Monte Carlo Algorithms

蒙特凯洛算法

蒙特卡罗算法是一种用随机数模拟问题的方法，可以近似计算圆周率和其他概率统计问题

Shusen Wang

Application 1: Calculating Pi

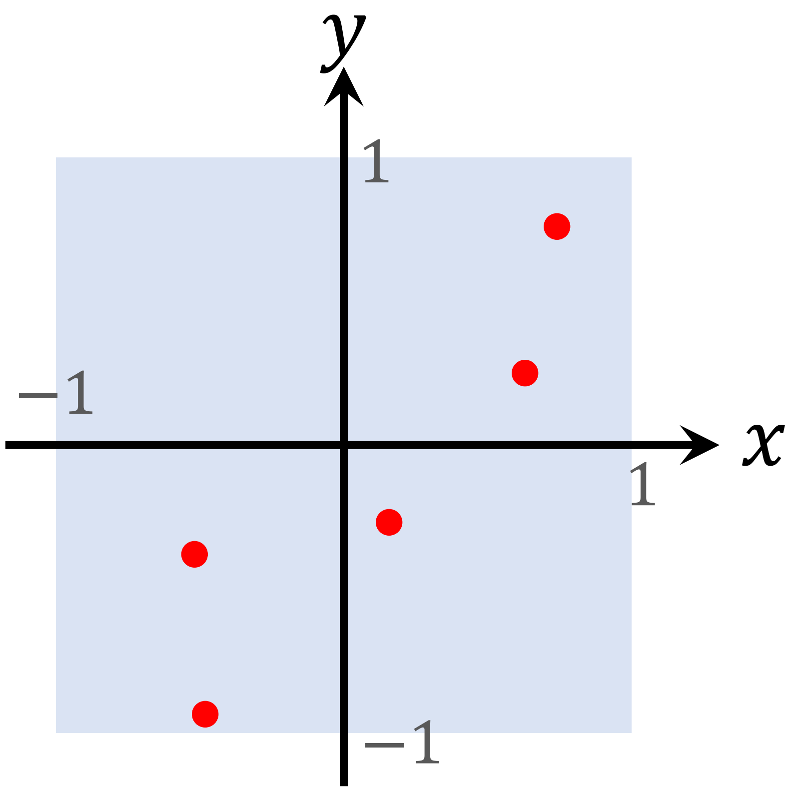
应用1：计算 π

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?

我们能用随机数生成器（近似）吗？

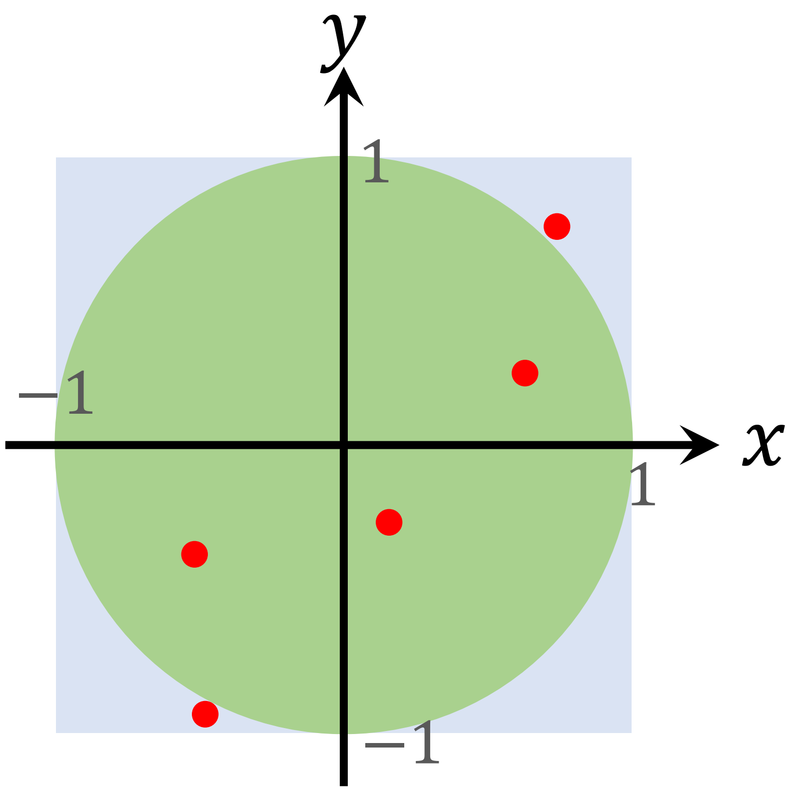
Calculating Pi



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

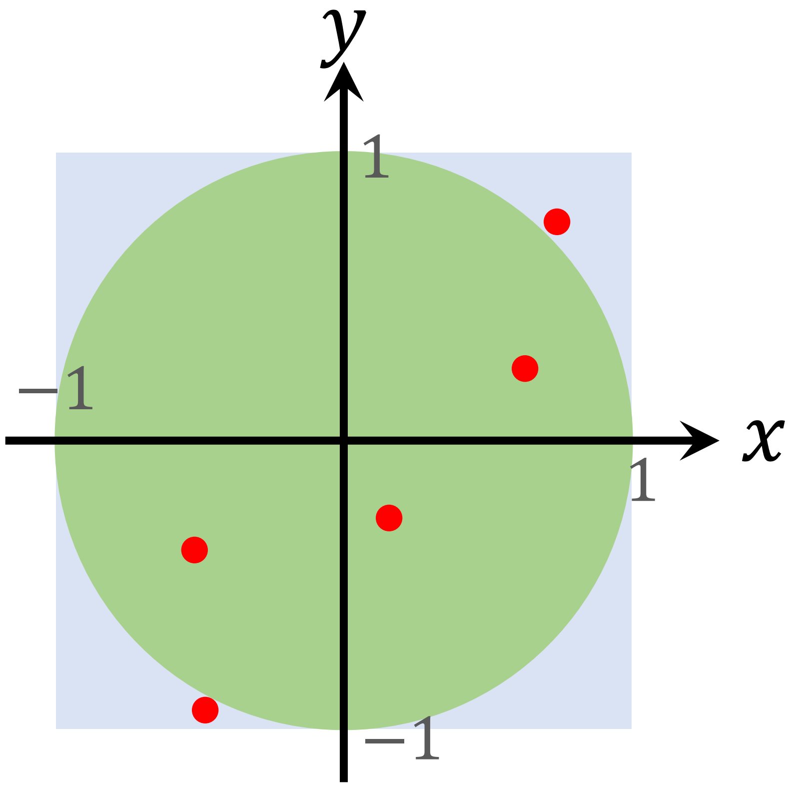
假设（x,y）是 方阵中 随机采样的 点

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?

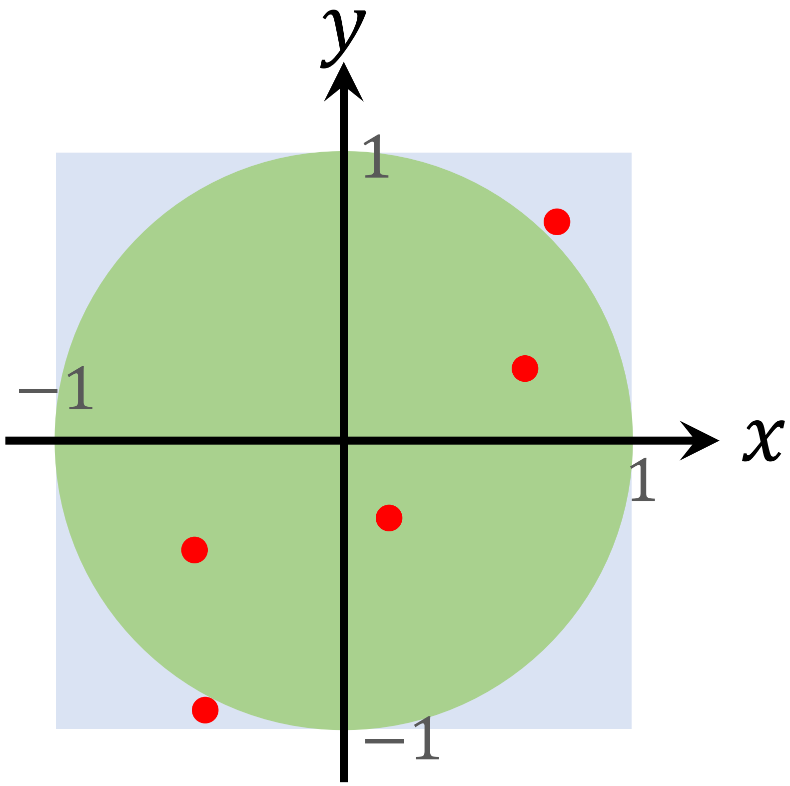
Calculating Pi



- 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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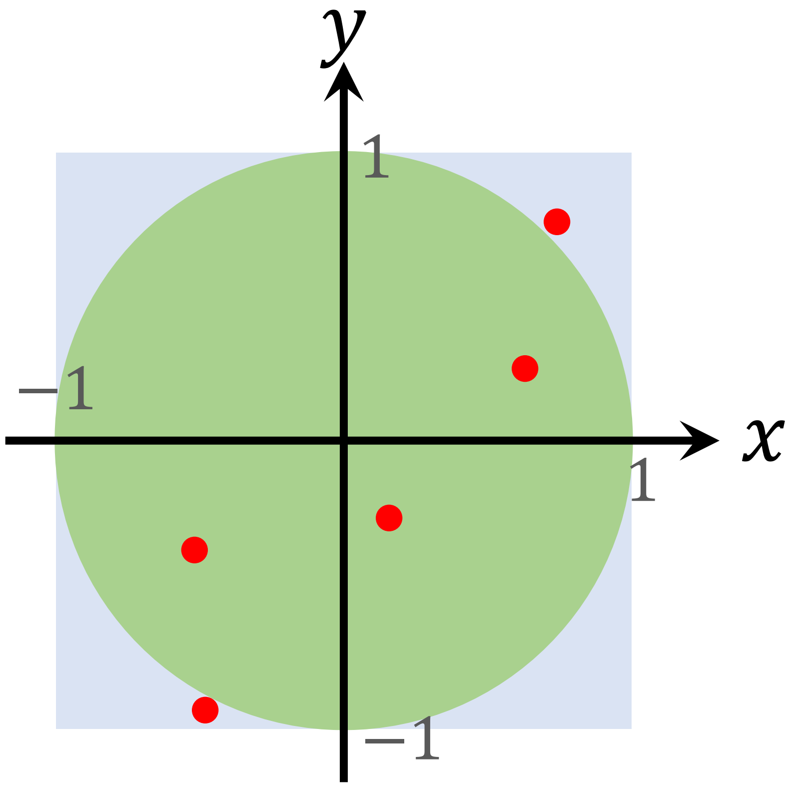

- Given a point (x, y), how do you know whether (x, y) is in the circle?
- If $x^2 + y^2 \leq 1$, then it is in the circle.

Calculating Pi

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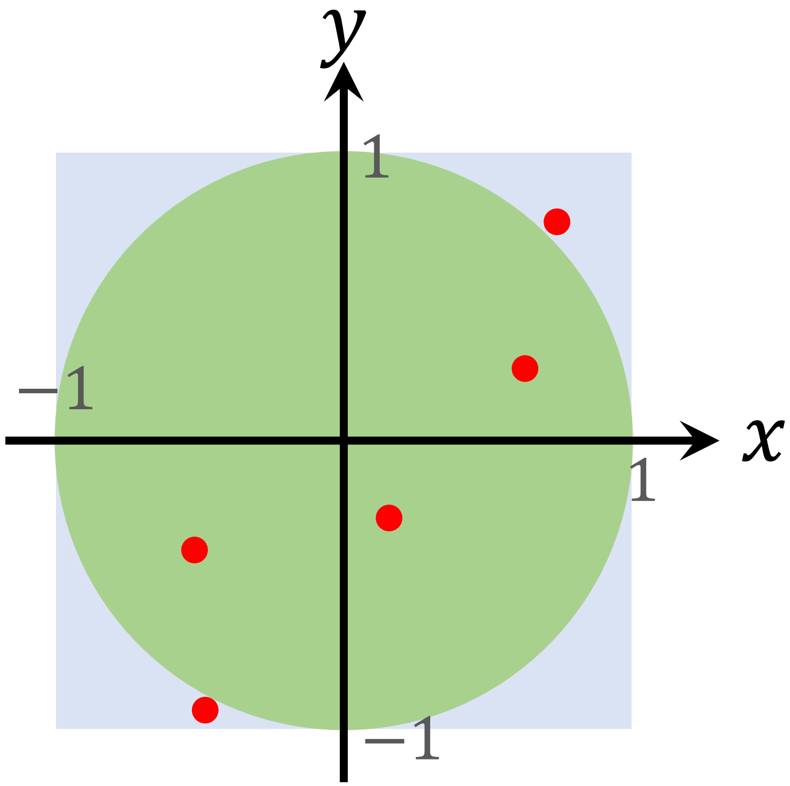
期望



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

n 个点 在方阵中
m 个点 在圆中

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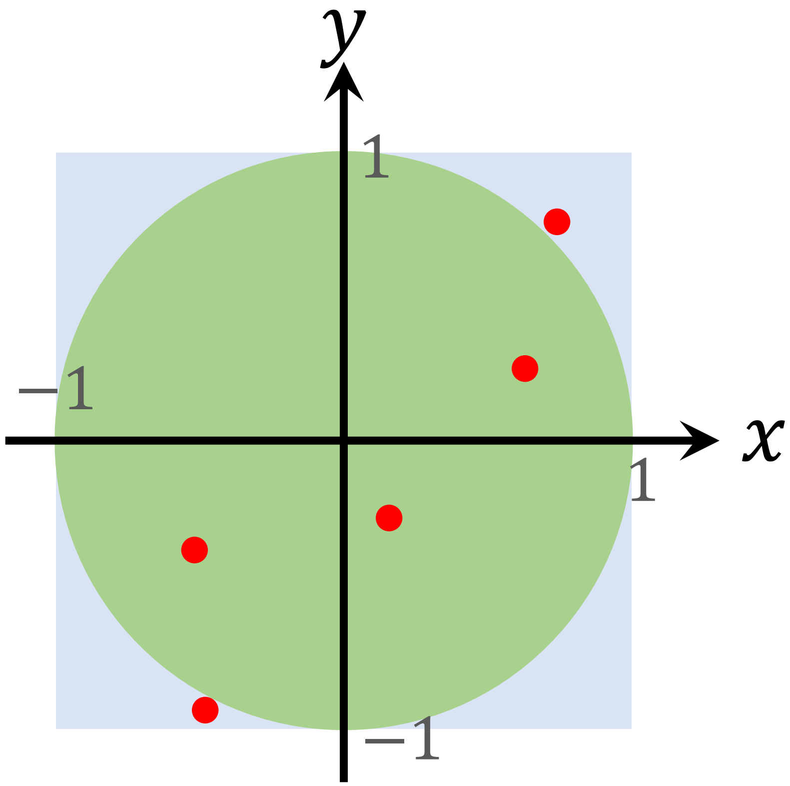

- Law of large numbers:

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

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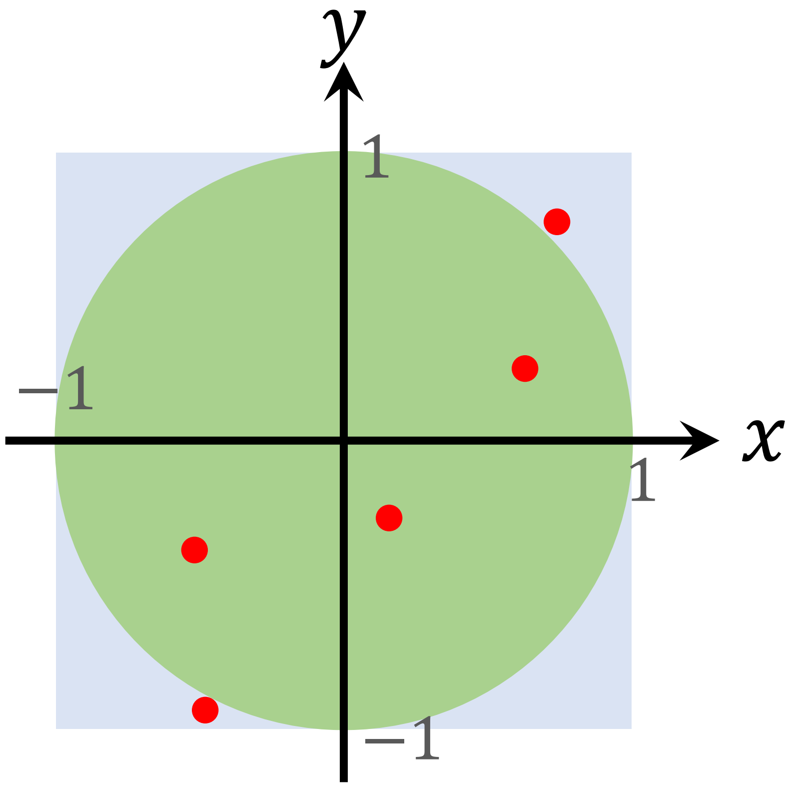


