Monte Carlo Algorithms

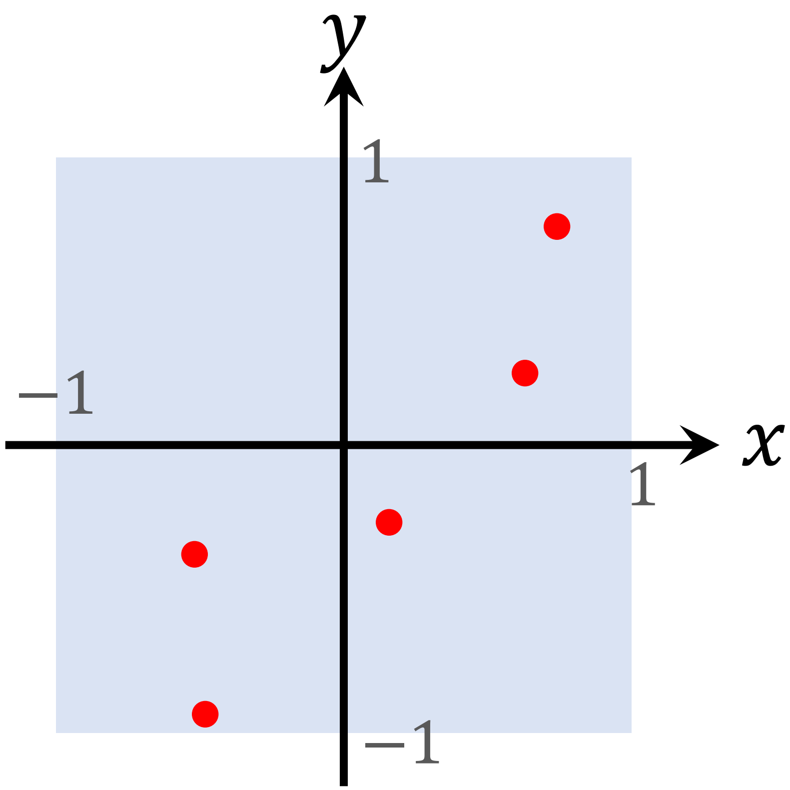
Shusen Wang

Application 1: Calculating Pi

Calculating Pi

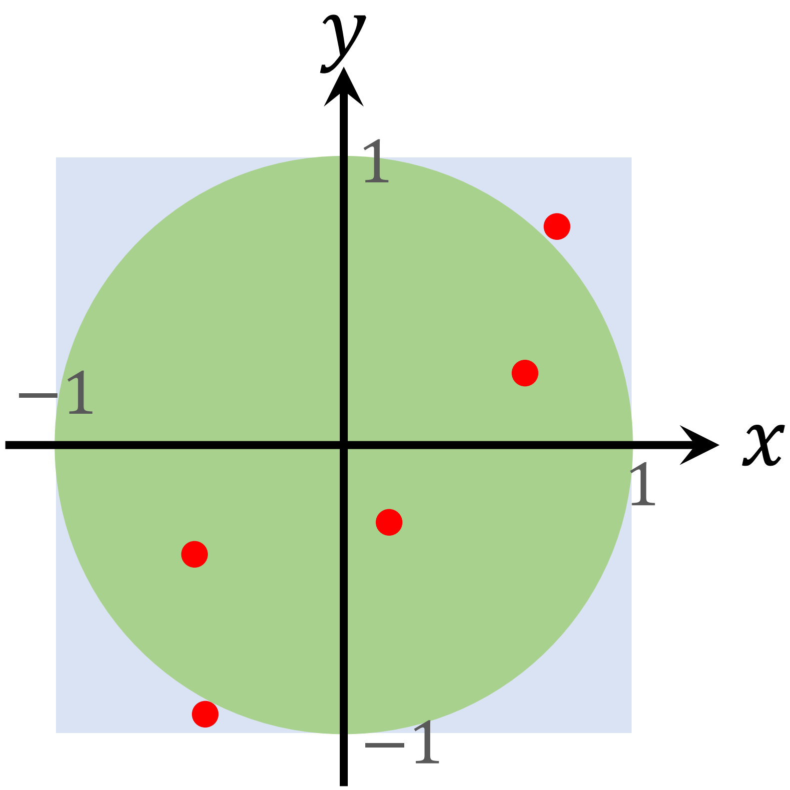
- We already know $\pi \approx 3.141592653589 \ldots$
- Pretend we do not know the value of π.
- Can we find it out (approximately) using a random number generator?

Calculating Pi



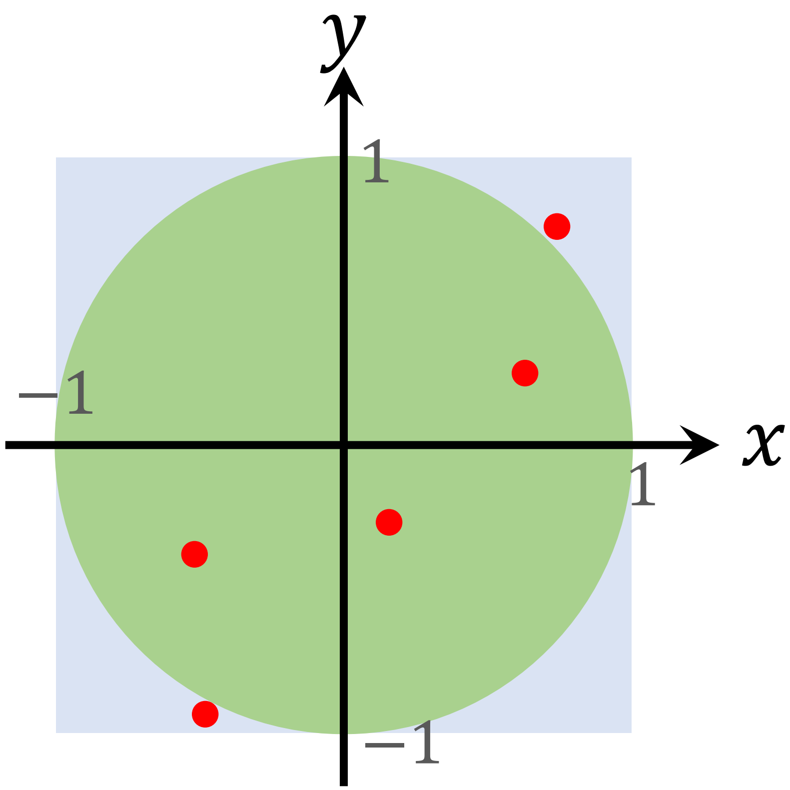
- Assume (x, y) is a point sampled from the square uniformly at random.

Calculating Pi



- Assume (x, y) is a point sampled from the square uniformly at random.
- What is the probability that (x, y) is in the circle?

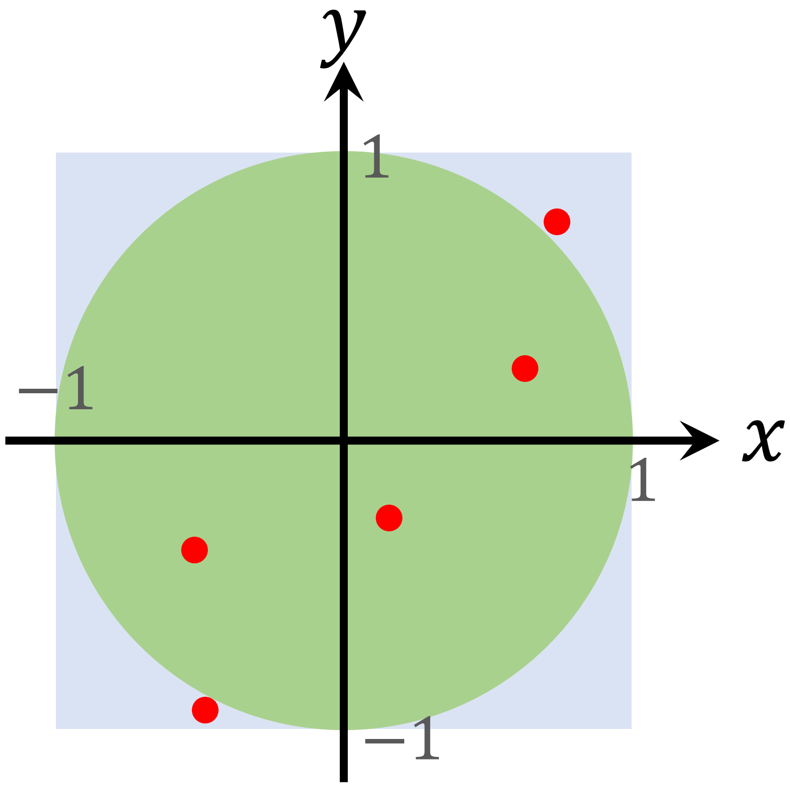
Calculating Pi



- Assume (x, y) is a point sampled from the square uniformly at random.
- What is the probability that (x, y) is in the circle?
- Area of the square is $A_1 = 2^2 = 4$.
- Area of the circle is $A_2 = \pi r^2 = \pi$.
- Probability: $P = \frac{A_2}{A_1} = \frac{\pi}{4}$.

Calculating Pi

- Suppose n points are uniformly sampled from $[-1,1]\times[-1,1]$.
- Then, in expectation, $Pn = \frac{\pi n}{4}$ points are in the circle.



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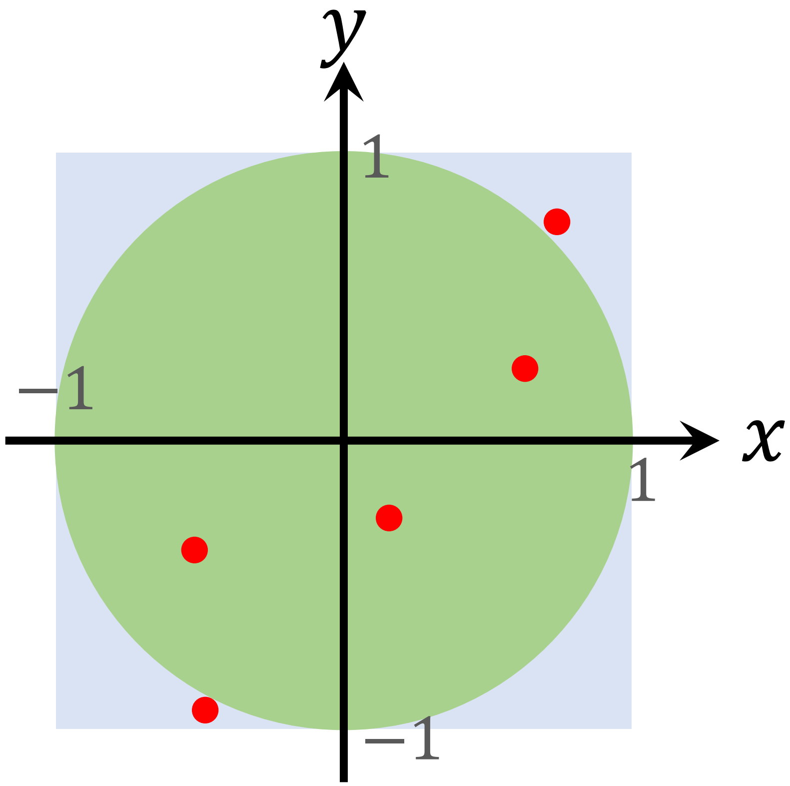

- Given a point (x, y), how do you know whether (x, y) is in the circle?
- If $x^2 + y^2 \leq 1$, then it is in the circle.

