Lecture 11

Integration

Quadrature and Monte Carlo methods

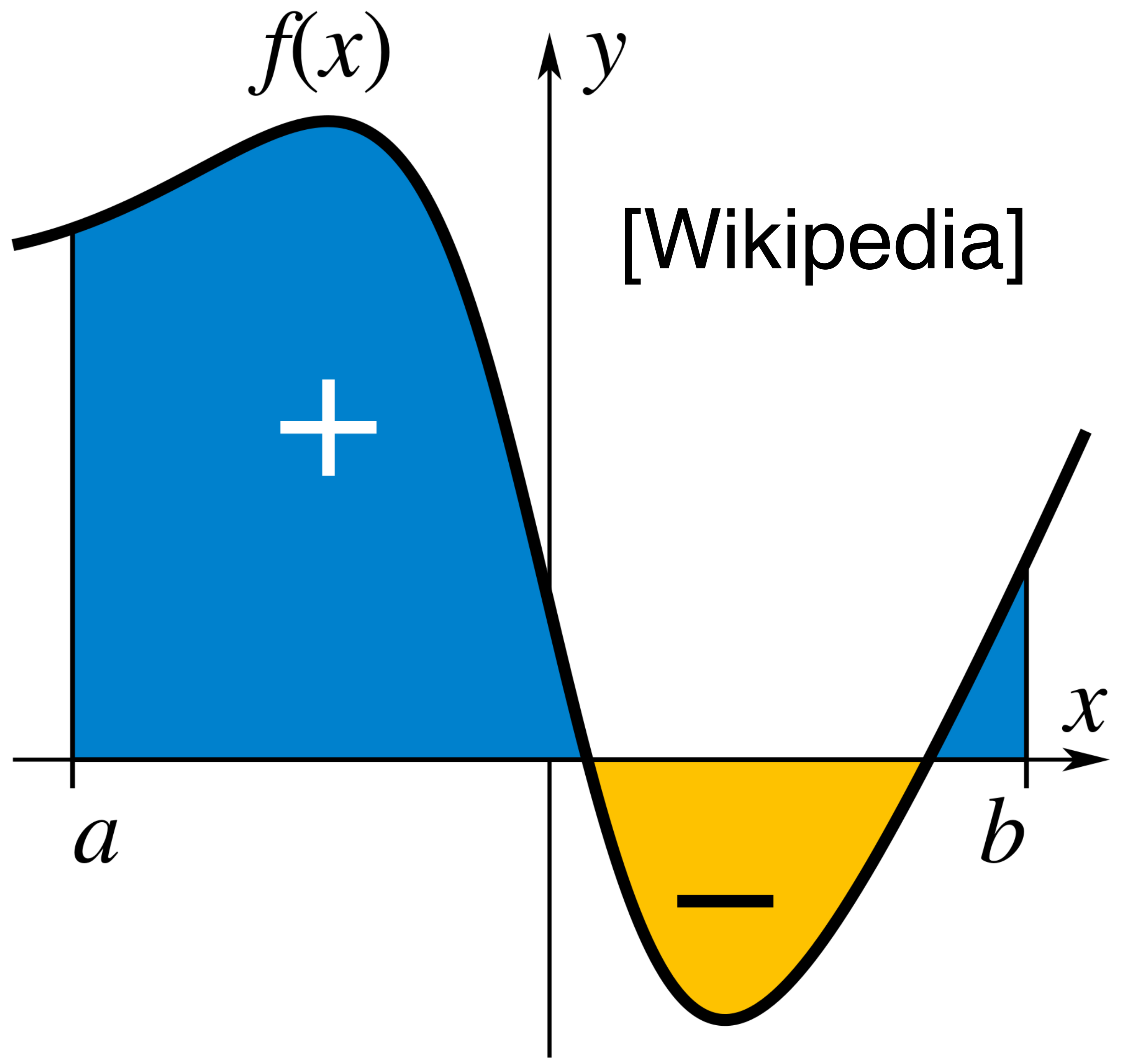
CS328 - Numerical Methods for Visual Computing and Machine Learning

Prof. Wenzel Jakob

EPFL RGL Realistic Graphics Lab

Definite integrals

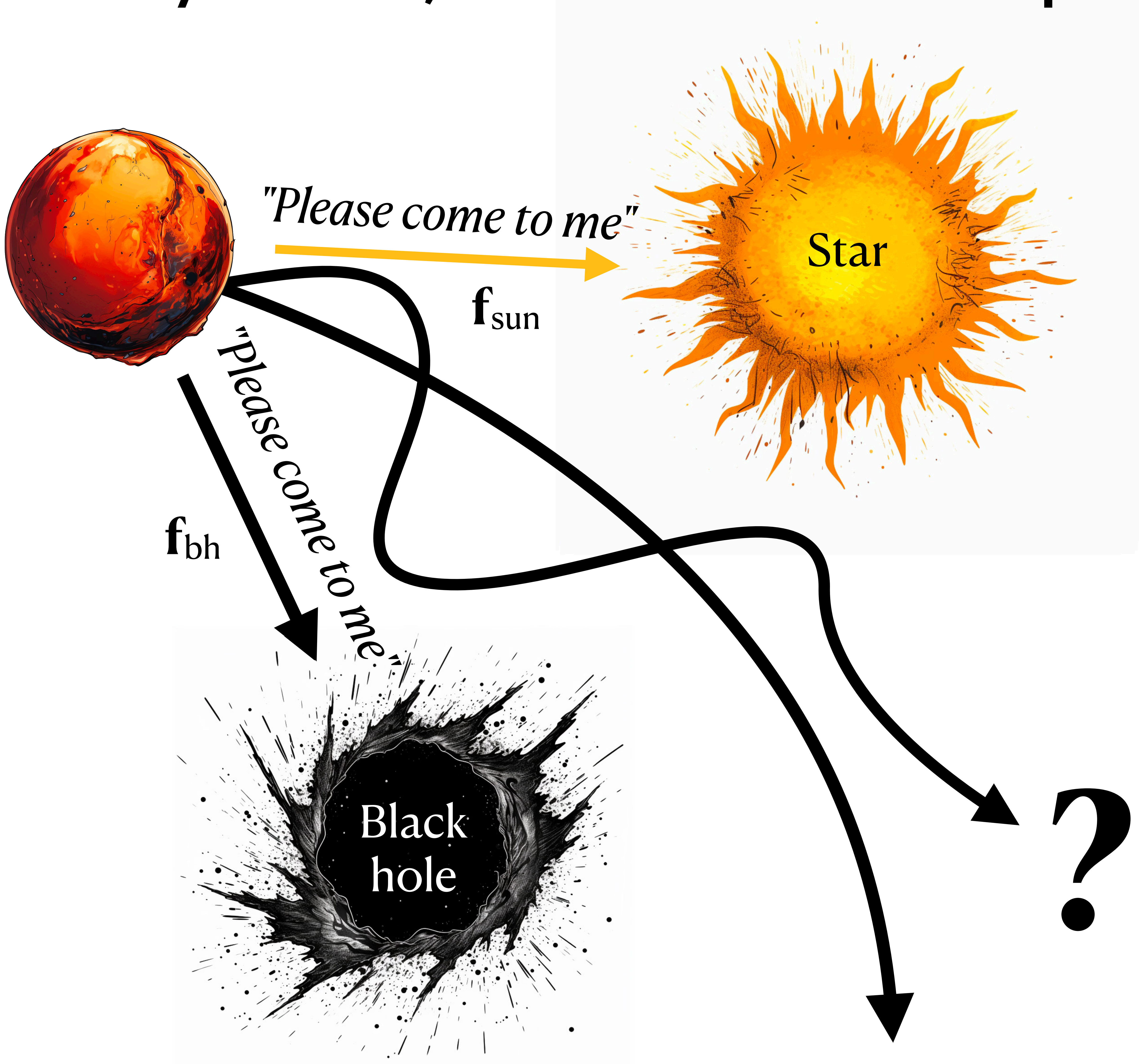
$$\int_a^b f(x)\,\mathrm{d}x$$



[Wikipedia]

Why do integrals arise?

.. for many reasons, but here are two examples of physical processes



MidJourney: {sun, black hole, red planet}, comic style on white background.

Velocity is the time derivative of **position**

$$\mathbf{v}(t) = \frac{\partial}{\partial t}\mathbf{x}(t)$$

Acceleration is the time derivative of **velocity**

$$\mathbf{a}(t) = \frac{\partial}{\partial t}\mathbf{v}(t)$$

Newton's 2_{nd} law relates **acceleration** to **forces**:

$$\mathbf{a}(t) = \frac{\mathbf{f}(t)}{m} = \frac{\mathbf{f}_{\text{sun}}(t) + \mathbf{f}_{\text{bh}}(t)}{m}$$

Mass of the planet

Why do integrals arise?

.. for many reasons, but here are two examples of physical processes

Wanted: **position** as a function of **time**

$$\mathbf{x}(t)$$

?

$\partial/\partial t$, $\int dt$

Velocity is the time derivative of **position**

$$\mathbf{v}(t) = \frac{\partial}{\partial t}\mathbf{x}(t)$$

Acceleration is the time derivative of **velocity**

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Newton's 2_{nd} law relates **acceleration** to **forces**:

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Mass of the planet

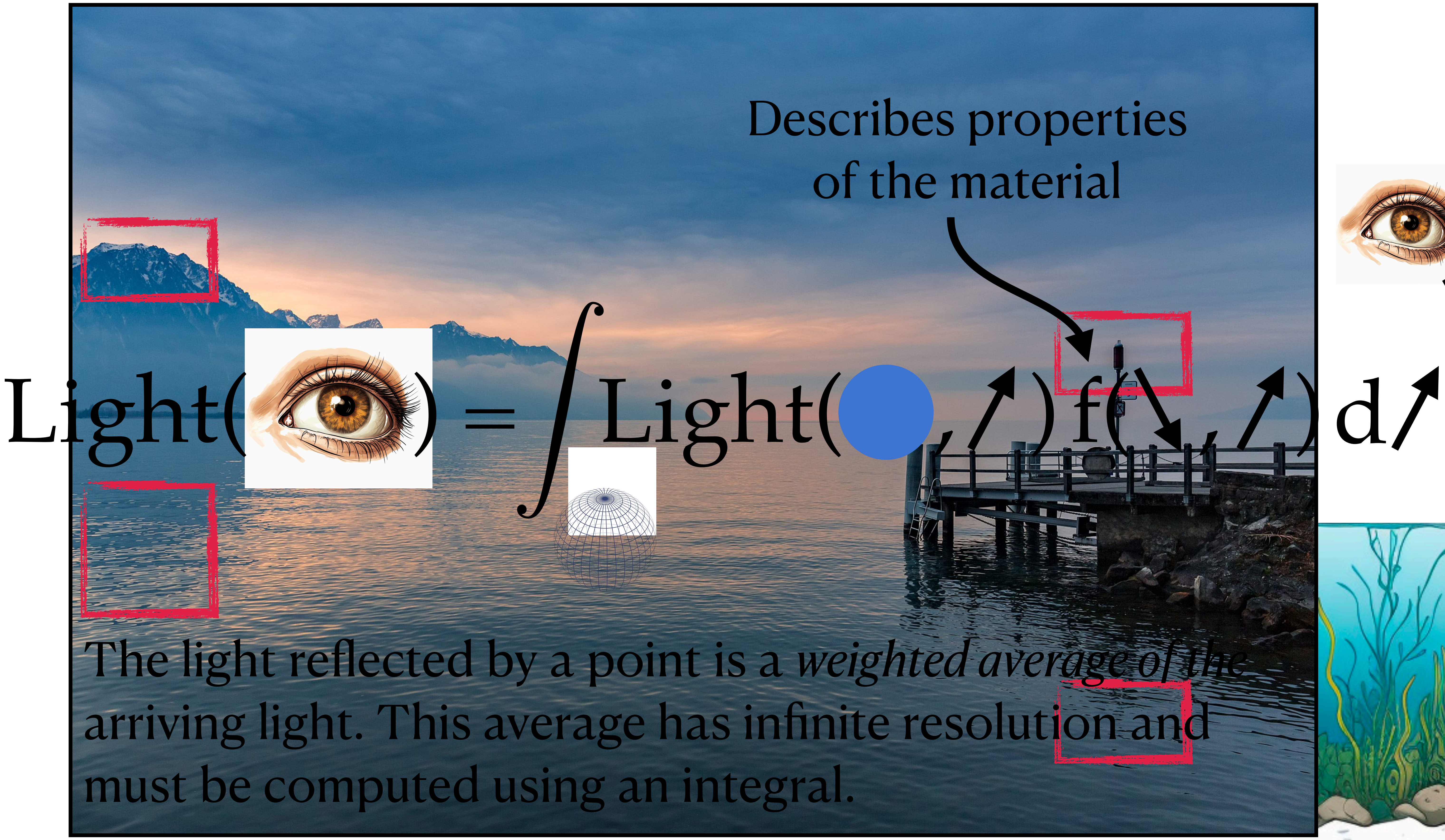
Physical equation models the evolution of the world as a *time average.*

This average is not discrete but has *infinite resolution*, hence an integral must be used to simulate physics.