- Law of large numbers:

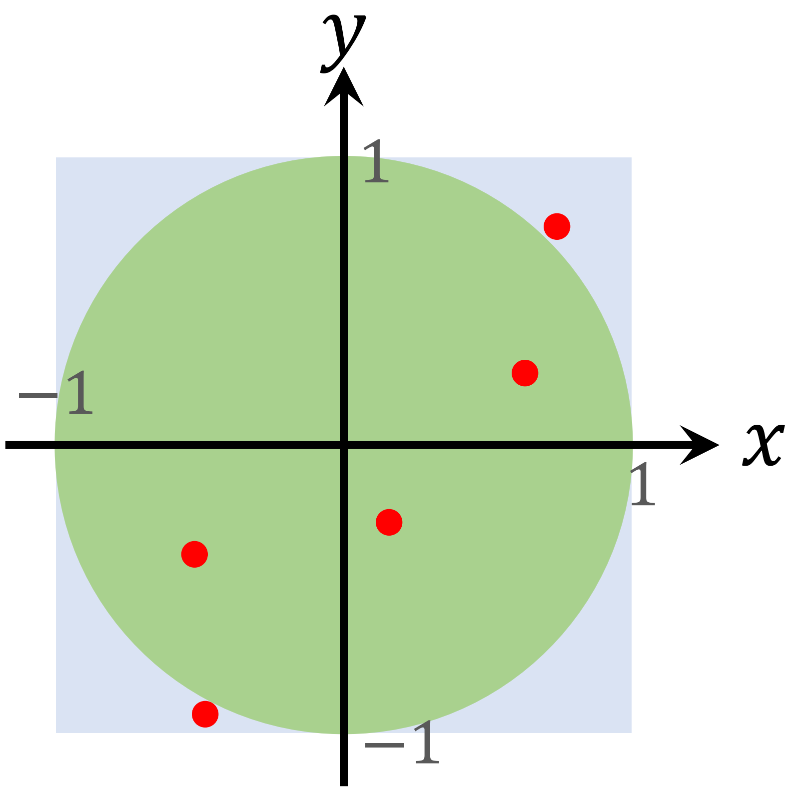
$$\frac{4m}{n} \to \pi, \quad \text{as } n \to \infty.$$

- Concentration bound:

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

Calculating Pi

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



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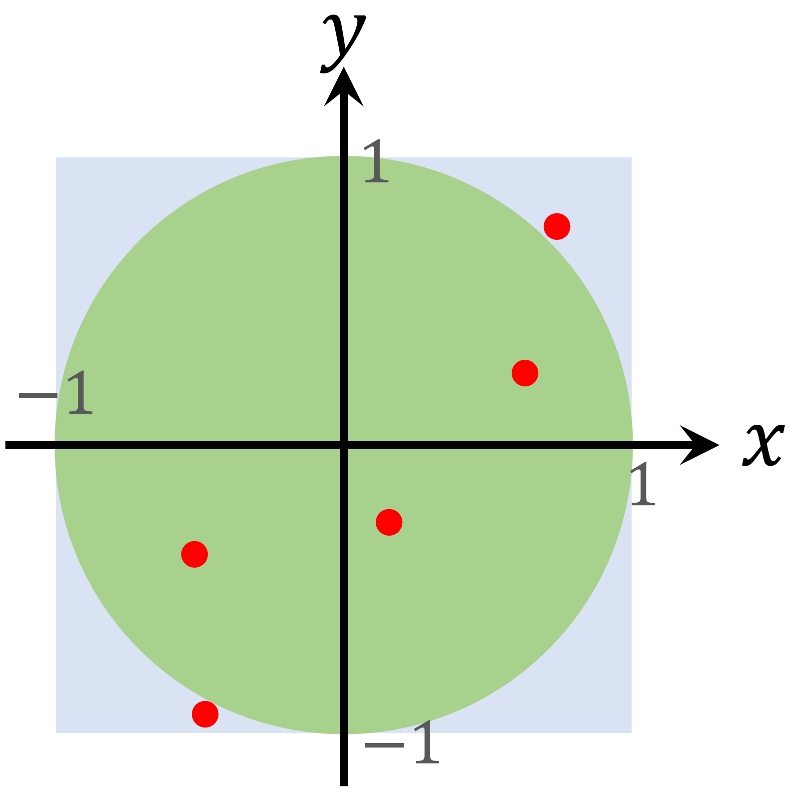

Algorithm

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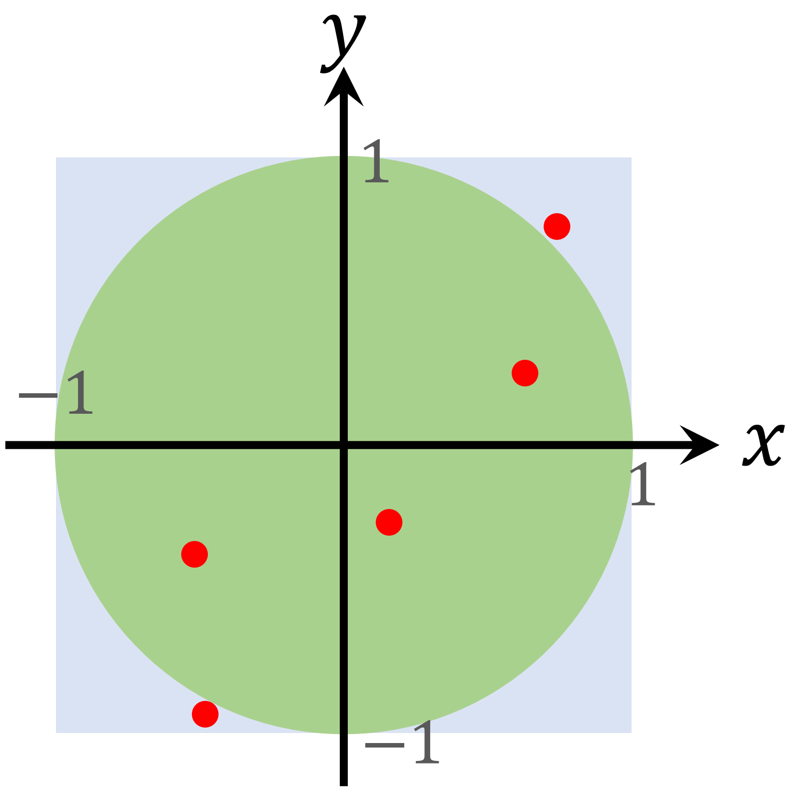


P3:随机数发生器

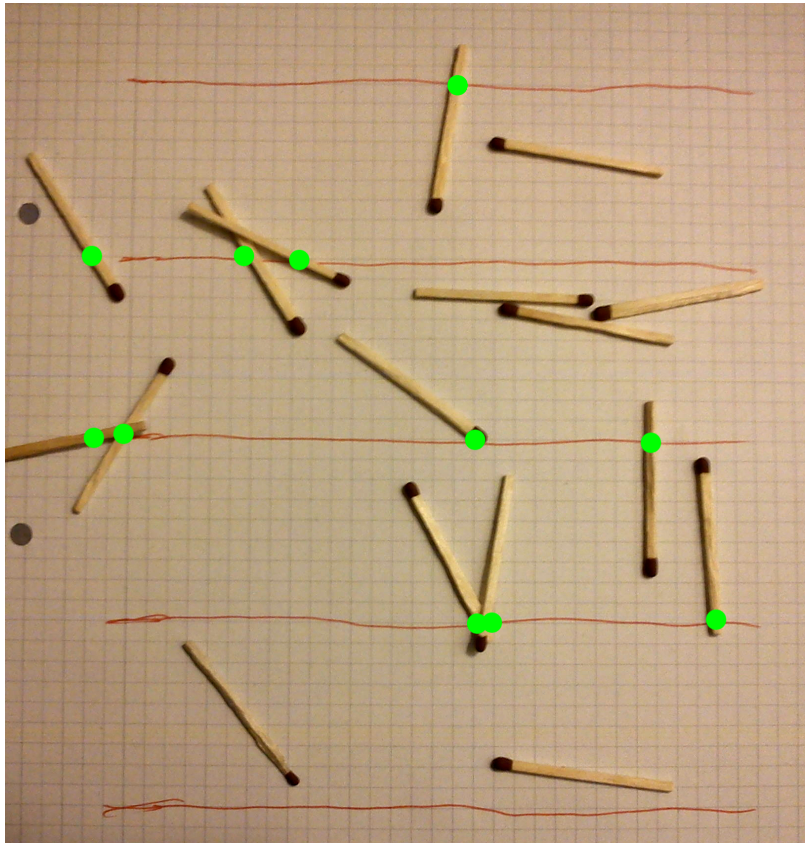
Algorithm

1. User specifies a big n; reset counter $m = 0$.
2. For $i = 1$ to n: 随机产生 n 个点（x,y），如果点在圆内 m计数+1
   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

Buffon's Needle Problem

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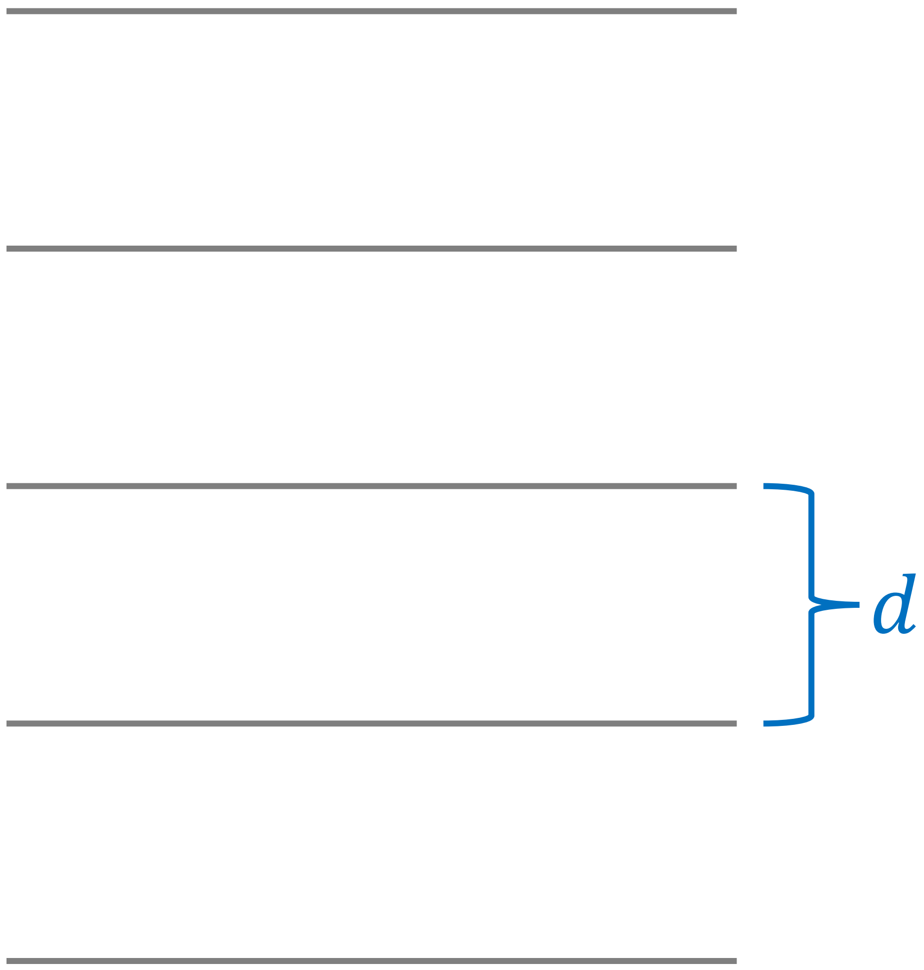
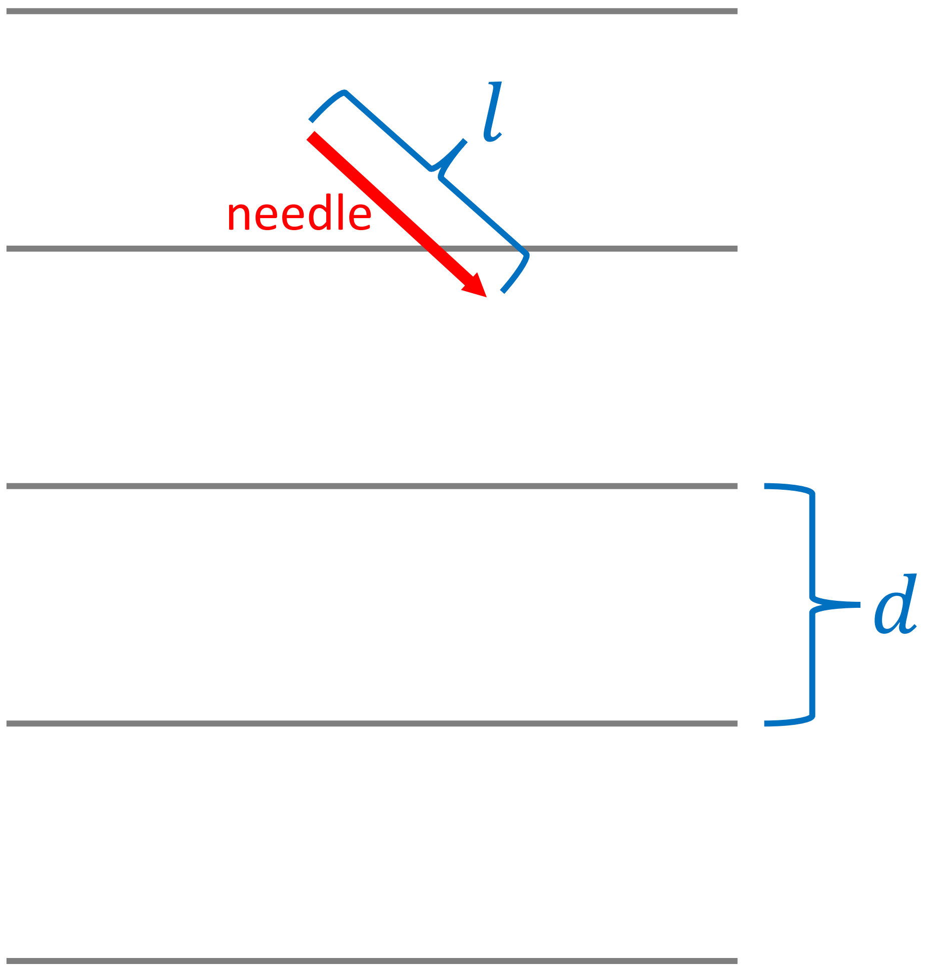


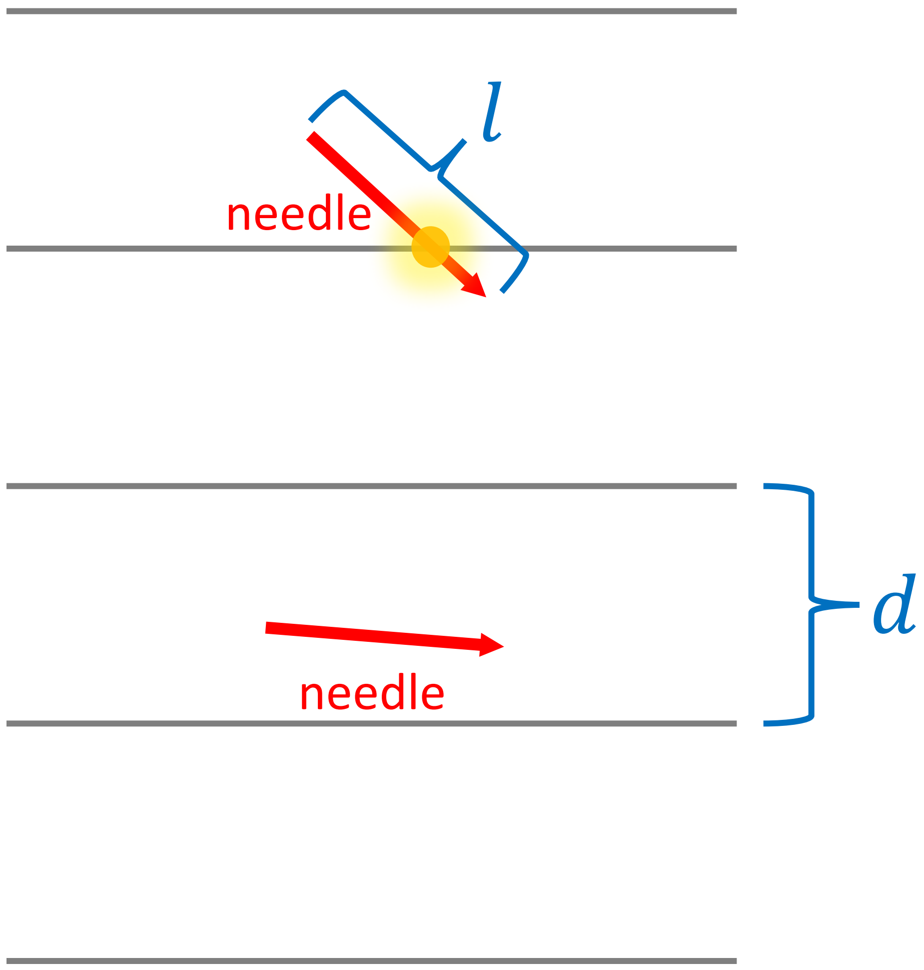
- The parallel lines have distance d.
- Needles have length l.