Calculating Pi

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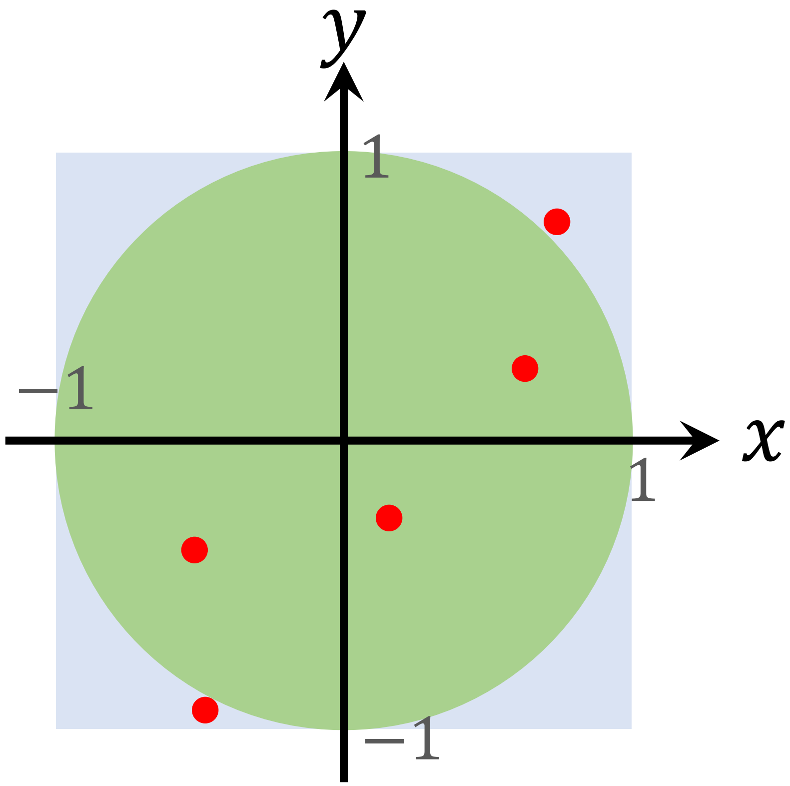

- We found m points in the circle.
- If n is big, then $m \approx \frac{\pi n}{4}$.
- Thus, $\pi \approx \frac{4m}{n}$.

Calculating Pi

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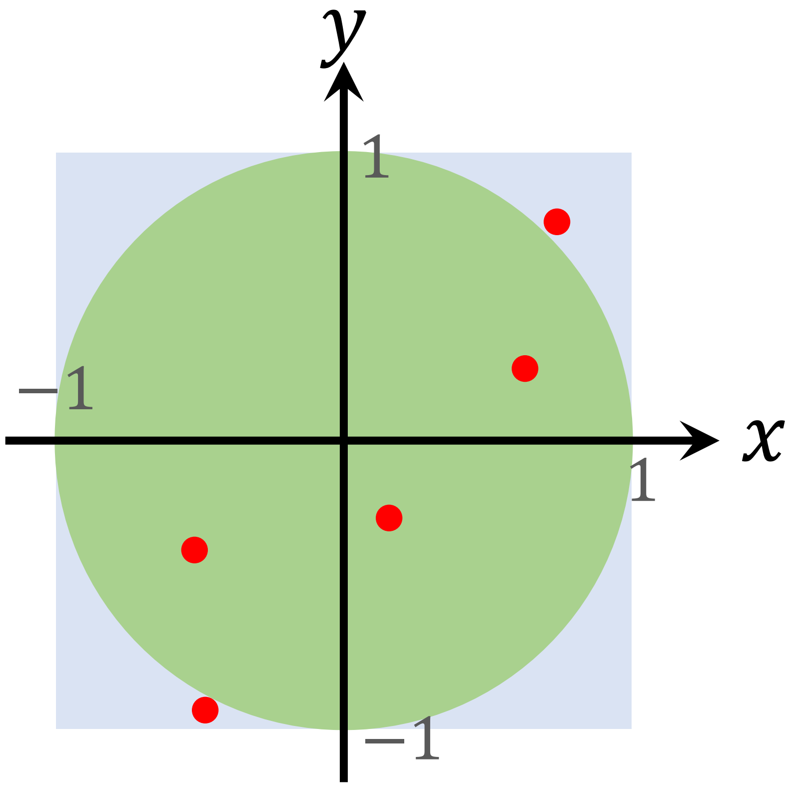

- Law of big number:

$$\frac{4m}{n} \to \pi, \quad \text{as } n \to \infty.$$

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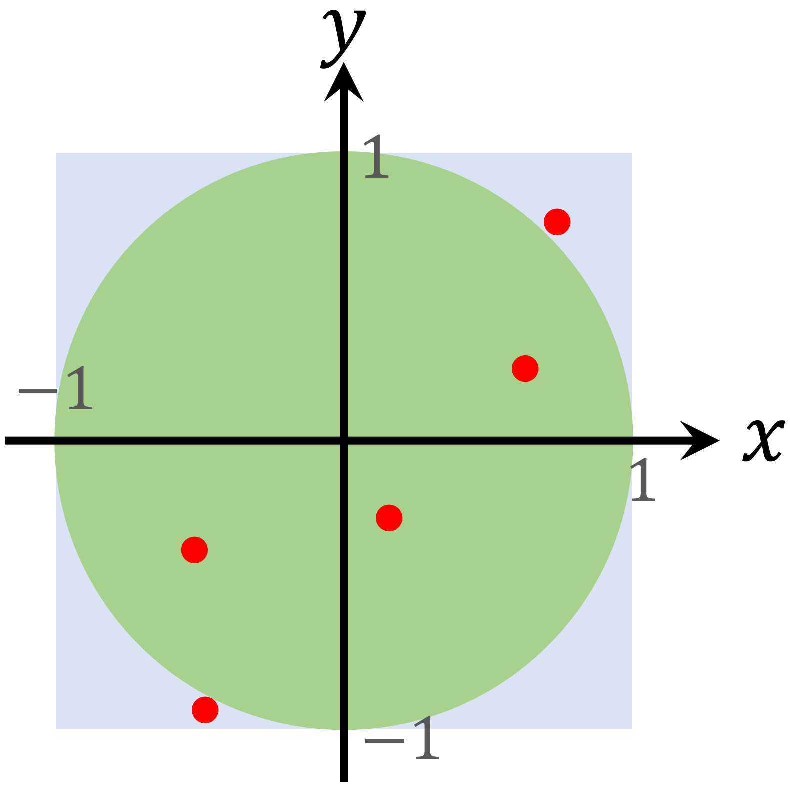


- Law of big number:

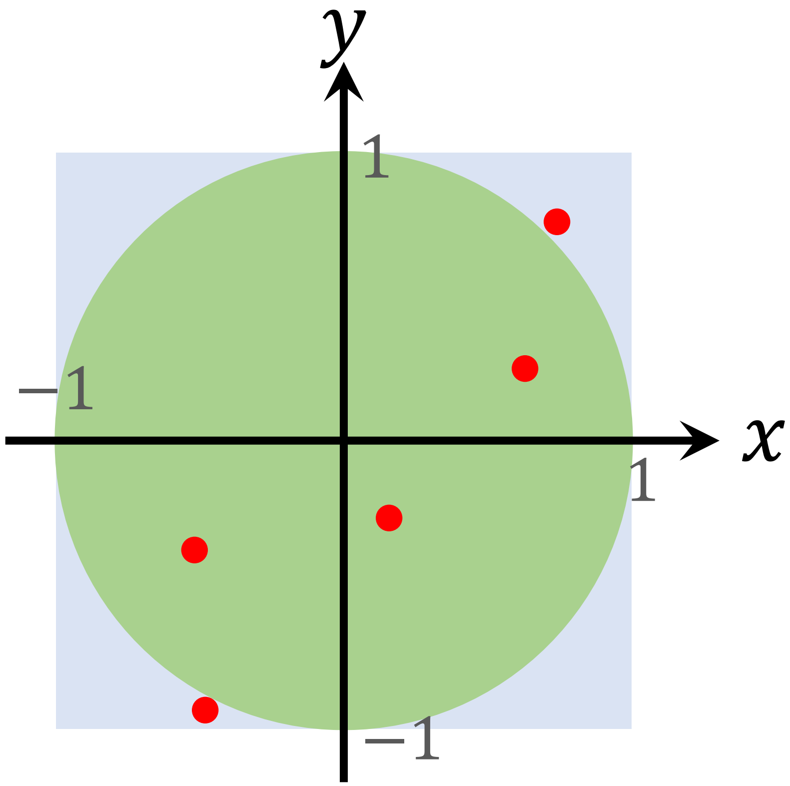
$$\frac{4m}{n} \to \pi, \quad \text{as } n \to \infty.$$

- Concentration bound:

$$\left|\frac{4m}{n} - \pi\right| = O\left(\frac{1}{\sqrt{n}}\right).$$

Calculating Pi

Totally n points sampled from the square; m are in the circle. Then $\pi \approx \frac{4m}{n}$.



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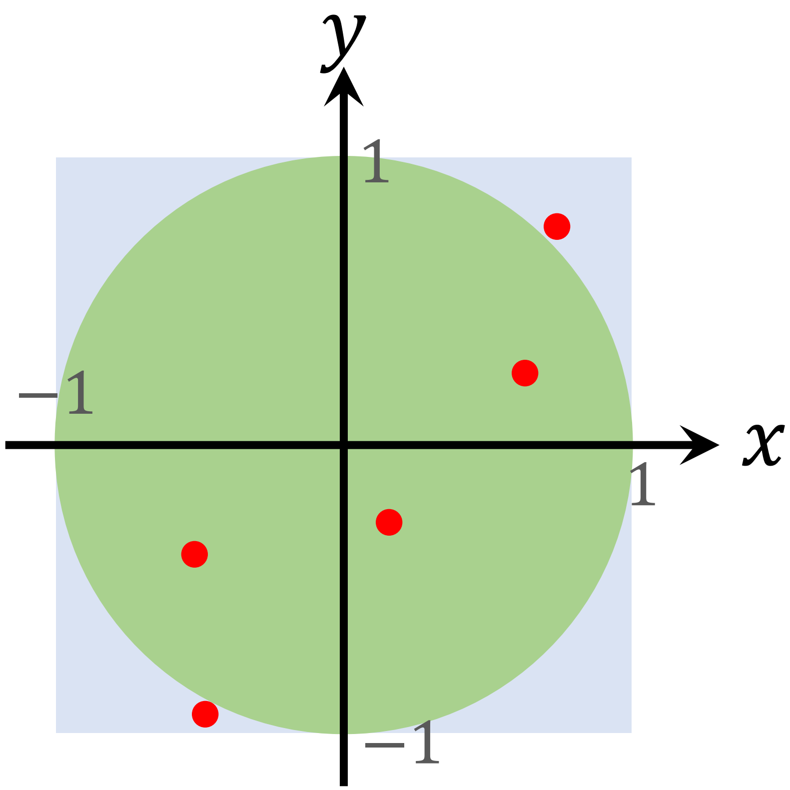


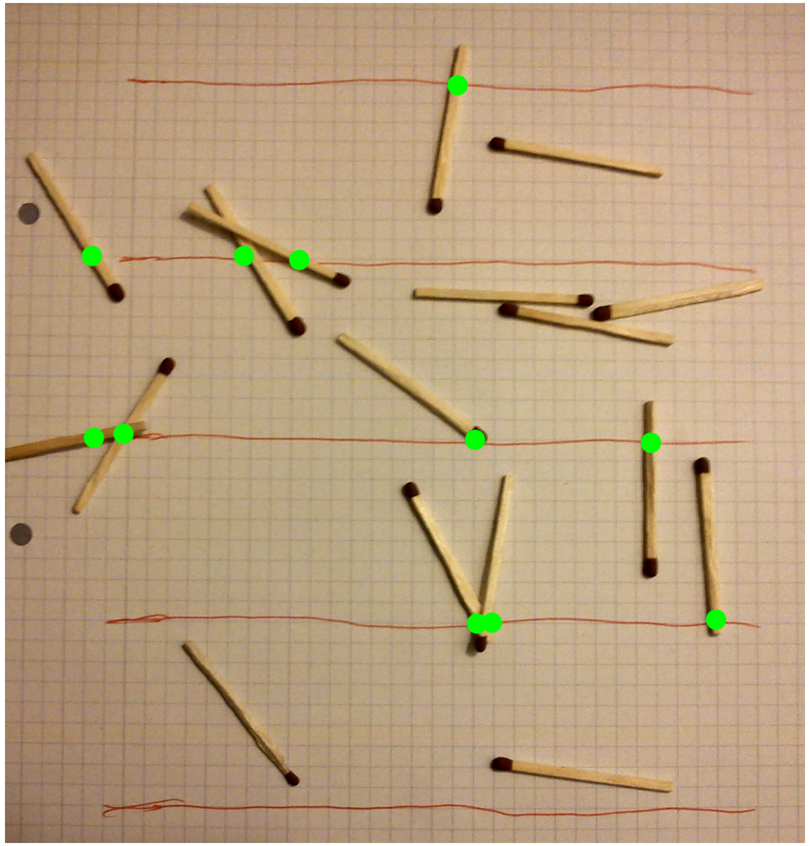
Algorithm

1. User specify a big n; reset counter $m = 0$.
2. For $i = 1$ to n:
   a) Randomly generate $x \in [-1, 1]$.
   b) Randomly generate $y \in [-1, 1]$.
   c) If $x^2 + y^2 \leq 1$, then $m \leftarrow m + 1$.
3. Return $\pi \approx \frac{4m}{n}$.

