

2019 Workshop on Gravitational Waves and High-Performance Computing

Geoffrey Lovelace

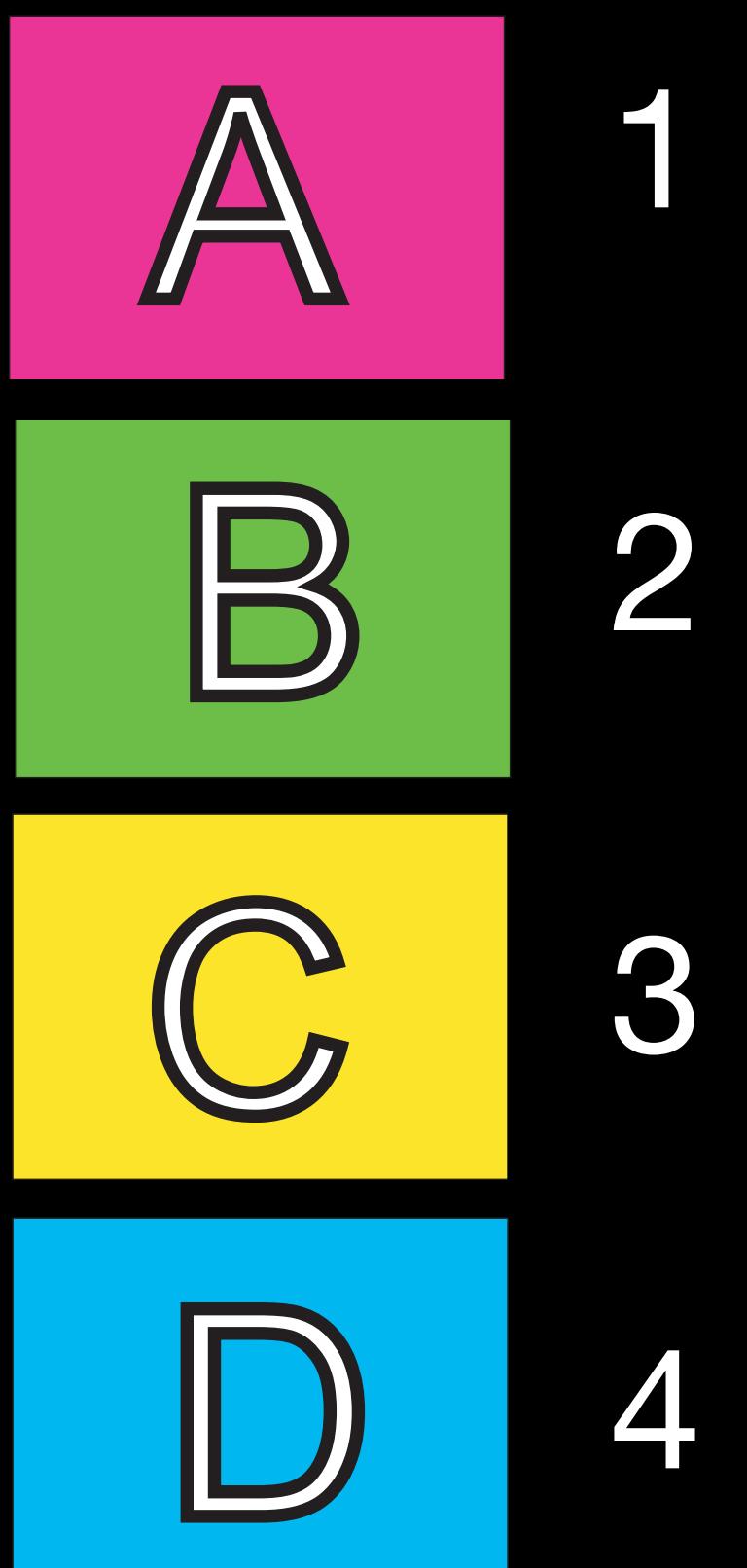
August 19, 2019 – August 23, 2019

Day 2

Clicker question #2.3

- What does this program print?

```
j = 1
while j < 3:
    j = j + 1
print(j)
```



Clicker question #2.4

- What does this program print?

```
product = 1
j = 1
while j < 3:
    product = product * j
    j = j + 1
print(product)
```

- A 1
- B 2
- C 6
- D 24

Clicker question #2.4b

- What does this program print?

```
product = 1
j = 1
while j < 4:
    product = product * j
    j = j + 1
print(product)
```

- A 1
- B 2
- C 6
- D 24

Clicker question #2.4c

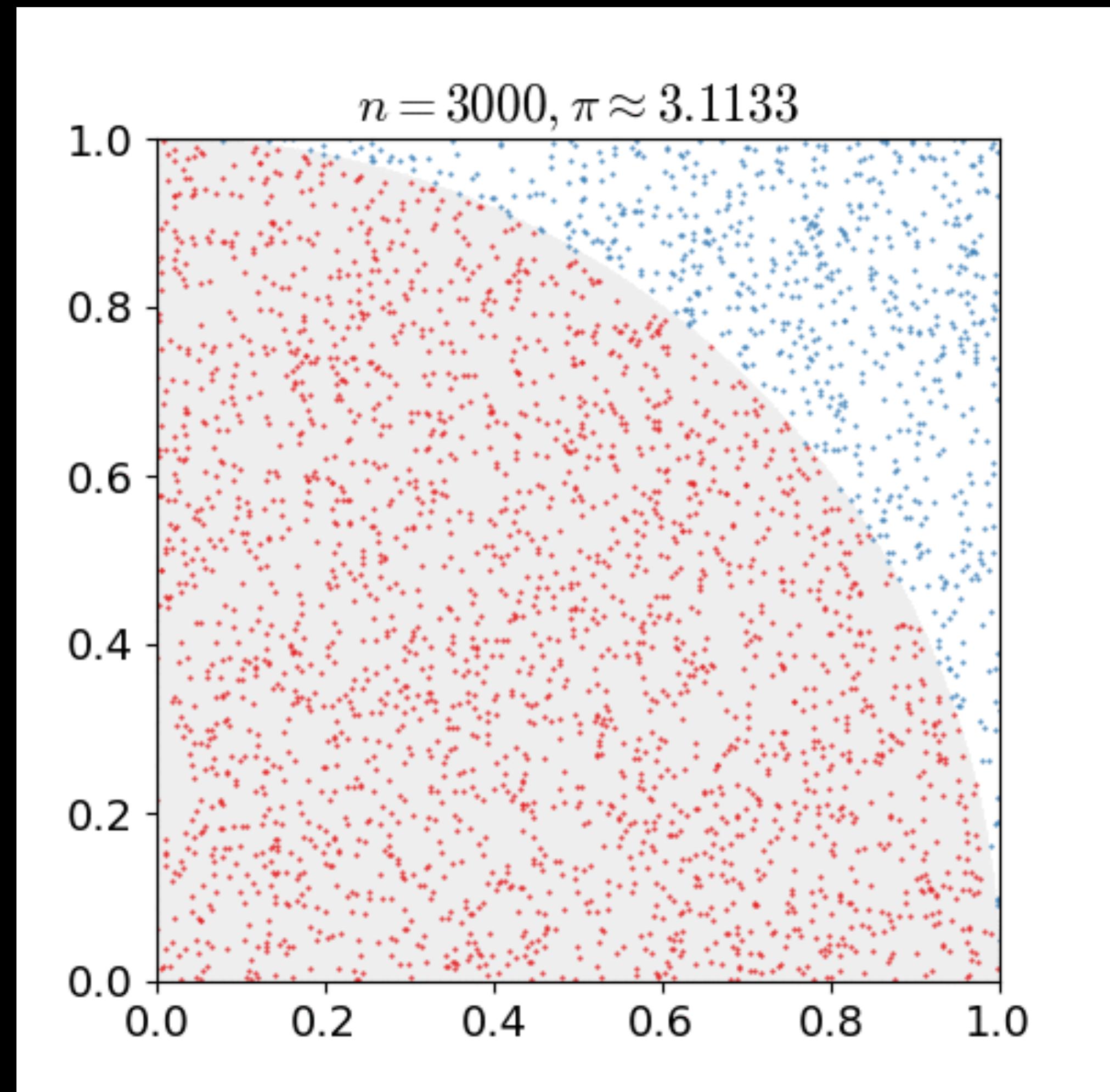
- What value of x makes the program print 24?

```
product = 1
j = 1
while j < x:
    product = product * j
    j = j + 1
print(product)
```

