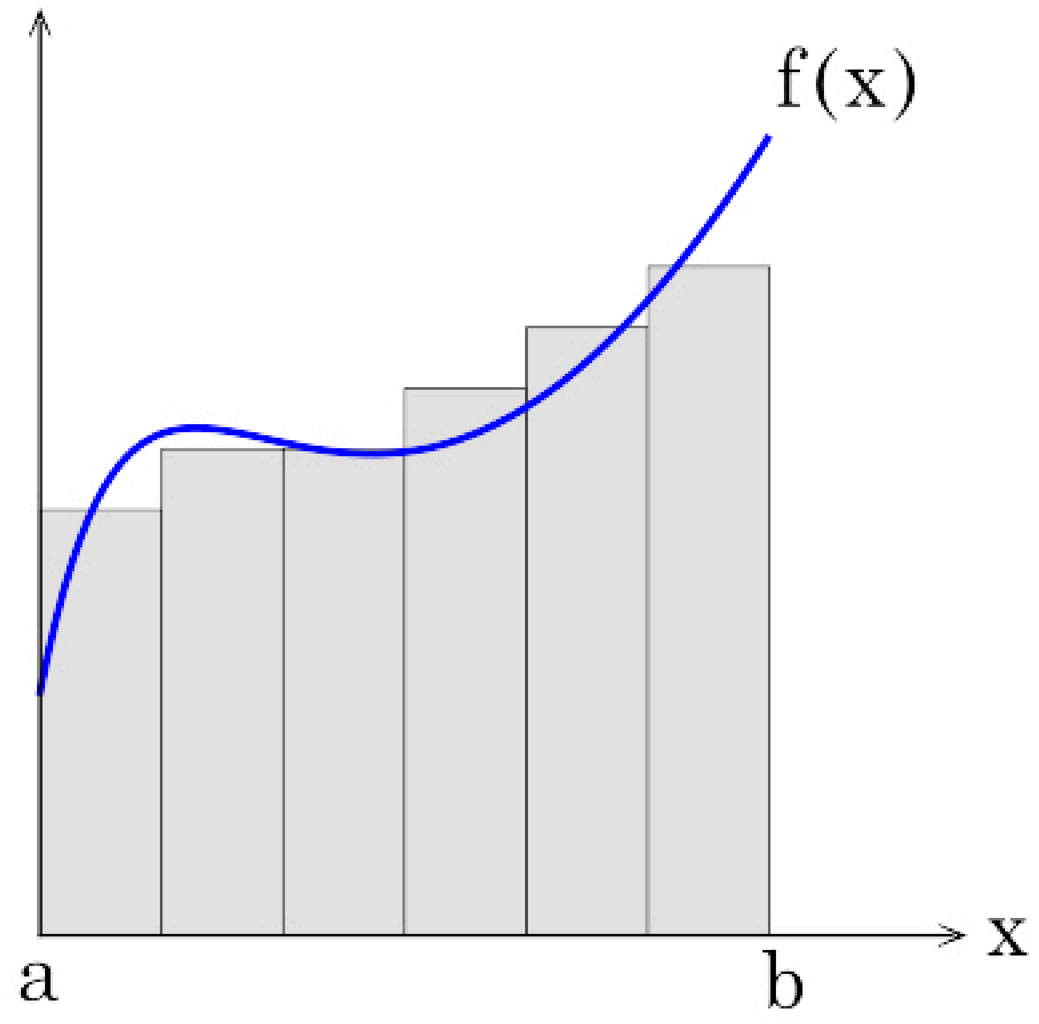
error $\sim m^{-1} \sim h$



discretization itself provides the first algorithm for integration: Euler method, i.e., rectangular scheme

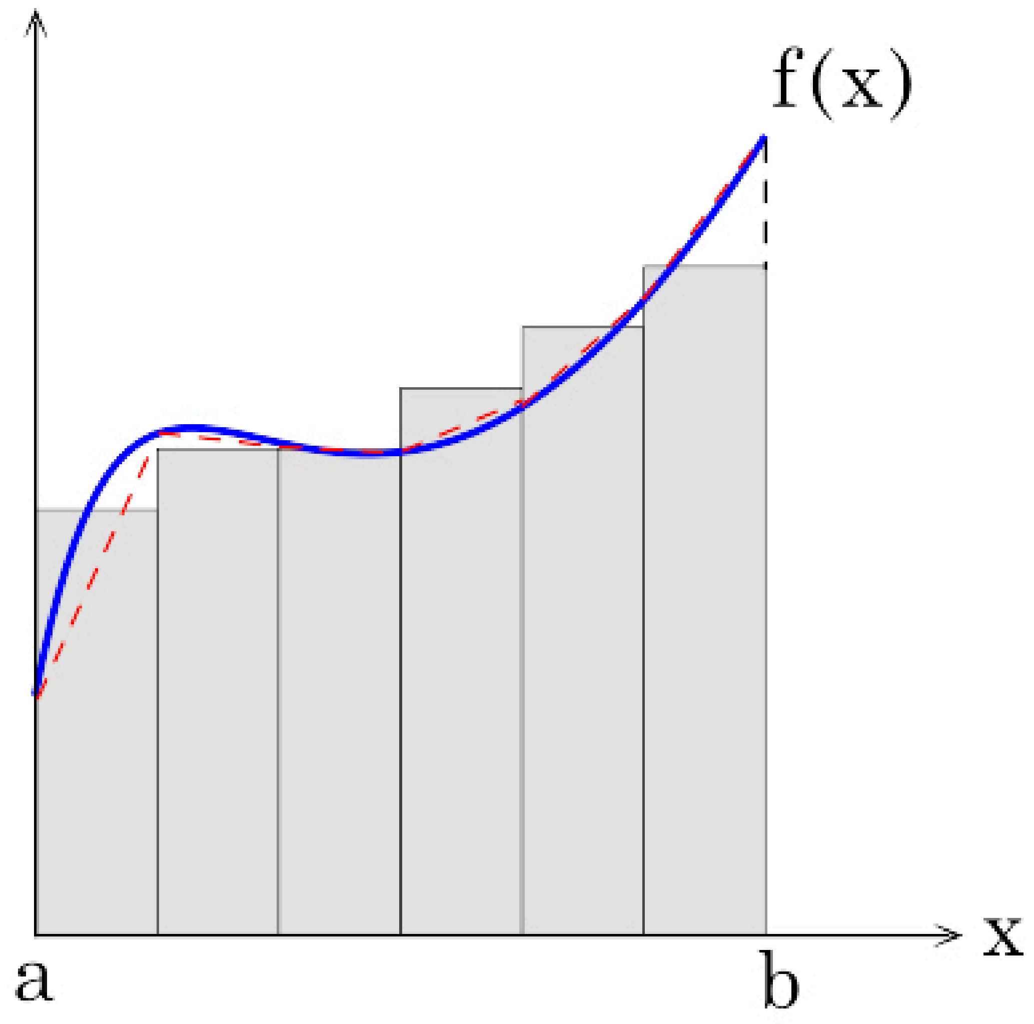
Newton-Cotes formula: geometrical meaning