Application 2: Buffon's Needle Problem

Buffon's Needle Problem

Buffon, 1707 – 1788
French scientist



Buffon's Needle Problem

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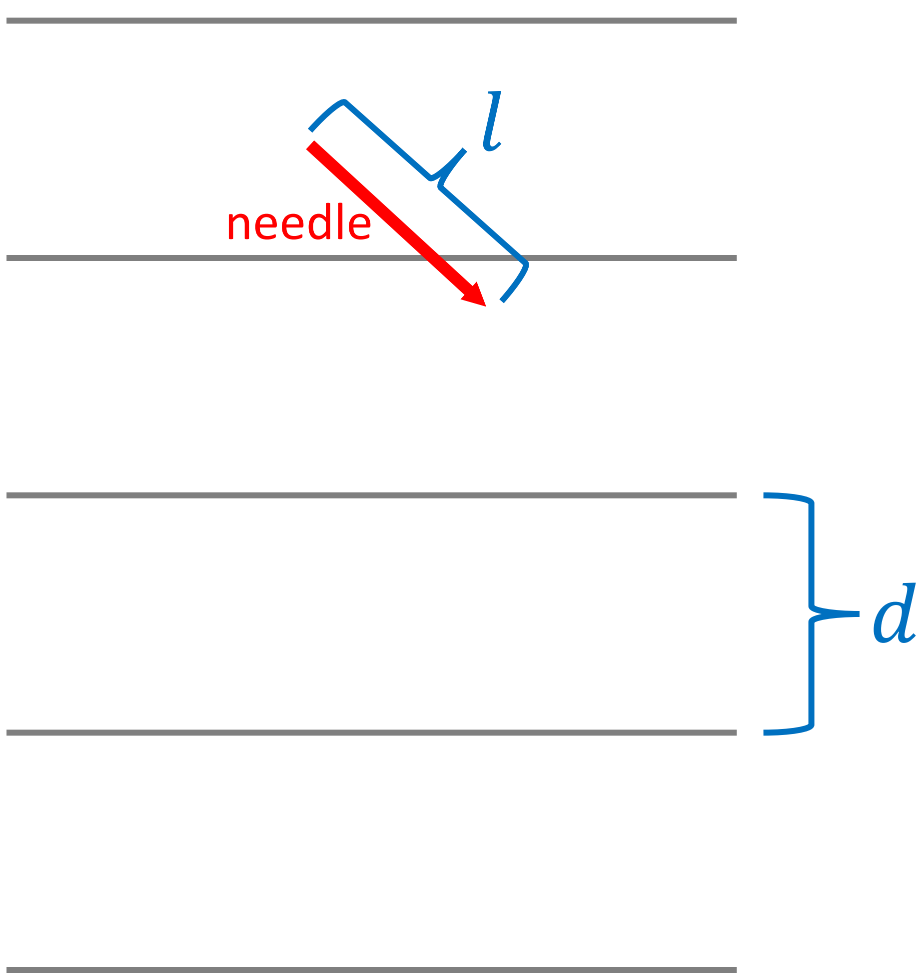
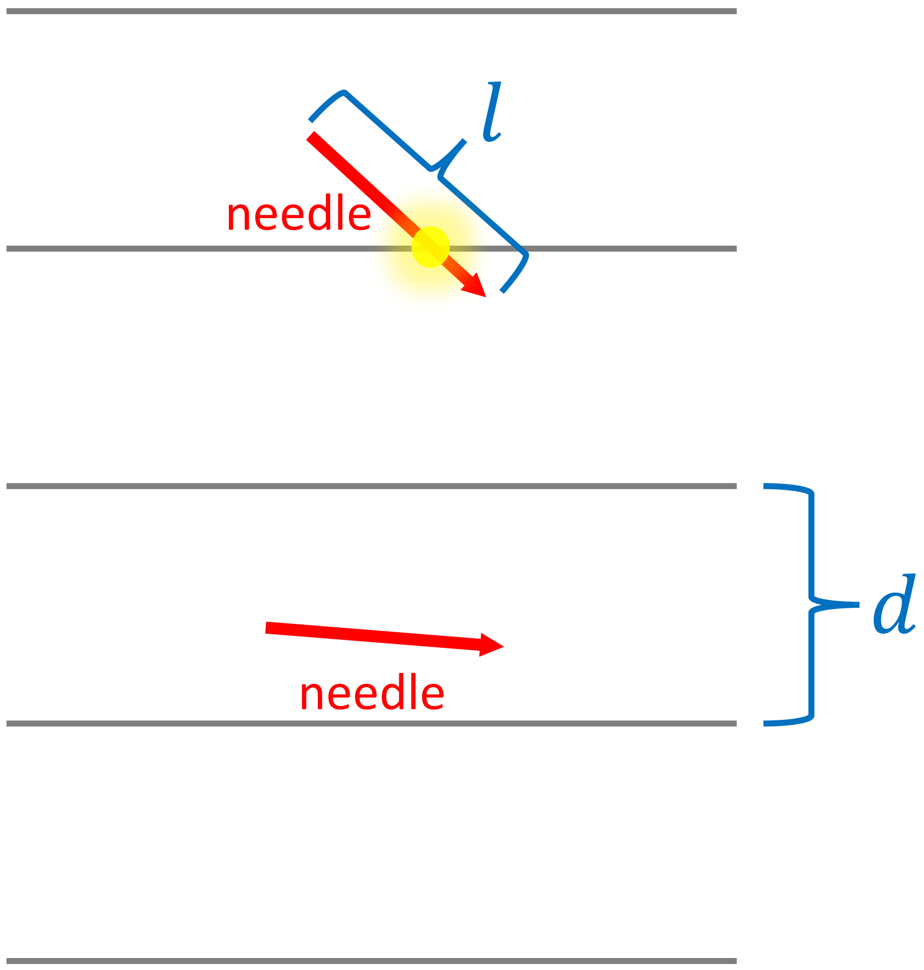


- The parallel lines have distance d.
- Needles have length l.
- Randomly throw a needle; the needle may or may not lie across a line.

Buffon's Needle Problem



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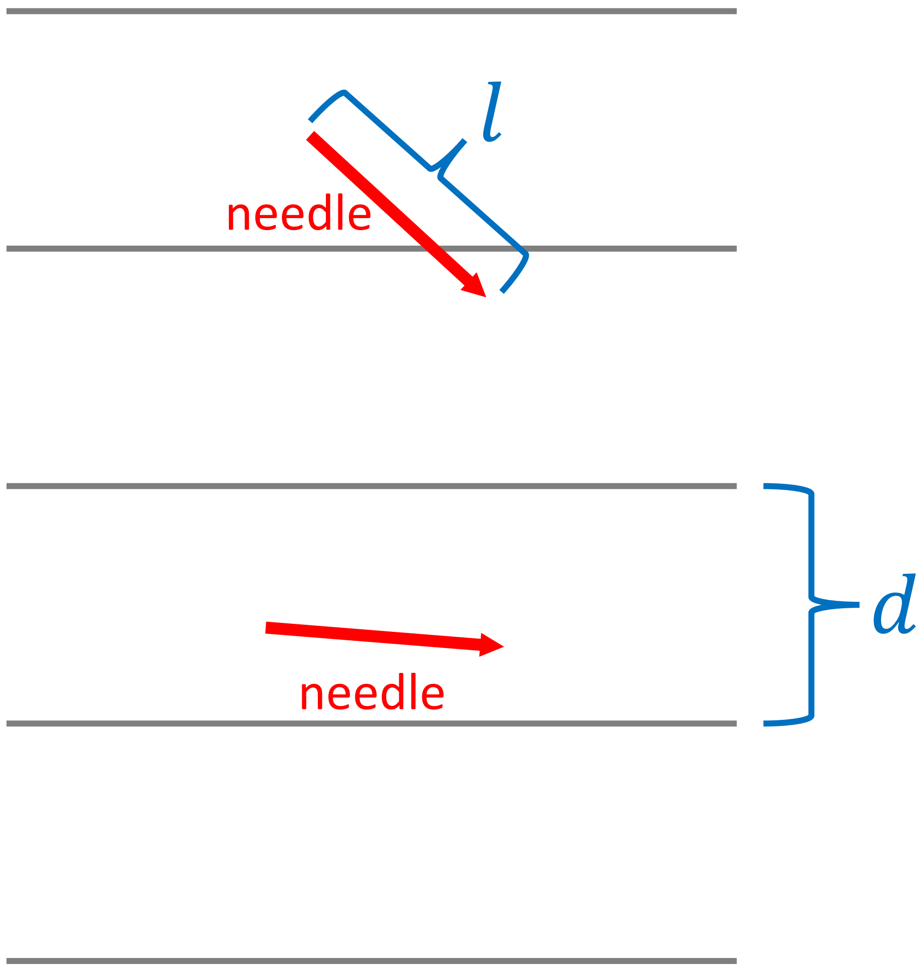
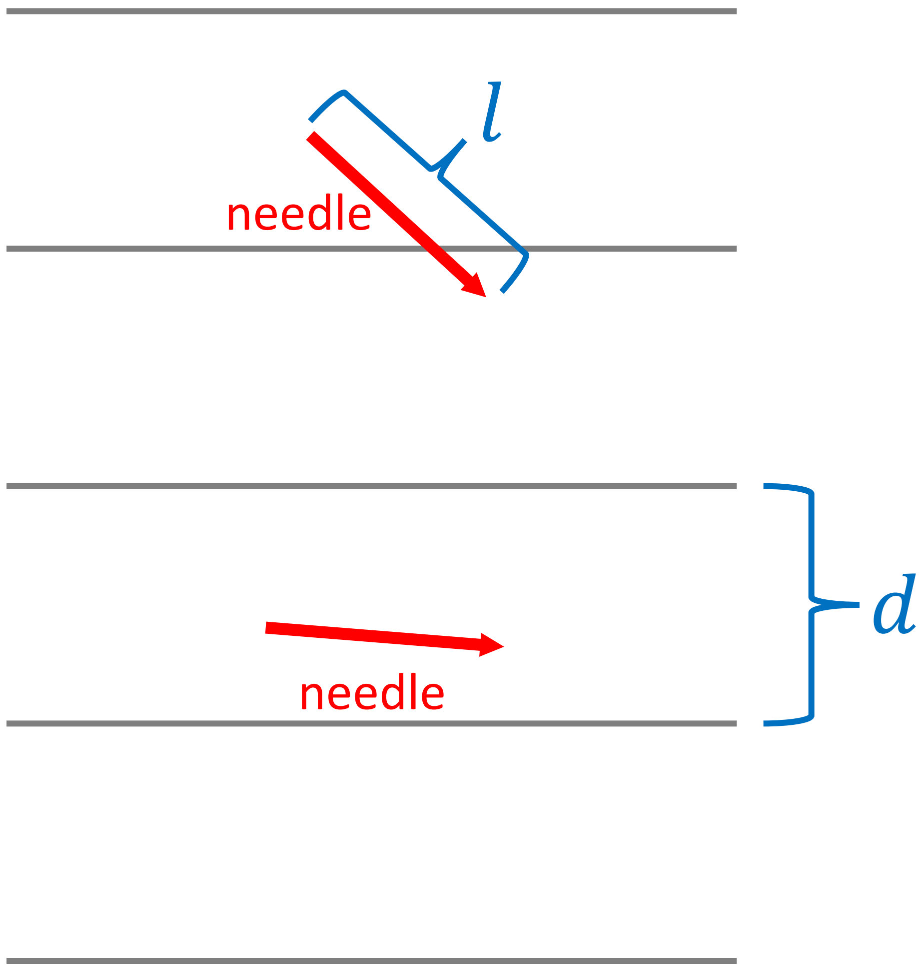


- The parallel lines have distance d.
- Needles have length l.
- Randomly throw a needle; the needle may or may not lie across a line.

With probability $P = \frac{2l}{\pi d}$, they are across.

- It can be proved using integral.