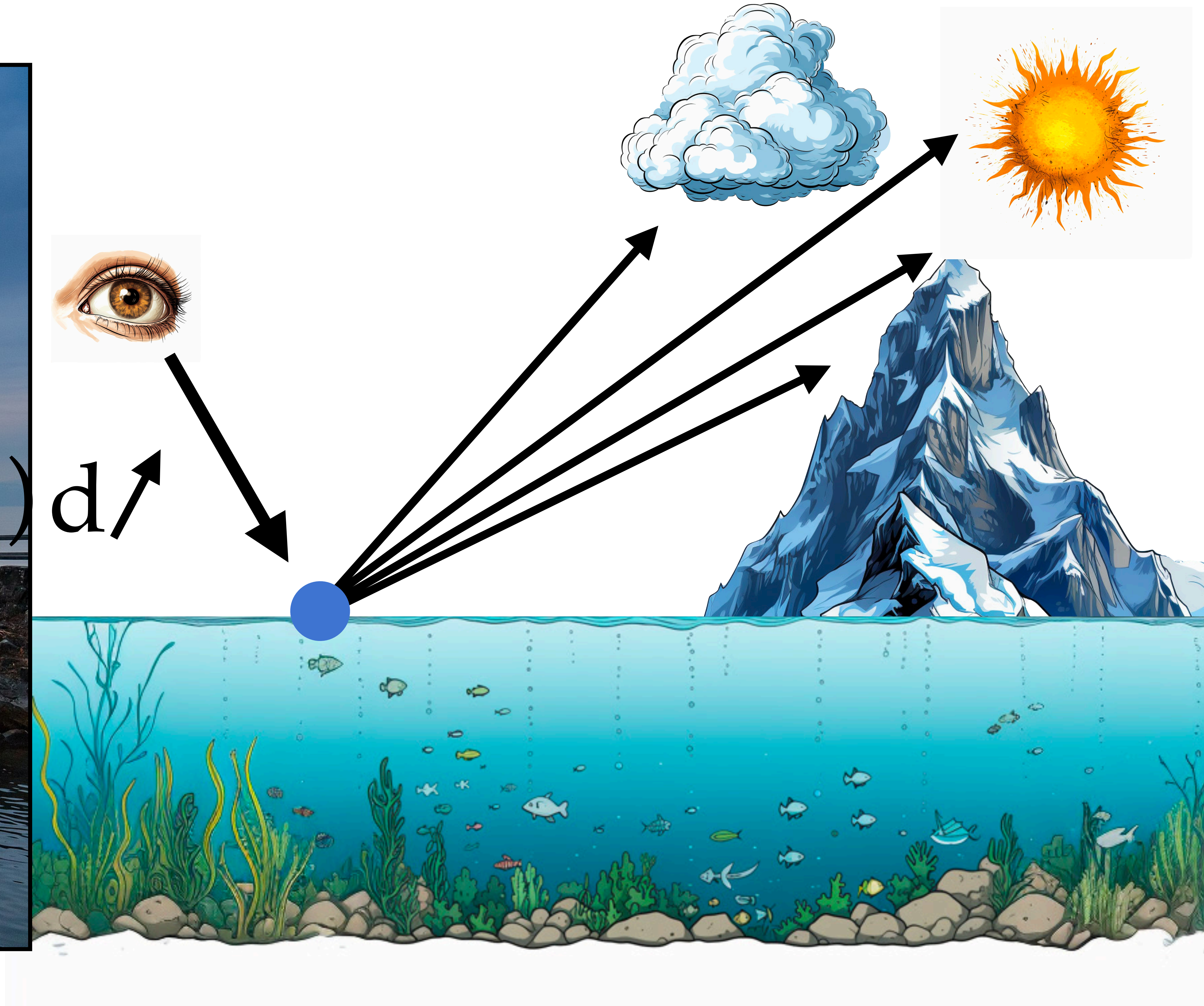
!

Why do integrals arise?

.. for many reasons, but here are two examples of physical processes

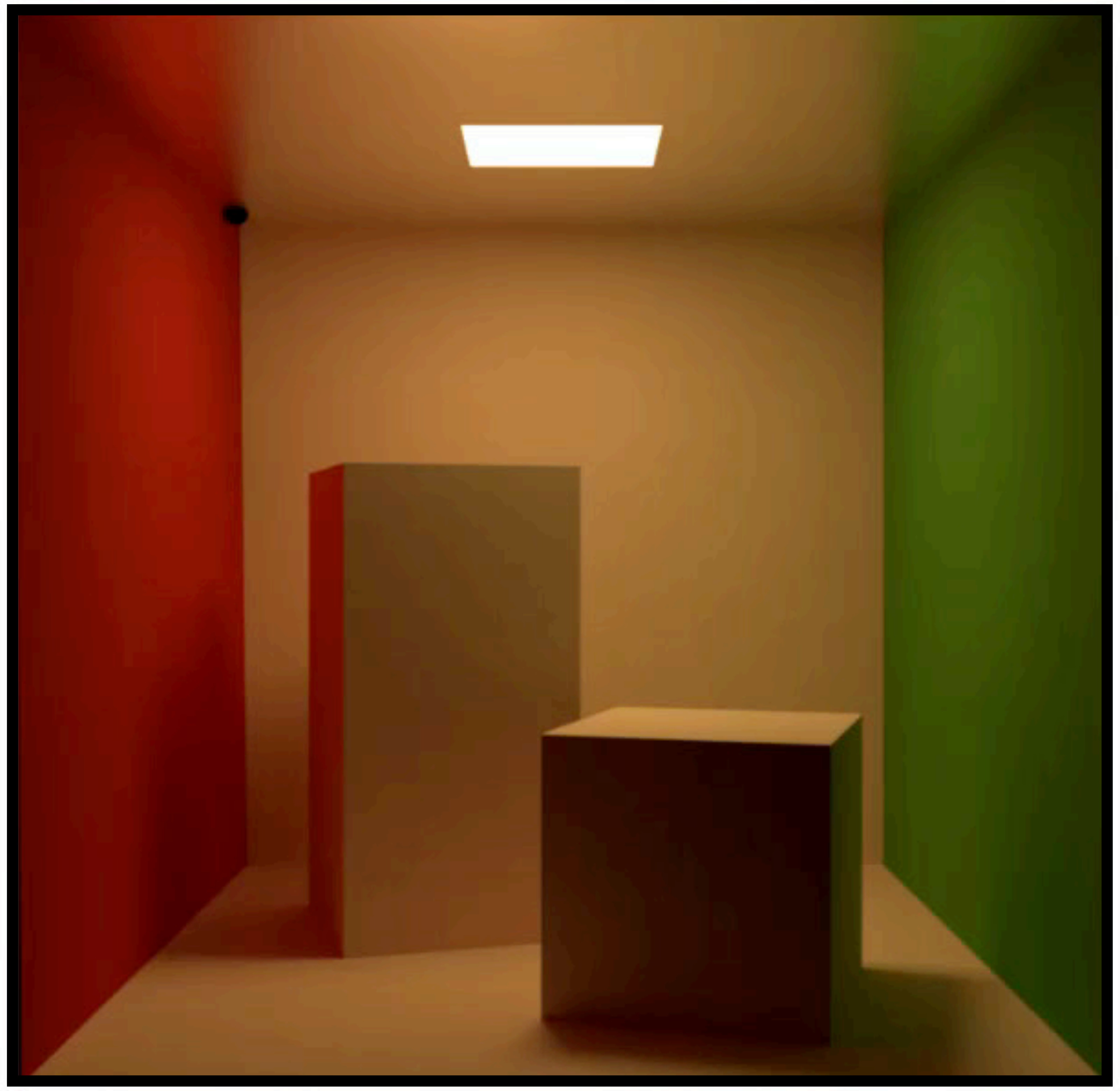


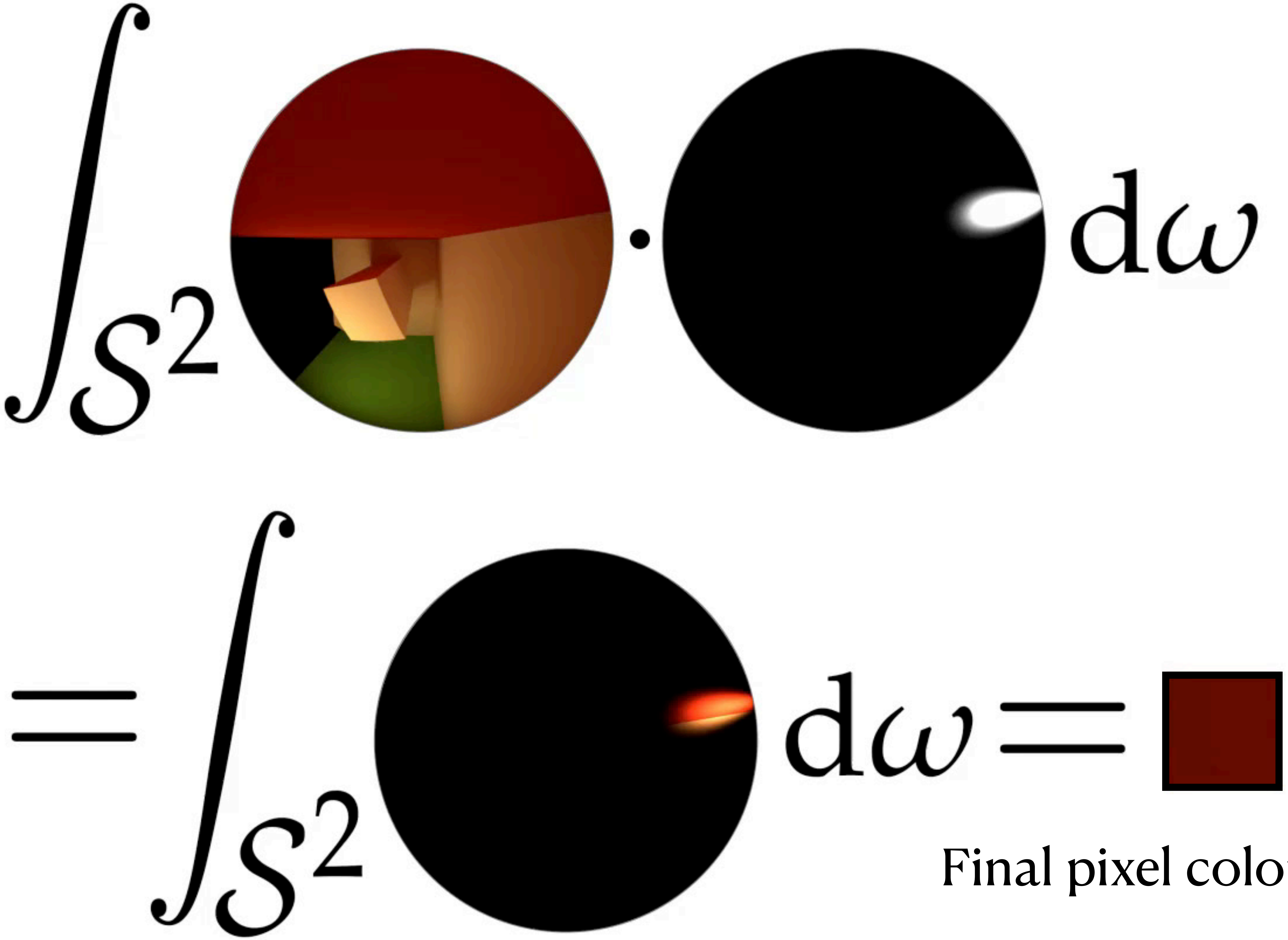
[Lake Geneva from Chillon Castle, Wikimedia commons]



MidJourney: all other images. (Too many prompts to list)

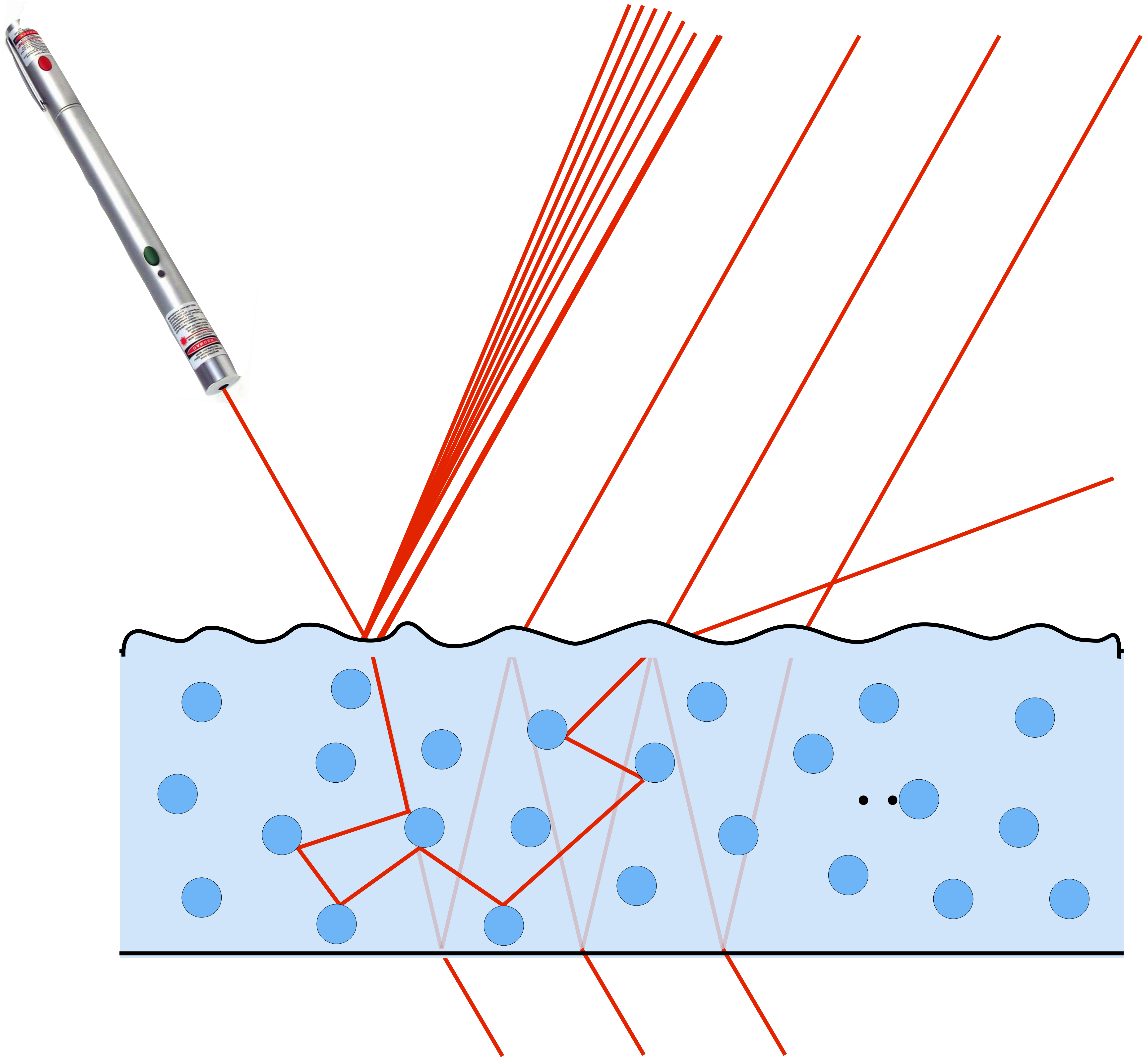
Computing integrals to create images





Final pixel color

Various types of materials and the effects they produce



[*Rendered* image made using Mitsuba Renderer]

Dawn of the Planet of the Apes , © 2013 Twentieth Century Fox Film Corporation. All Rights Reserved.
Image provided by Weta Digital.