Buffon's Needle Problem



- 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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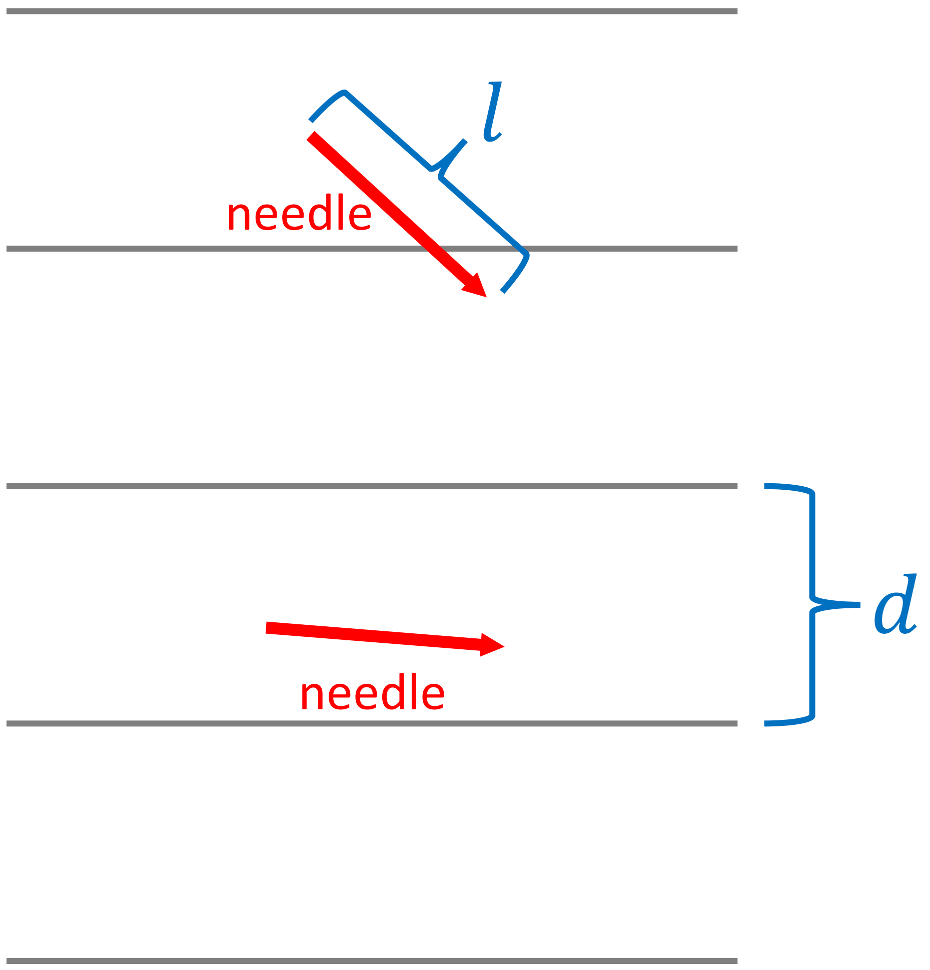
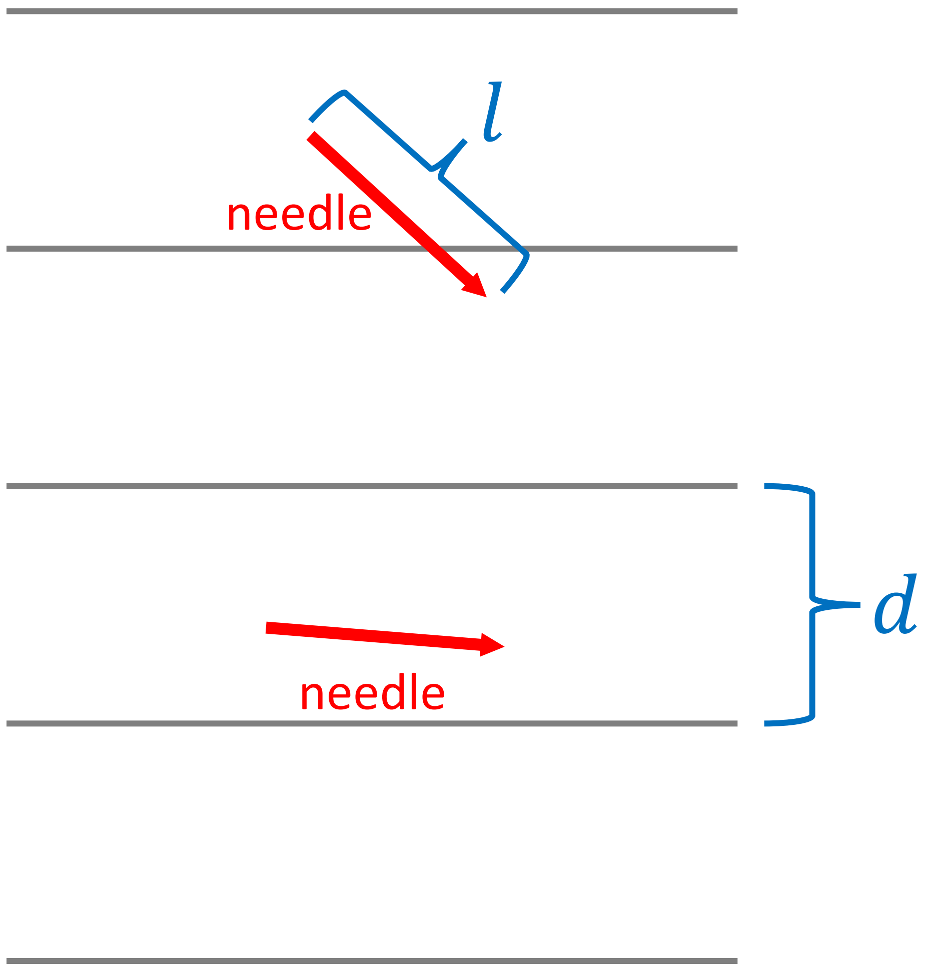


- The parallel lines have distance d.
- Needles have length l.
- Randomly throw a needle; the needle may or may not lie across a line.

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

- It can be proved using integral.

Buffon's Needle Problem



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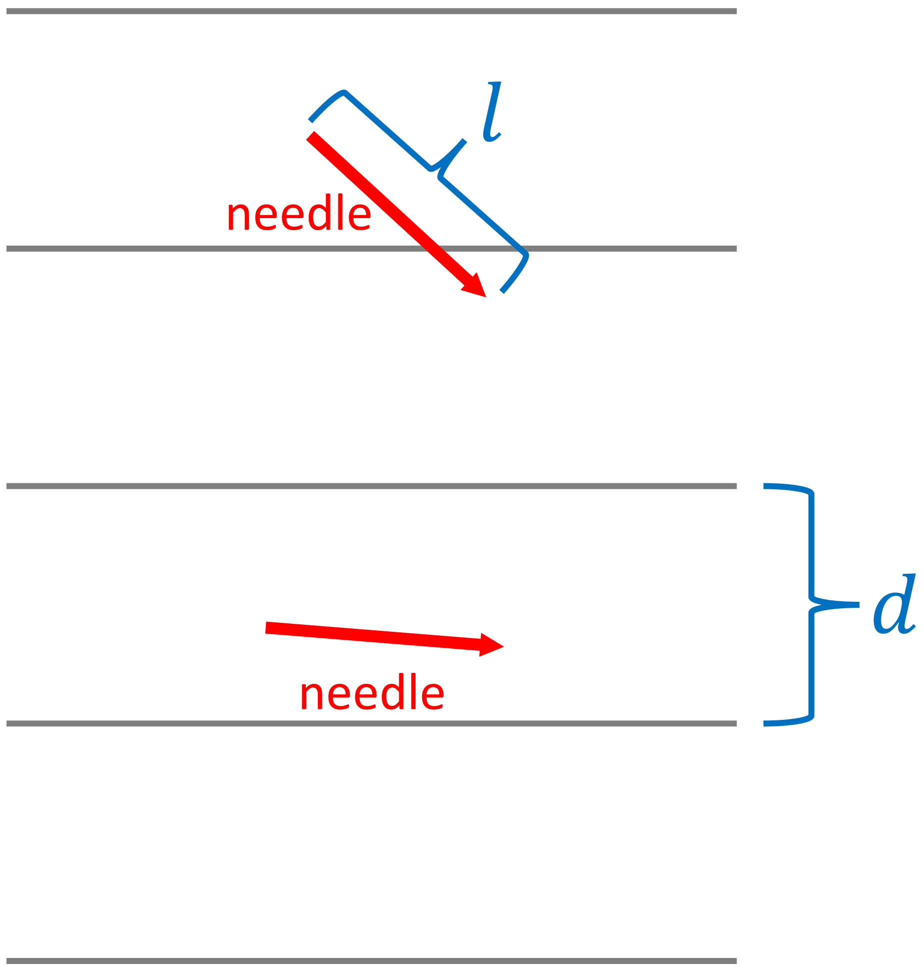
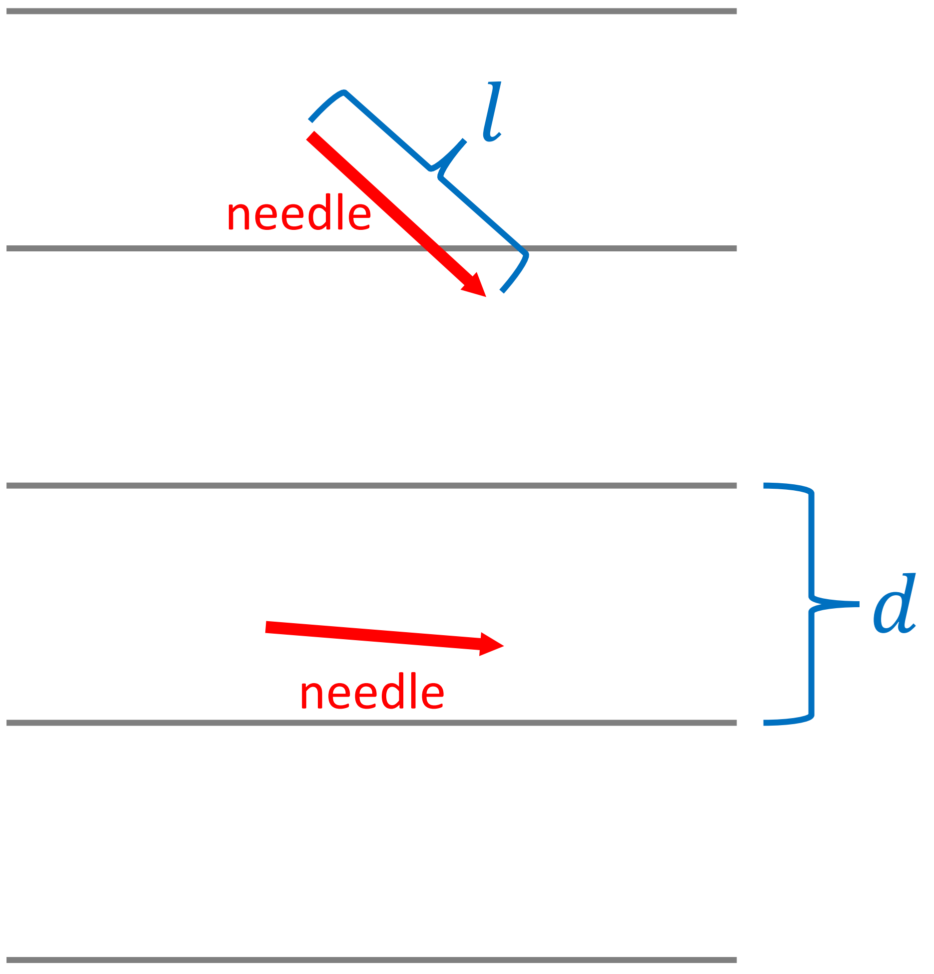


With probability $P = \frac{2l}{\pi d}$, they are across.

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

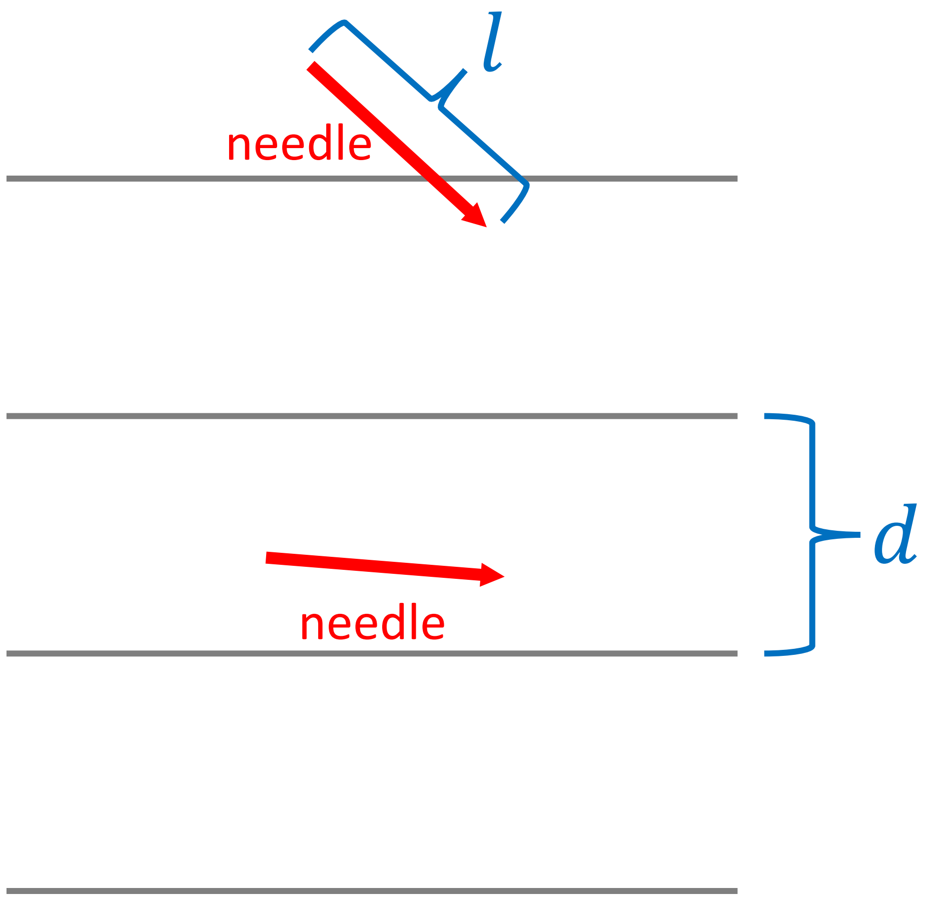
Buffon's Needle Problem



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, $m \approx \frac{2\,l\,n}{\pi\,d}$.