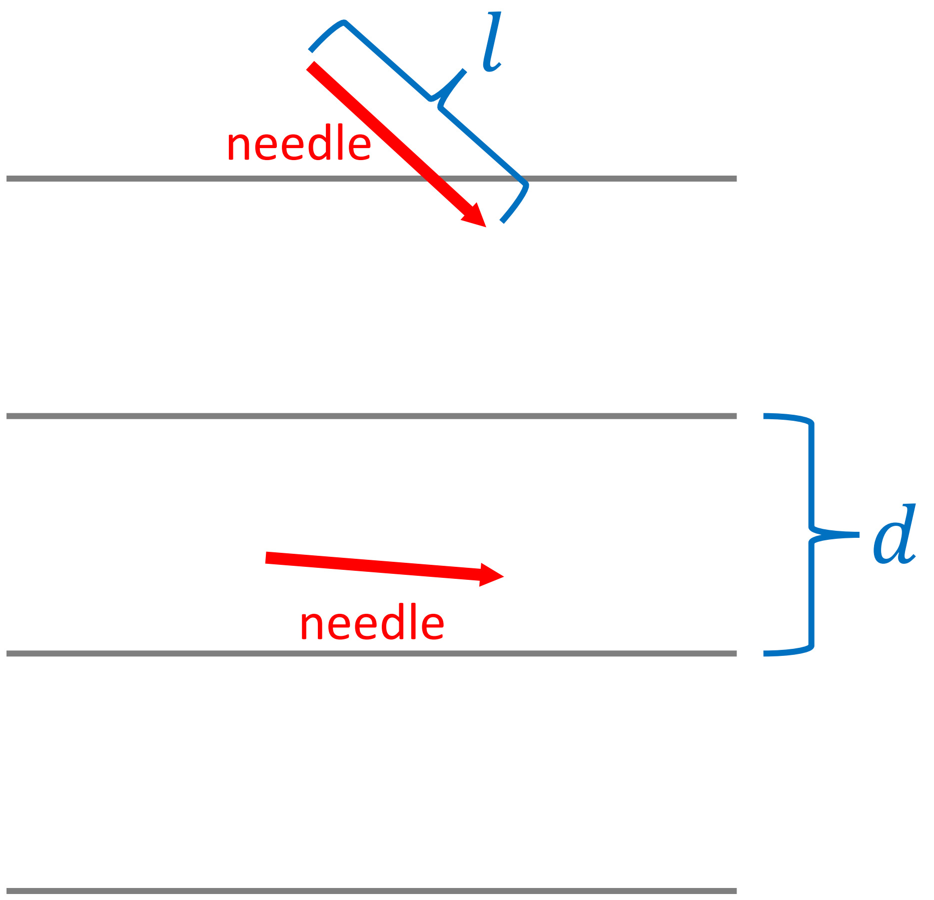
Buffon's Needle Problem



With probability $P = \frac{2l}{\pi d}$, they are across.

- Randomly throw a total of n needles.
- In expectation, $Pn = \frac{2ln}{\pi d}$ needles lie across the lines.

Buffon's Needle Problem



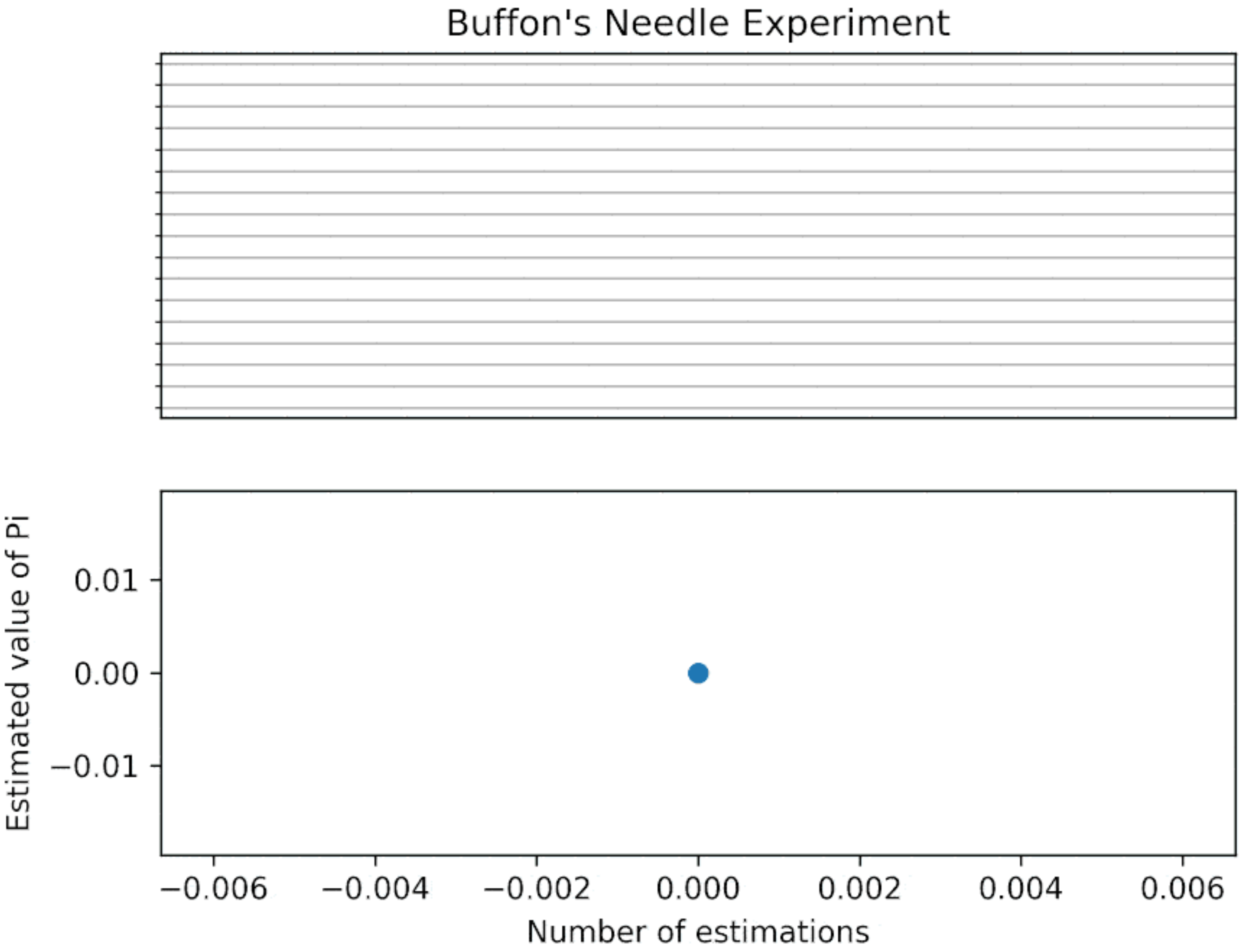
With probability $P = \frac{2l}{\pi d}$, they are across.

- Randomly throw a total of n needles.
- In expectation, $Pn = \frac{2ln}{\pi d}$ needles lie across the lines.
- Actually observe m needles across the lines.
- If n is big, $m \approx \frac{2\ l\ n}{\pi\ d}$.
- Thus, $\pi \approx \frac{2\ l\ n}{d\ m}$.

Buffon's Needle Problem

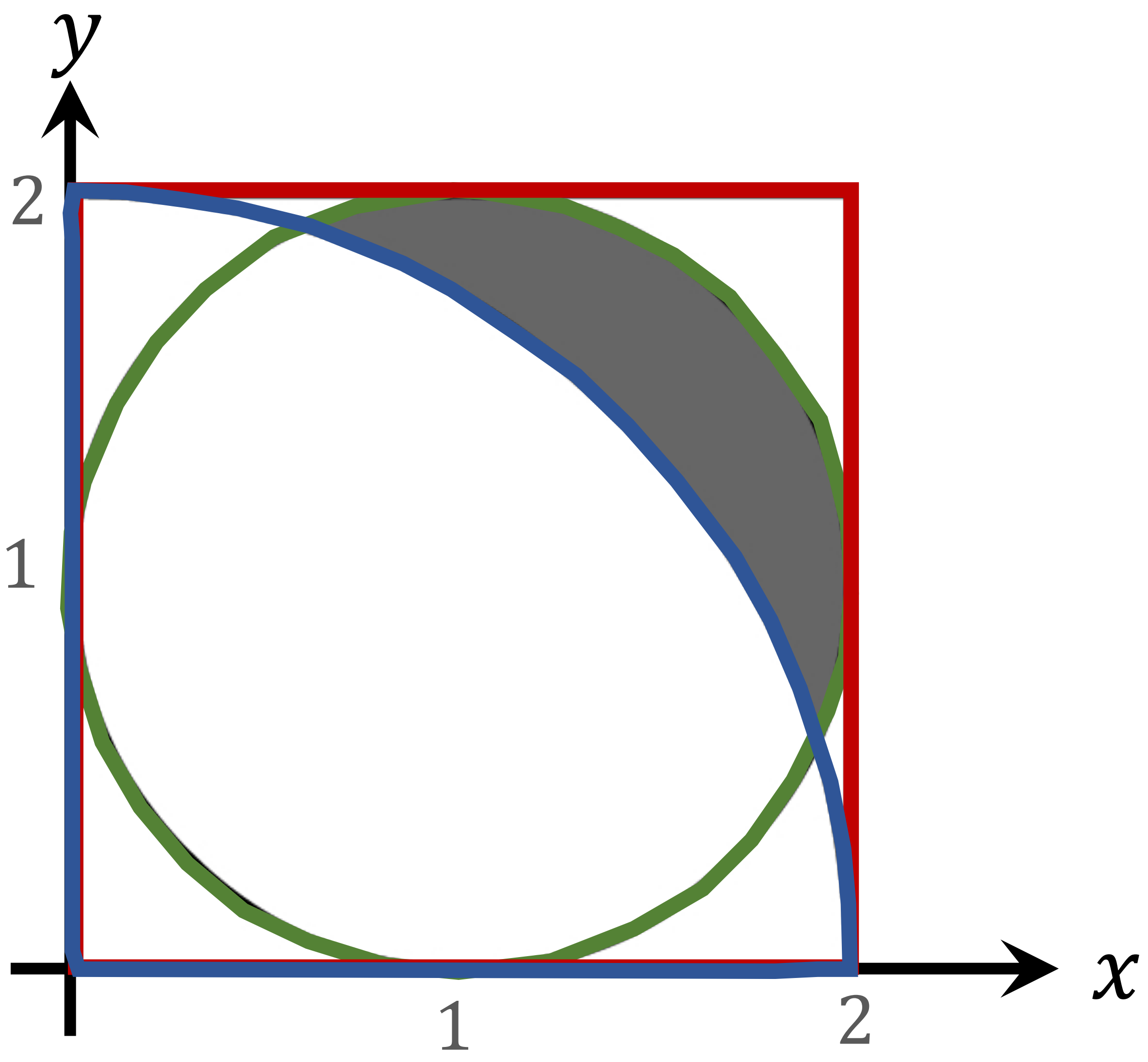
Researcher	Year	$n =$	$m =$	Estimate of π
Wolf	1850	5000	2532	3.1596
Smith	1855	3204	1218	3.1554
De Morgan	1860	600	382	3.137
Fox	1884	1030	489	3.1595
Lazzerini	1901	3408	1808	3.1415929
Reina	1925	2520	859	3.1795

Buffon's Needle Problem



Application 3: Area of A Region

What is the area of the grey region?