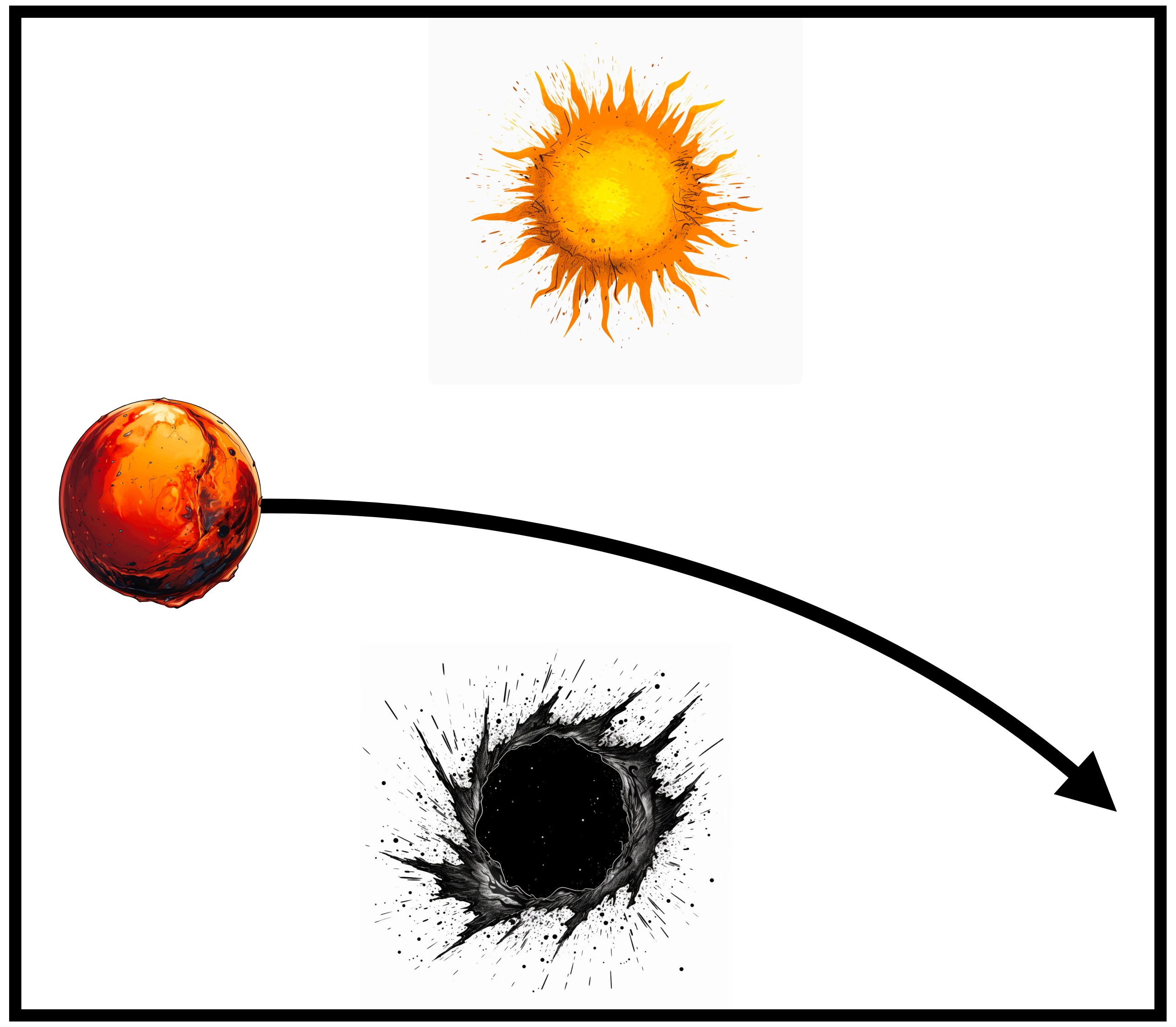
Today's topics

- **Why is integration harder than differentiation?**

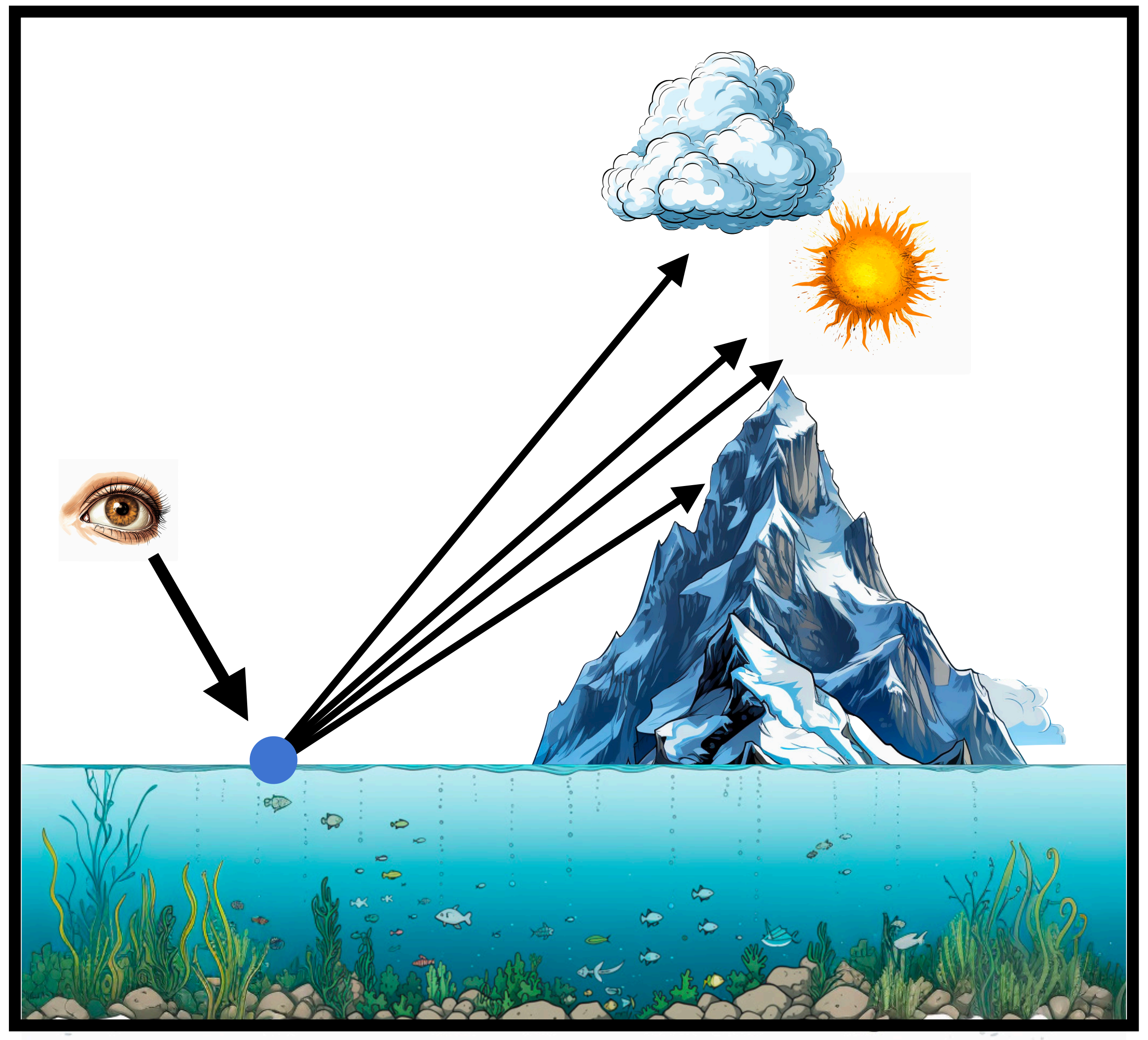
- Approach 1: Quadrature
  - Riemann integration
  - Rules: midpoint, trapezoid, Simpson.
  - The curse of dimensionality

- Approach 2: Monte Carlo
  - History
  - Computing integrals using random numbers
  - Importance sampling

Low dimensional integration



High dimensional integration



Integration, MATH-101 style

1. Find **antiderivative** using "rules of the game"

$$F(x) := \int f(x)\mathrm{d}x$$

(*indefinite* integral)

2. Apply fundamental theorem of calculus

$$\int_a^b f(x)\mathrm{d}x = F(b) - F(a)$$

(*definite* integral)

The rules of the game, aka. calculus

Rules for specific functions:

$$\int x^a \, dx = \frac{x^{a+1}}{a+1} + C \qquad \text{(for } a \neq -1\text{)}$$

$$\int \frac{1}{x} \, dx = \ln |x| + C \qquad \int e^{ax} \, dx = \frac{1}{a} e^{ax} + C$$

$$\int \sin x \, dx = -\cos x + C$$

Meta-rules: integration by parts:

$$\int_a^b u(x)v'(x) \, dx = [u(x)v(x)]_a^b - \int_a^b u'(x)v(x) dx$$

$$= u(b)v(b) - u(a)v(a) - \int_a^b u'(x)v(x) \, dx$$

Integration versus differentiation

Differentiation

Analytic & numerical approaches **OK** 😊

$$\int f(x)\,\mathrm{d}x$$

$$f(x)$$

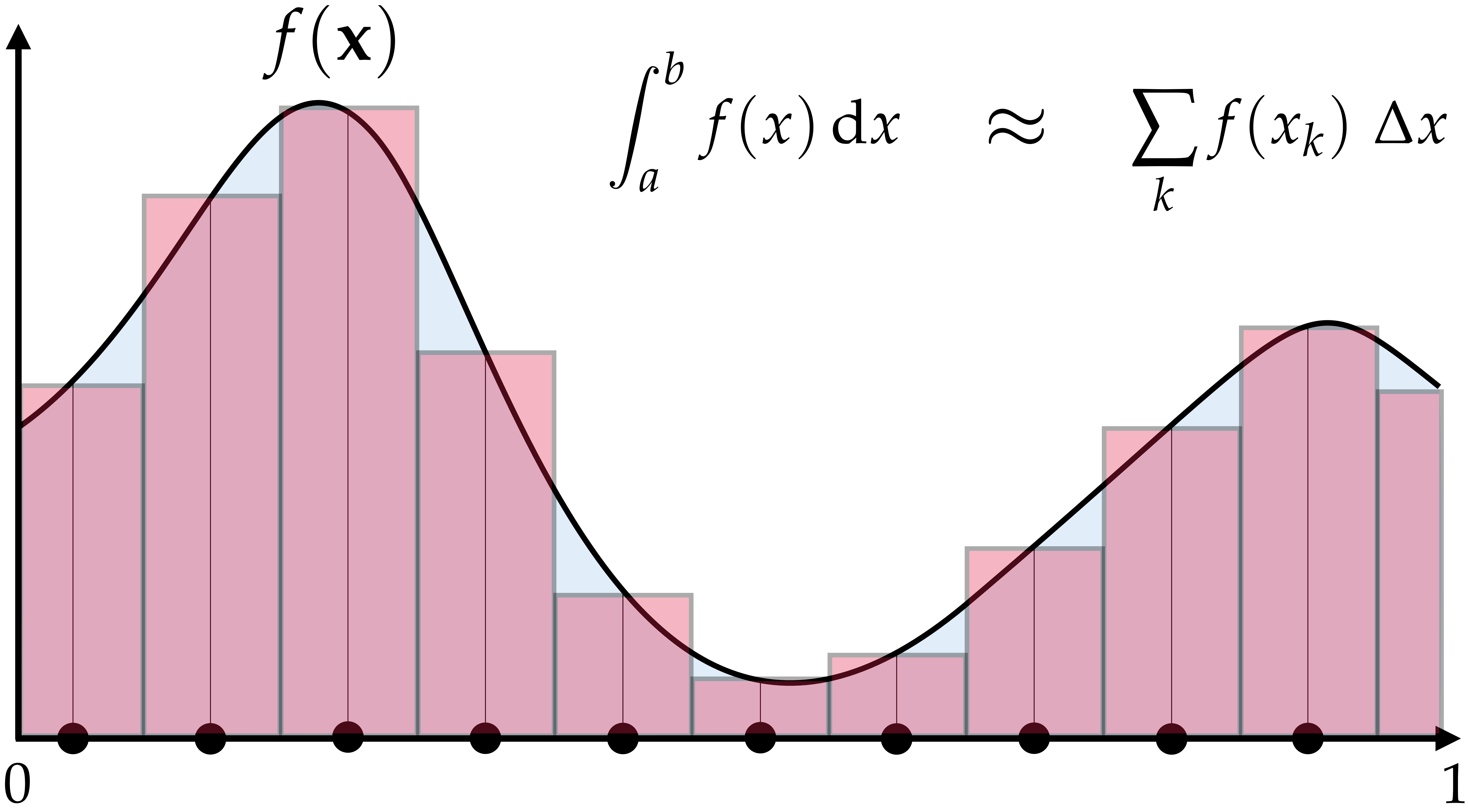
$$f'(x)$$

Integration

Analytic approaches **almost always fail** 😳

Numerical approaches **OK** 😊

Approximating integrals using Riemann sums



$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_k f(x_k)\,\Delta x$$

Quadrature

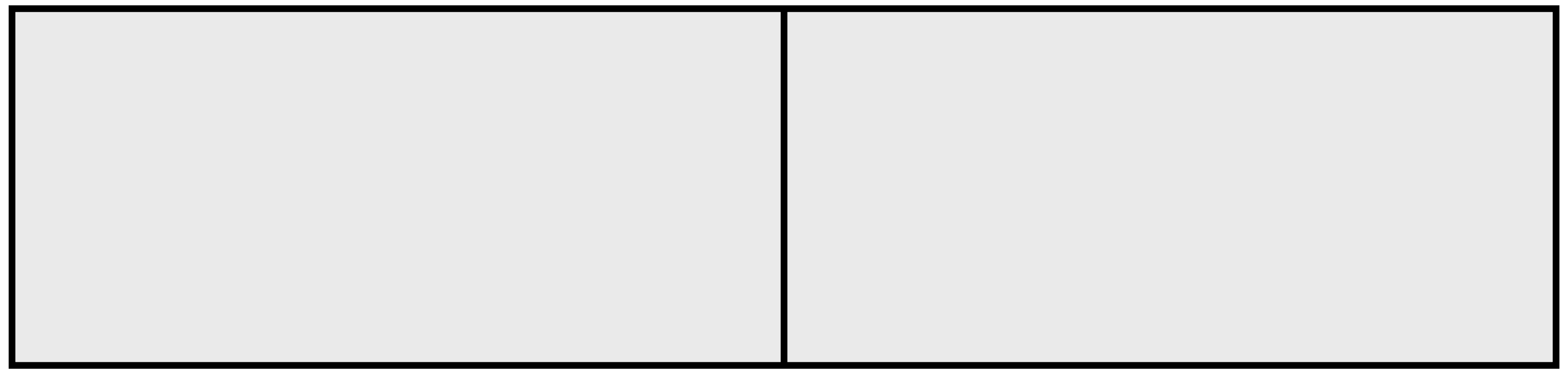
- **High level idea**:
  - Build an approximation of the original function *(Riemann sum: piecewise constant)*
  - Must be possible to create/fit this approximation from a function evaluations
  - Approximation must have an *analytic integral*.
  - Use integral of the approximation as approximation of the *original* analytic integral.