- A 3
- B 4
- C 5
- D 6

A silly way to compute π

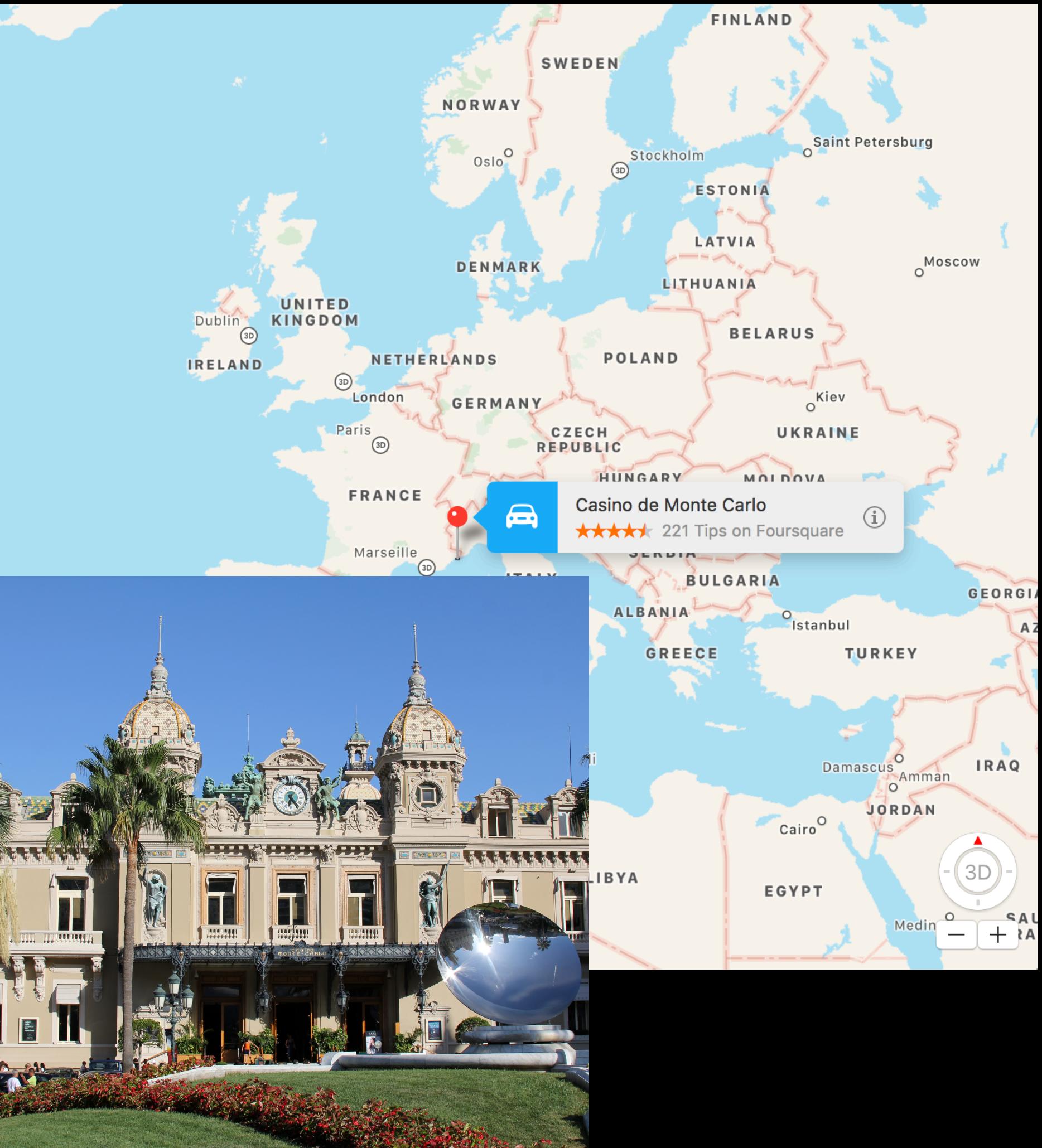
- Throw darts in square
 - $(\text{circle area}) \div (\text{square area}) \approx \text{darts in circle} \div \text{darts in square} = \pi/4$