$h * f(x^{(i)})$



retangular

$h * [f(x^{(i)}) + f(x^{(i+1)})]/2$



trapezoidal

aim: $\mathcal{I}(a,b) = \int_a^b f(x)dx$

trapezoidal rule:

$$\mathcal{I}(a,b) \approx h\left[\frac{f(a)+f(b)}{2} + \sum_{i=1}^{m-1} f(a+ih)\right]$$

error $\sim \mathcal{O}(h^2)$

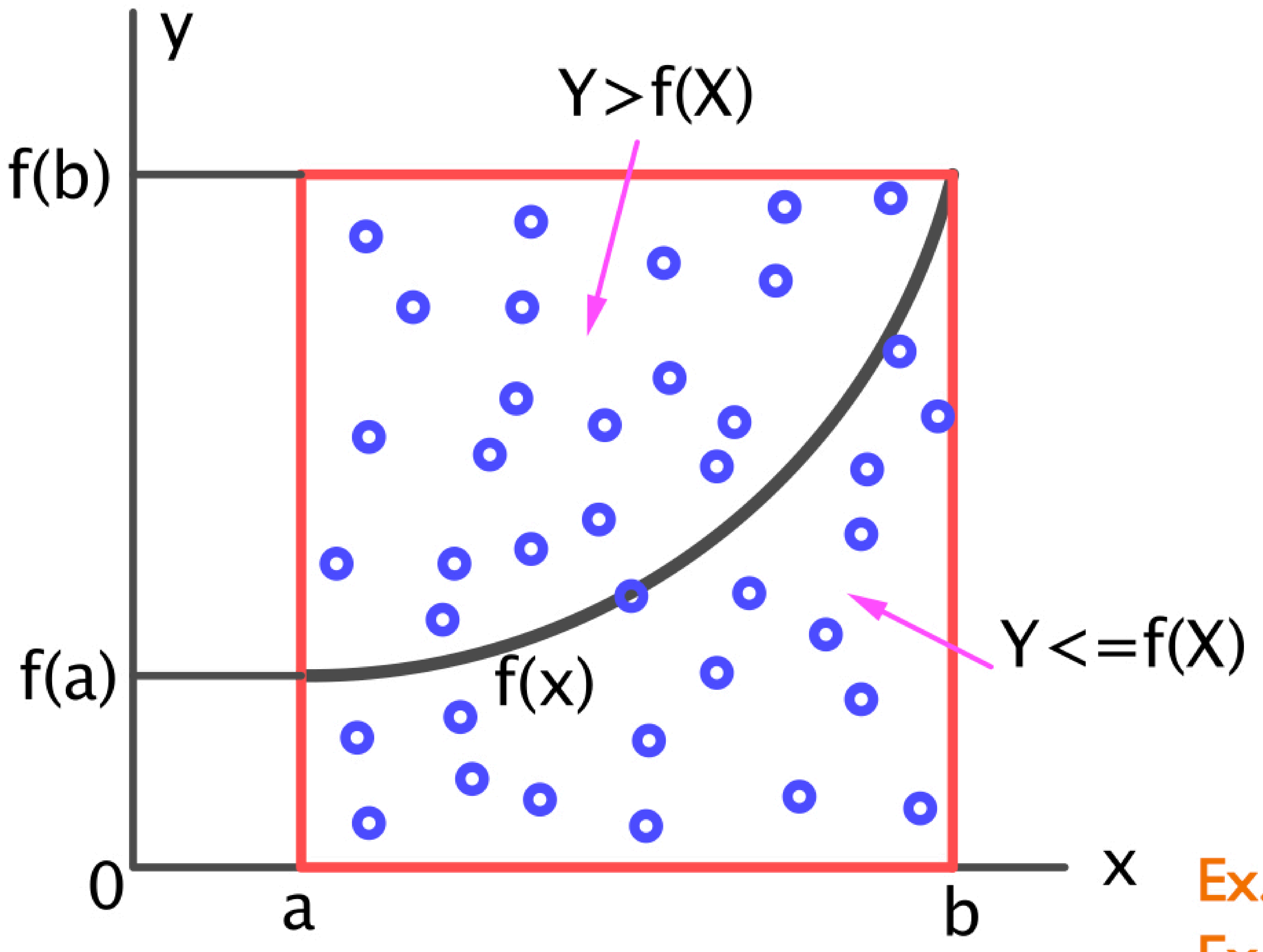
Ex.: Work out the explicit form of the error.

Simpson'srule: 3 points->parabola

$$\mathcal{I}(a,b) \approx \frac{1}{3}h\left[f(a)+f(b) + 4\sum_{i=1}^{m/2} f(a+(2i-1)h) + 2\sum_{i=1}^{m/2-1} f(a+2ih)\right]$$

error $\sim \mathcal{O}(h^4)$

Idea of using random numbers



random estimator

$$\frac{m'}{m} \approx \frac{\mathcal{I}(a,b)}{(b-a)f(b)}$$

m: number of samples

m': number of samples under $f(x)$

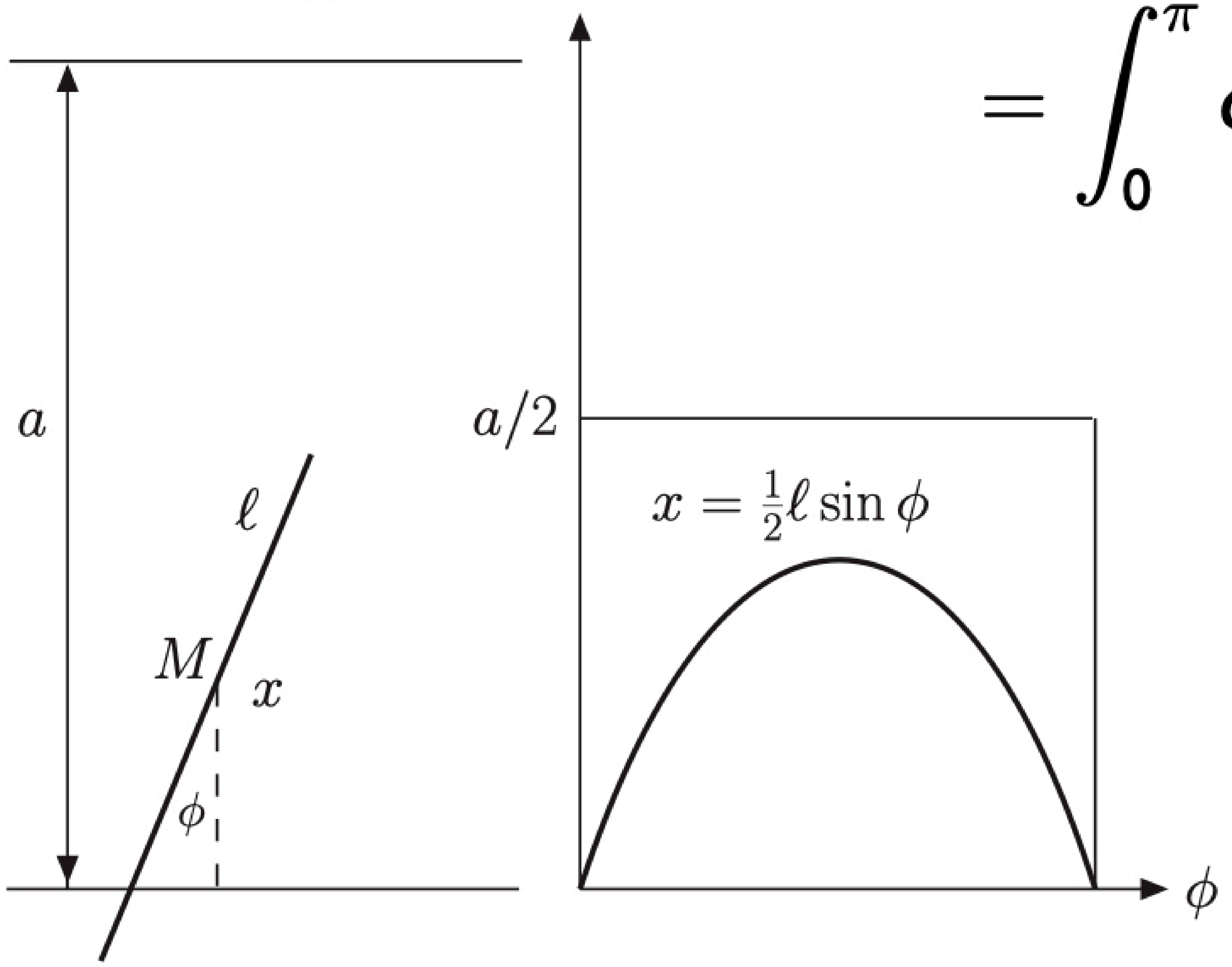
$$\mathcal{I}(a,b) \approx \frac{m'}{m} \times (b-a)f(b)$$

Ex.: How to estimate pi using this method?