- **Two flavors**:
  - **Quadrature rule**: applies to small part of the function
  - **Composite quadrature**: repeatedly applies the rule to integrate the *entire* function.

Midpoint rule

$$\int_a^b f(x)\,dx \approx (b-a)f\left(\frac{a+b}{2}\right)$$

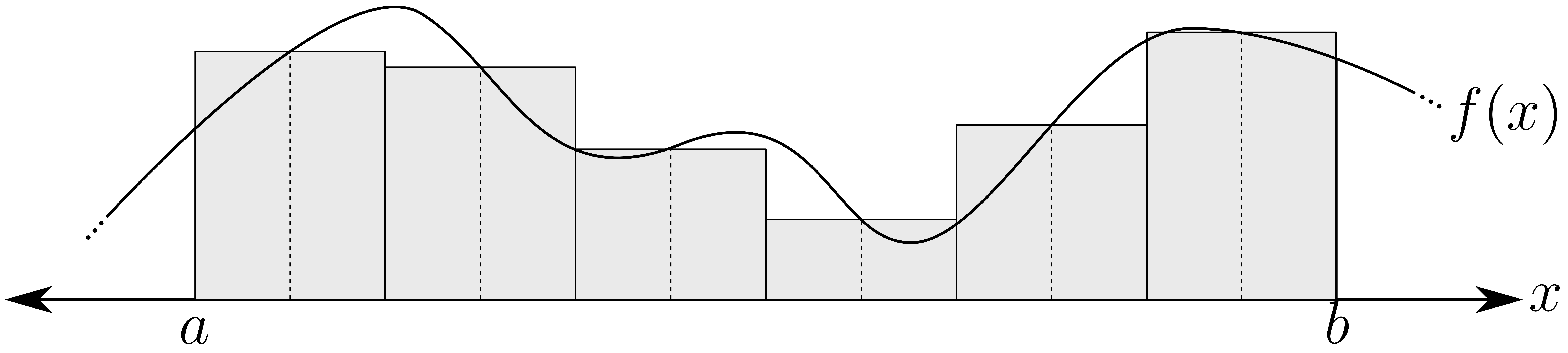
$$f\left(\frac{a+b}{2}\right)$$



[Figure by Justin Solomon]

Composite midpoint rule

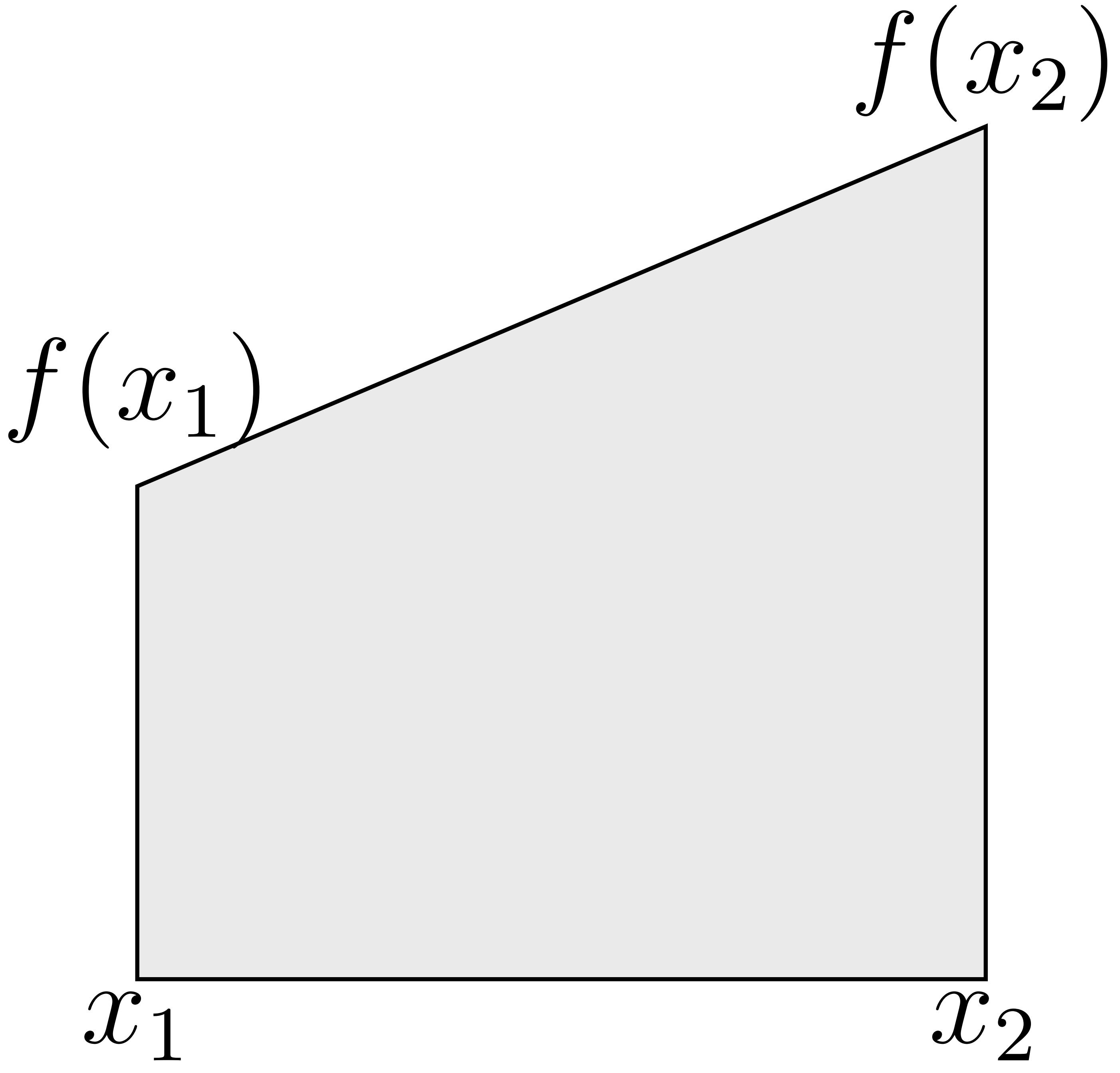
$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{k} f\left(\frac{x_{i+1}+x_i}{2}\right)\Delta x$$



[Figure by Justin Solomon]

Trapezoid rule

$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

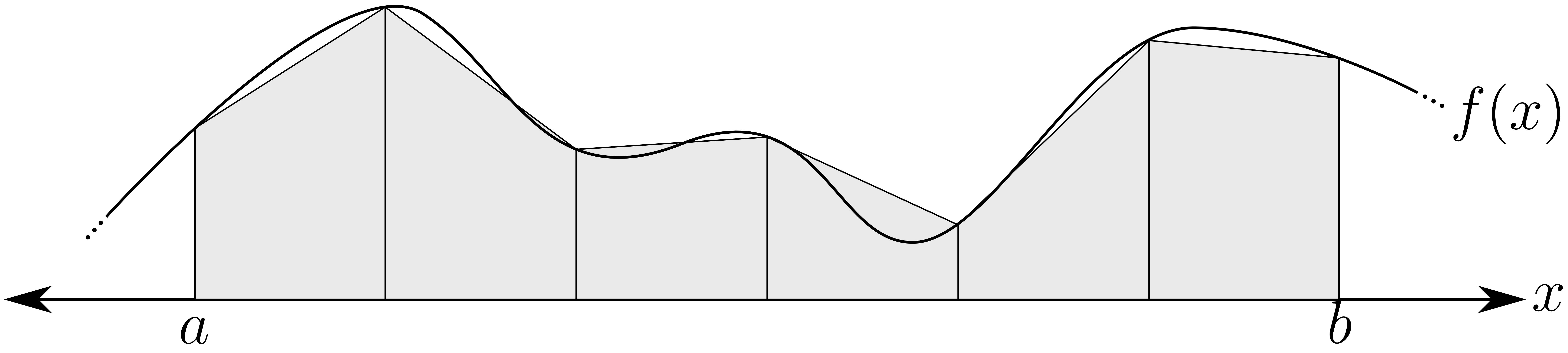


[Figure by Justin Solomon]

Composite trapezoid rule

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{k} \left(\frac{f(x_i) + f(x_{i+1})}{2} \right) \Delta x$$

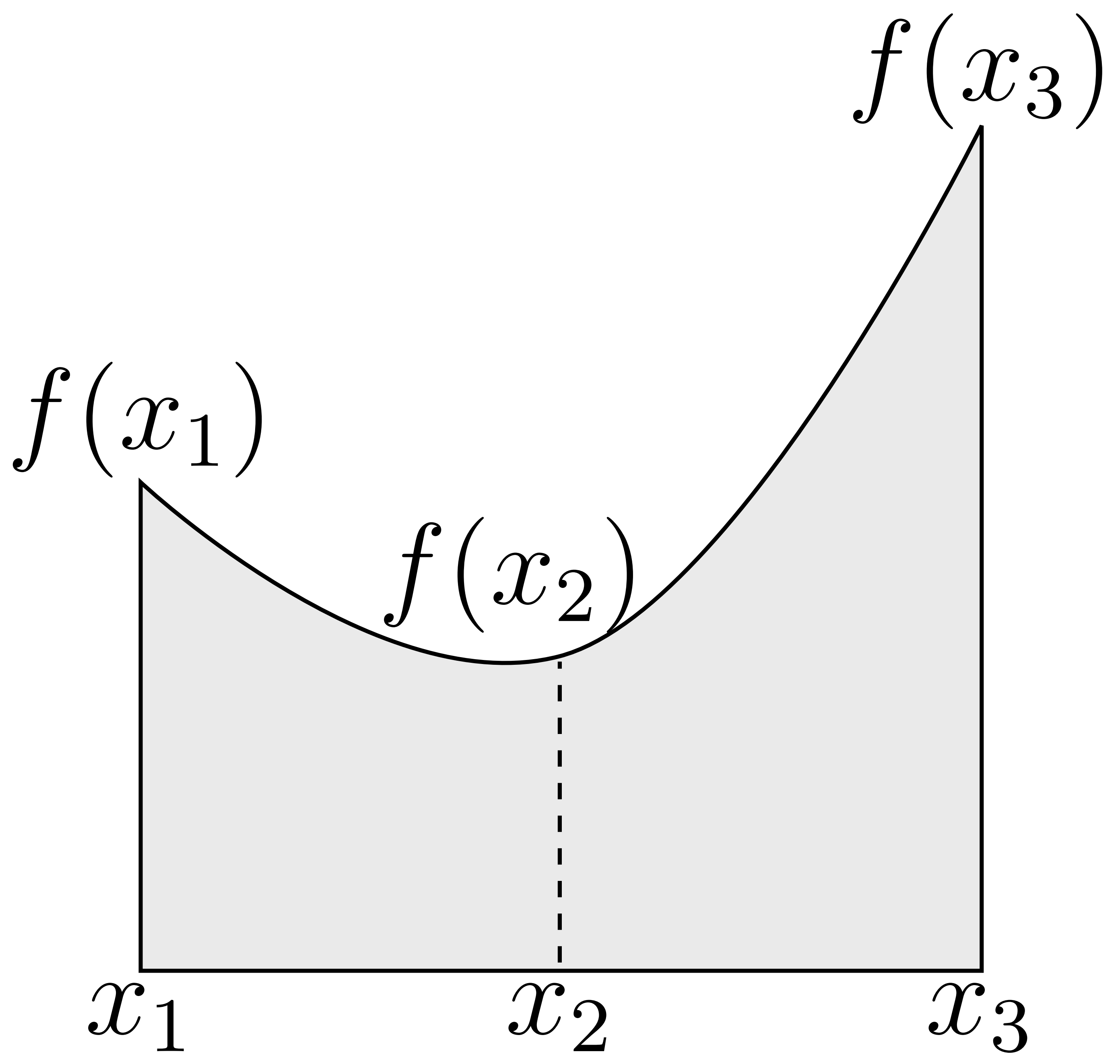
$$= \Delta x \left(\frac{1}{2} f(a) + f(x_1) + \cdots + f(x_{k-1}) + \frac{1}{2} f(b) \right)$$



[Figure by Justin Solomon]