Buffon's Needle Problem



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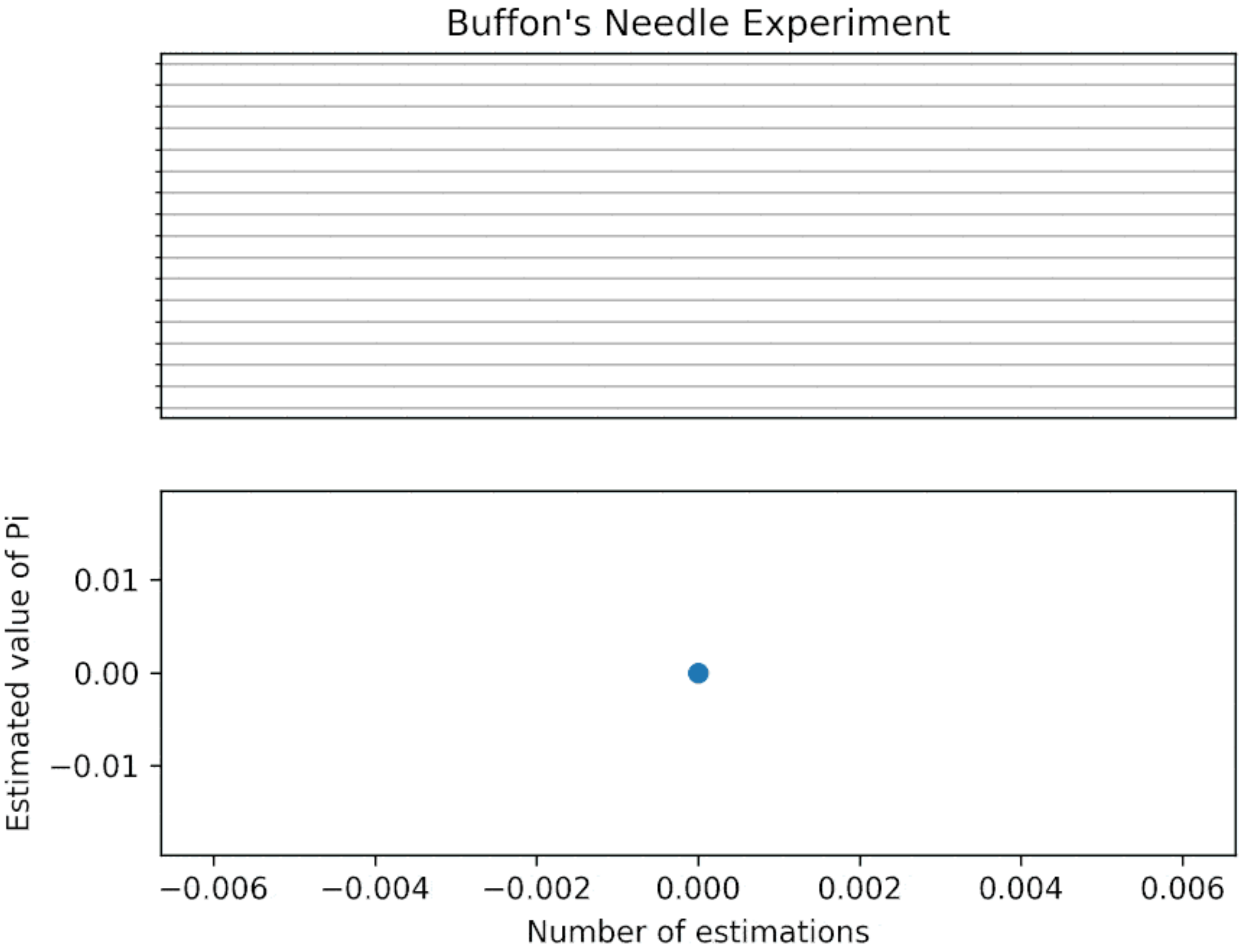
- Randomly throw a total of n needles.
- In expectation, $Pn = \frac{2ln}{\pi d}$ needles lie across the lines.
- Actually observe m needles across the lines.
- If n is big, $m \approx \frac{2\,l\,n}{\pi\,d}$.
- Thus, $\pi \approx \frac{2\,l\,n}{d\,m}$.

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

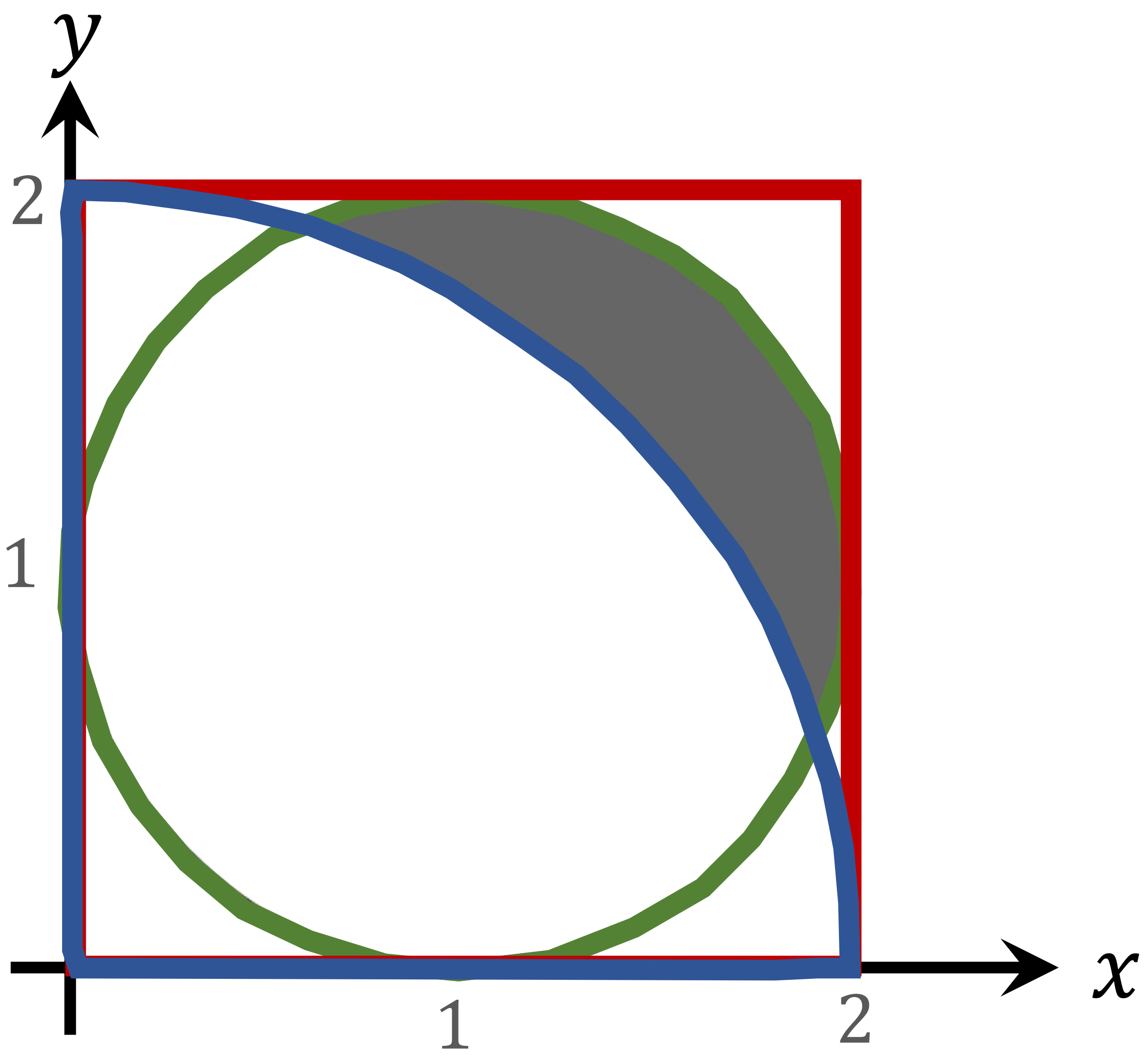
Buffon's Needle Problem



Application 3: Area of A Region

区域面积

What is the area of the grey region?



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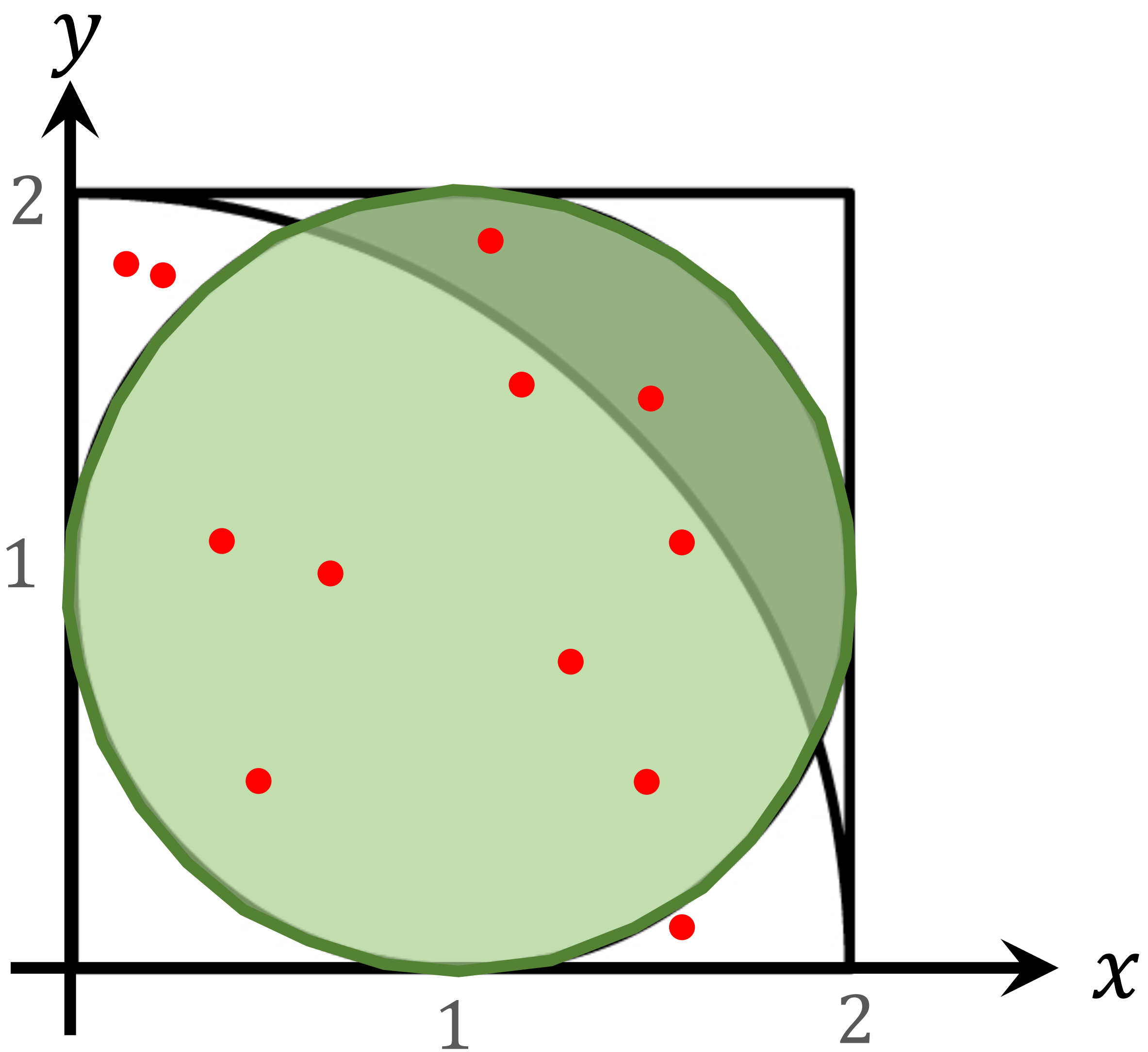

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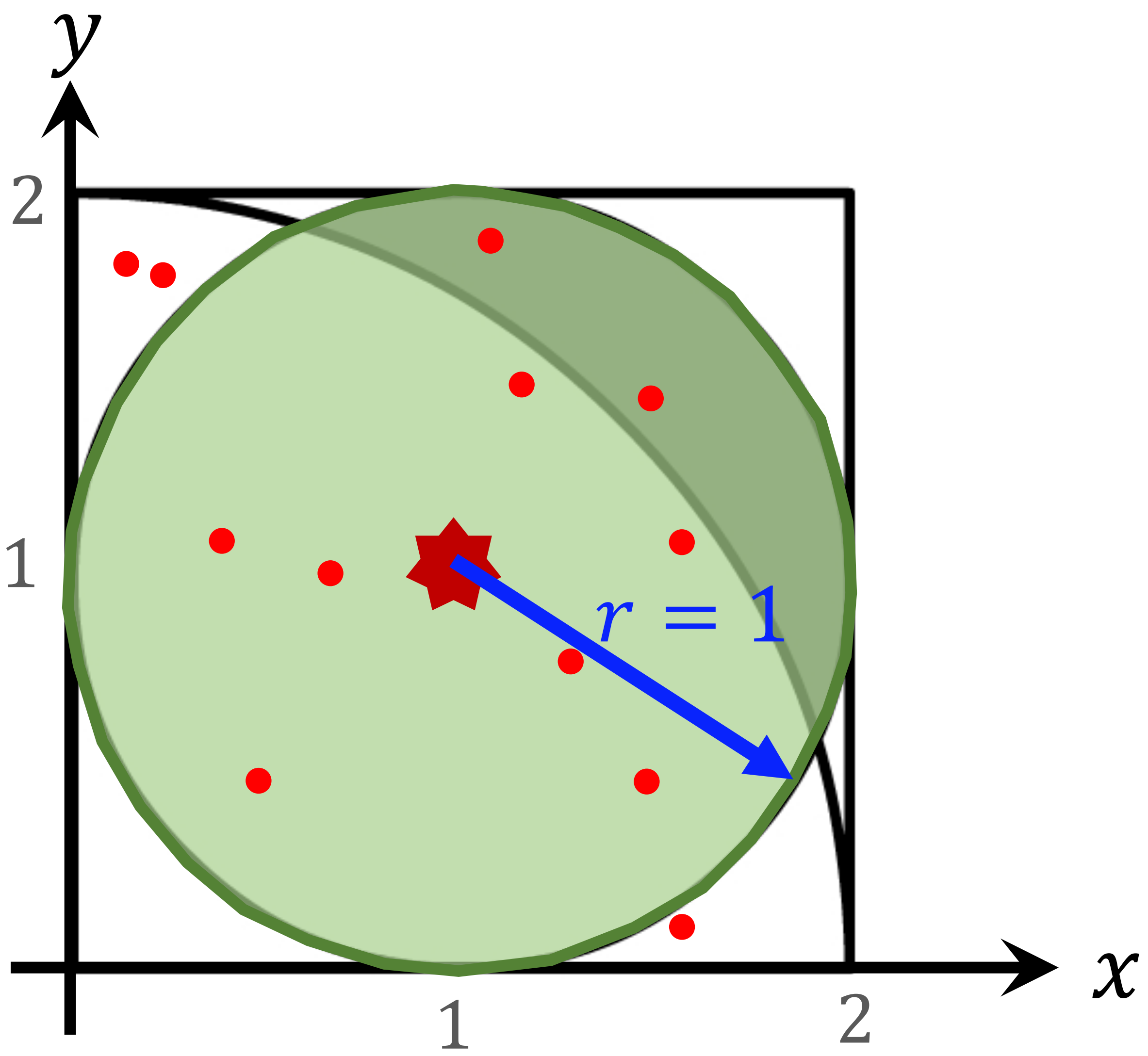
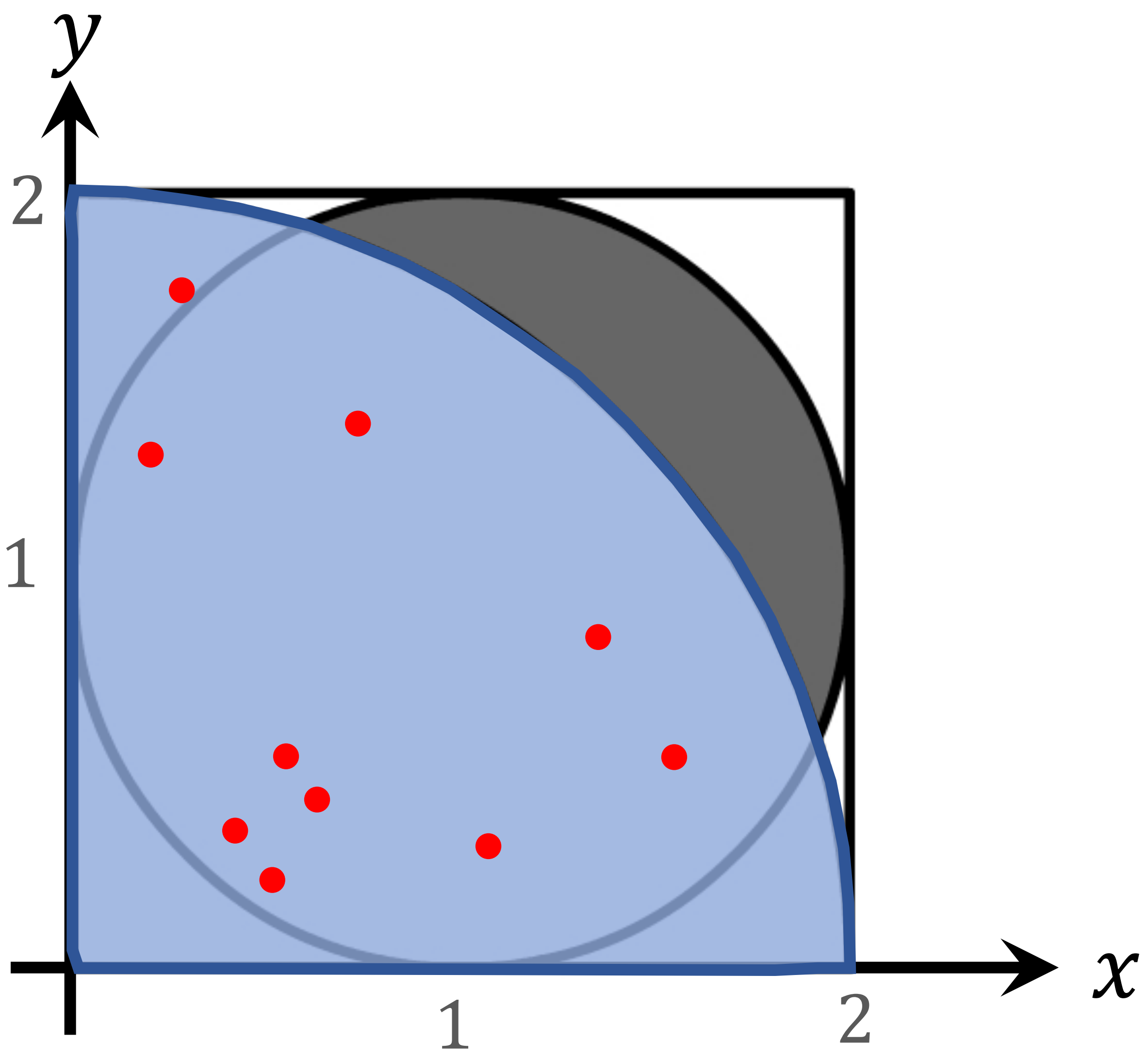