Courtesy wikipedia

Monte Carlo methods

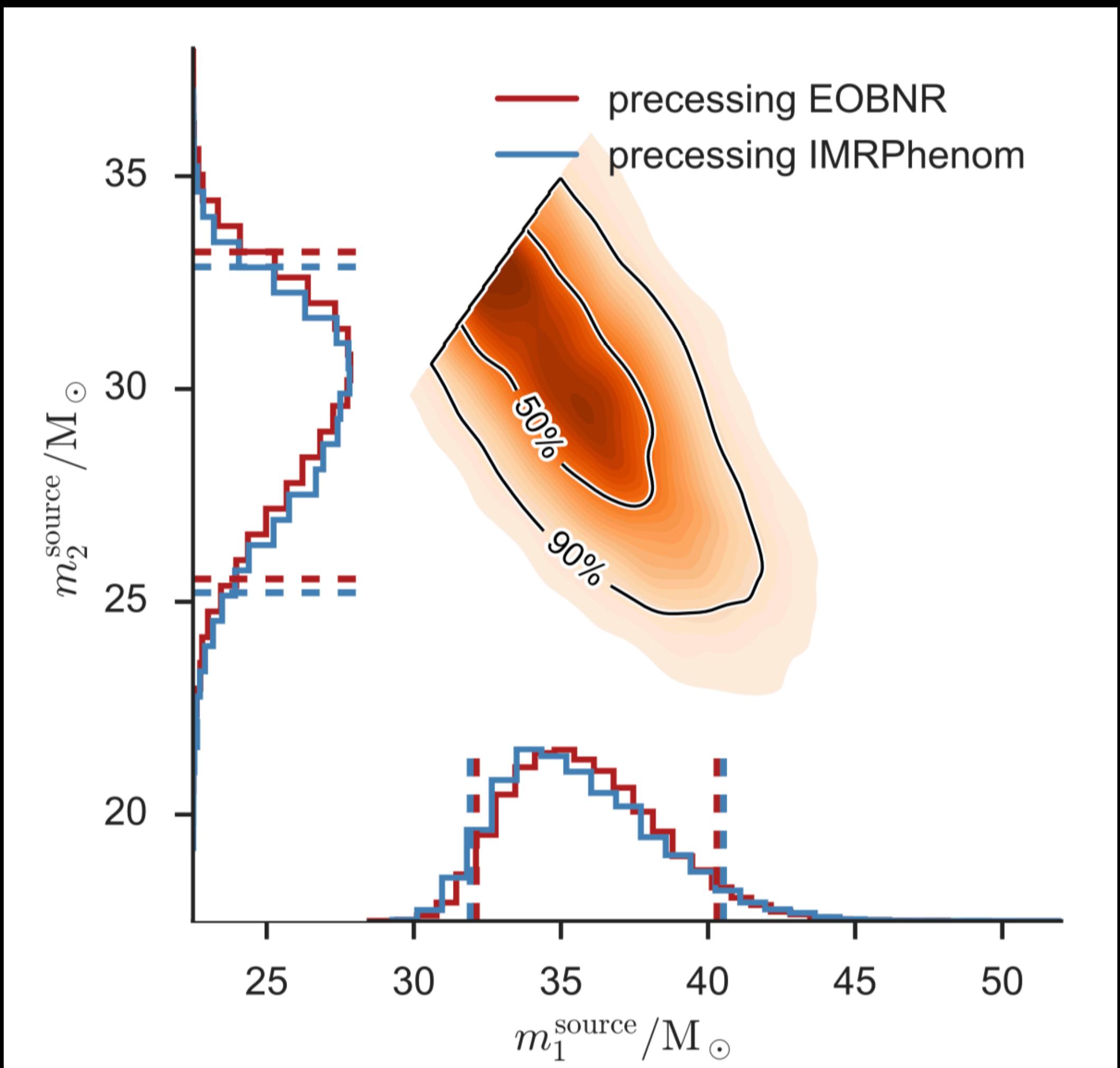
- This idea might seem silly, but it actually has a lot of uses in physics
- **Monte Carlo methods: use repeated random numbers to get results**
- Min/max of functions
especially functions of many variables
- Integrals
especially high dimensional
- Explore probability distributions



Images courtesy Wikipedia, Apple Maps

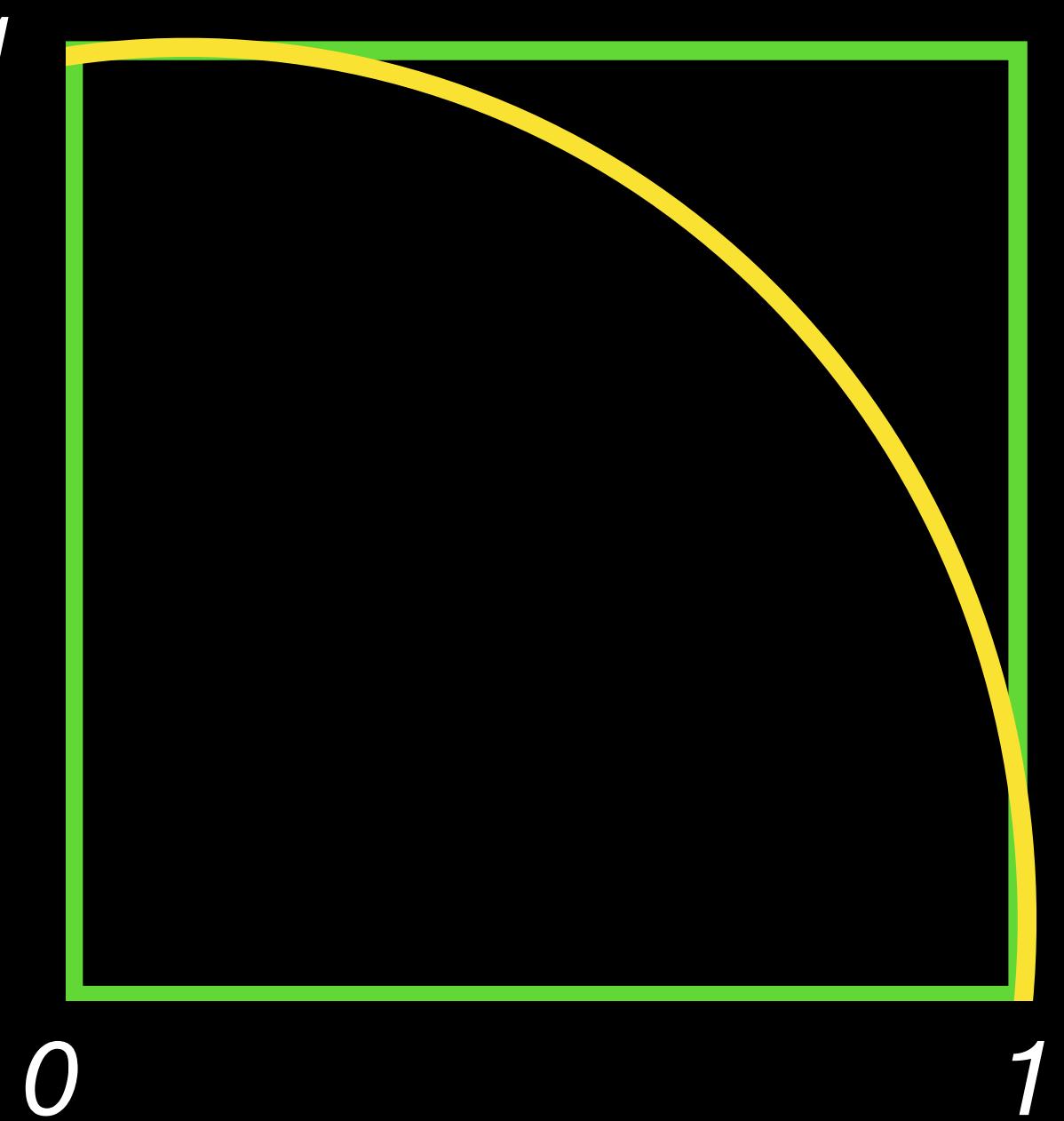
Monte Carlo methods

- This idea might seem silly, but it actually has a lot of uses in physics
- When we observe a gravitational wave from merging black holes...
 - What kinds of black holes made the waves?
 - Choose random parameters (masses, spins, ...)
 - Compute the corresponding grav. wave
 - More likely to call the wave a “hit” the better it matches—vs. the last wave “hit”