Simpson's rule

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$



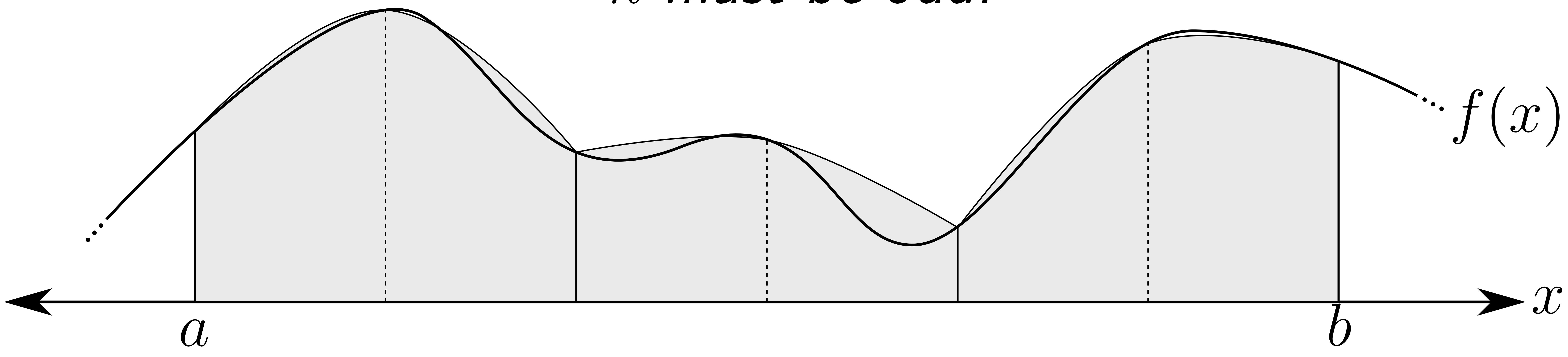
[Figure by Justin Solomon]

Composite Simpson's rule

$$\int_a^b f(x)\,dx \approx \frac{\Delta x}{3}\left[f(a) + 2\sum_{i=1}^{n-2-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(b)\right]$$

$$= \frac{\Delta x}{3}\left[f(a) + 4f(x_1) + 2f(x_2) + \cdots + 4f(x_{n-1}) + f(b)\right]$$

n *must be odd!*

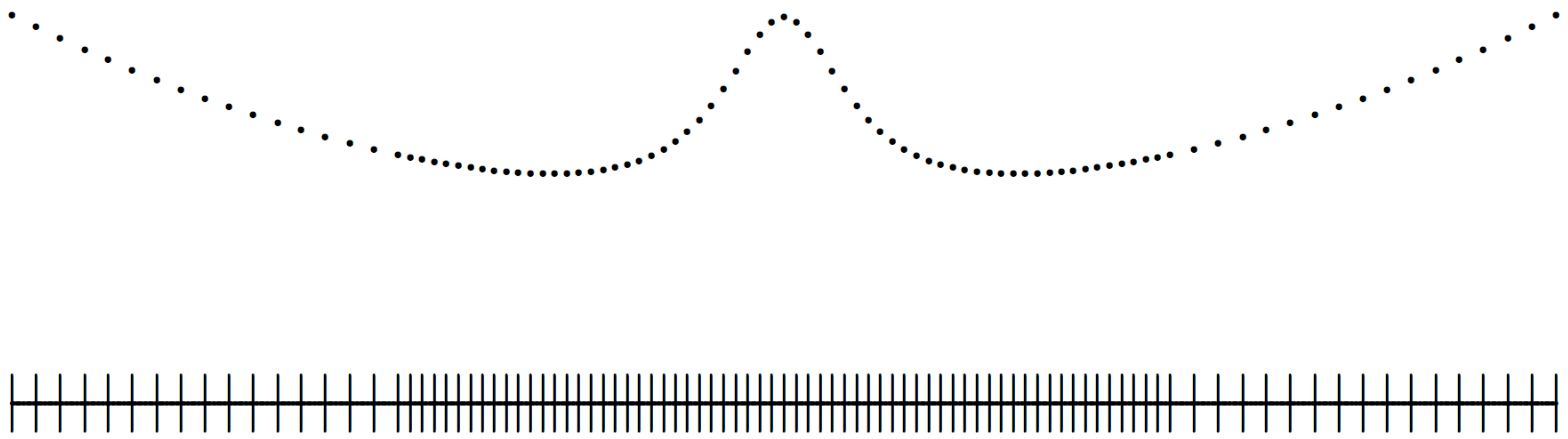


[Figure by Justin Solomon]

Demo time

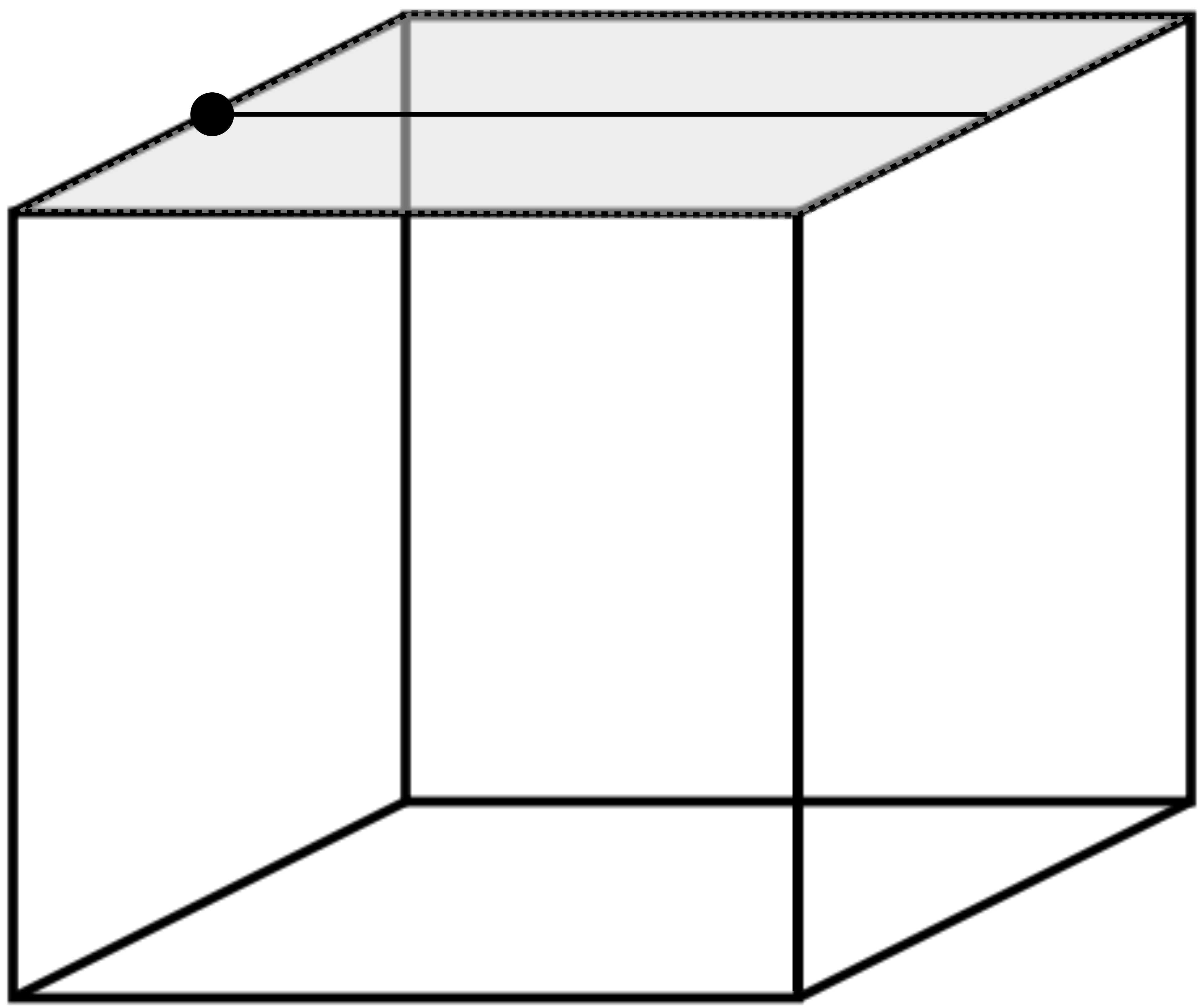
Adaptive quadrature

```
# High-level idea
def integrate(f, a, b):
    i_t = trapezoid(f, a, b)
    i_s = simpson(f, a, b)

    if abs(i_s - i_t) > ε * abs(i_t):
        mid = (a + b) / 2
        return integrate(f, a, mid) + integrate(f, mid, b)
    else:
        return i_s
```



[Heath]

Higher-dimensional quadrature

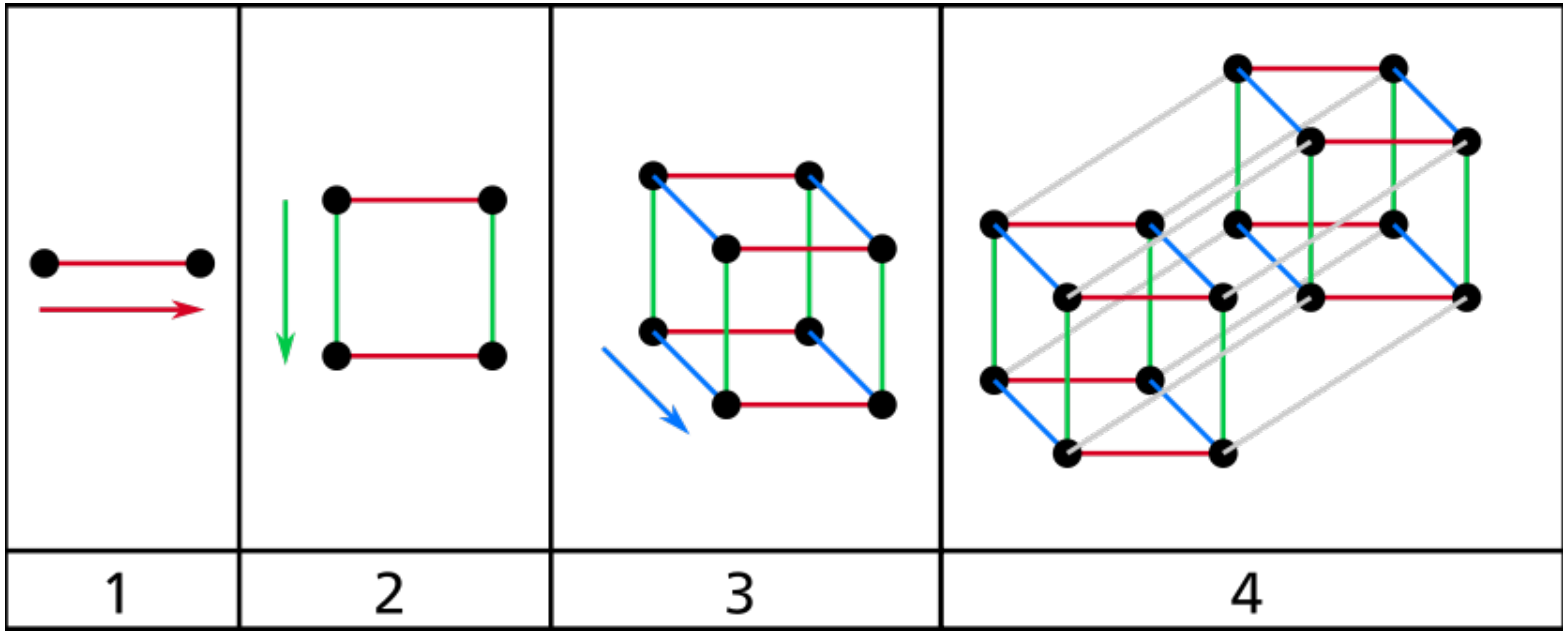


Fubini's theorem:

$$\int_{X\times Y\times Z} f(x,y,z)\,\mathrm{d}(x,y,z) = \int_Z \left(\int_Y \left(\int_X f(x,y,z)\,\mathrm{d}x\right)\,\mathrm{d}y\right)\,\mathrm{d}z = \ldots$$

The curse of dimensionality

Sampling a function on a regular grid becomes completely impractical in higher dimensions.