- If a point (x, y) is in the circle, it must satisfy

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

What is the area of the grey region?



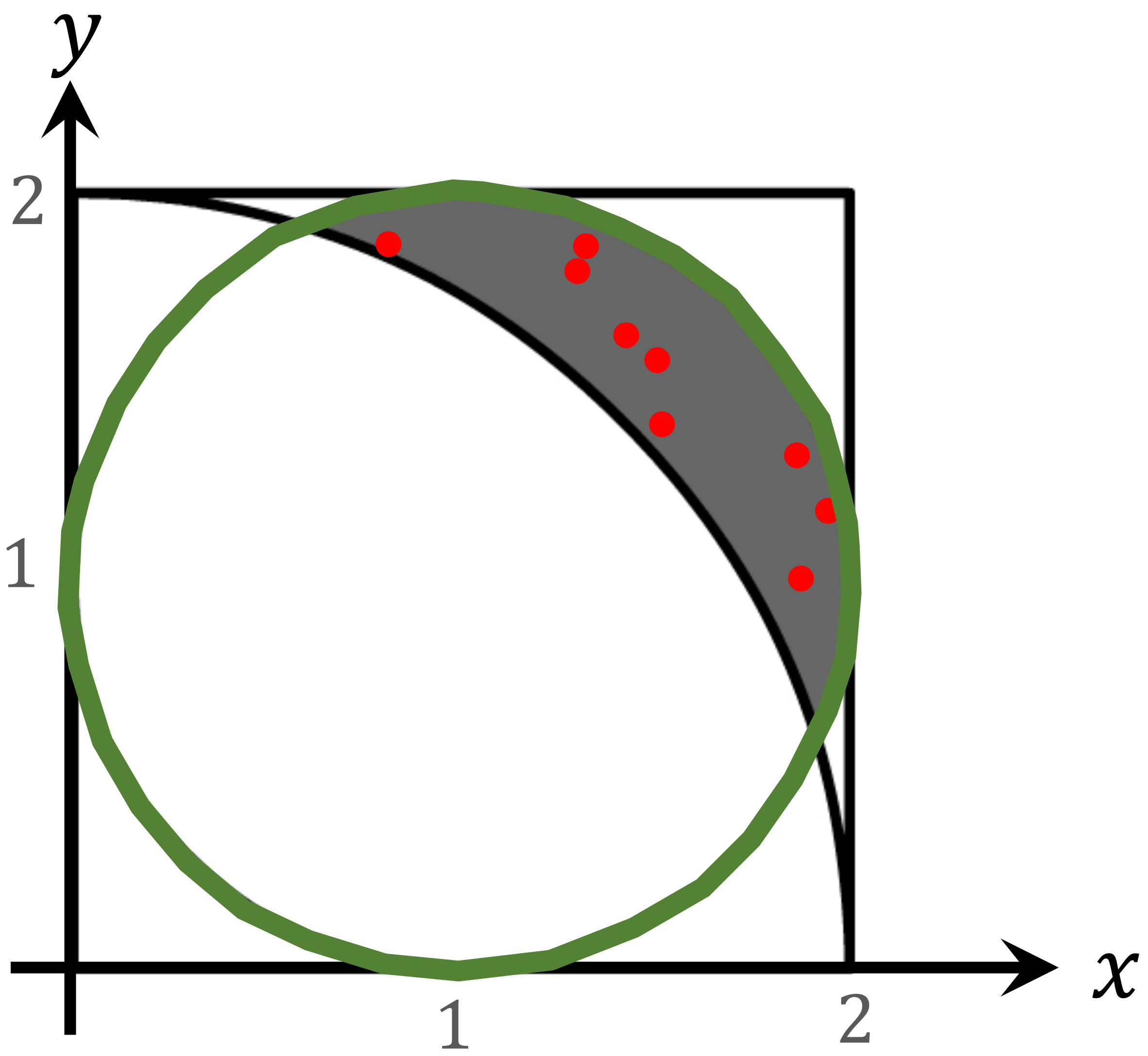
- If a point (x, y) is in the circle, it must satisfy

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

- 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?

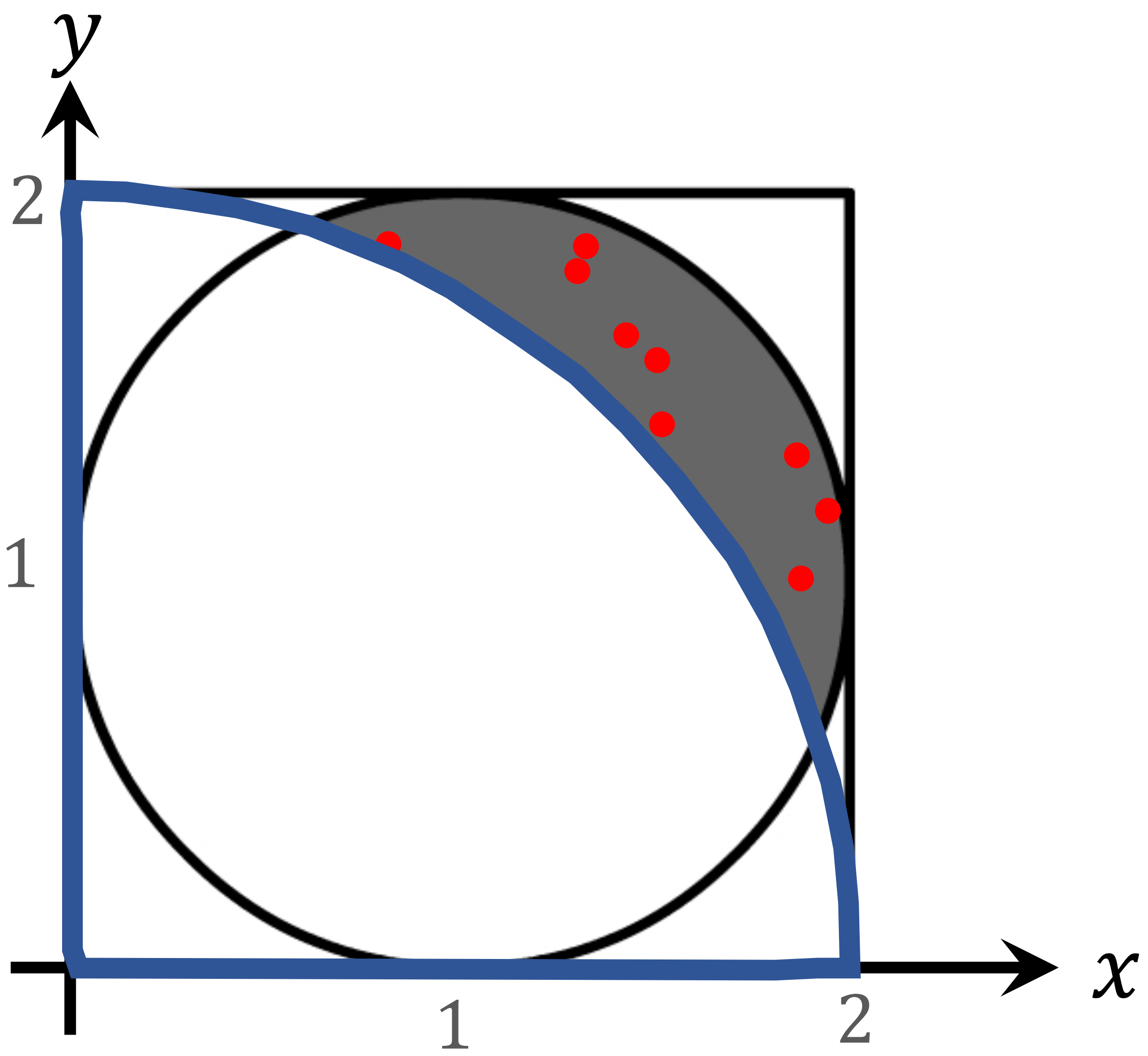


- A point (x, y) in the grey region satisfies both of

$$\boxed{1.\ (x-1)^2 + (y-1)^2 \le 1,}$$

2. $x^2 + y^2 > 2^2$.

What is the area of the grey region?



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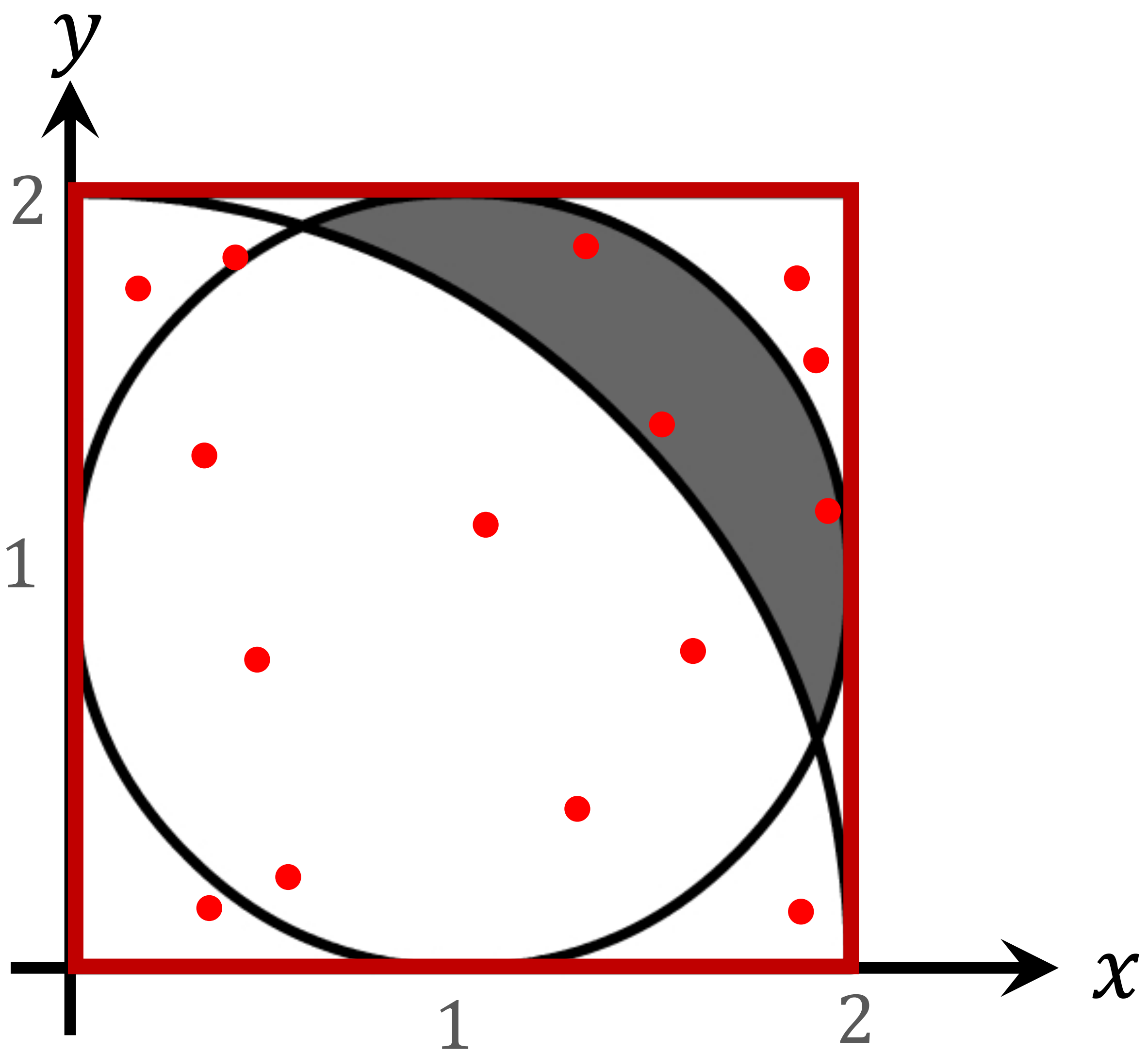
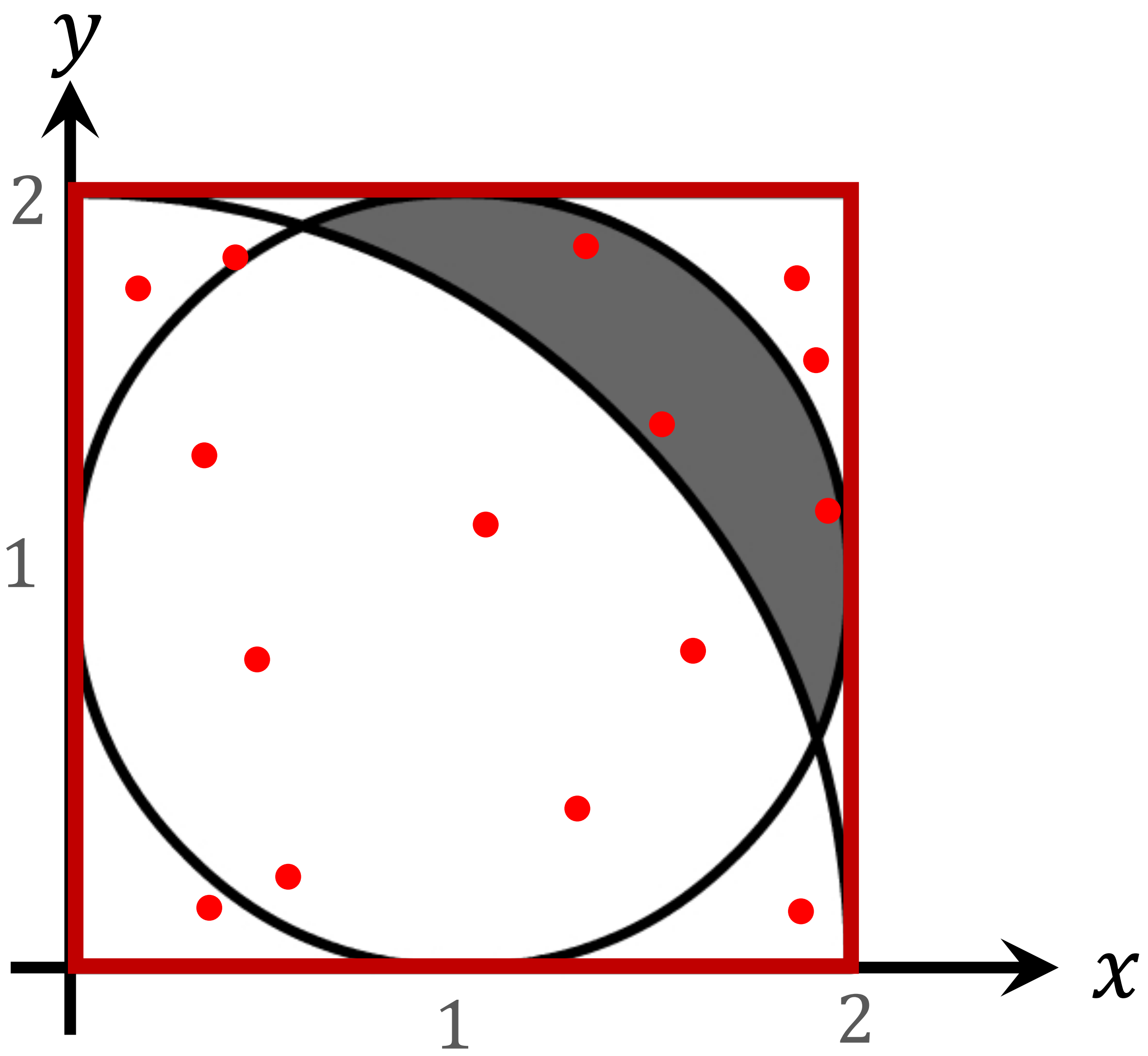