GW150914: Abbott+ (2016)

Pi Dartboard 1



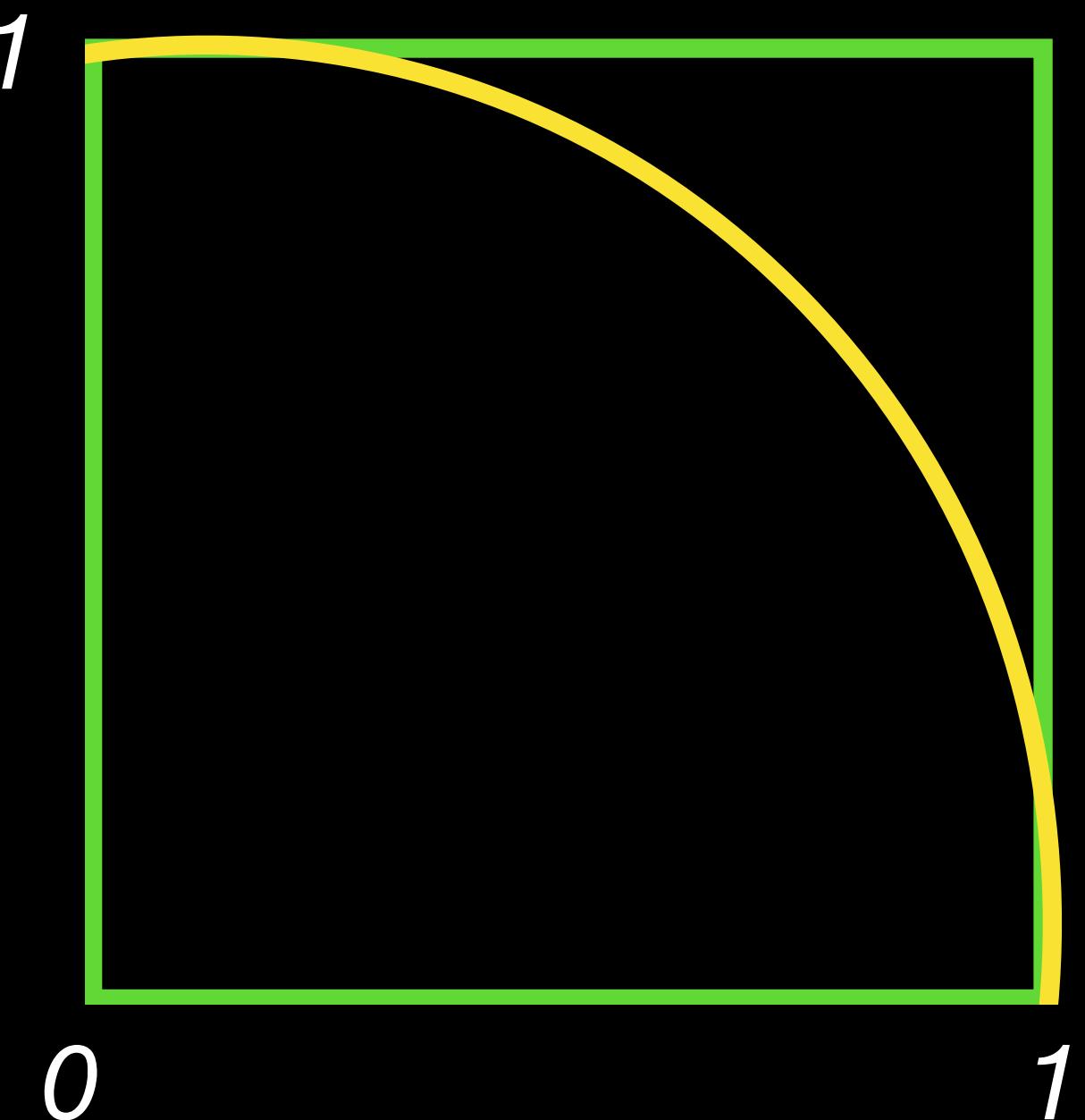
- Write a program that prints one random number between 0 and 1

```
import math  
import random  
print(random.random())
```

Pi Dartboard 2

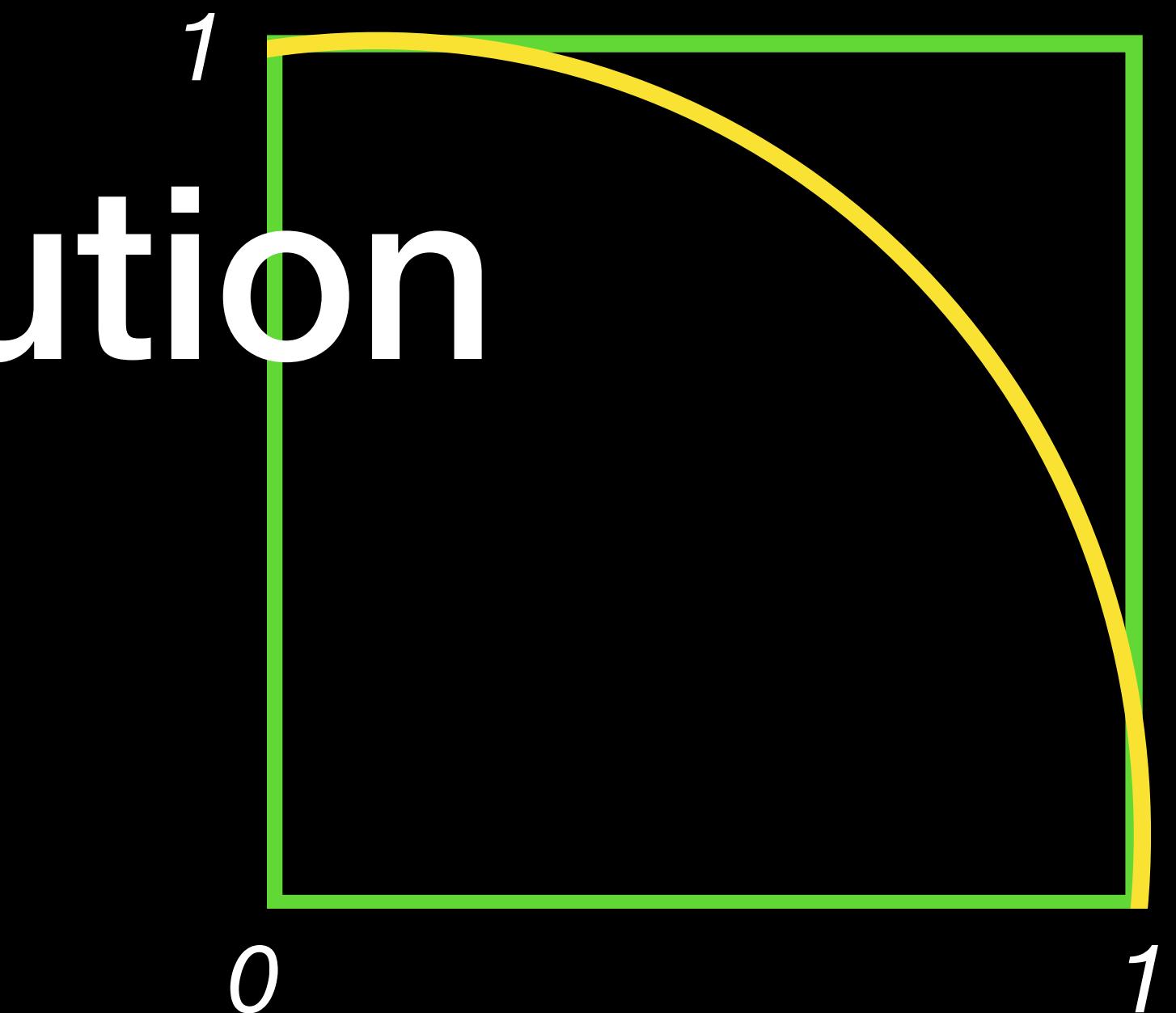
- **Challenge:** Modify your program
 - Store the random number in a variable x
 - Store a second random number in a variable y
 - Print x and y

```
import math  
import random  
print(random.random())
```