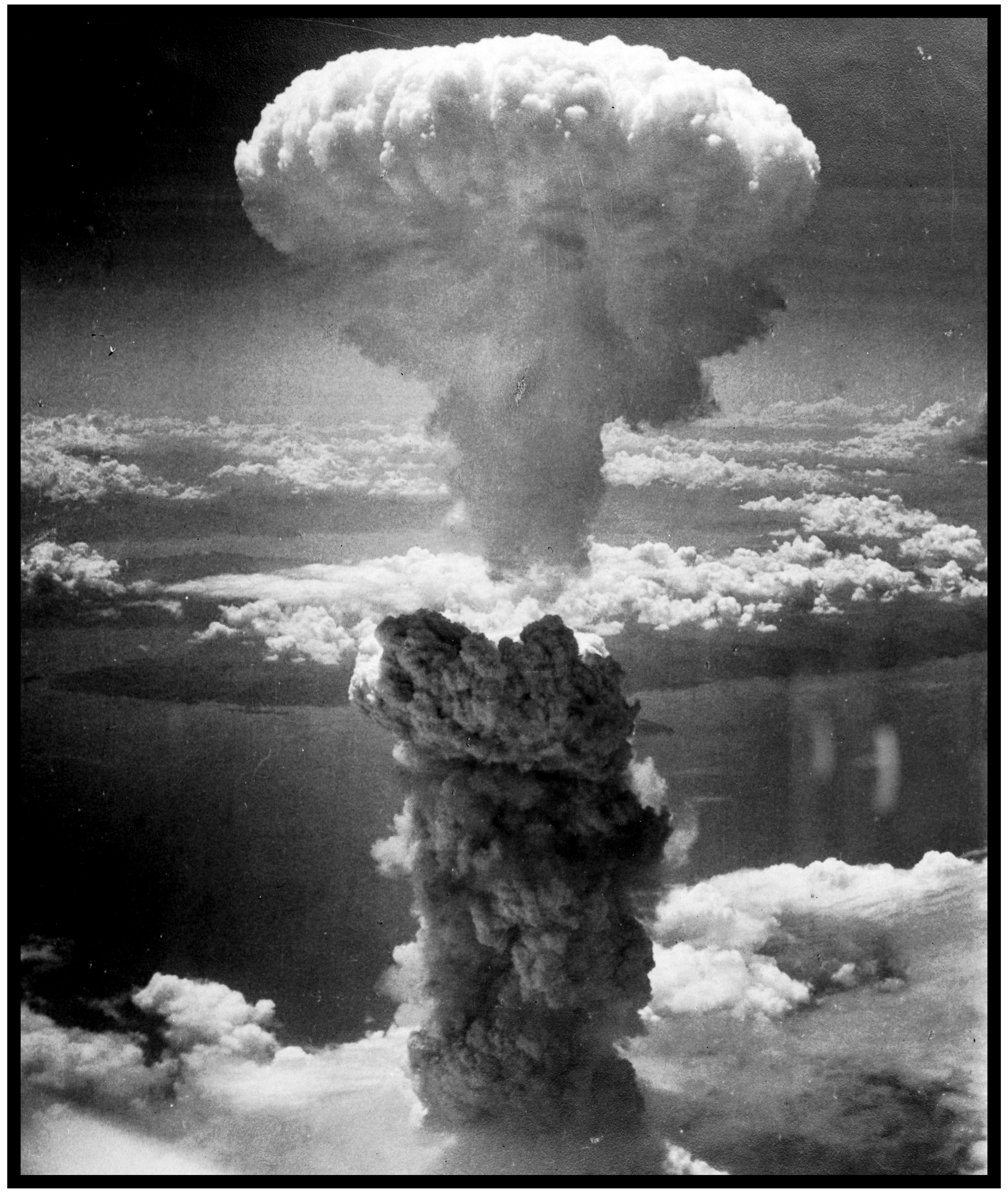
A 100-dimensional cube has
1267650600228229401496703205376 corners

(!!!!)

Monte Carlo Integration

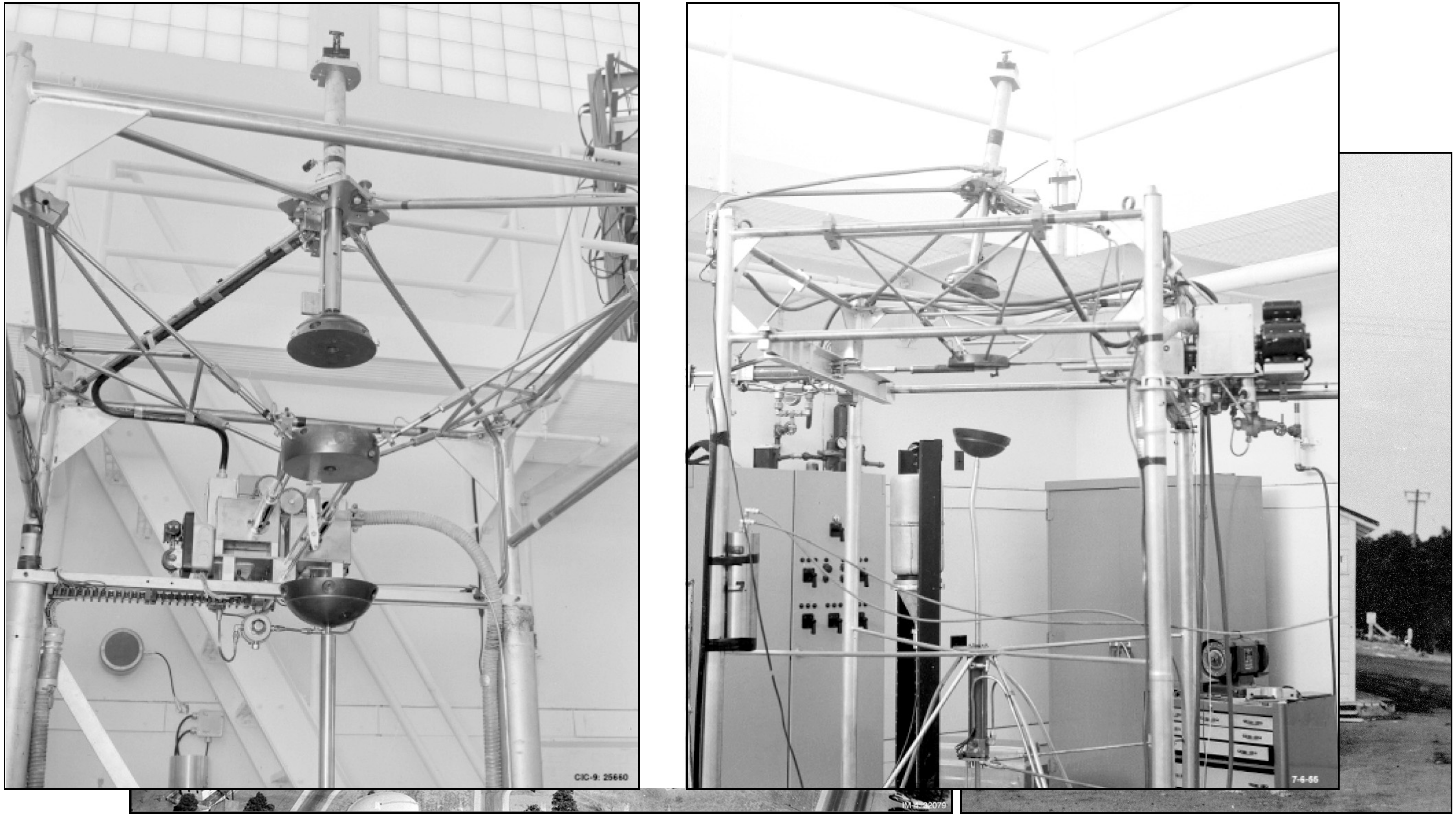
History of the Monte Carlo method

- Developed in the 1940s in the context of the development of the atomic bomb
- General & very easy to implement.
- Uses randomness to simulate many possible realizations of a complex process
- Very slow convergence

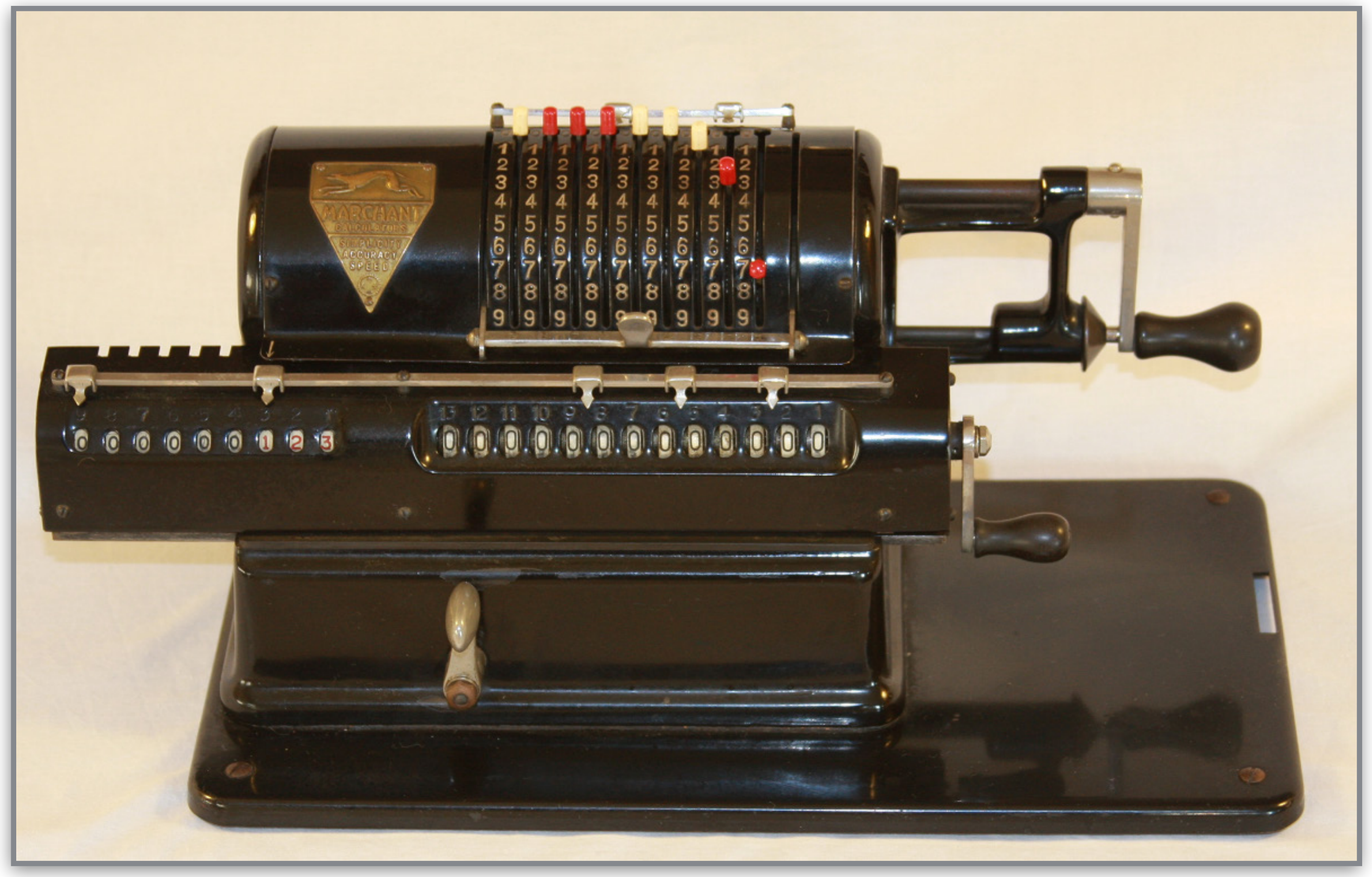


The Manhattan Project

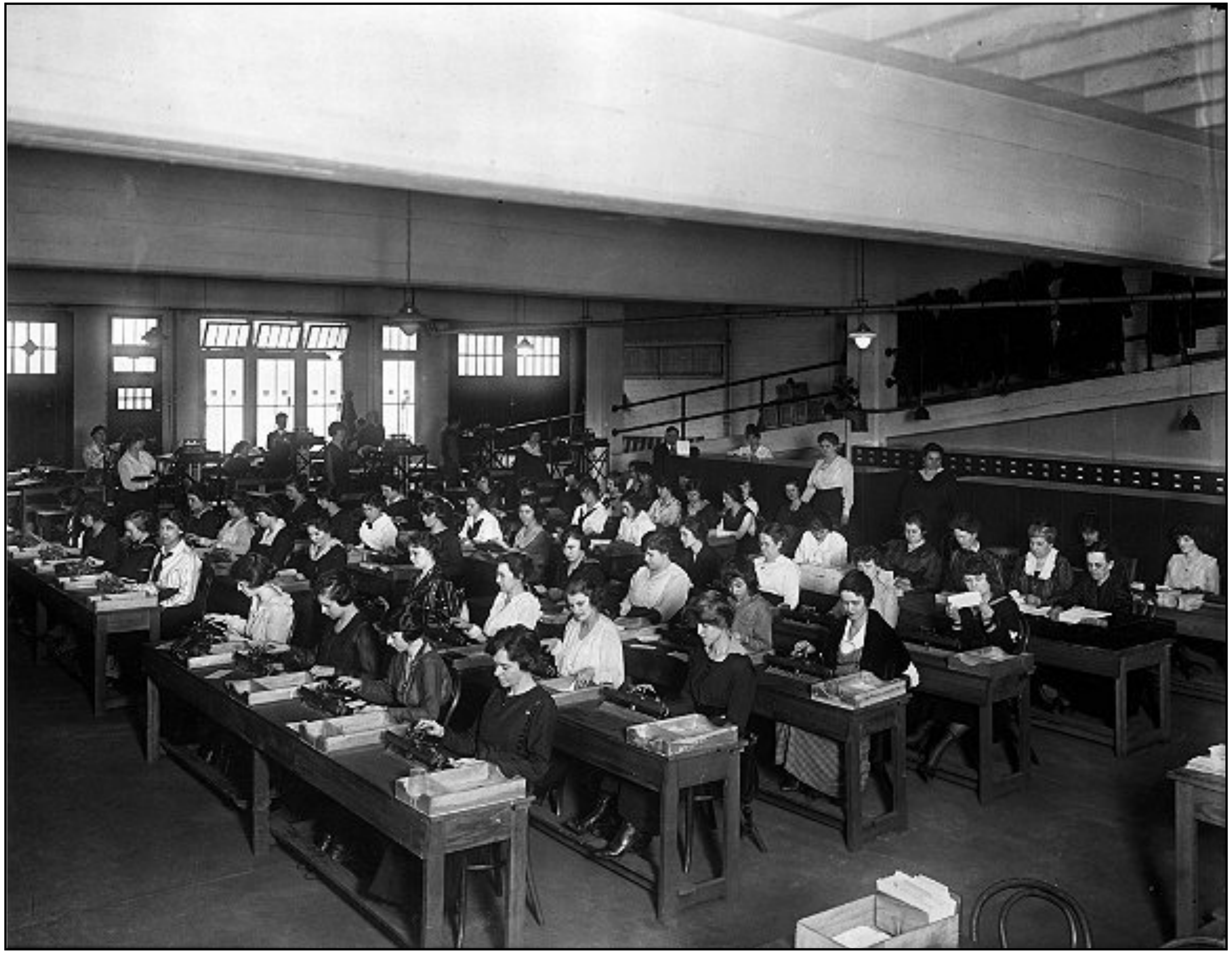
[Godiva device, Wikipedia commons]



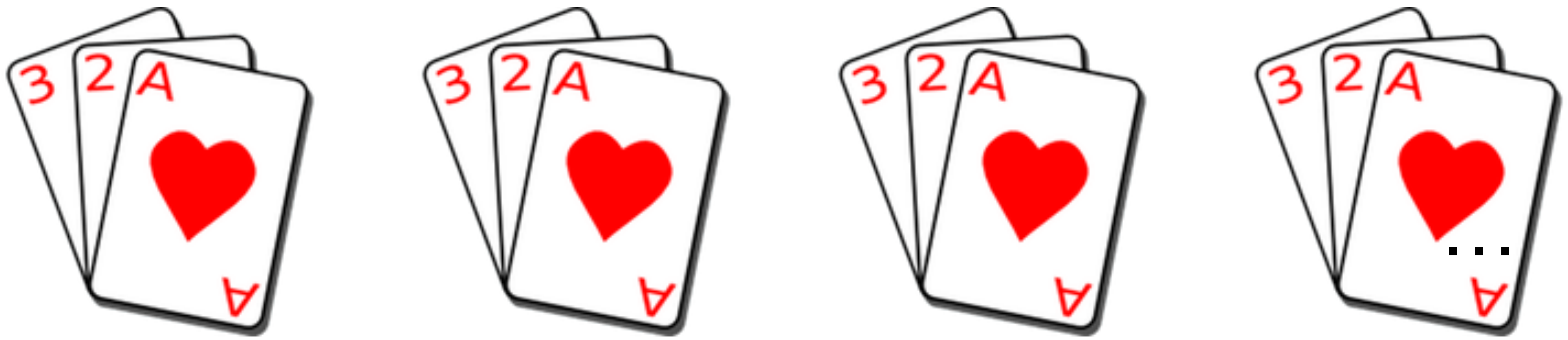
Human computers



Marchant desk calculator



Stanisław Ulam's hospital stay



Lose Win Win Lose

Stanisław Ulam

What's the chance of winning with a properly shuffled deck?