Ex.: Comment this method for multi-integration.

Buffon's needle experiment

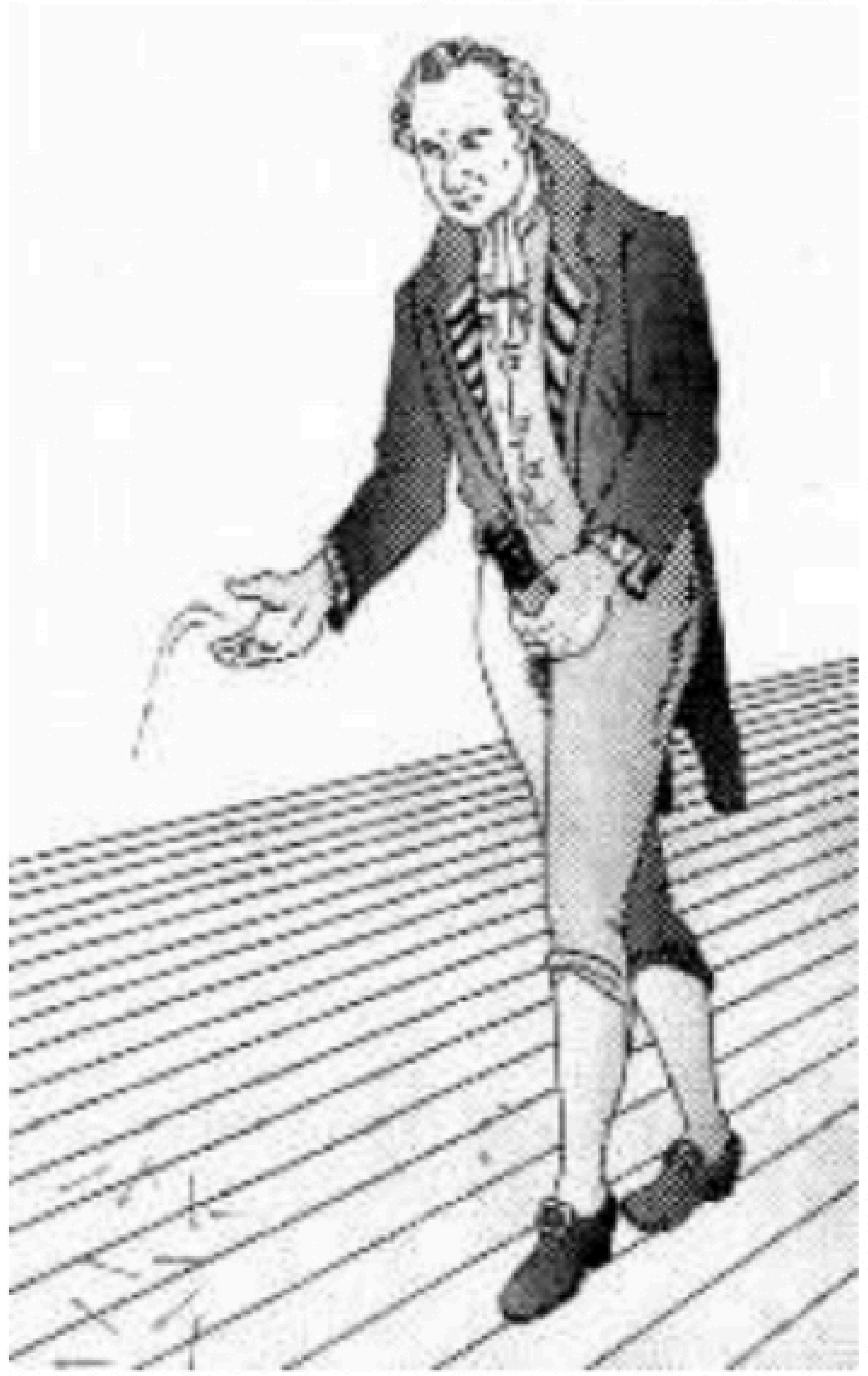
$0 \leq x \leq \frac{a}{2}, \; x \leq \frac{\ell \sin\phi}{2}$