Pi Dartboard 2 Solution

- **Challenge:** Modify your program
 - Store the random number in a variable x
 - Store a second random number in a variable y
 - Print x and y

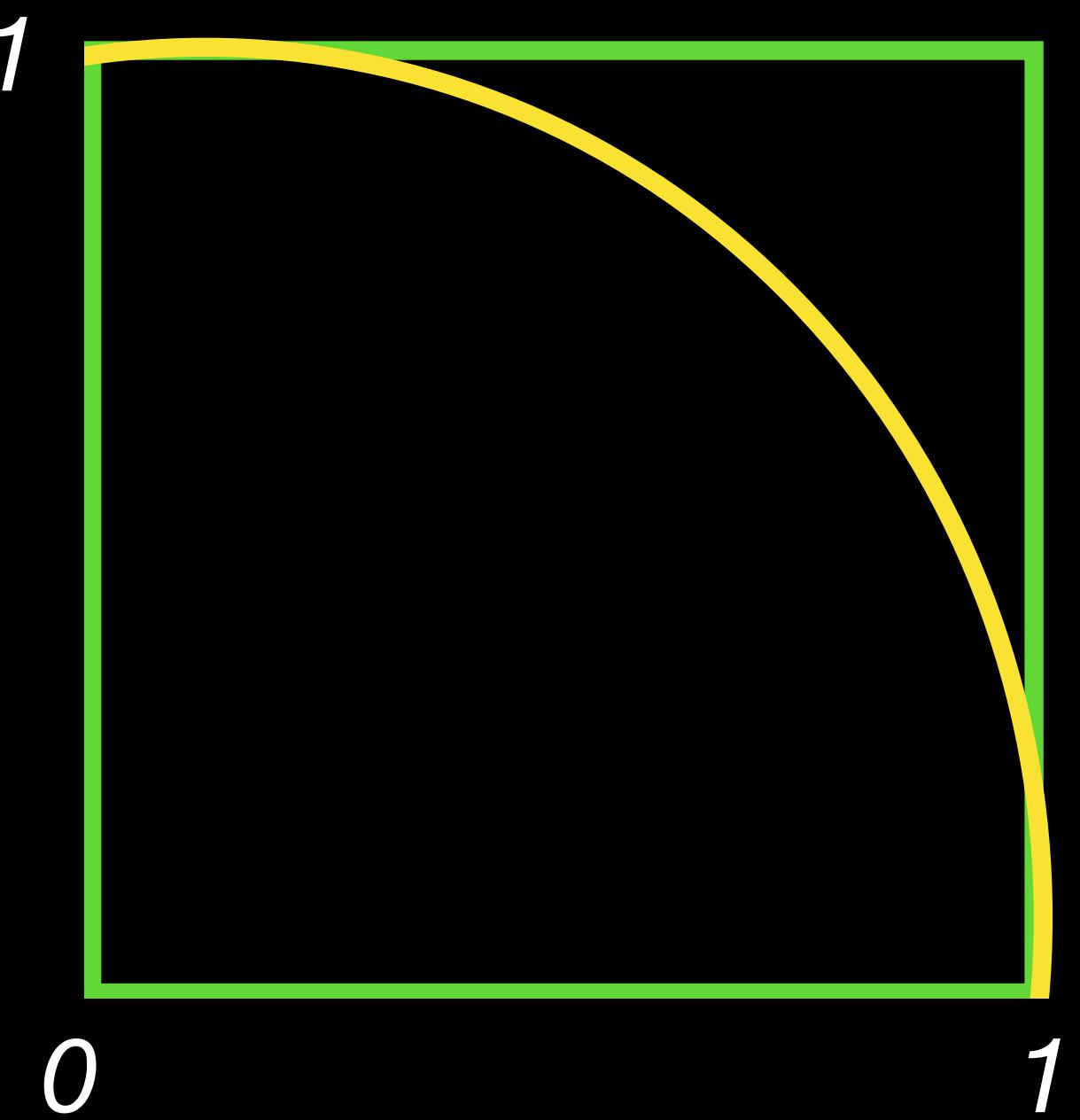


```
import math  
import random  
  
x = random.random()  
y = random.random()  
  
print(x)  
print(y)
```

Pi Dartboard 3

- **Challenge:** Modify your program
 - Compute $x^2 + y^2$ and store it in a variable rSquared
 - Print rSquared instead of just x and y