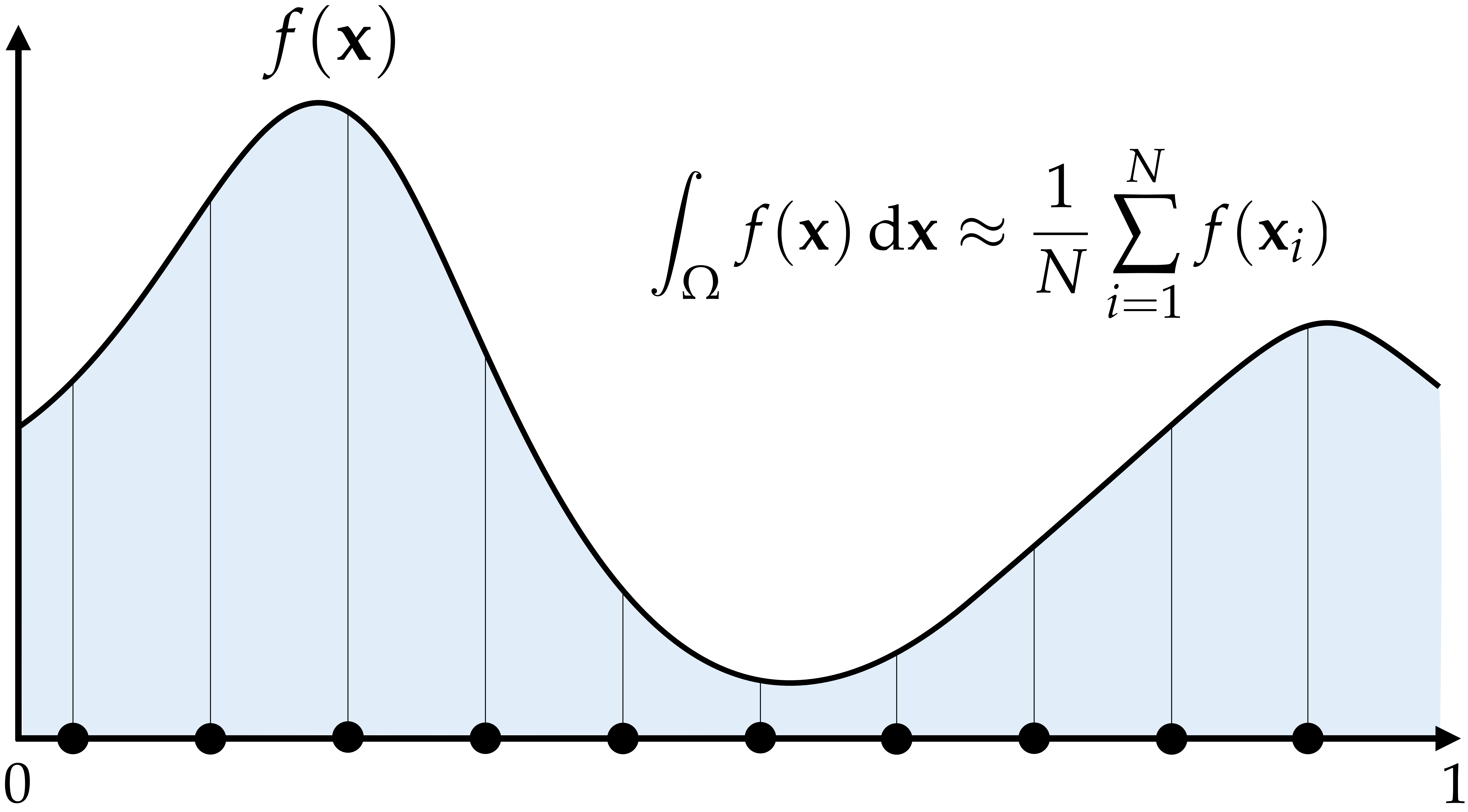
$$P = \lim_{n\to\infty} P_n \quad \text{where} \quad P_n = \frac{1}{n}\sum_{i=1}^{n}\begin{cases}1, & \text{game } i \text{ is won,}\\ 0, & \text{game } i \text{ is lost}\end{cases}$$

Recap: Birthday Paradox

You have **already used** a Monte Carlo method in CS328!

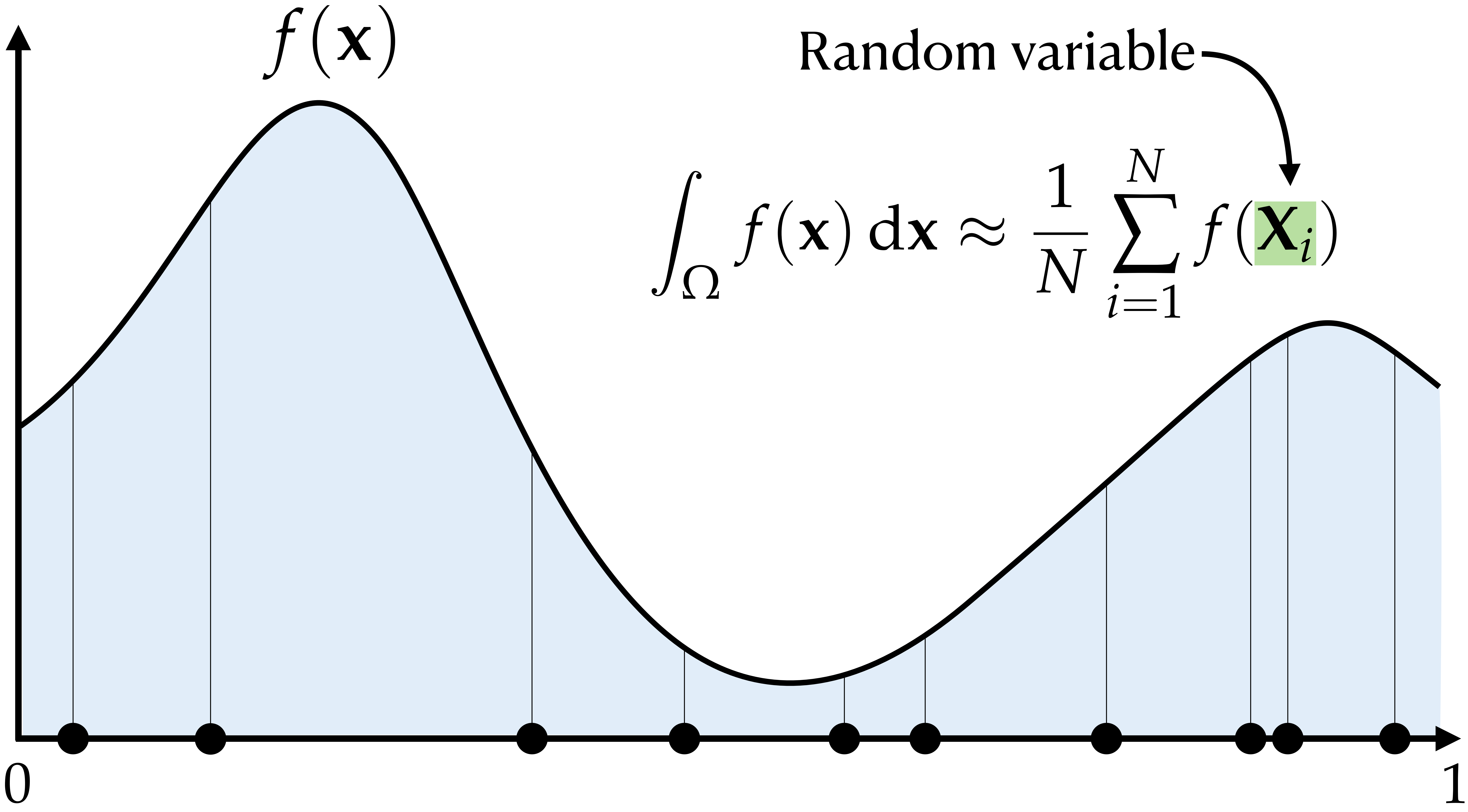
```
In [7]: # For n people, compute an approximation of the probability that two people share the same birthday, using K iterations
        def birtyday_paradox(n, K):
            s = 0 # Keep track of how often the statement is true

            # Perform K iterations of the same experiment.
            for it in range(K):
                dates = [rnd.randint(0, 365) for i in range(n)]
                if len([x for x in dates if dates.count(x) > 1]) > 0:
                    s += 1

            # Return average probability
            return s / K
```

Recap: Riemann sums & quadrature



$$\int_\Omega f(\mathbf{x})\,\mathrm{d}\mathbf{x} \approx \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i)$$

Monte Carlo integration



Does Monte Carlo integration work?

$$\cancel{\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{X}_i)} \overset{?}{\approx} \int_\Omega f(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$E\left[\frac{1}{N}\sum_{i=1}^{N} f(\mathbf{X}_i)\right] = \frac{1}{N}\sum_{i=1}^{N} E\left[f(\mathbf{X}_i)\right]$$

Linearity of the expected value

$$= \frac{1}{N}\sum_{i=1}^{N}\int_\Omega f(\mathbf{x})\,p_{\mathbf{X}_i}(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

Expectation over the continuous set Ω of possible outcomes

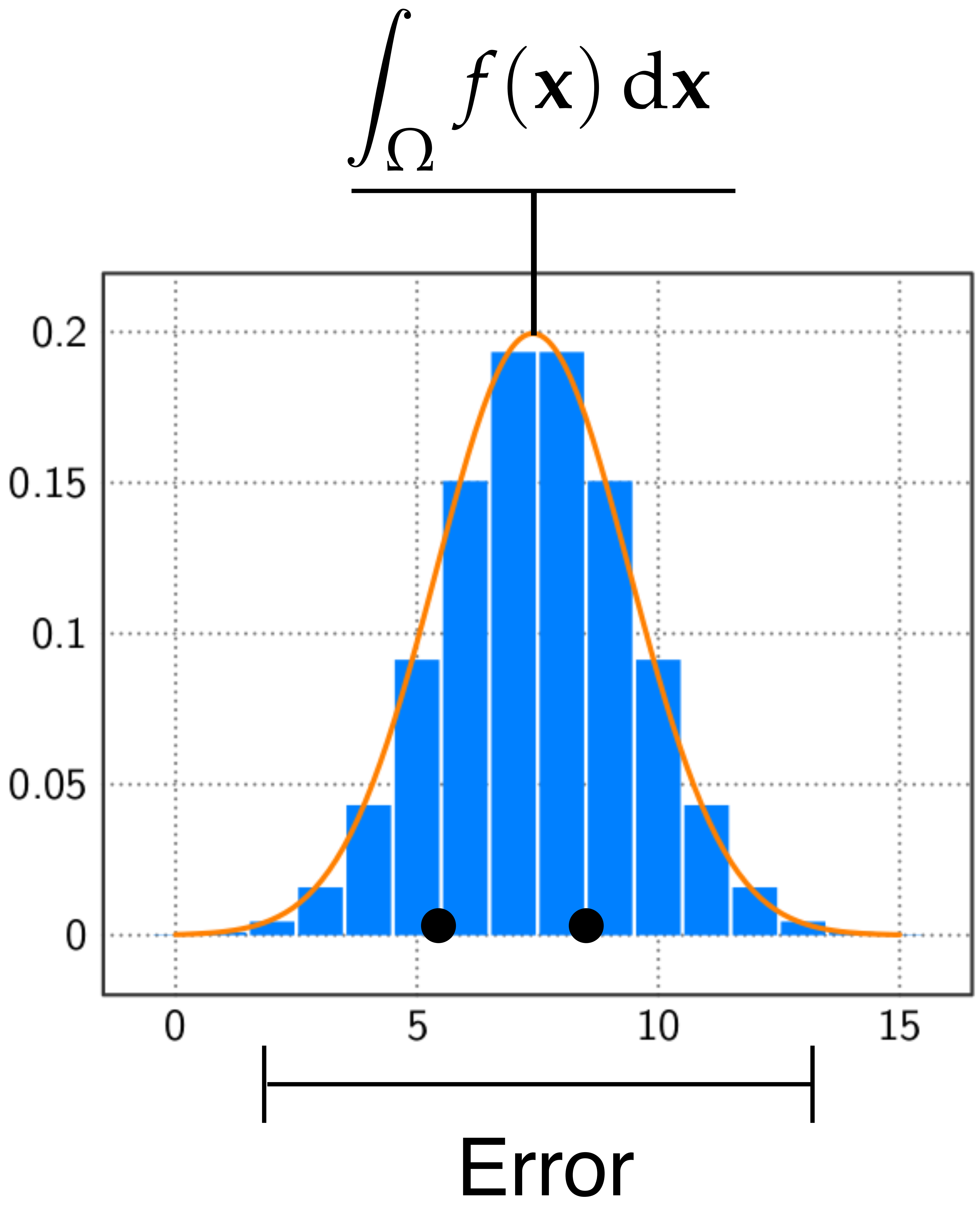
(Suppose that $p_{\mathbf{X}_i} = 1$ and volume of $\Omega = 1$)

$$= \int_\Omega f(\mathbf{x})\mathrm{d}\mathbf{x}$$

Uniform distribution

Characteristics

- Result obtained by averaging many samples
- **Central limit theorem** says: the result will tend to a normal distribution.
- Previous slide showed that the distribution is centered around the correct answer.
- **But**: algorithm will give a random answer, so there is always some error. This can be characterized using the variance.