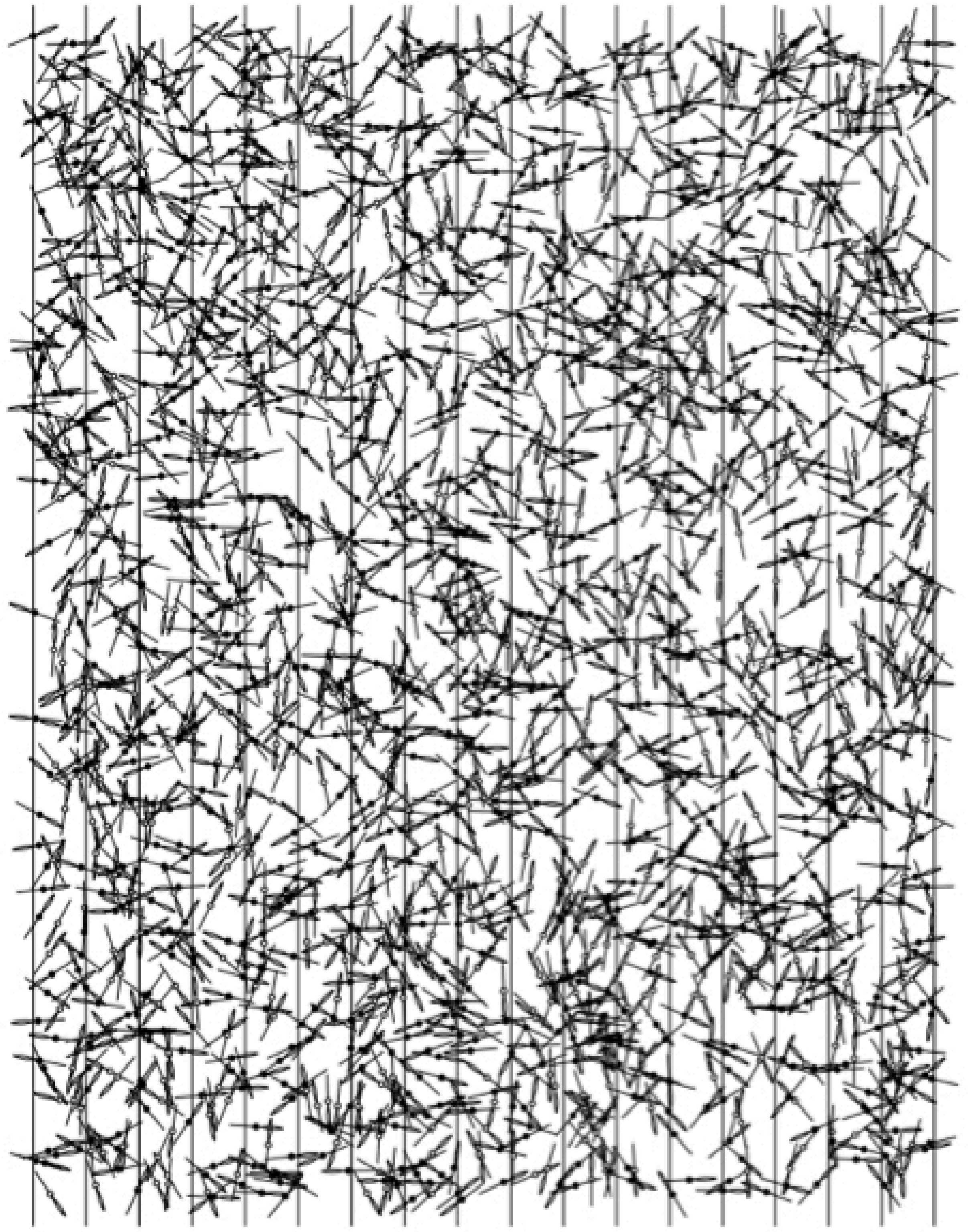


$P = P(\text{intersection between needle and line})$

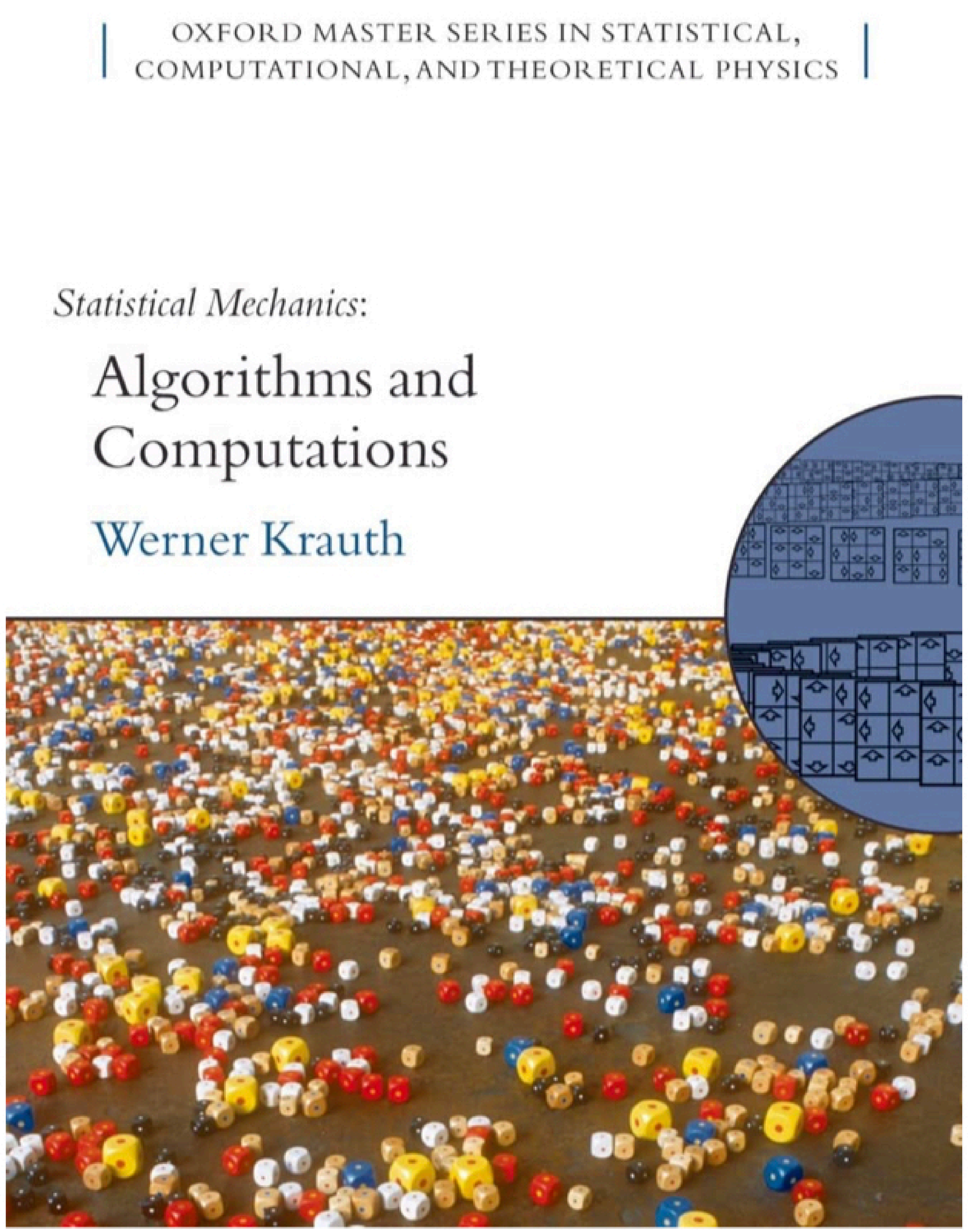
$$= \int_0^{\pi} d\phi \frac{\ell \sin\phi}{2} \Big/ \int_0^{\pi} d\phi \int_0^{a/2} dx = \frac{2\ell}{a\pi} \rightarrow \pi = \frac{2}{P}\frac{\ell}{a}$$

estimator for $\pi \approx \left(\frac{\ell}{a}\right) \frac{2N}{N_{\text{Buffon}}}$





Random algorithms in statistical physics



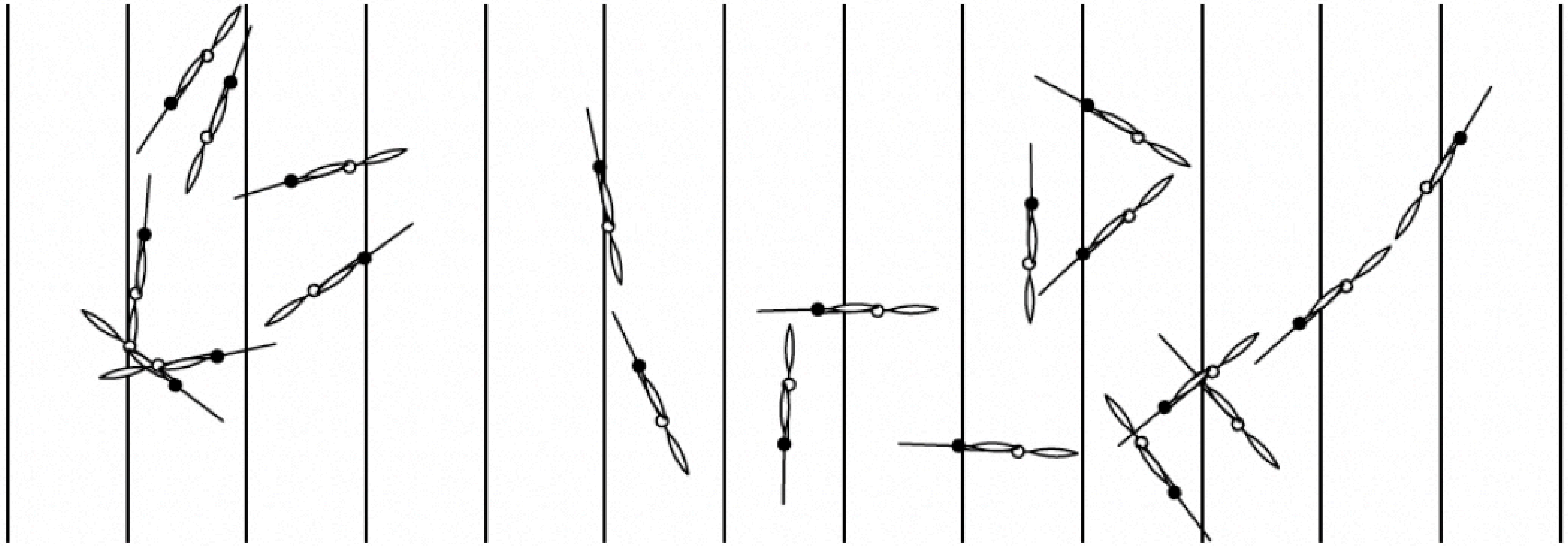
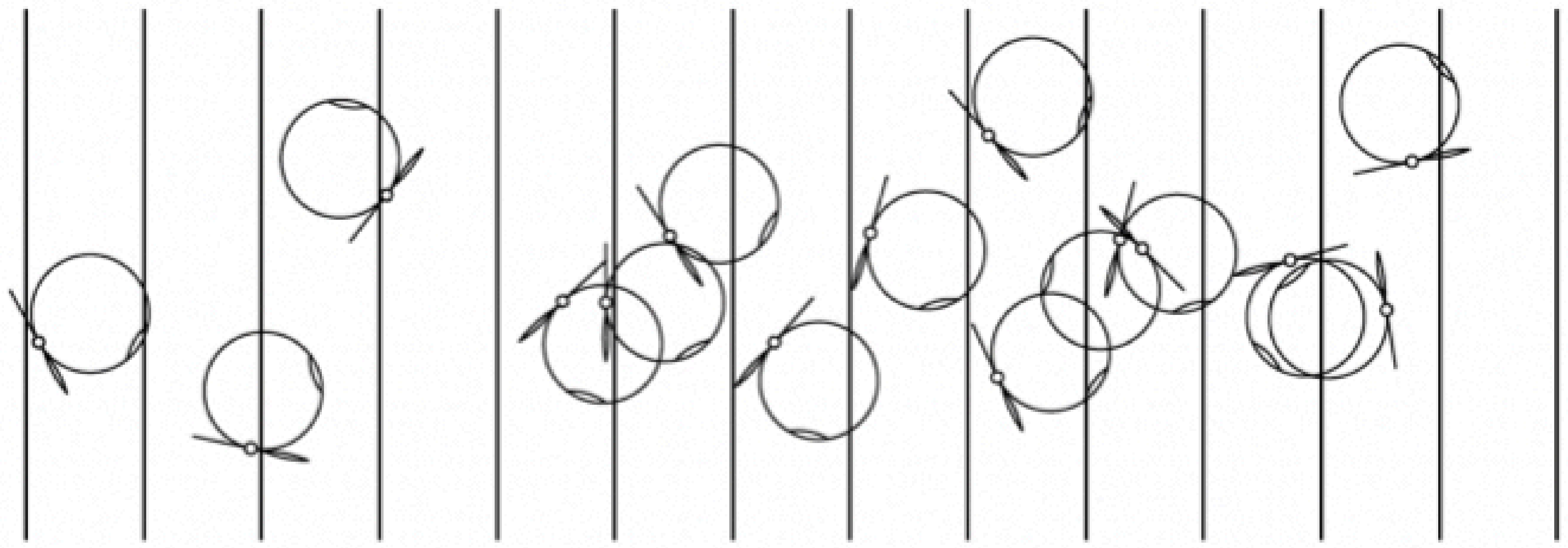