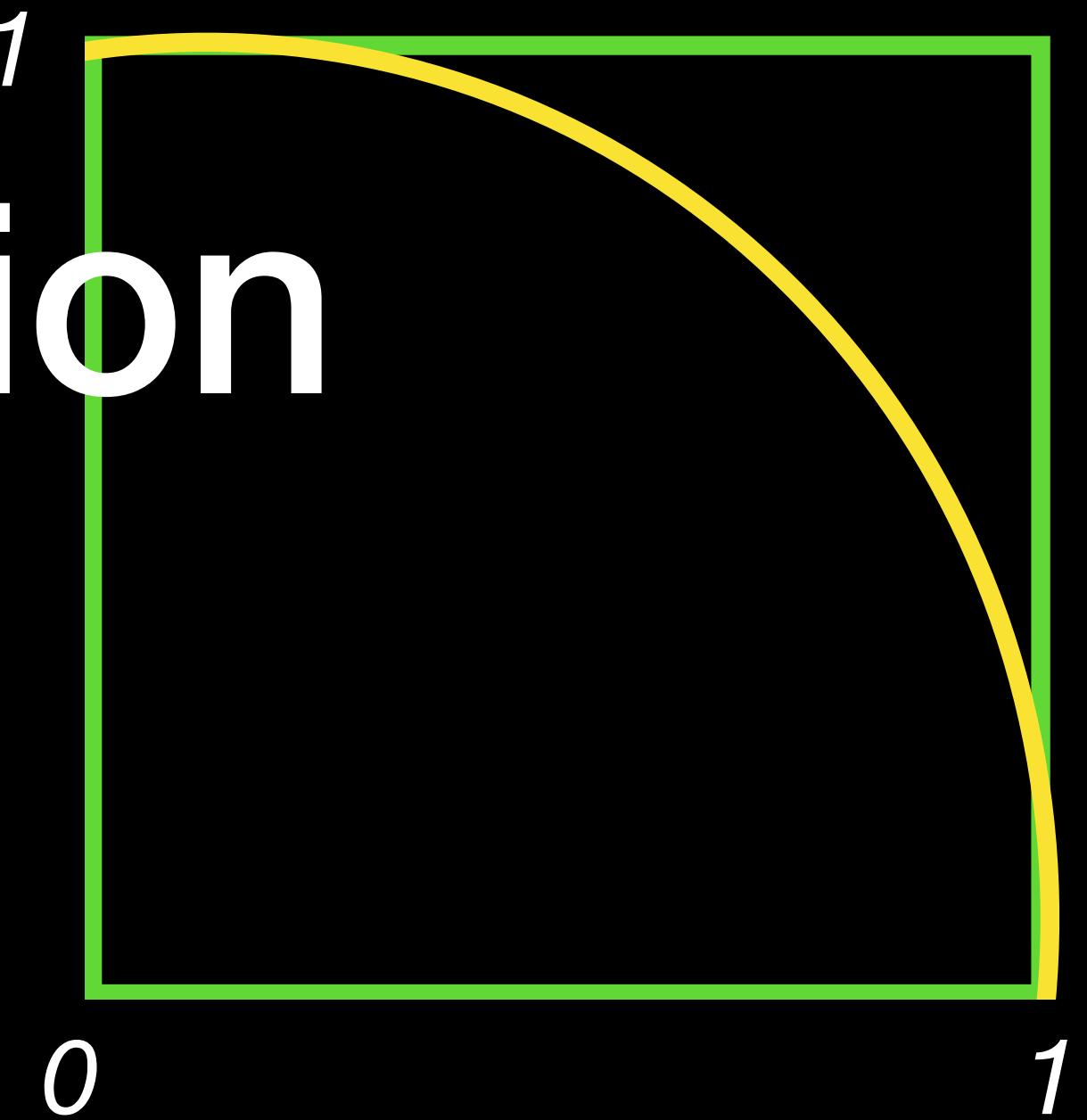
```
import math  
import random  
  
x = random.random()  
y = random.random()  
  
print(x)  
print(y)
```



Pi Dartboard 3 Solution

- **Challenge:** Modify your program
 - Compute $x^2 + y^2$ and store it in a variable rSquared
 - Print rSquared instead of just x and y

```
import math  
import random  
  
x = random.random()  
y = random.random()  
rSquared = x**2 + y**2  
print(rSquared)
```

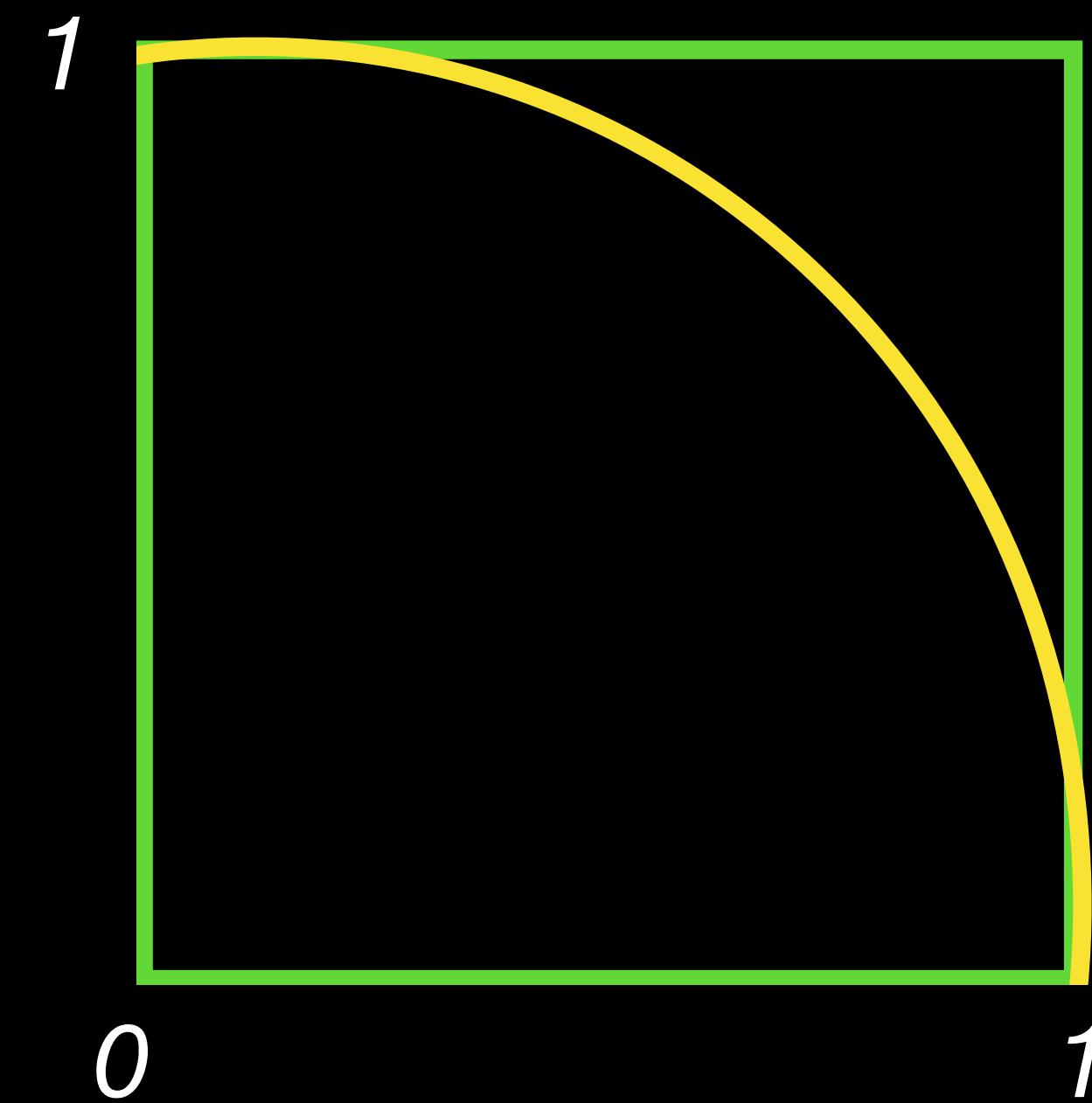


Clicker question #2.5

- Which could be a number the program prints?

```
import math  
import random  
  
x = random.random()  
y = random.random()  
  
rSquared = x**2 + y**2  
print(rSquared)
```

- | | |
|---|-------|
| A | -1.51 |
| B | 2.43 |
| C | -0.32 |
| D | 1.01 |



Clicker question #2.5

- If the dart is inside the **circle**, which could be the number printed by the program?