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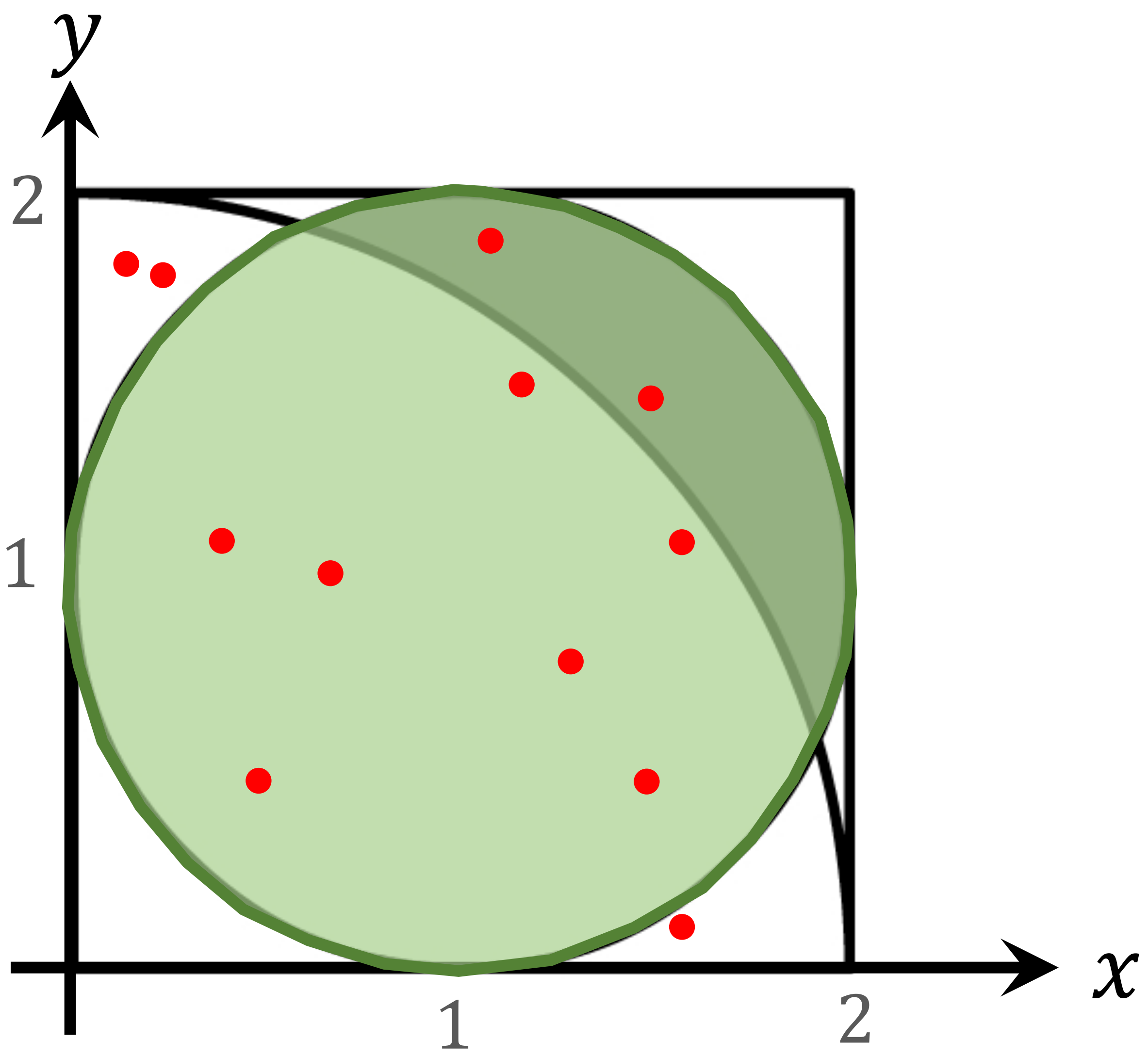

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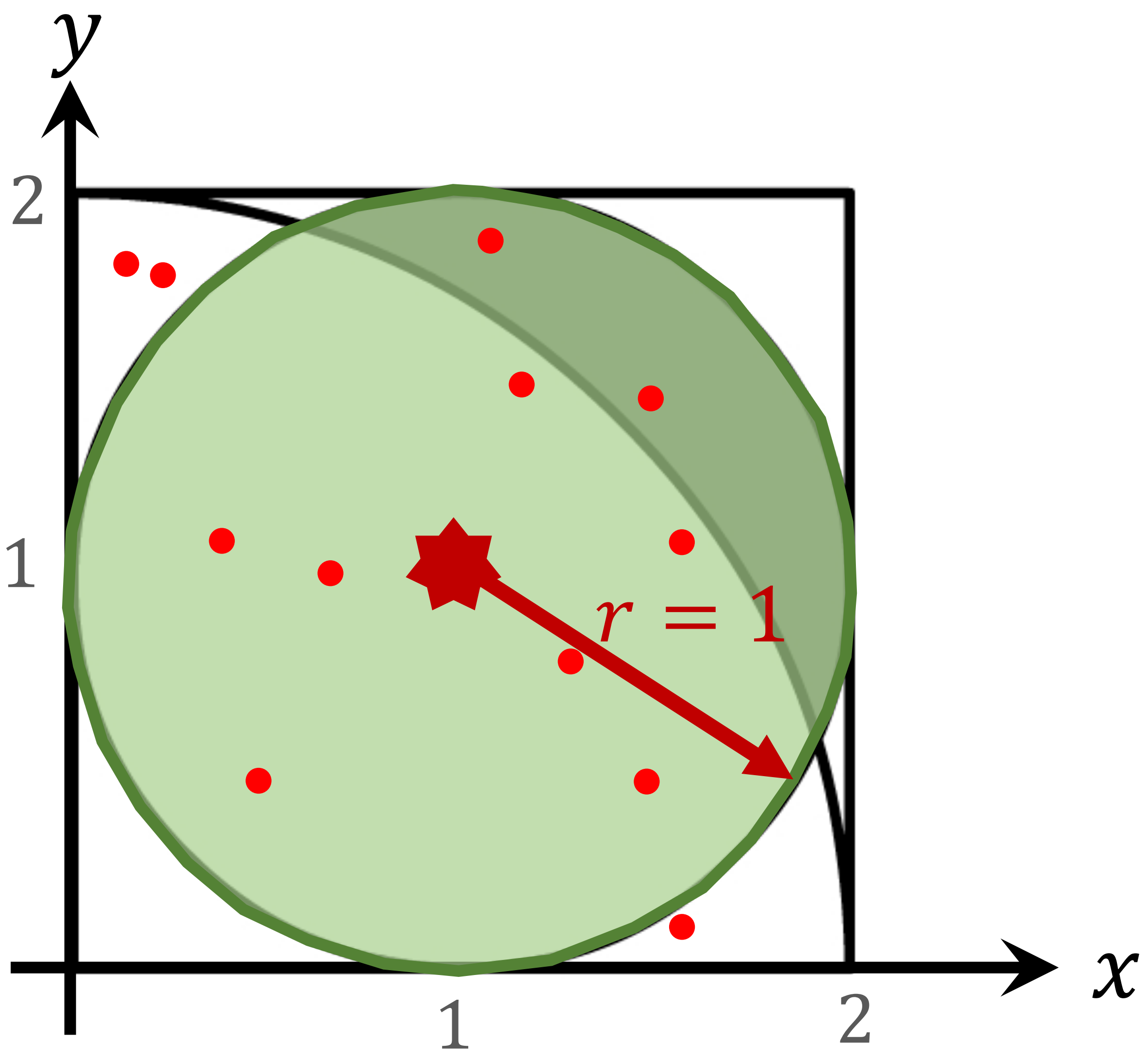

- If a point (x, y) is in the circle, it must satisfy

$$(x-1)^2 + (y-1)^2 \leq 1.$$

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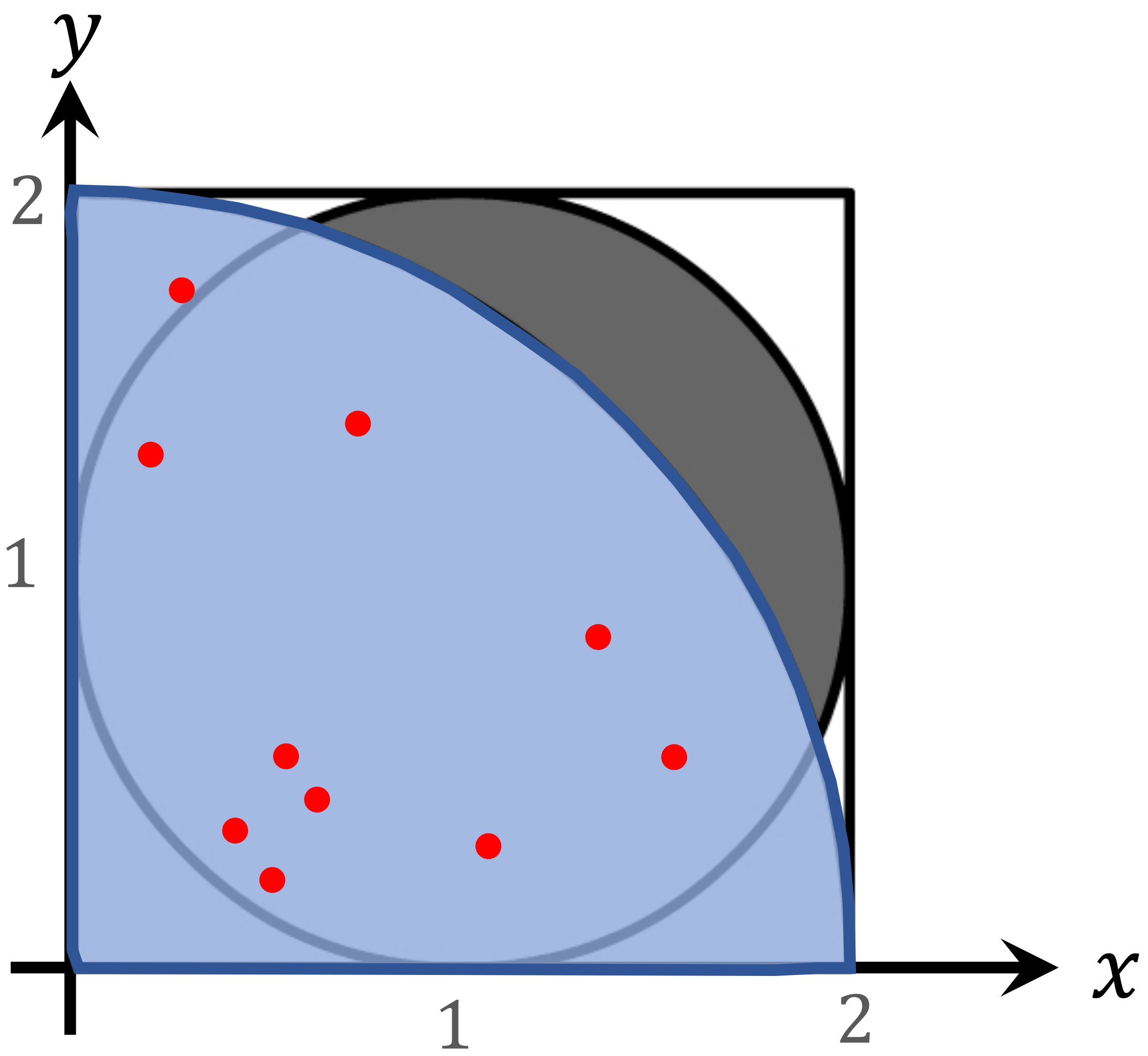


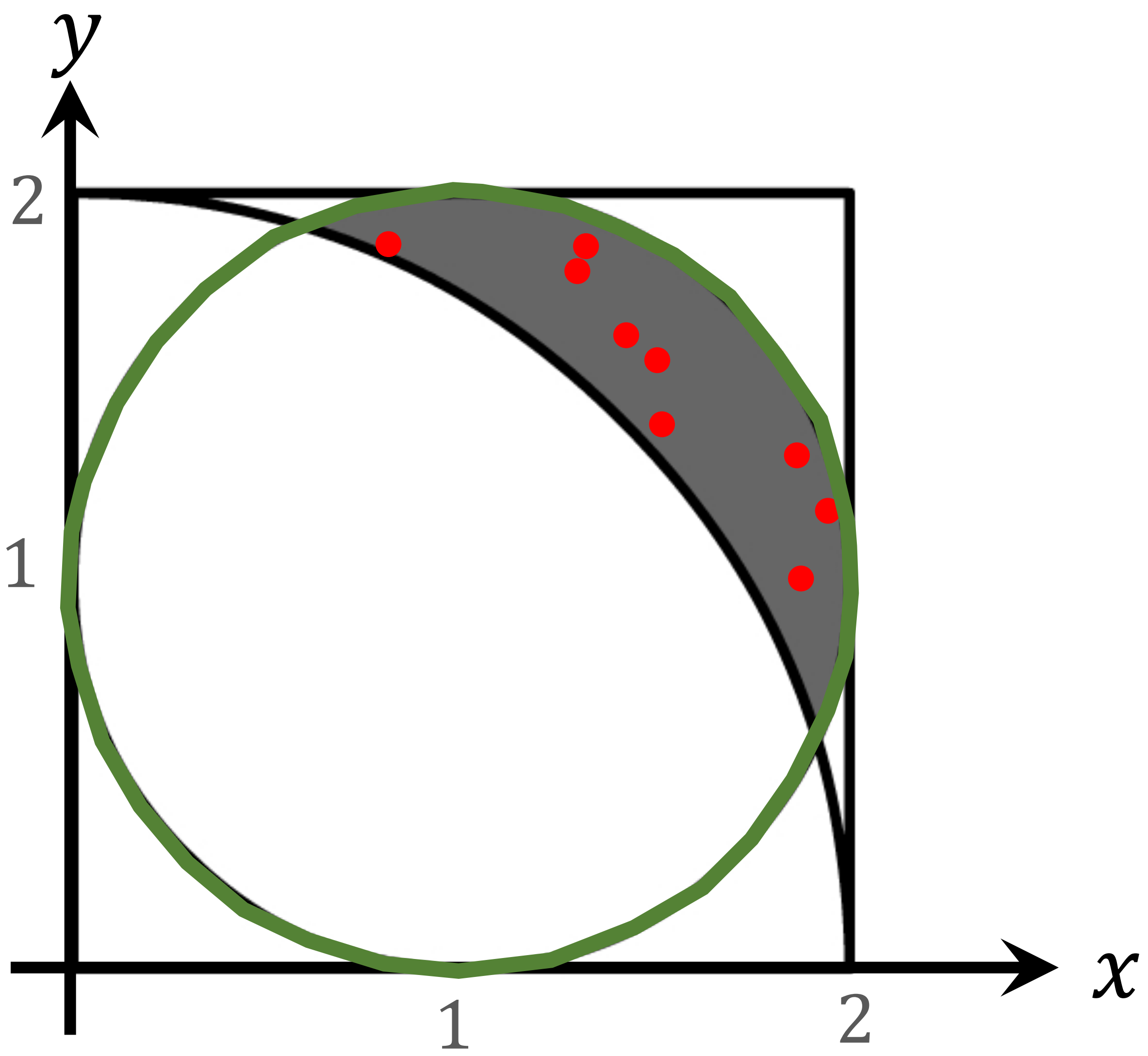
- If a point (x, y) is in the circle, it must satisfy