- Area of the square: $A_1 = 2^2 = 4.$

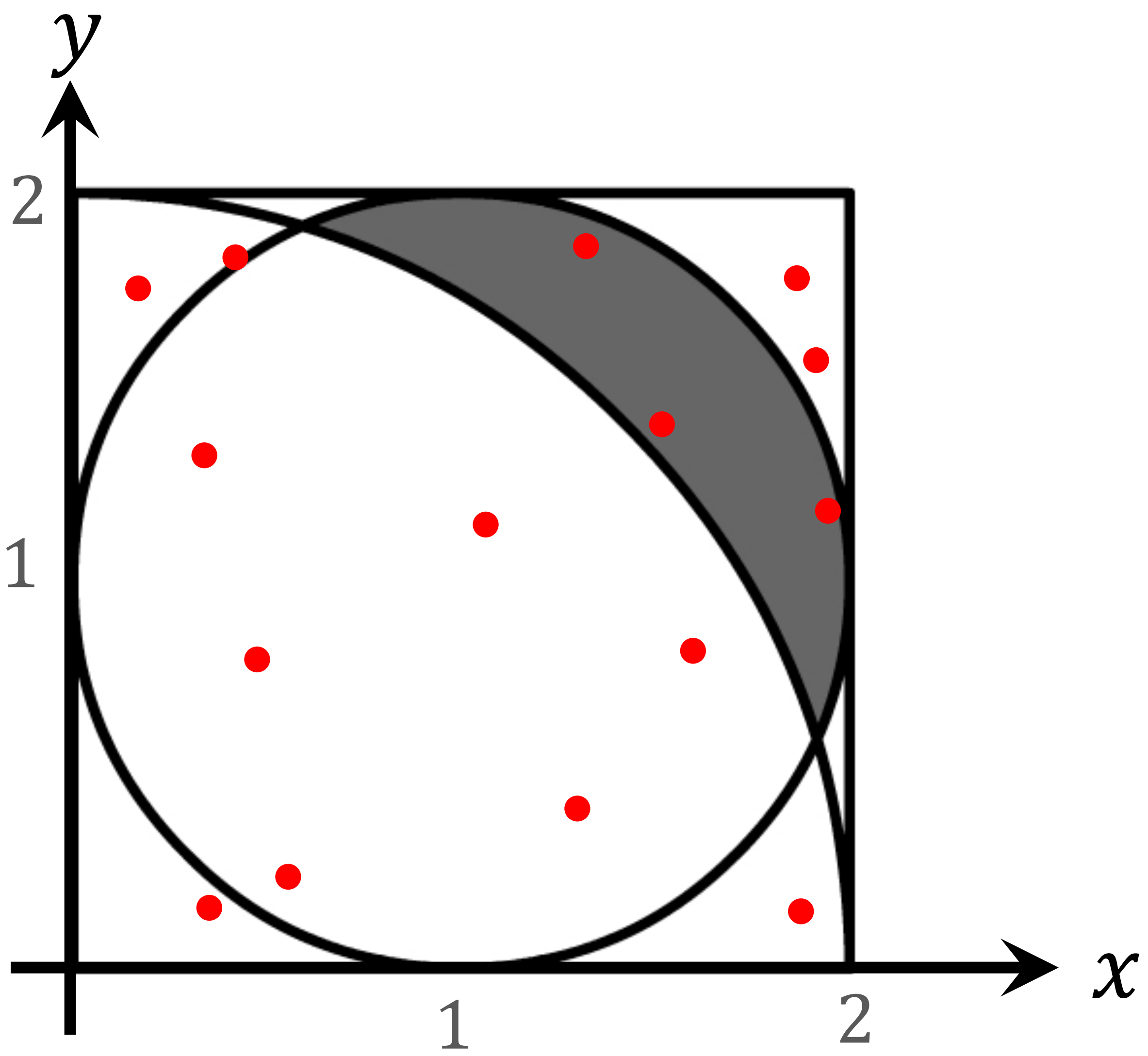
What is the area of the grey region?



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

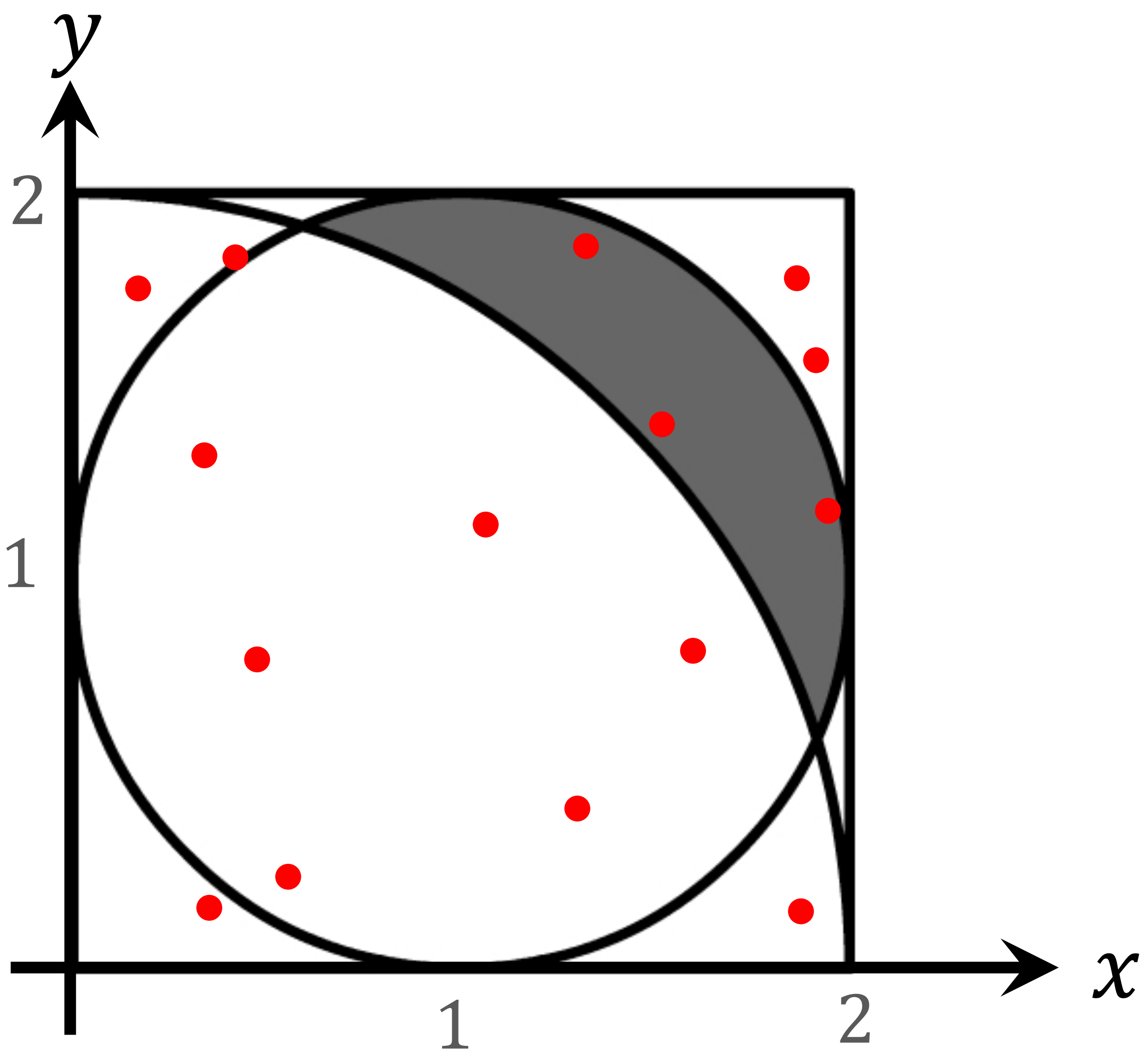
$$P = \frac{A_2}{A_1} = \frac{A_2}{4}.$$

What is the area of the grey region?



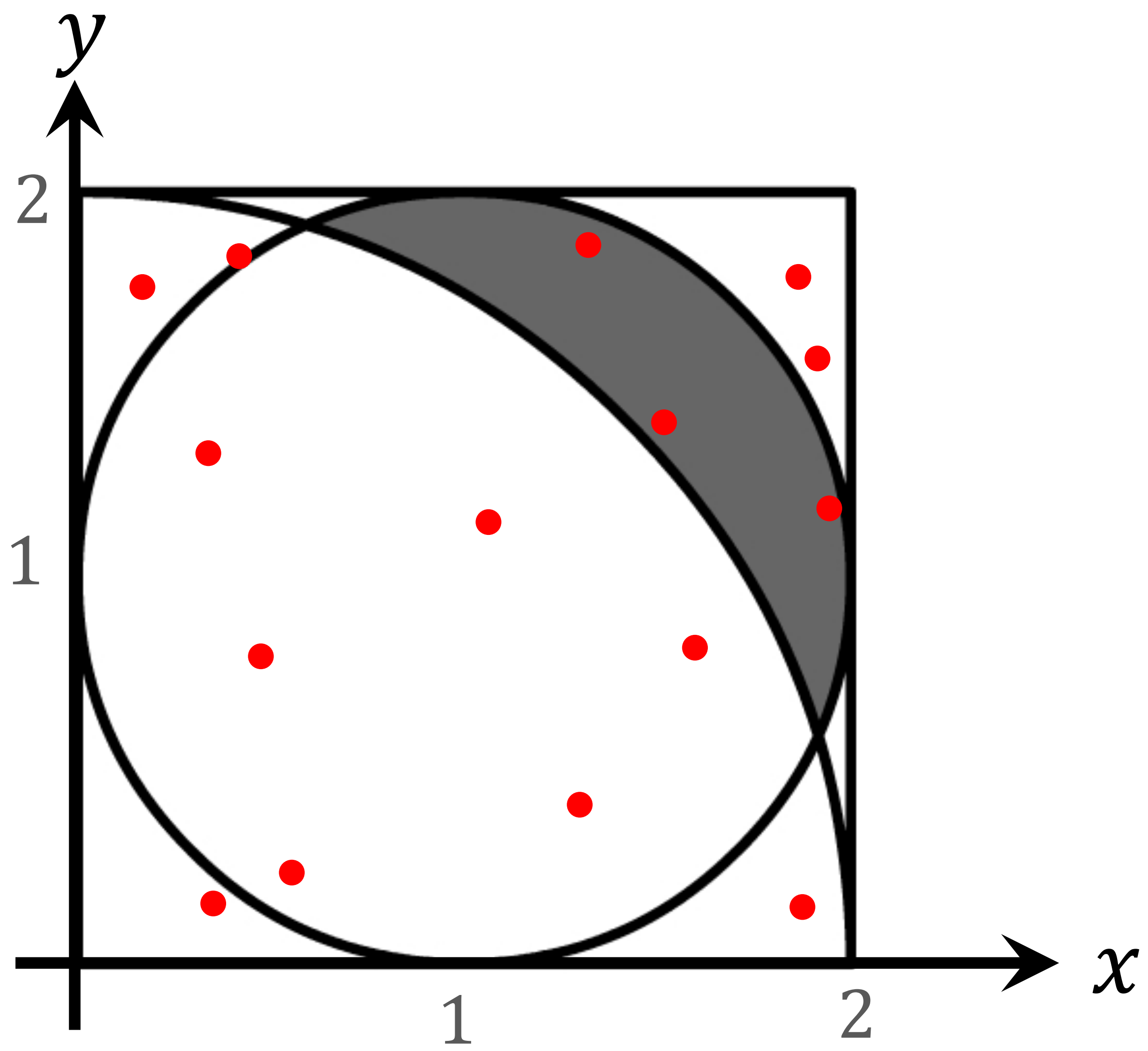
- Uniformly sample n points from the square $[0, 2]\times[0, 2]$.
- In expectation, $\boxed{nP} = \boxed{\frac{n\, A_2}{4}}$ points fall in the grey region.

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 $\boxed{m \approx \frac{n\,A_2}{4}}$.
- Thus, $\boxed{A_2 \approx \frac{4m}{n}}$.

What is the area of the grey region?