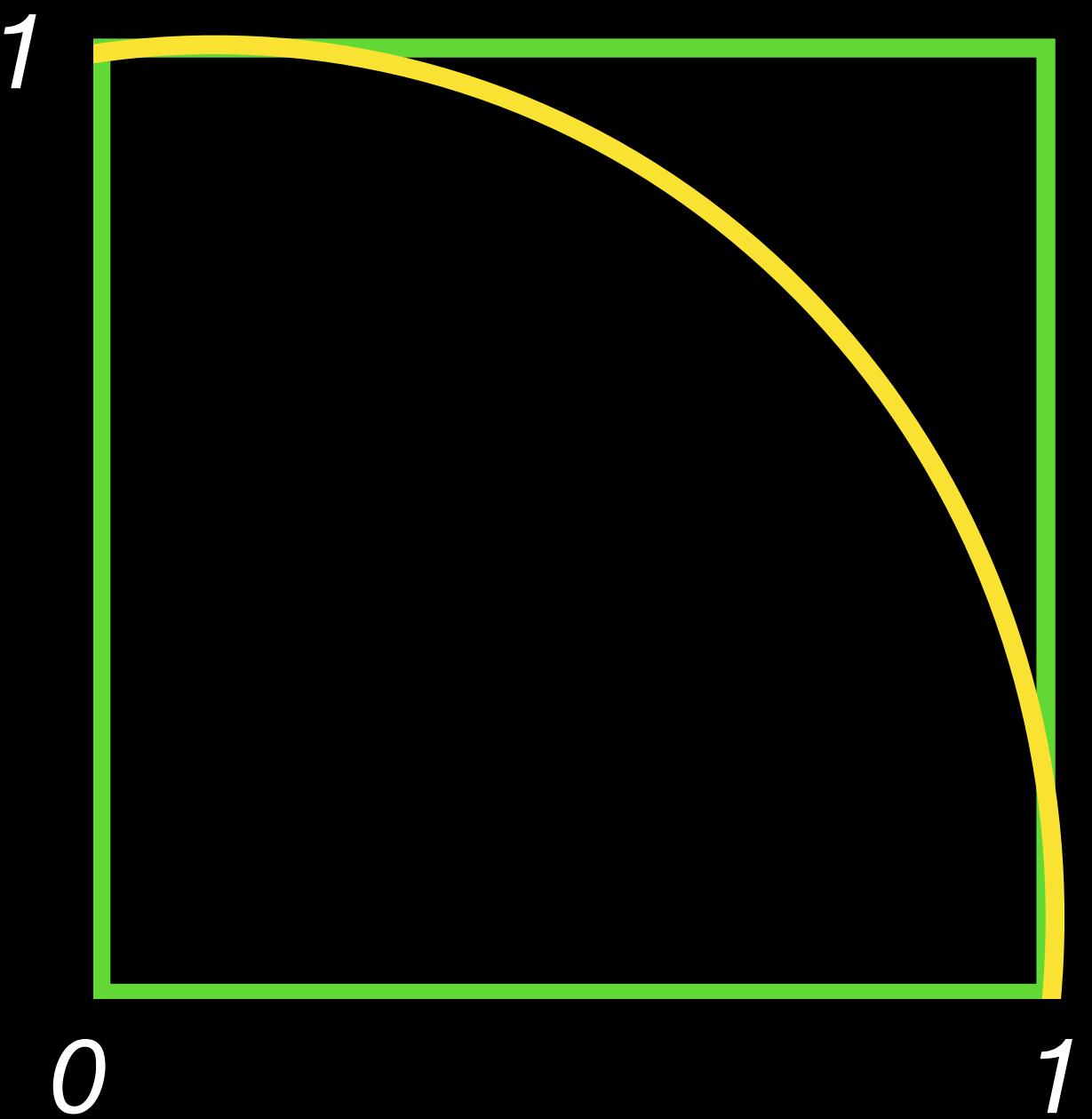
```
import math  
import random  
  
x = random.random()  
y = random.random()  
rSquared = x**2 + y**2  
print(rSquared)
```



Pi Dartboard 4

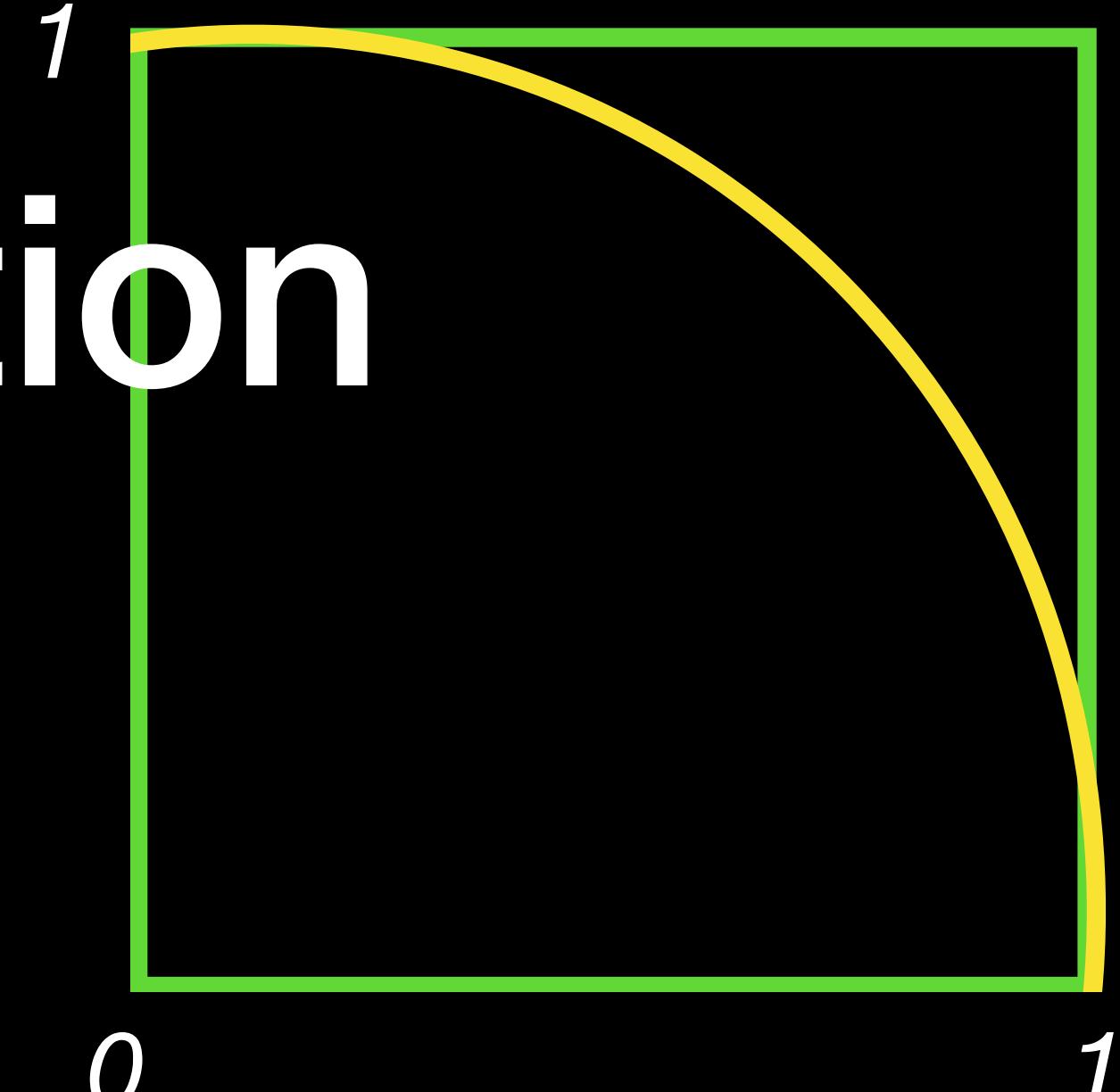
- **Challenge:** Modify your program
 - Just below import random, make a new variable called “hits”, set to 0
 - If rSquared < 1, add 1 to hits
 - Print hits instead of rSquared

```
import math  
import random  
  
x = random.random()  
y = random.random()  
  
rSquared = x**2 + y**2  
print(rSquared)
```