$$(x-1)^2 + (y-1)^2 \leq 1.$$

- If a point (x, y) is in the quarter circle, it must satisfy

$$x^2 + y^2 \leq 2^2.$$

What is the area of the grey region?



- A point (x, y) in the grey region satisfies both of

1. $(x-1)^2 + (y-1)^2 \leq 1.$
2. $x^2 + y^2 > 2^2.$

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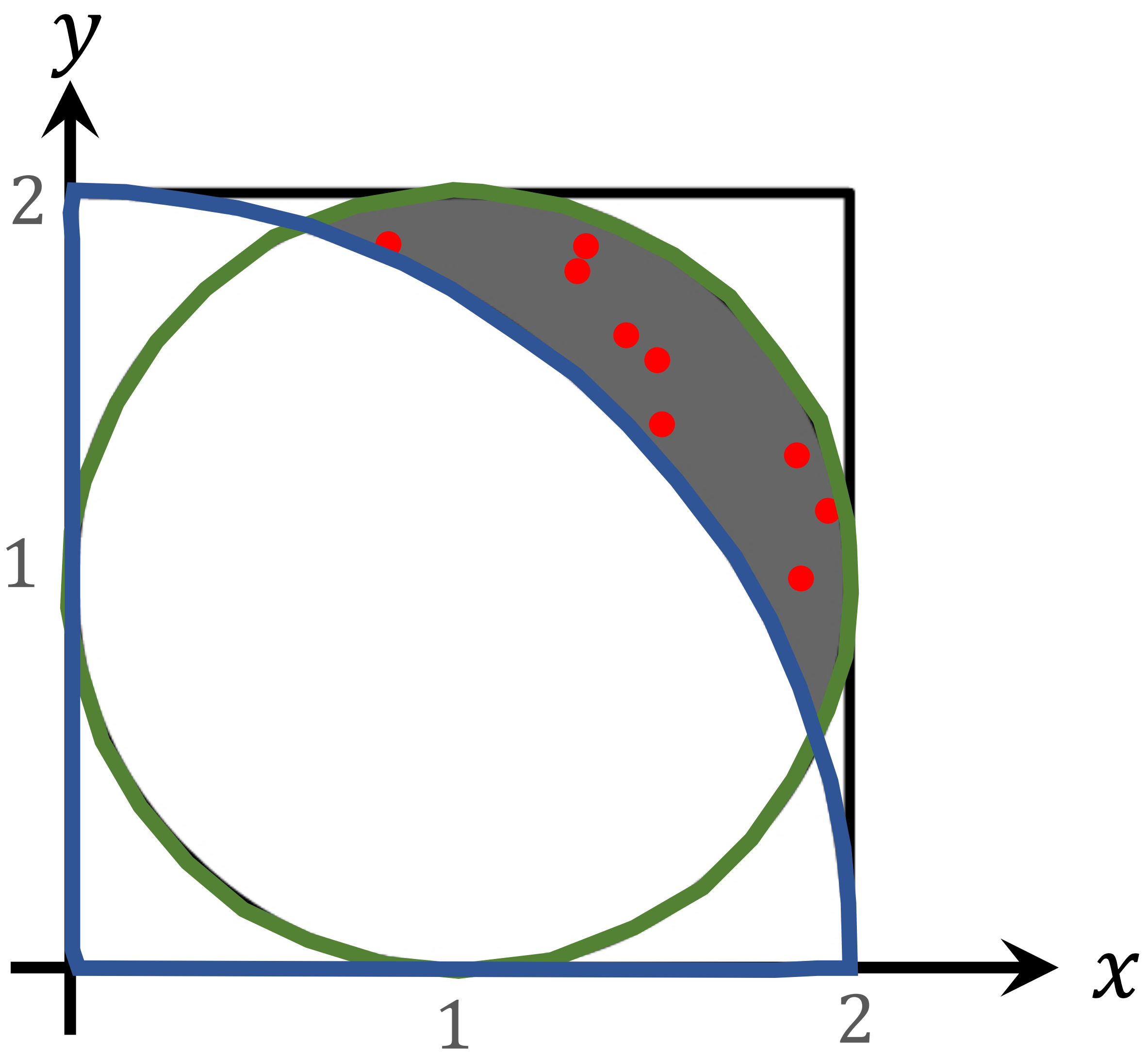

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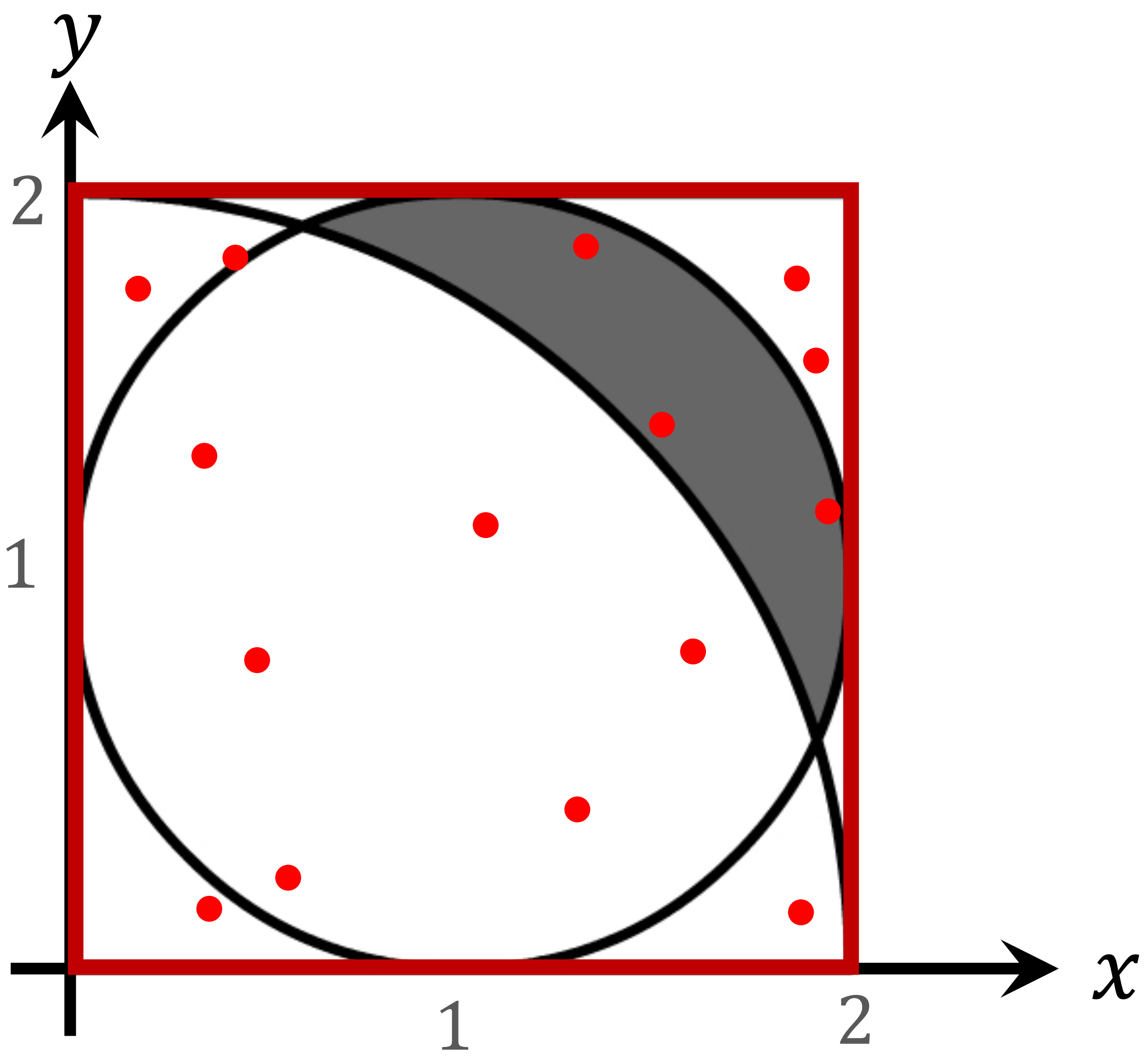
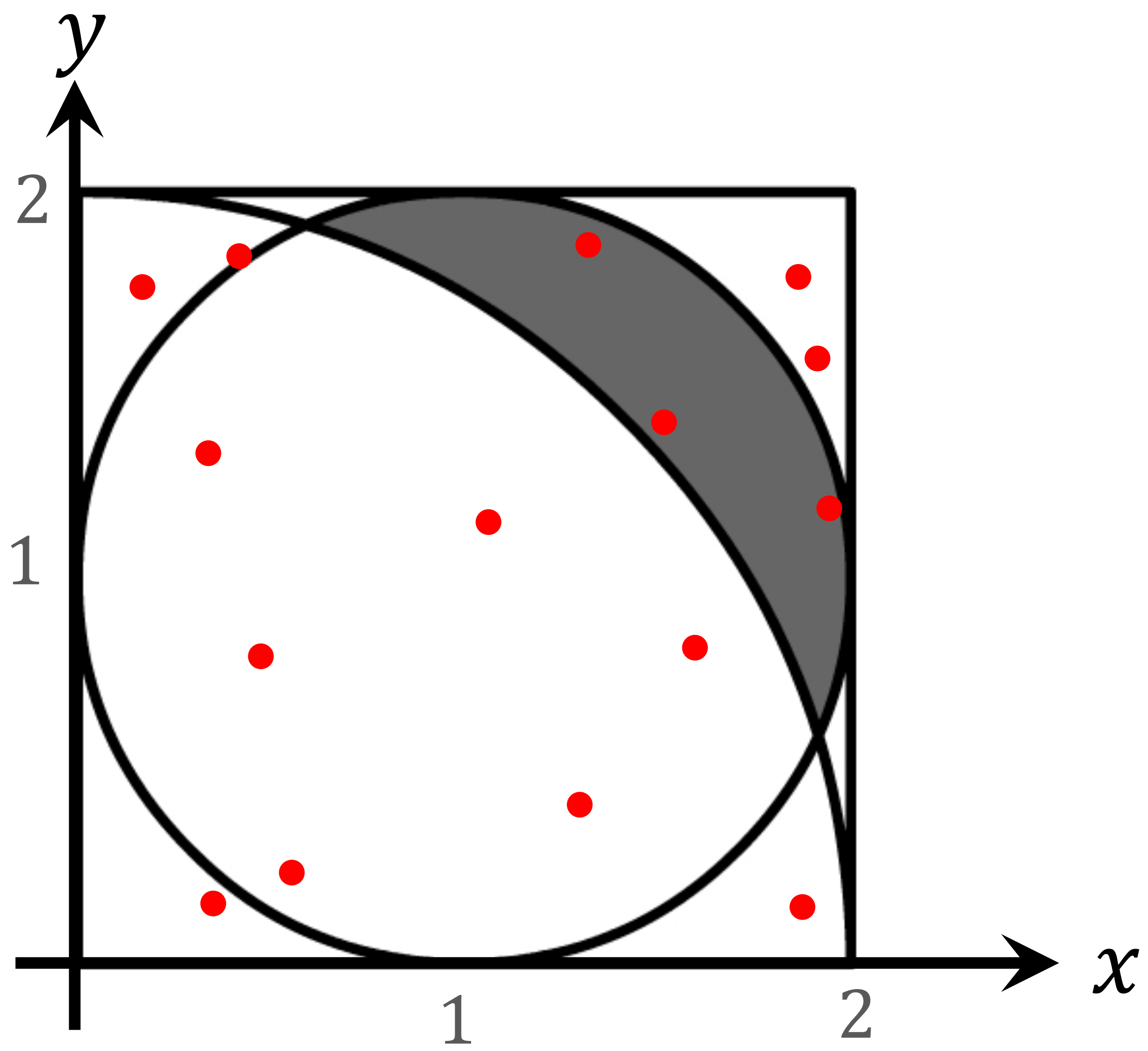


- Area of the square: $A_1 = 2^2 = 4$.
- Area of the grey region: A_2.
- A point uniformly sampled from the square falls in the grey region w.p.