Fig. 1.12 Buffon's experiment performed with Gadget No. 1. It is impossible to tell whether black or white needles were thrown randomly.



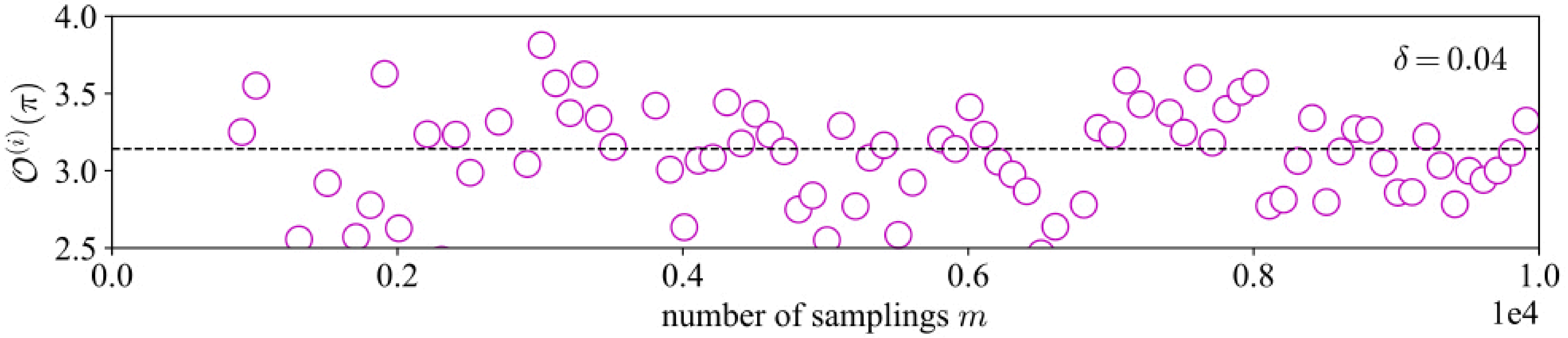
Random walk: a first glimpse

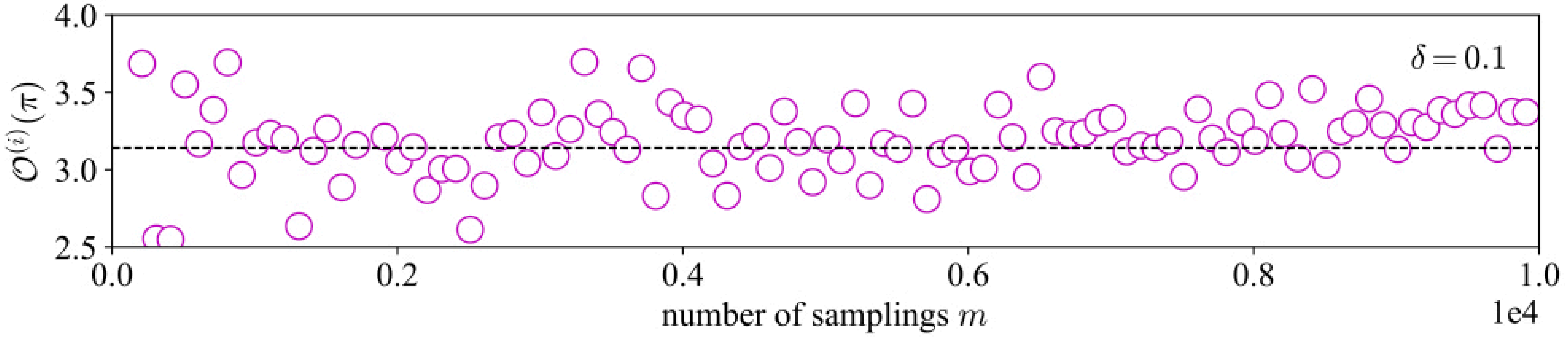
$x + \delta x \to x, y + \delta y \to y$