Algorithm

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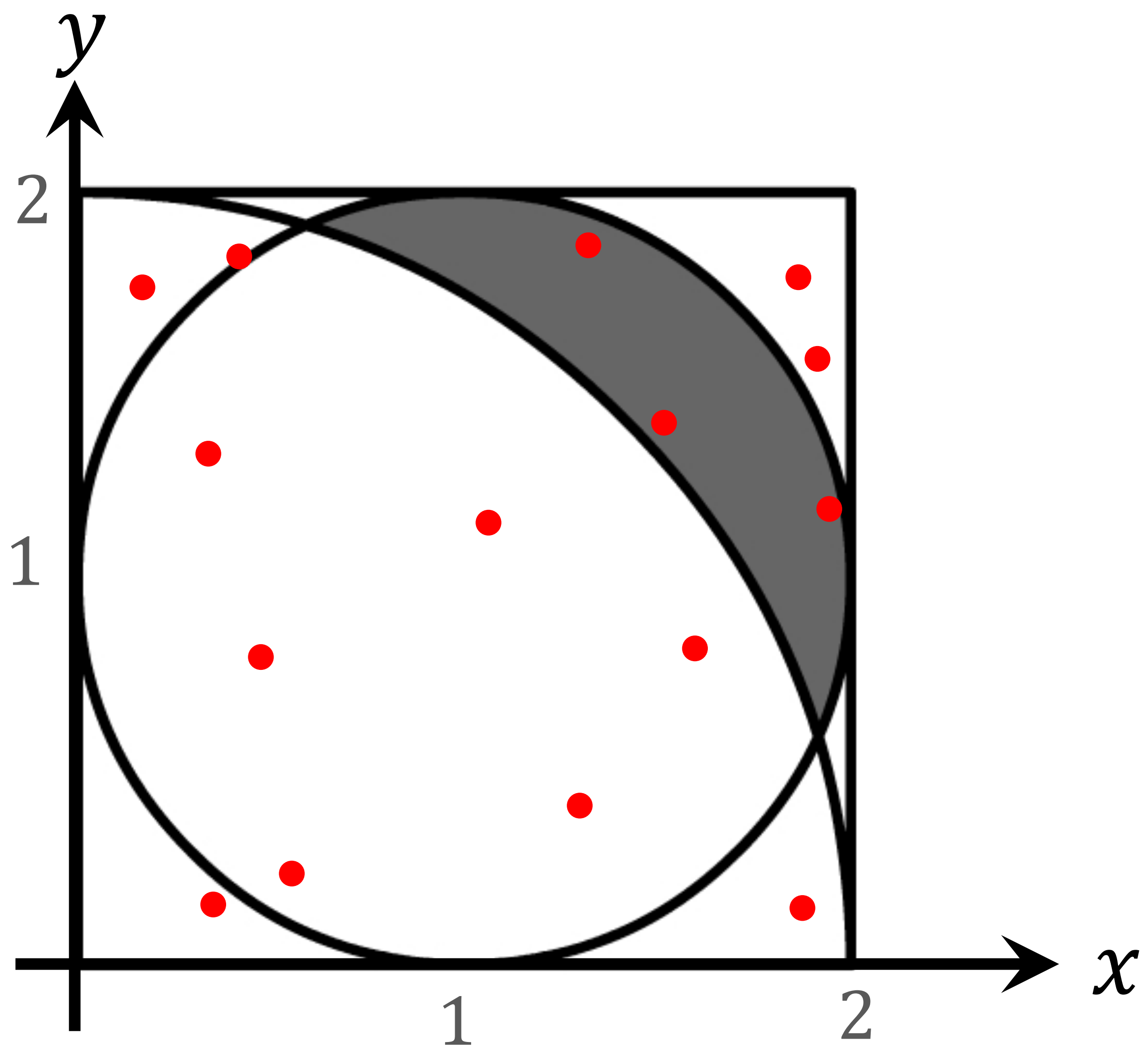

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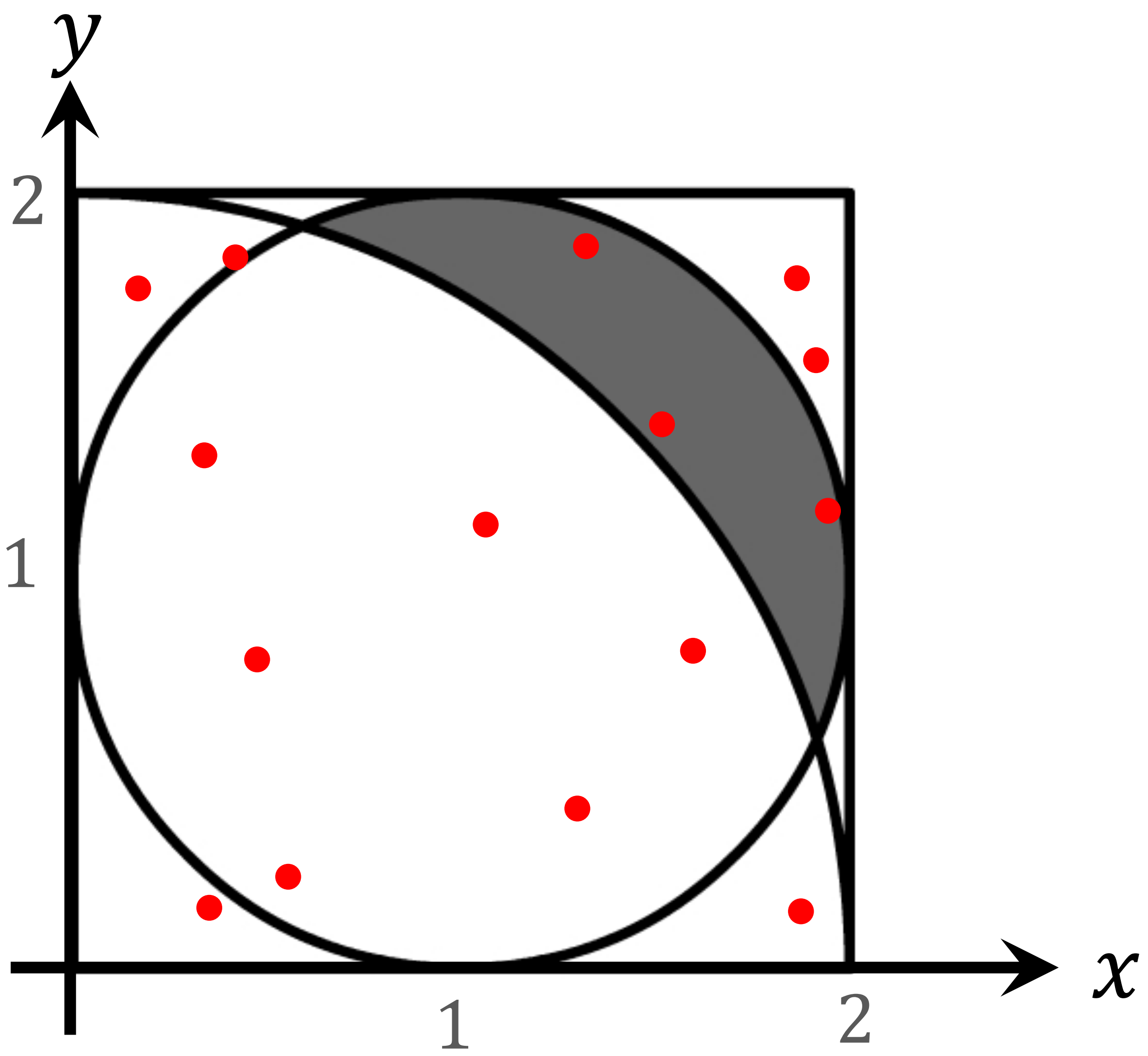

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   a) Randomly generate $x \in [0, 2]$.
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   c) If both of the following conditions are satisfied, then $m \leftarrow m + 1$:
      i. $(x-1)^2 + (y-1)^2 \leq 1$.
      ii. $x^2 + y^2 > 2^2$.
3. Return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

Application 4: Integration

Integration

- We are given a function, e.g. $\boxed{f(x) = \frac{1}{1+\sin(x)\cdot(\log_{\mathrm{e}} x)^2}.}$
- Calculate the integral: $I = \int_{0.8}^{3} f(x)\, dx$.

Integration

- We are given a function, e.g., $f(x) = \frac{1}{1+\sin(x)\cdot(\log_e x)^2}$.
- 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.
  非常复杂的
- Using Monte Carlo to approximate the integral.

Monte Carlo Integration (Univariate)

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

Monte Carlo Integration (Univariate)

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1. Draw n samples from $[a, b]$ uniformly at random; denote them by $x_1, \cdots, x_n$.

Monte Carlo Integration (Univariate)

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

1. Draw n samples from $[a, b]$ uniformly at random; denote them by $x_1, \cdots, x_n$.
2. Calculate $\boxed{Q_n} = \boxed{(b-a)} \cdot \boxed{\frac{1}{n}\sum_{i=1}^{n}} \boxed{f(x_i)}$

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2. Calculate $Q_n = (b - a) \cdot \frac{1}{n} \sum_{i=1}^{n} f(x_i)$.
3. Return $\boxed{Q_n}$ as an approximation to the integral $\boxed{I = \int_a^b f(x)\,dx}$

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3. Return Q_n as an approximation to the integral $I = \int_a^b f(x)\,dx$.

Theory: Law of large numbers guarantees $\boxed{Q_n \to I}$, as $\boxed{n \to \infty}$

Monte Carlo Integration (Univariate): Example

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

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 $x_1, \cdots, x_n$.

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 $Q_n = \boxed{2.2}\ \boxed{\frac{1}{n}\sum_{i=1}^{n}}\boxed{f(x_i)}$

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 $I = \int_\Omega f(\mathbf{x})\, d\mathbf{x}$.

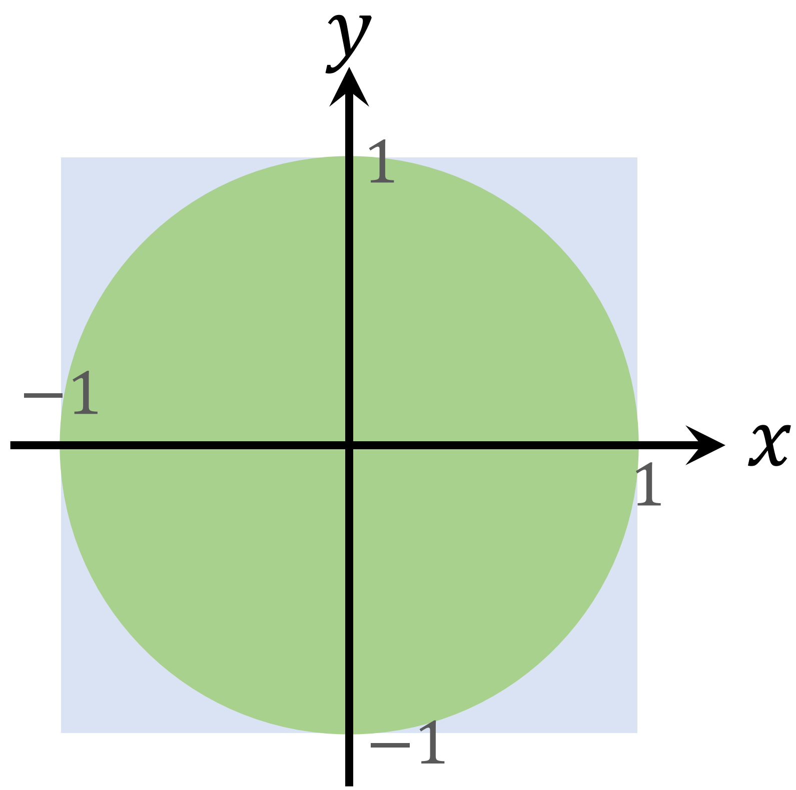
1. Draw n samples from set Ω uniformly at random; denote them by $\mathbf{x}_1, \cdots, \mathbf{x}_n$.
2. Calculate $V = \int_\Omega d\mathbf{x}$.

Monte Carlo Integration (Multivariate)

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

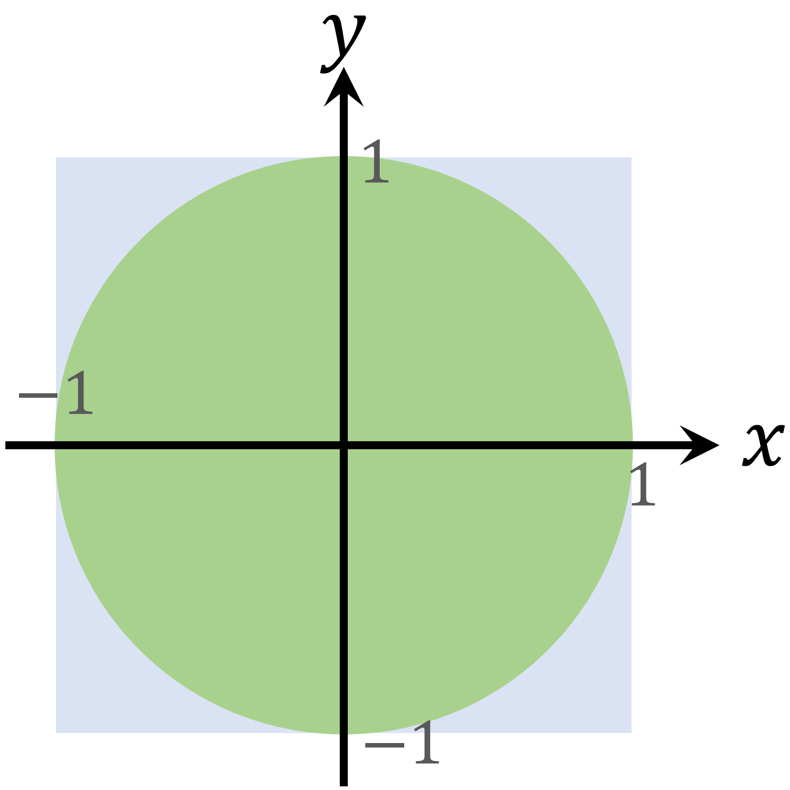
1. Draw n samples from set Ω uniformly at random; denote them by $\mathbf{x}_1, \cdots, \mathbf{x}_n$.
2. Calculate $V = \int_\Omega d\mathbf{x}$.
3. Calculate $\boxed{Q_n} = \boxed{V}\, \boxed{\frac{1}{n}\sum_{i=1}^{n}}\, \boxed{f(\mathbf{x}_i)}$
4. Return Q_n as an approximation to the integral $I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

Monte Carlo Integration: Bivariate Example



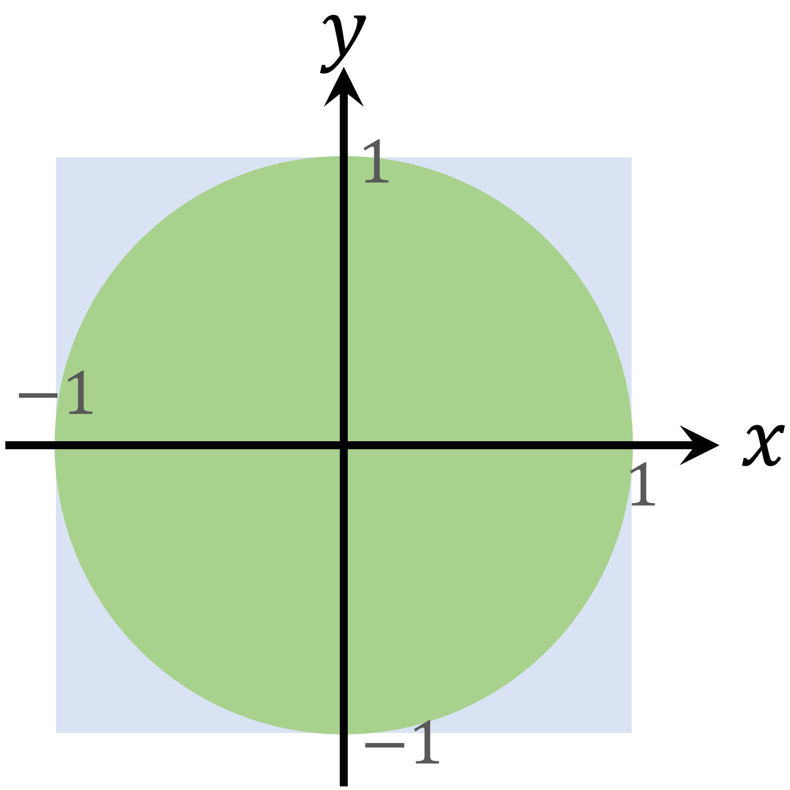
- Let $\boxed{f(x,y)} = \begin{cases} 1, \text{if } x^2 + y^2 \le 1; \\ 0, \quad \text{otherwise.} \end{cases}$