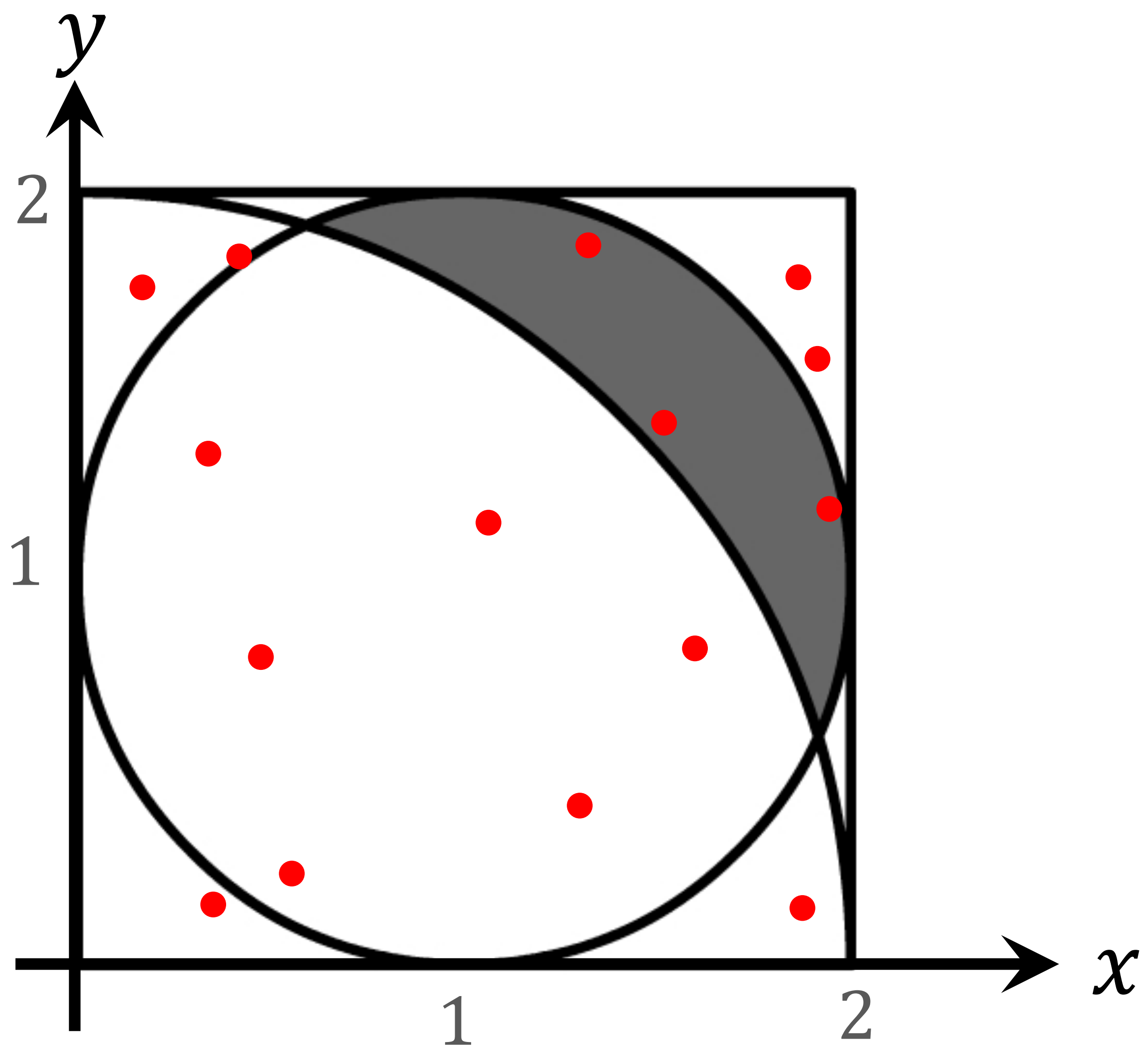
$$P = \frac{A_2}{A_1} = \frac{A_2}{4}.$$

What is the area of the grey region?



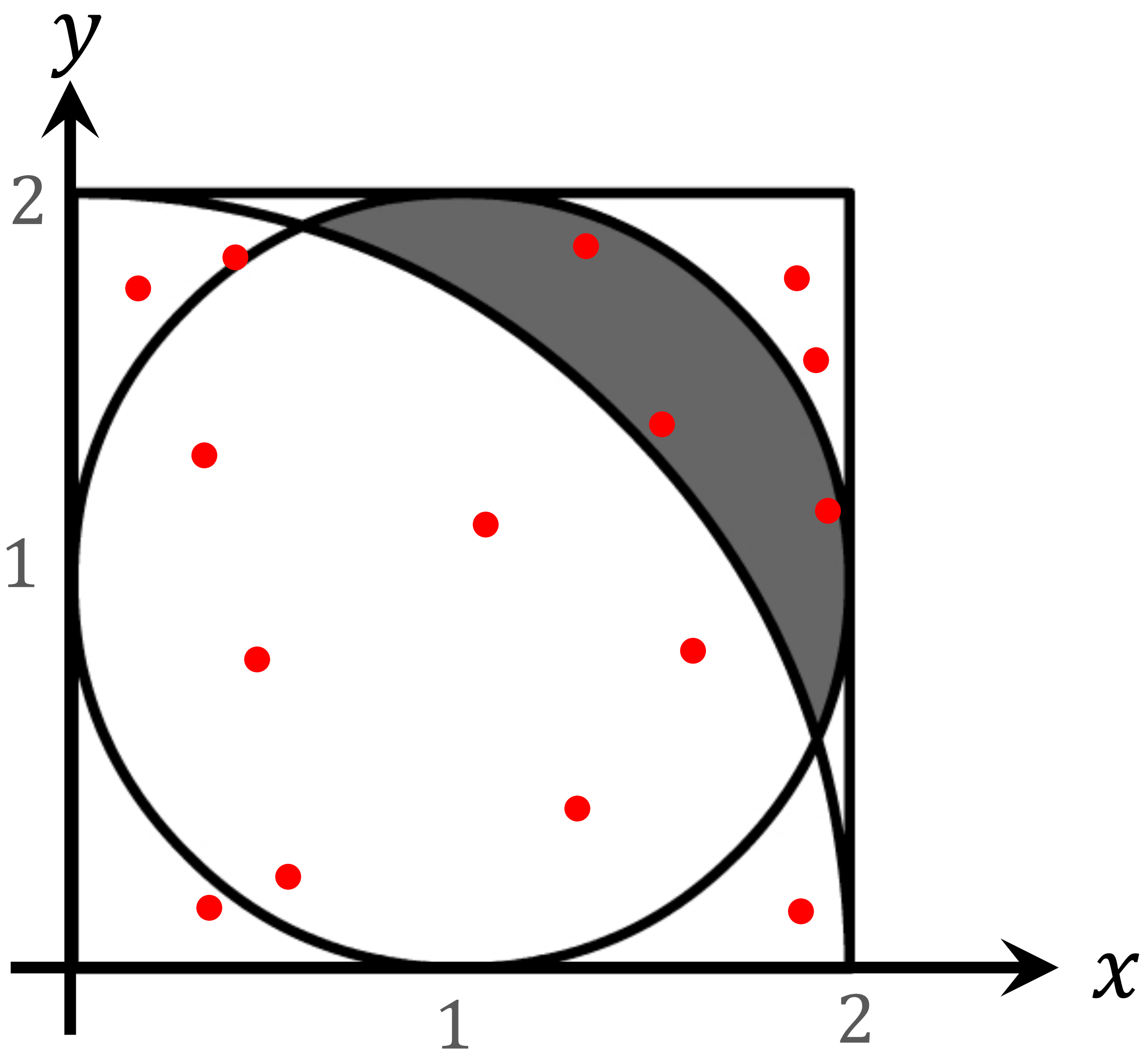
- Uniformly sample n points from the square $[0,2]\times[0,2]$.
- In expectation, $nP = \frac{n\,A_2}{4}$ points fall in the grey region.

What is the area of the grey region?



- Uniformly sample n points from the square $[0, 2]\times[0, 2]$.
- In expectation, $nP = \frac{n\,A_2}{4}$ points fall in the grey region.
- We actually observe m points in the grey region.
- If n is big, then $m \approx \frac{n\,A_2}{4}$.
- Thus, $A_2 \approx \frac{4m}{n}$.

What is the area of the grey region?



Algorithm

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2. For $i = 1$ to n:
   a) Randomly generate $x \in [0, 2]$.
   b) Randomly generate $y \in [0, 2]$.
   c) If both of the following conditions are satisfied, then $m \leftarrow m + 1$:
      i. $(x - 1)^2 + (y - 1)^2 \leq 1$.
      ii. $x^2 + y^2 > 2^2$.
3. Return $\text{area} = \frac{4m}{n}$.

Application 4: Integration

Integration

- We are given a function, e.g., $f(x) = \frac{1}{1+\sin(x)\cdot(\log_{\mathrm{e}} x)^2}$.
- Calculate the integral: $I = \int_{0.8}^{3} f(x)\, dx$.
- If $f(x)$ is very involved, there is no way to analytically calculate the integral.
- Using Monte Carlo to approximate the integral.

Monte Carlo Integration (Univariate)

Task: Given a univariate function $f(x)$, calculate $I = \int_a^b f(x)\, dx$.

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1. Draw n samples from $[a, b]$ uniformly at random; denote them by $x_1, \cdots, x_n$.
2. Calculate $Q_n = (b - a) \cdot \frac{1}{n} \sum_{i=1}^{n} f(x_i)$.
3. Return Q_n as an approximation to the integral $I = \int_a^b f(x)\,dx$.

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Theory: Law of large numbers guarantees $Q_n \rightarrow I$, as $n \rightarrow \infty$.

Monte Carlo Integration (Univariate): Example

Task: Given function $f(x) = \frac{1}{1+\sin(x)\cdot(\log_e x)^2}$, calculate $I = \int_{0.8}^{3} f(x)\, dx$.

1. Draw n samples from $[0.8, 3]$ uniformly at random; denote them by $x_1, \cdots, x_n$.
2. Calculate $Q_n = 2.2 \cdot \frac{1}{n}\sum_{i=1}^{n} f(x_i)$.
3. Return Q_n as an approximation to the integral $I = \int_{0.8}^{3} f(x)\, dx$.

Monte Carlo Integration (Multivariate)

Task: Given a multivariate function $f(\mathbf{x})$, calculate $I = \int_{\Omega} f(\mathbf{x})\, d\mathbf{x}$.