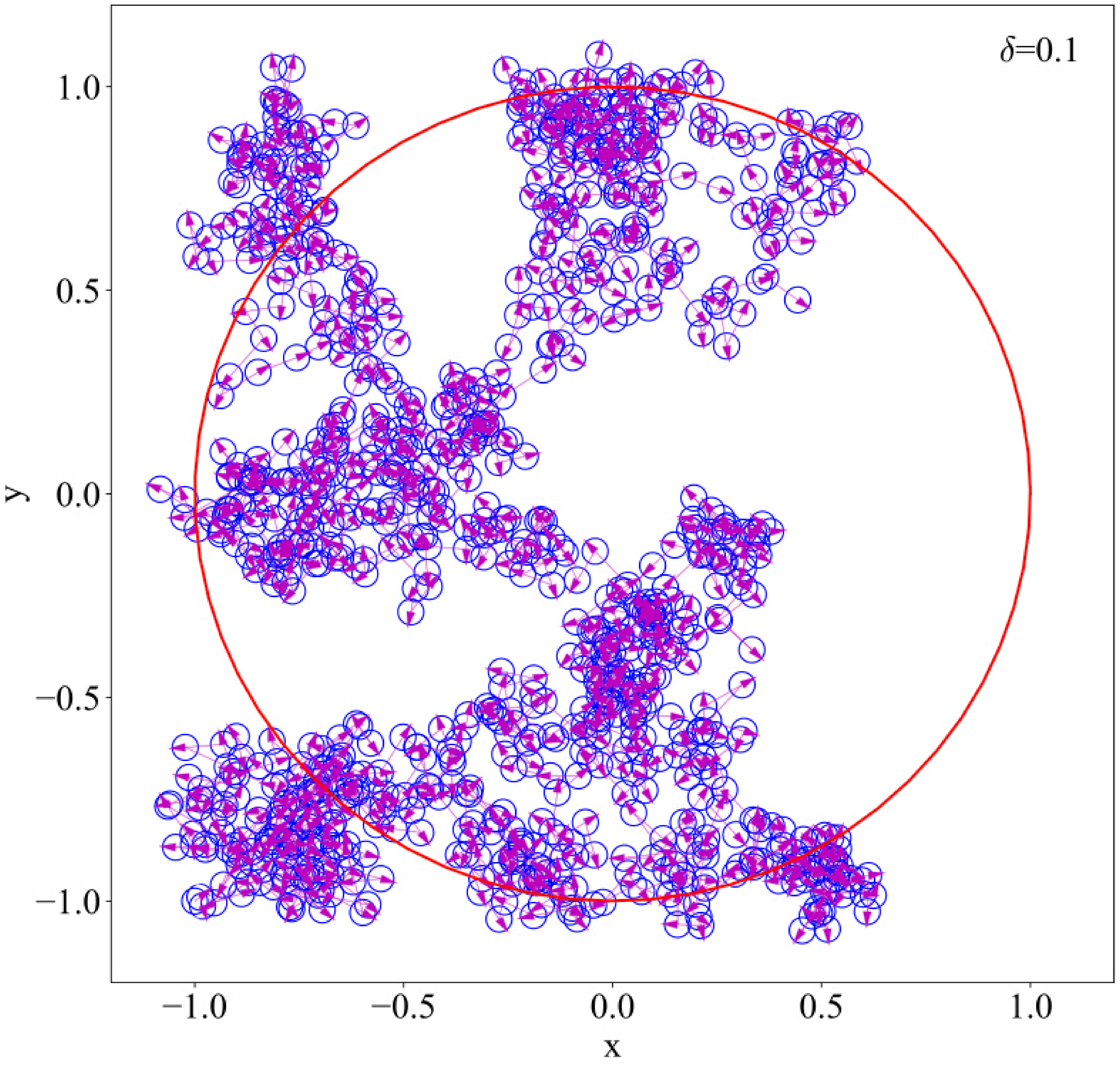
under $x^2 + y^2 \leq 1$

$$\langle f \rangle \approx \frac{1}{m} \sum_{i=1}^{m} \tilde{f}^{(i)}$$

Markov chain Monte Carlo (MCMC)