How well does it work?

Remarkable about this:

<u>Dimension doesn't influence the convergence rate!</u>

A word of caution

> *Monte Carlo is an extremely bad method. It should be used only when all alternative methods are worse.*

- Alan Sokal

Rough guideline:

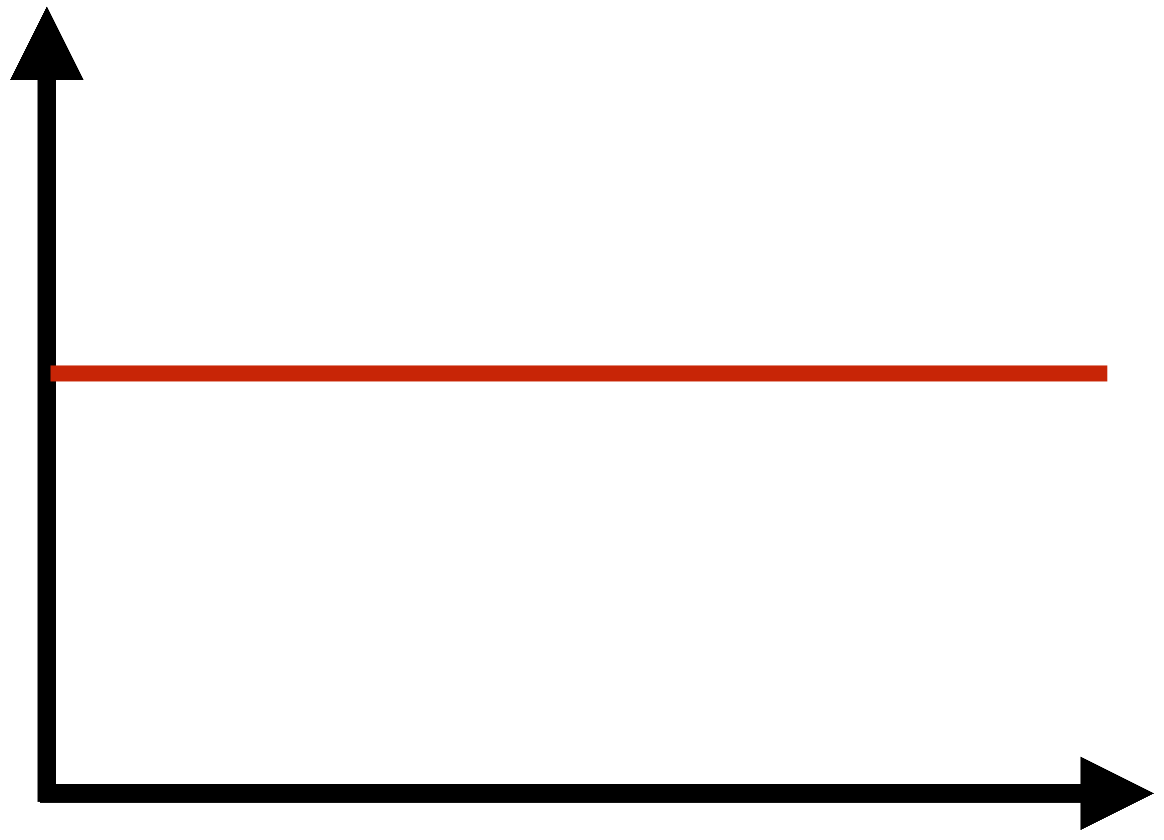
1-3 dimensions: quadrature & adaptive quadrature
4 dimensions+: Monte Carlo integration

Demo time

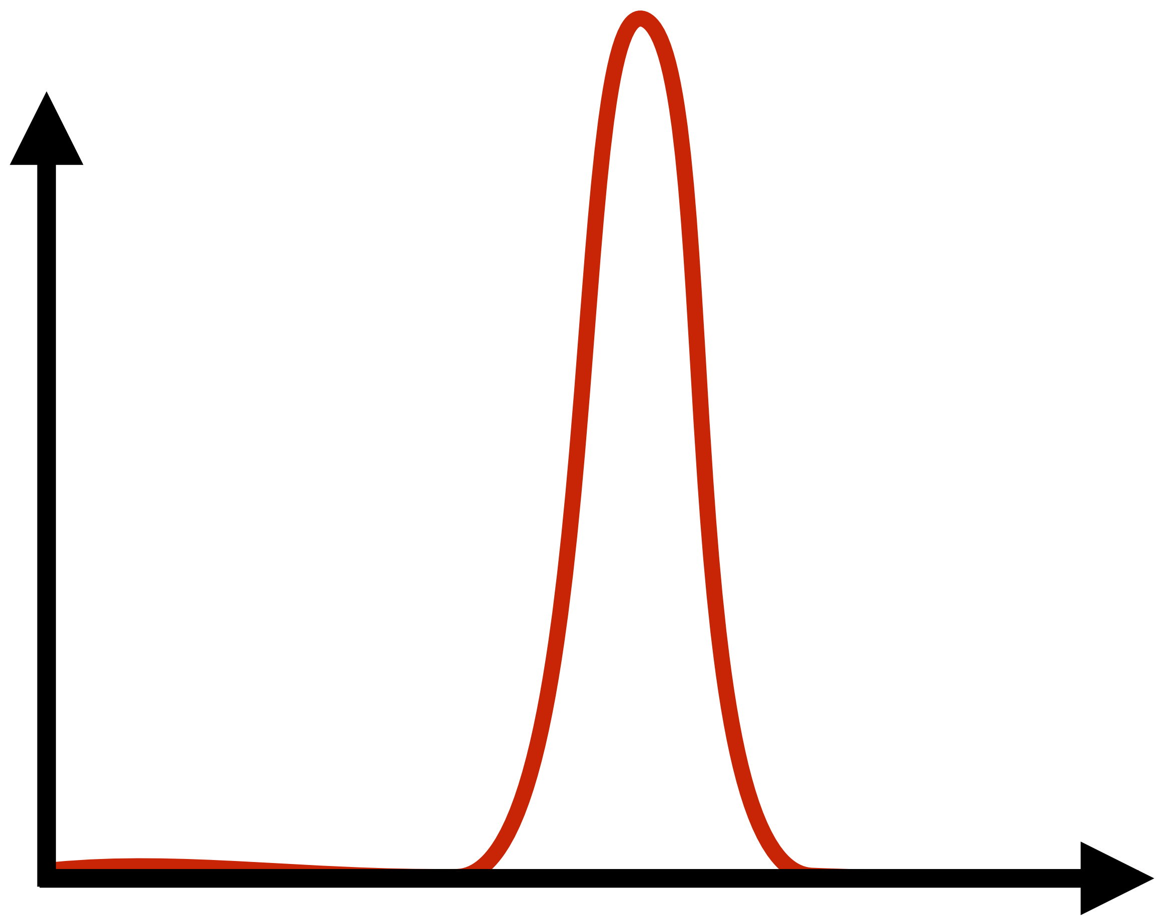
How much error do we expect?

$$\text{Error} \approx \sqrt{\frac{1}{N}\text{Var}[f(\mathbf{X}_i)]}$$

How big is $\text{Var}[f(\mathbf{X}_i)]$?

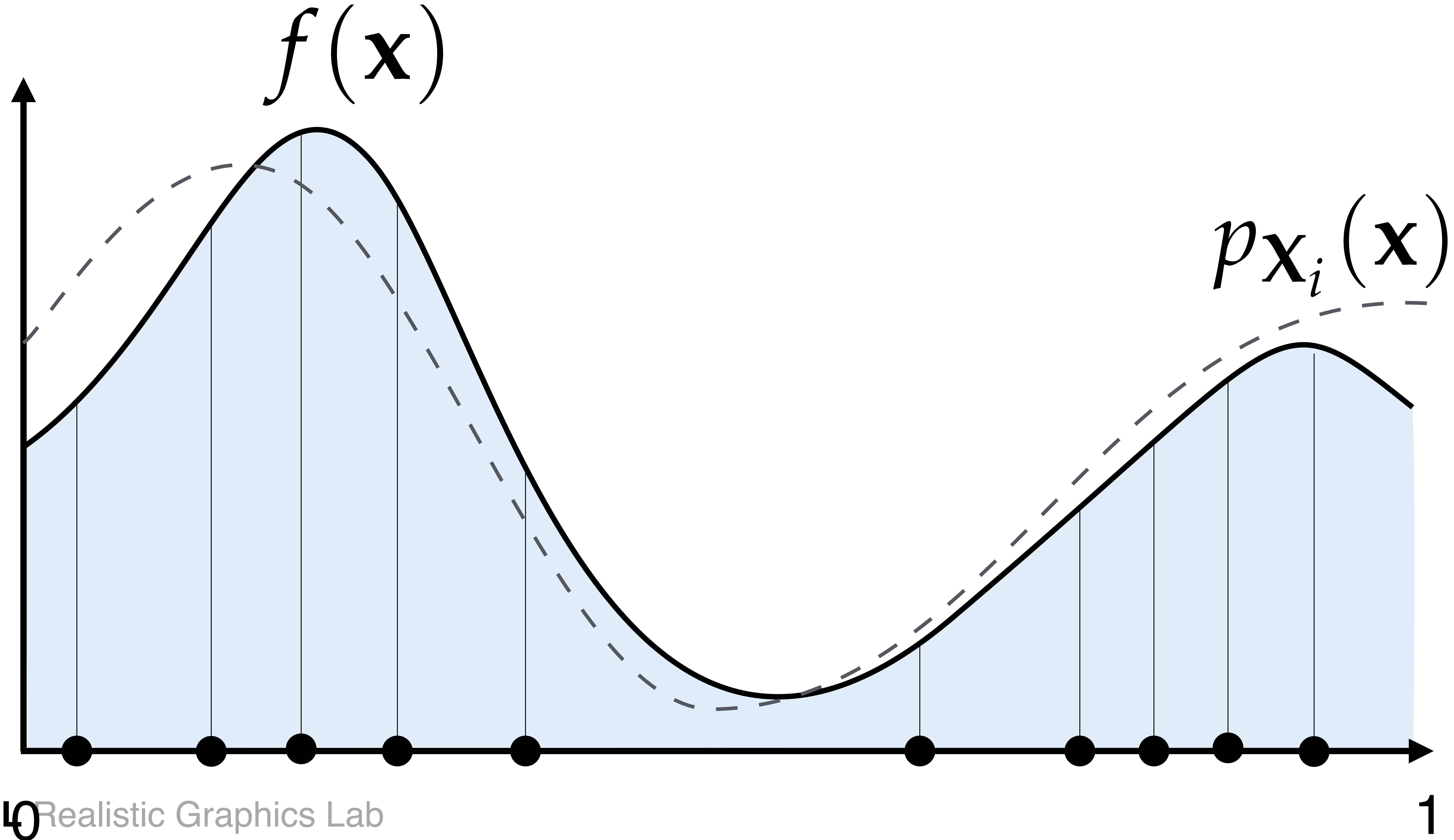


Example 1



Example 2

Importance sampling



Derivation

$$E\left[\frac{1}{N}\sum_{i=1}^{N}\frac{f(\mathbf{X}_i)}{p_{\mathbf{X}}(\mathbf{X}_i)}\right] = \frac{1}{N}\sum_{i=1}^{N}E\left[\frac{f(\mathbf{X}_i)}{p_{\mathbf{X}}(\mathbf{X}_i)}\right]$$

Linearity of the expected value

$$= \frac{1}{N}\sum_{i=1}^{N}\int_{\Omega}\frac{f(\mathbf{x})p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}(\mathbf{x})}\,\mathrm{d}\mathbf{x}$$

Expectation over the continuous set Ω of possible outcomes

~~(Suppose that $p_{\mathbf{X}} \equiv 1$ and Volume of $\Omega \equiv 1$)~~

~~$= \int_{\Omega} f(\mathbf{x})\mathrm{d}\mathbf{x}$~~

~~Uniform distribution~~

$$= \int_{\Omega}\frac{f(\mathbf{x})p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}(\mathbf{x})}\,\mathrm{d}\mathbf{x} \neq \int_{\Omega} f(\mathbf{x})\mathrm{d}\mathbf{x}$$

Importance sampling

$$E\left[\frac{1}{N}\sum_{i=1}^{N}\frac{f(\mathbf{X}_i)}{p_{\mathbf{X}}(\mathbf{X}_i)}\right] = \int_{\Omega} f(\mathbf{x})\mathrm{d}\mathbf{x}$$

This is known as **Importance Sampling**.

Requirement: $p_{\mathbf{X}}(\mathbf{x}) > 0$ for all $\mathbf{x}$ with $f(\mathbf{x}) \neq 0$.

How to find the sampling distribution?

- Picking a good sampling distribution p is a crucial step to effectively use Monte Carlo methods. Ideally as close as possible to f.
- The typical recipe is:
  - Start with *uniformly distributed* random numbers
  - Transform these random numbers by a sequence of mathematical operations, which changes their distribution.
  - Details depend on the application/integral.
- CS440, my master-level course about graphics will teach you all about this.

Monte Carlo methods in the film industry

Monte Carlo noise!!!

Next lecture:
Inverse Graphics

(last lecture of the semester)