$\mathbf{x} \in \mathbb{R}^d$ is a vector

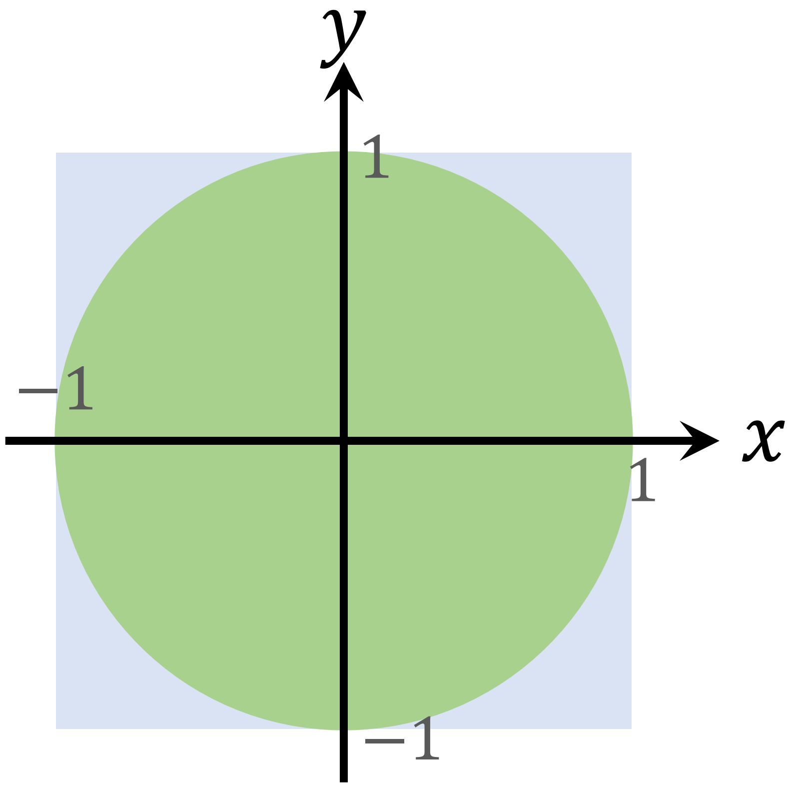
Ω is a subset of $\mathbb{R}^d$

Monte Carlo Integration (Multivariate)

Task: Given a multivariate function $f(\mathbf{x})$, calculate $I = \int_{\Omega} f(\mathbf{x})\, d\mathbf{x}$.

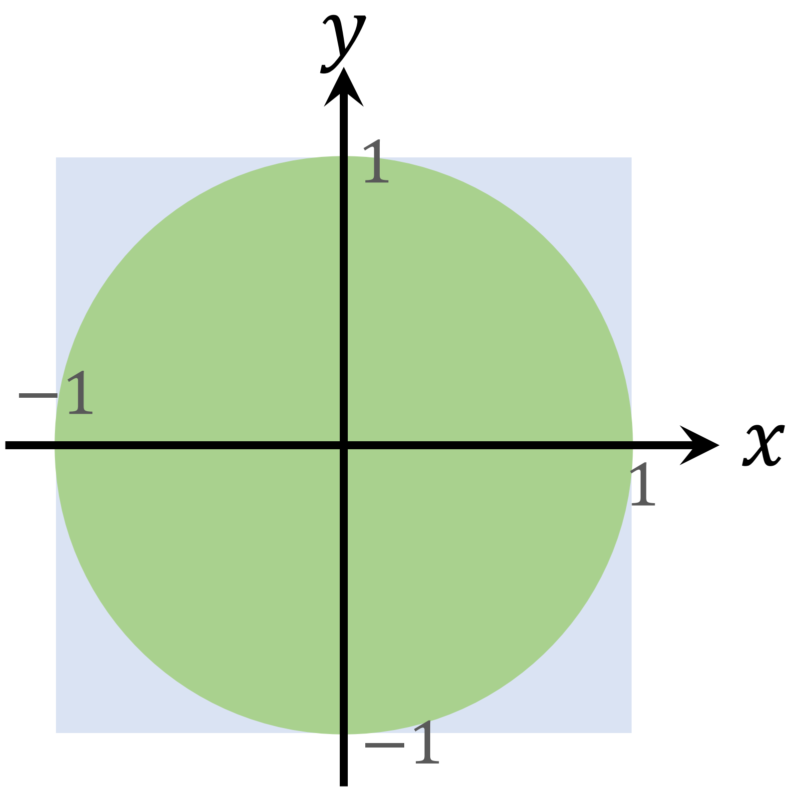
1. Draw n samples from set Ω uniformly at random; denote them by $\mathbf{x}_1, \cdots, \mathbf{x}_n$.
2. Calculate $V = \int_{\Omega} d\mathbf{x}$.
3. Calculate $Q_n = V \cdot \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{x}_i)$.
4. Return Q_n as an approximation to the integral $I = \int_{\Omega} f(\mathbf{x})\, d\mathbf{x}$.

Monte Carlo Integration: Bivariate Example



- Let $f(x,y) = \begin{cases} 1, \text{if } x^2 + y^2 \leq 1; \\ 0, \quad \text{otherwise.} \end{cases}$
- Let $\Omega = [-1,1]\times[-1,1]$.
- What is $I = \int_\Omega f(x,y)\, dx\, dy$?

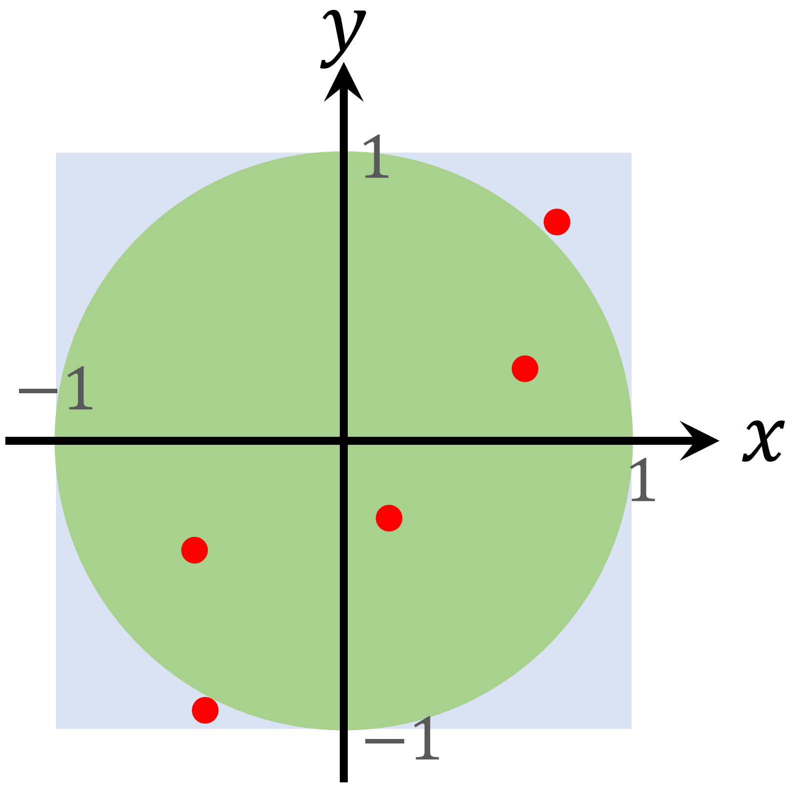
Monte Carlo Integration: Bivariate Example



- Let $f(x,y) = \begin{cases} 1, \text{if } x^2 + y^2 \le 1; \\ 0, \quad \text{otherwise.} \end{cases}$
- Let $\Omega = [-1,1]\times[-1,1]$.
- What is $I = \int_{\Omega} f(x,y)\, dx\, dy$?
- Obviously, I is the area of the circle:

$$I = \pi r^2 = \pi.$$

Monte Carlo Integration: Bivariate Example

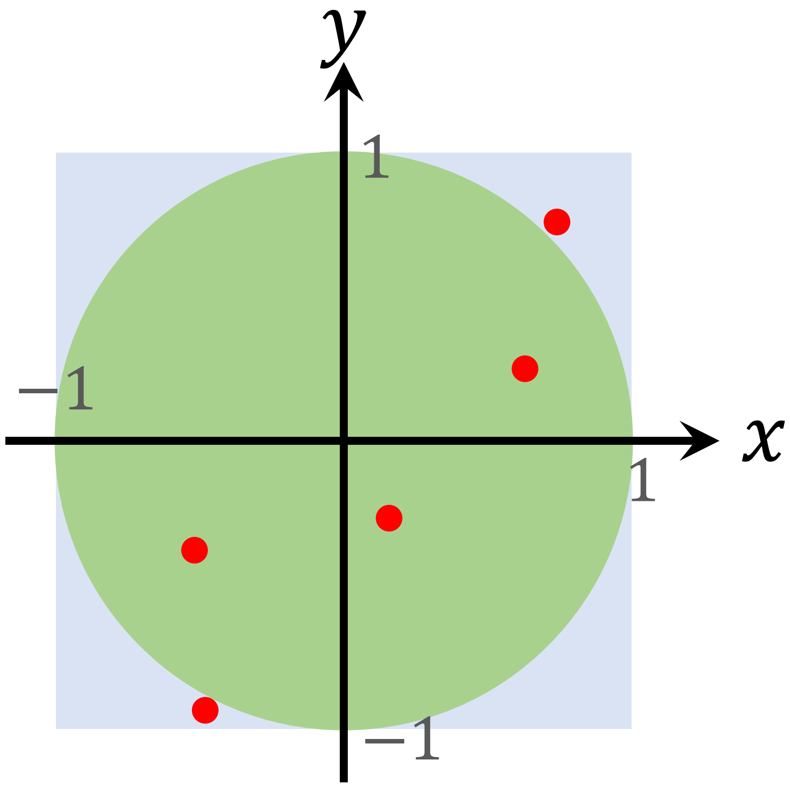


1. Draw n samples from set Ω uniformly at random; denote them by

$$(x_1, y_1), \cdots, (x_n, y_n).$$

2. Calculate $V = \int_{\Omega} dx\, dy = 4$. (It is the area of set Ω.)

Monte Carlo Integration: Bivariate Example



1. Draw n samples from set Ω uniformly at random; denote them by
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2. Calculate $V = \int_\Omega dx\, dy = 4$. (It is the area of set Ω.)
3. Calculate $Q_n = V \cdot \frac{1}{n} \sum_{i=1}^{n} f(x_i, y_i)$.
4. Return Q_n as an approximation to the integral $\pi = \int_\Omega f(x, y)\, dx\, dy$.

Application 5: Estimate of Expectation

Expectation

- Let X be a d-dimensional random vector.
- Let $p(\mathbf{x})$ be a probability density function (PDF).
  - Property: $\int_{\mathbb{R}^d} p(\mathbf{x})\, d\mathbf{x} = 1$.
  - E.g., PDF of uniform distribution is $p(x) = \frac{1}{t}$, for $x \in [0, t]$.
  - E.g., PDF of univariate Gaussian is $p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]$.

Expectation

- Let X be a d-dimensional random vector.
- Let $p(\mathbf{x})$ be a probability density function (PDF).
- Let $f(\mathbf{x})$ be any function of vector variable.
- **Expectation**: $\mathbb{E}_{X\sim p}[f(X)] = \int_{\mathbb{R}^d} f(\mathbf{x}) \cdot p(\mathbf{x})\, d\mathbf{x}$.

Monte Carlo Estimate of Expectation

Task: Estimate the expectation $\mathbb{E}_{X\sim p}[f(X)] = \int_{\mathbb{R}^d} f(\mathbf{x}) \cdot p(\mathbf{x})\, d\mathbf{x}$.

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Task: Estimate the expectation $\mathbb{E}_{X\sim p}[f(X)] = \int_{\mathbb{R}^d} f(\mathbf{x}) \cdot p(\mathbf{x})\, d\mathbf{x}$.

1. Draw n random samples from the probability distribution $p(\mathbf{x})$; denote them by $\mathbf{x}_1, \cdots, \mathbf{x}_n$.
2. Calculate $Q_n = \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{x}_i)$.
3. Return Q_n as an approximation to $\mathbb{E}_{X\sim p}[f(X)]$.

Monte Carlo and Beyond

Monte Carlo

Casino de Monte-Carlo, Monaco

- The term “Monte Carlo method" was first introduced in 1947 by Nicholas Metropolis.

Reference

- Metropolis. The beginning of the Monte Carlo method. *Los Alamos Science*, 125–130, 1987.

Monte Carlo Algorithms

- Monte Carlo refers to algorithms that rely on repeated random sampling to obtain numerical results.
- The output of Monte Carlo algorithms can be incorrect.
  - In all of our examples, the algorithms’ outputs are incorrect.
  - But they are close to the correct solution.

Monte Carlo Algorithms

- Monte Carlo refers to algorithms that rely on repeated random sampling to obtain numerical results.
- The output of Monte Carlo algorithms can be incorrect.
- Las Vegas algorithms are those always produce the correct answers.
  - E.g., random quicksort.
- Atlantic City algorithms are polynomial-time randomized algorithms that answer correctly w.p. greater than 75%.

Thank you!