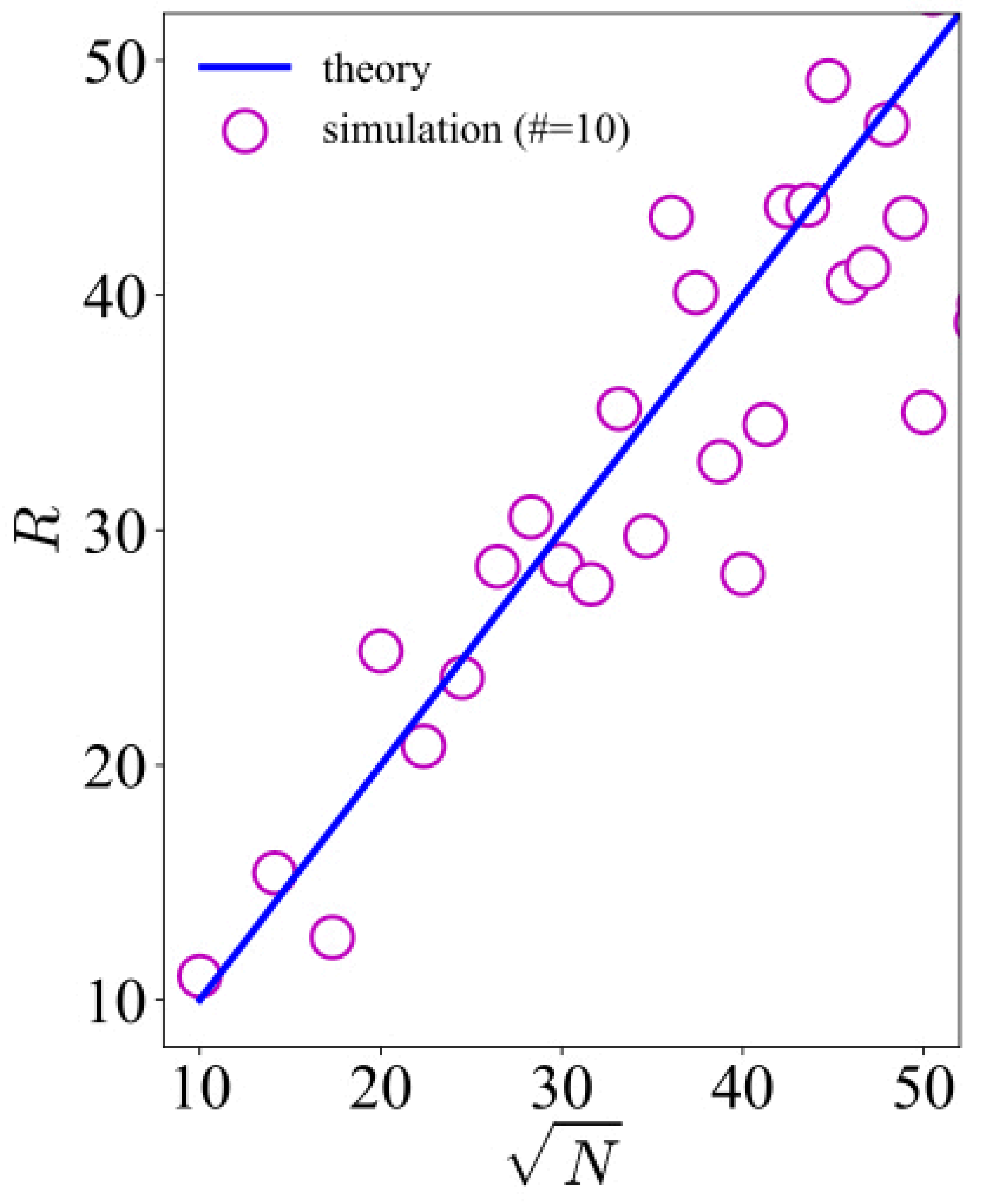


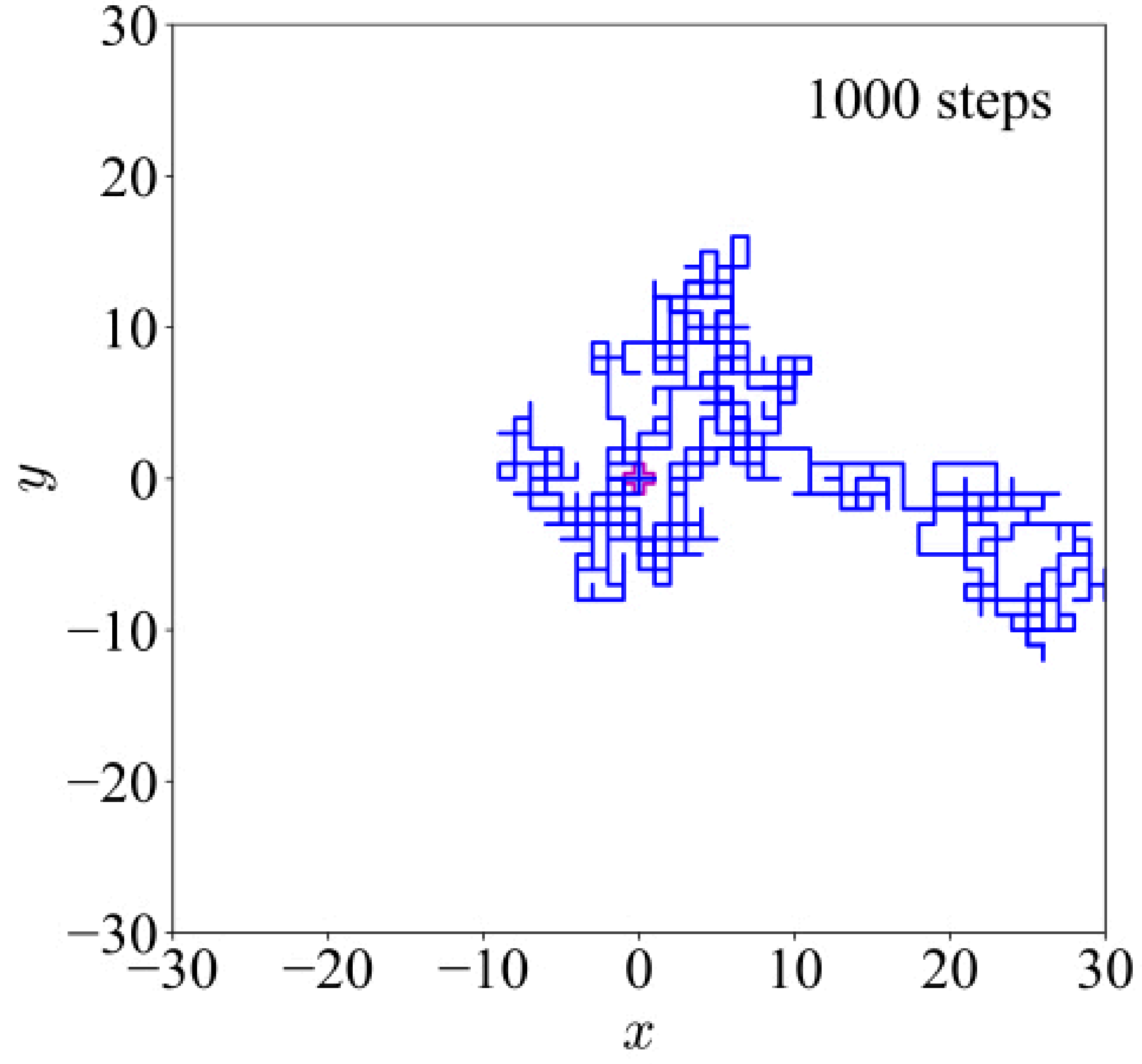
Random walk: basic properties

$$R^2 = \left(\delta x^{(1)} + \delta x^{(2)} + \cdots + \delta x^{(N)}\right)^2 + \left(\delta y^{(1)} + \delta y^{(2)} + \cdots + \delta y^{(N)}\right)^2$$

$$= \delta x^{(1),2} + \delta x^{(2),2} + \cdots + \delta x^{(N),2} + \underbrace{2\sum_{i<j} \delta x^{(i)}\delta x^{(j)}}_{\text{random}\to 0} + (x \leftrightarrow y)$$

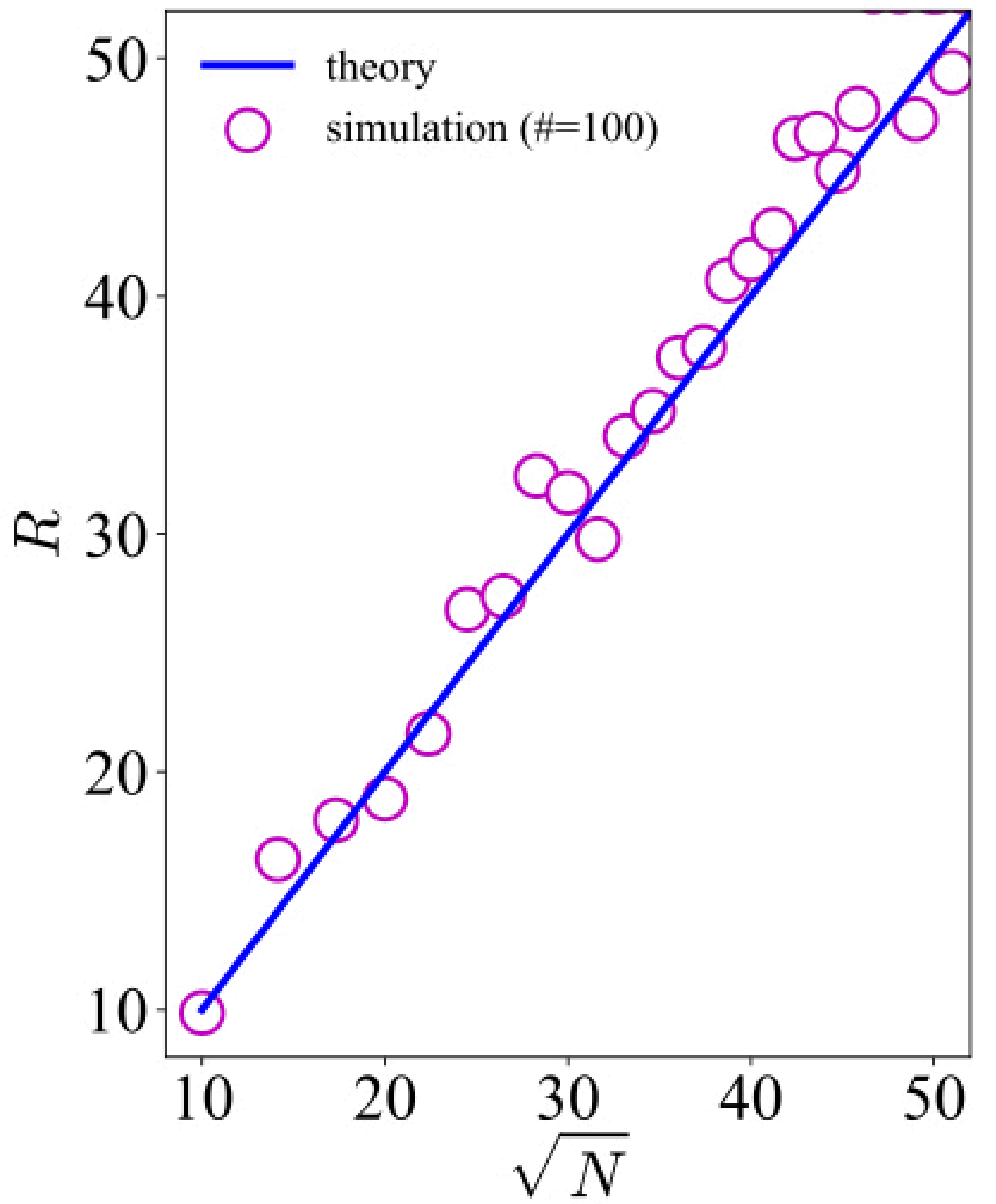
$$\approx \delta x^{(1),2} + \delta x^{(2),2} + \cdots + \delta x^{(N),2} + (x \leftrightarrow y)$$





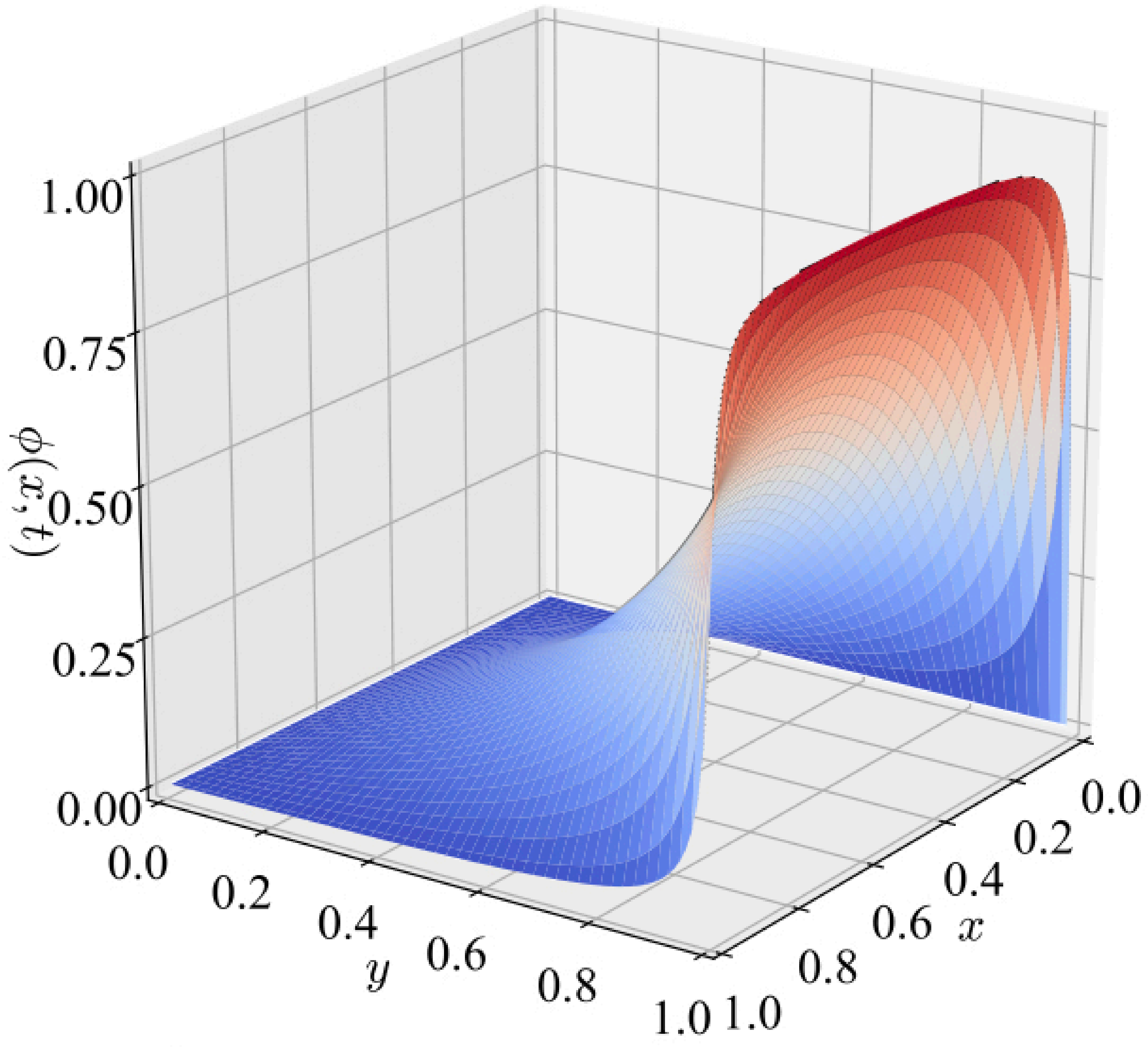
$$r_{\text{rms}}^2 = \langle \delta x \rangle^2 + \langle \delta y \rangle^2$$