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



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- Let $\Omega = [-1,1]\times[-1,1]$.
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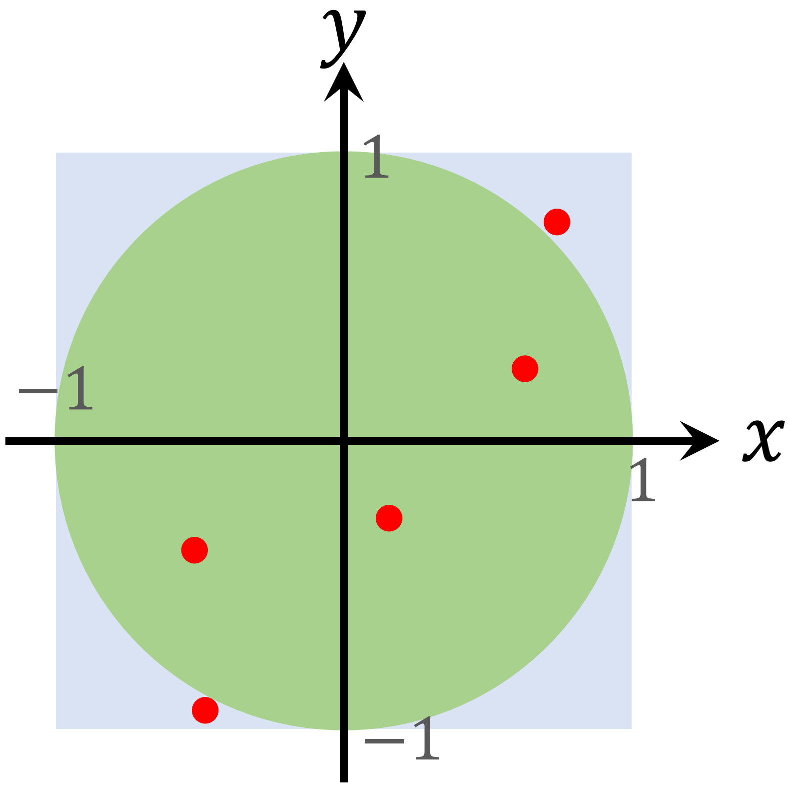
- I is the area of the circle:

$$\boxed{I = \pi r^2 = \pi.}$$

Monte Carlo Integration: Bivariate Example



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

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

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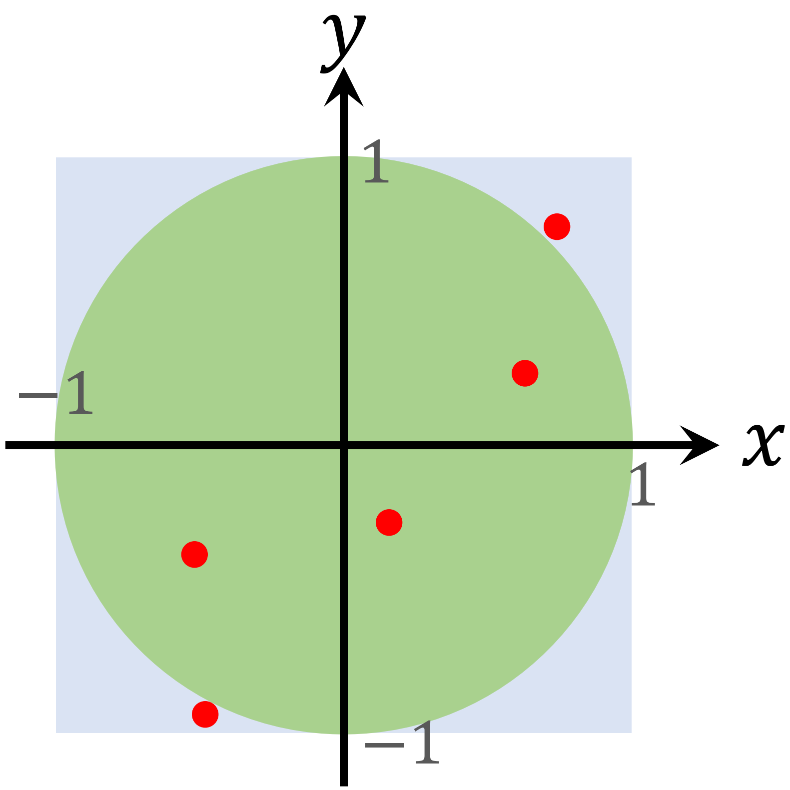

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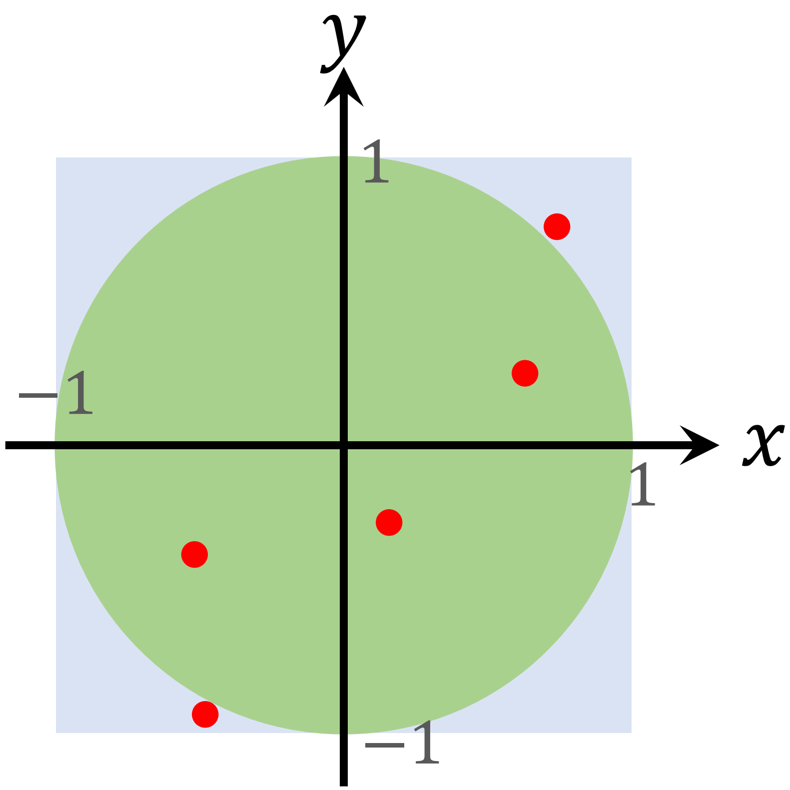
Monte Carlo Integration: Bivariate Example



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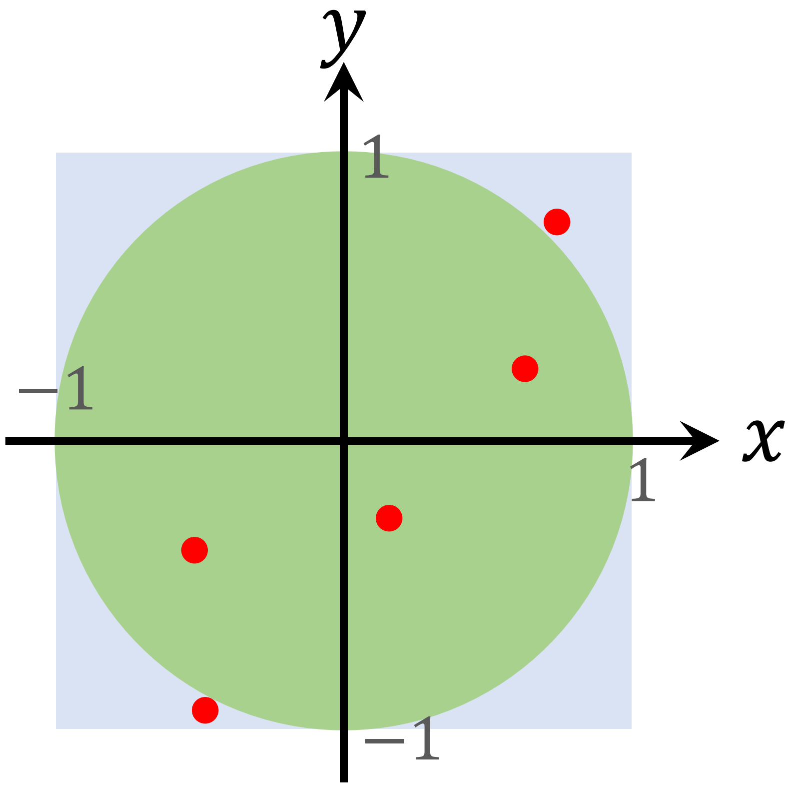
Monte Carlo Integration: Bivariate Example



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3. Calculate $Q_n = V \cdot \frac{1}{n} \sum_{i=1}^{n} f(x_i, y_i)$.
4. Return $\boxed{Q_n}$ as an approximation to the integral $\boxed{\pi = \int_\Omega f(x, y)\, dx\, dy}$

Application 5: Estimate of Expectation

期望估计

Expectation

- Let X be a d-dimensional random vector.
- Let $p(\mathbf{x})$ be a probability density function (PDF).

概率密度函数

Expectation

- Let X be a d-dimensional random vector.
- Let $p(\mathbf{x})$ be a probability density function (PDF).
  - Property: $\boxed{\int_{\mathbb{R}^d} p(\mathbf{x})\, d\mathbf{x} = 1}$

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 $\boxed{p(x) = \frac{1}{t}}$ for $\boxed{x \in [0, t]}$

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 $\boxed{p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right]}$.

Expectation

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

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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Monte Carlo Estimate of Expectation

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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

蒙特卡洛及其他

Monte Carlo

Casino de Monte-Carlo, Monaco

- The term “Monte Carlo method" was firstly 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. 蒙特卡罗是指依靠重复随机抽样来获得数值结果的算法
- The output of Monte Carlo algorithms can be incorrect. 蒙特卡罗算法的输出可能会不正确
  - In all of our examples, the algorithms' outputs are incorrect. 在我们所有的例子中，算法的输出都是不正确的。
  - But they are close to the correct solution. 但它们已经接近于正确的解决方案

Monte Carlo Algorithms

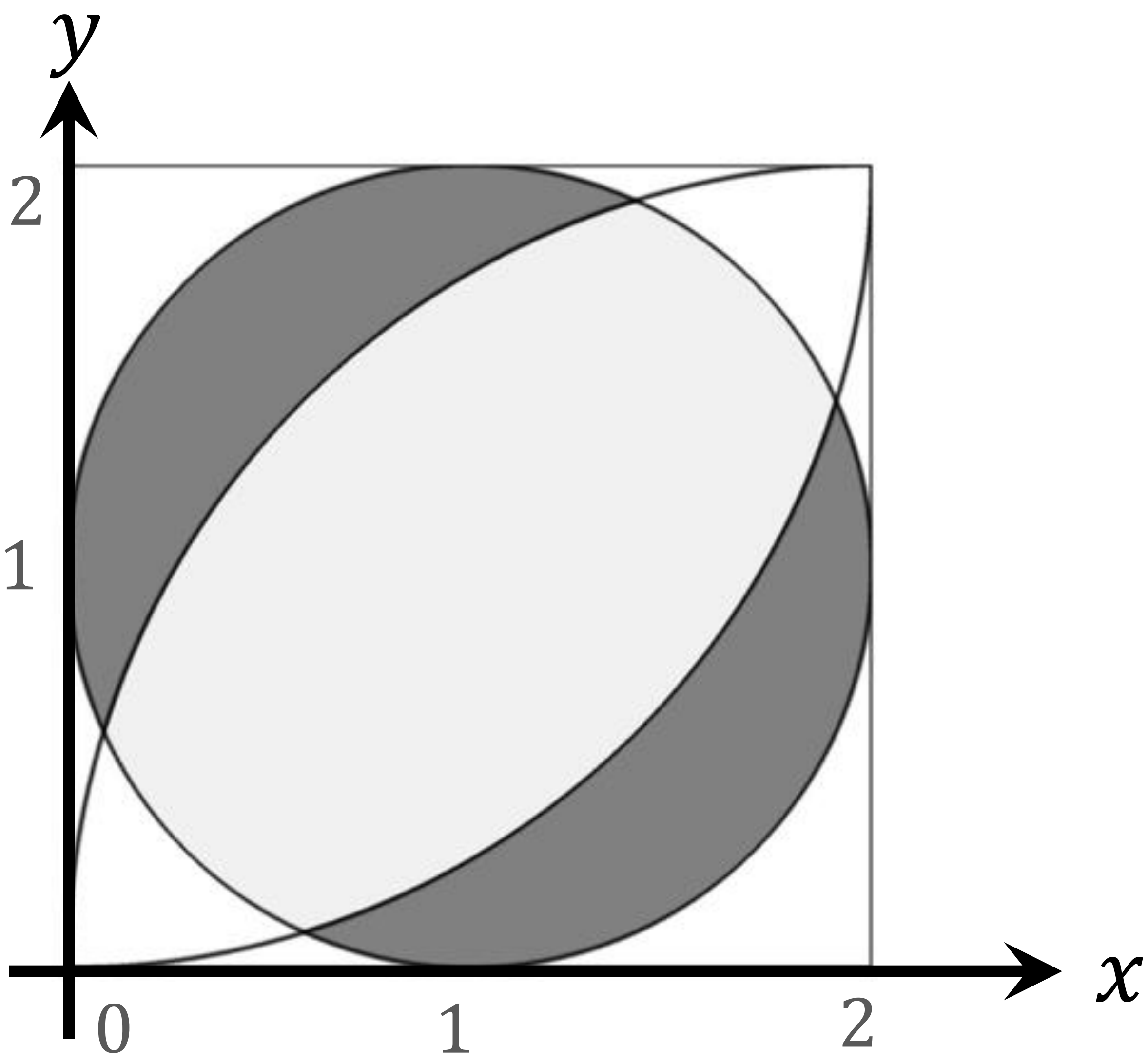
- Monte Carlo refers to algorithms that rely on repeated random sampling to obtain numerical results.
- The output of Monte Carlo algorithms can be incorrect.
- Las Vegas algorithms are those always produce the correct answers.
  - E.g., random quicksort.

拉斯维加斯的算法总是能产生正确的答案

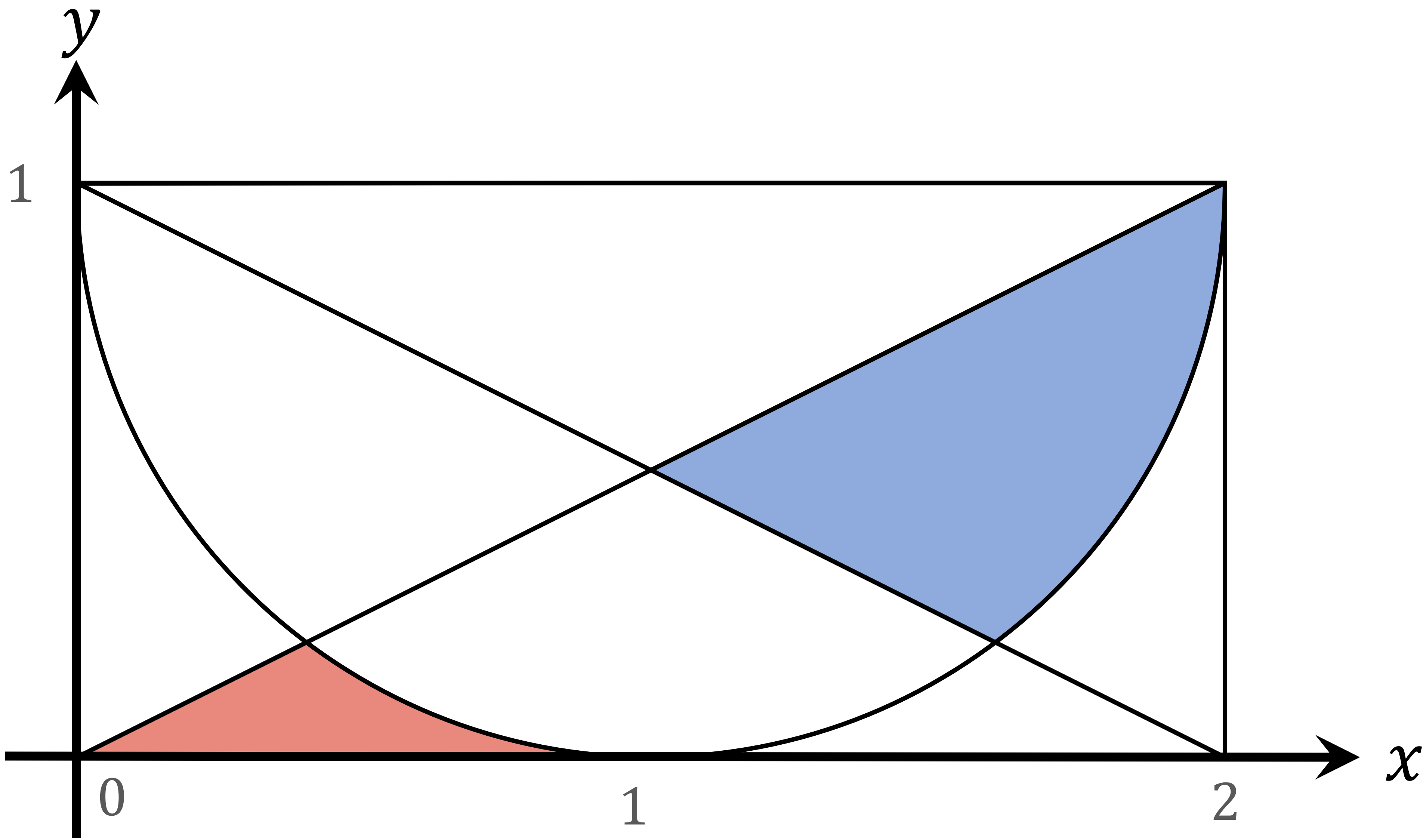
- Atlantic City algorithms are polynomial-time randomized algorithms that answer correctly w.p. greater than 75%.

Question

What is the area of the grey region?



What are the areas of the red and blue regions?



Thank you!