$$R^2 \approx N r_{\text{rms}}^2 \rightarrow R \approx \sqrt{N} r_{\text{rms}} \sim \sqrt{N}$$



Ex.: Does the scaling depend on dimension?

Multi-variate functions



Laplacian: $\Delta \equiv \nabla \cdot \nabla$; Poisson equation: $\nabla^2 \Phi = -\rho/\epsilon_0$

$$\delta\vec{x} = \vec{x} - \vec{x}_0, \ \vec{x} \in \mathrm{R}^d$$

$$f(\vec{x}) \approx f(\vec{x}_0) + \delta\vec{x}^\top \left.\frac{\partial f(\vec{x})}{\partial \vec{x}}\right|_{\vec{x}=\vec{x}_0} + \frac{1}{2}\delta\vec{x} \left.\frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top}\right|_{\vec{x}=\vec{x}_0} \delta\vec{x}^\top + \cdots$$

notations:

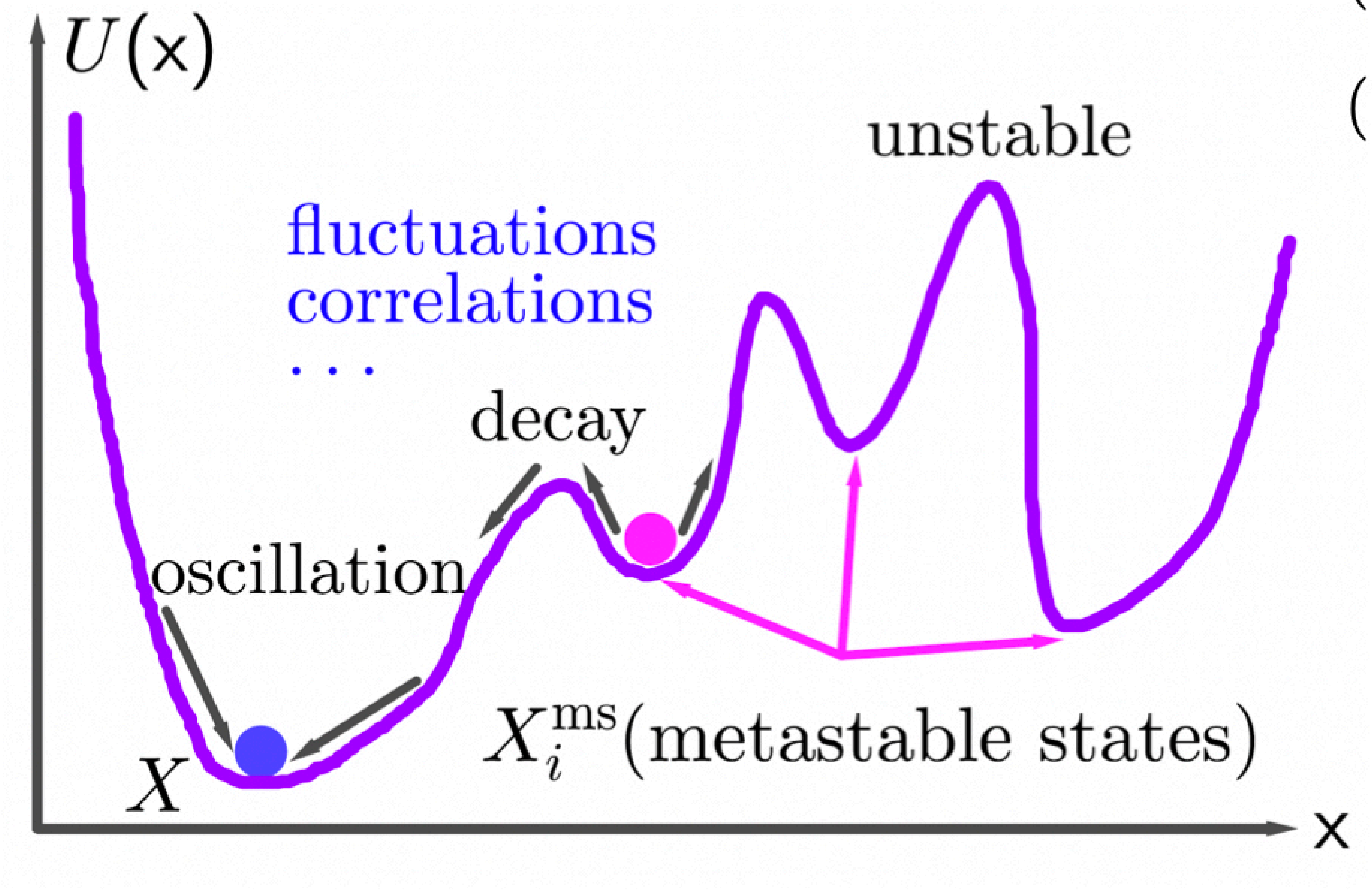
harmonic expansion

$$\vec{g} = \frac{\partial f(\vec{x})}{\partial \vec{x}} = \left(\frac{\partial f}{\partial x^1}, \frac{\partial f}{\partial x^2}, \cdots, \frac{\partial f}{\partial x^d}\right)^\top, \ H(\vec{x}) \equiv \frac{\partial^2 f}{\partial \vec{x} \partial \vec{x}^\top} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_d \partial x_1} & \frac{\partial^2 f}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_d \partial x_d} \end{pmatrix}$$

Ex.: If $f(x, y) = x^2 + 3xy + 2y^2$, what is $\vec{g}$ and $\vec{H}$?

Harmonic approximation

$$U_{\mathrm{harm}}(\delta x) \approx \frac{1}{2}\omega^2 \delta x^2 + \mathrm{const.}$$



Examples:

(1) anharmonic potential $a\delta x^3 + b\delta x^4$

(2) quantum harmonic oscillator $H = \hbar\omega(a^\dagger a + 1/2)$

(3) ϕ^4-scalar field $\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{1}{24}\lambda\phi^4$

frequently-used method in physical problems: firstly obtaining the solution via the simple approximation, the terms like this are often called the non-interacting terms, and then perturbatively computing the high order effects based on the simple solution