Pi Dartboard 4 Solution

- **Challenge:** Modify your program
 - Just below import random, make a new variable called “hits”, set to 0
 - If rSquared < 1, add 1 to hits
 - Print hits instead of rSquared

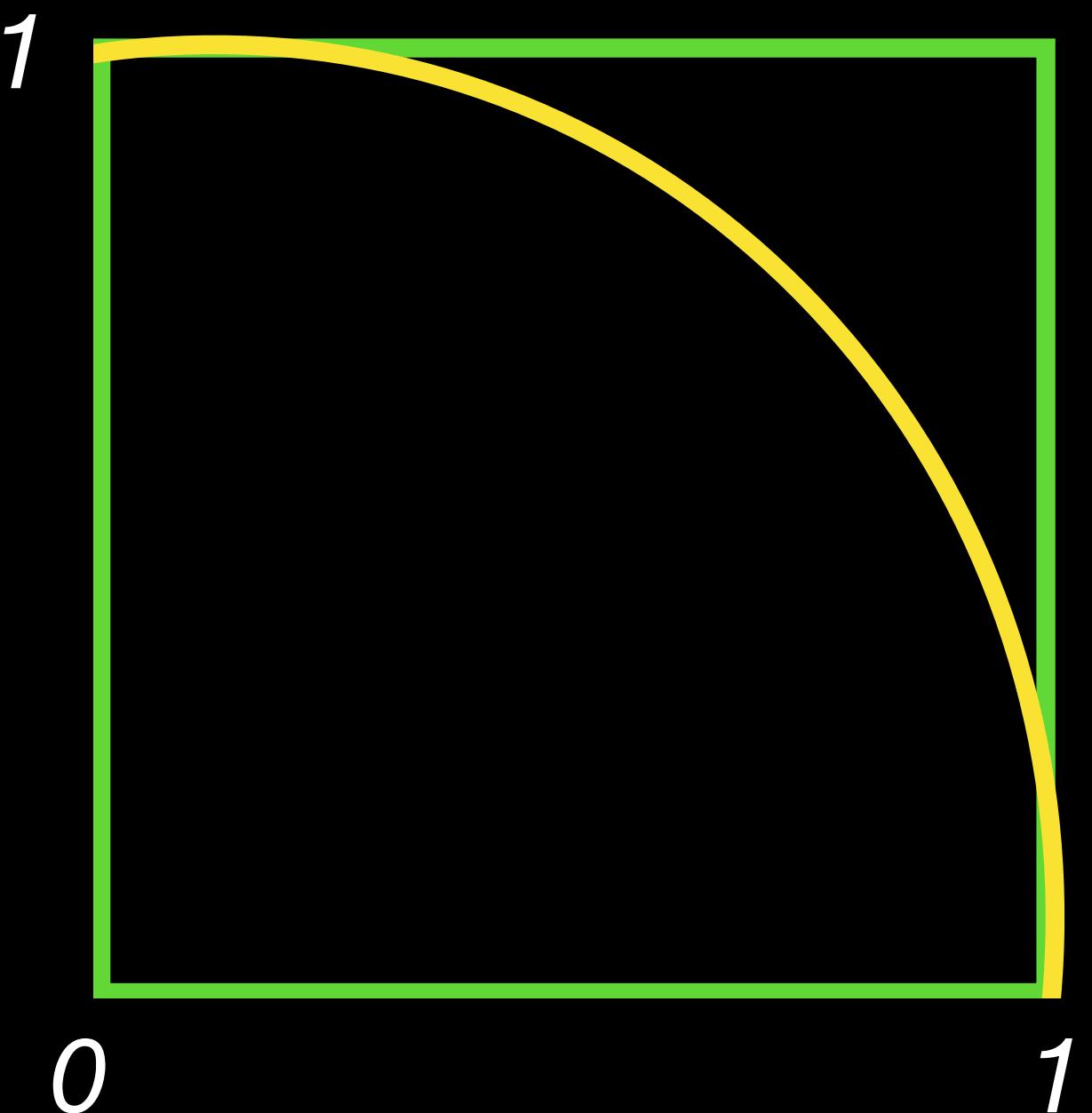


```
import math 0
import random
hits = 0
x = random.random()
y = random.random()
rSquared = x**2 + y**2
if rSquared < 1:
    hits = hits + 1
print(hits)
```

Pi Dartboard 4.5

- **Challenge:** Modify your program
 - Add a new variable, just below hits, called throws. Set it equal to 10.
 - Add a while loop just below your new variable, throws.
 - Make a counter variable (i or j or ...) and set it equal to zero. Then make a while loop. While your counter variable is less than throws, each time through the while loop, add 1 to your counter variable.

```
import math
import random
hits = 0
x = random.random()
y = random.random()
rSquared = x**2 + y**2
if rSquared < 1:
    hits = hits + 1
print(hits)
```



Pi Dartboard 4.5 solution

- **Challenge:** Modify your program
 - Add a new variable, just below hits, called throws. Set it equal to 10.
 - Add a while loop just below your new variable, throws.
 - Make a counter variable (i or j or ...) and set it equal to zero. Then make a while loop. While your counter variable is less than throws, each time through the while loop, add 1 to your counter variable.

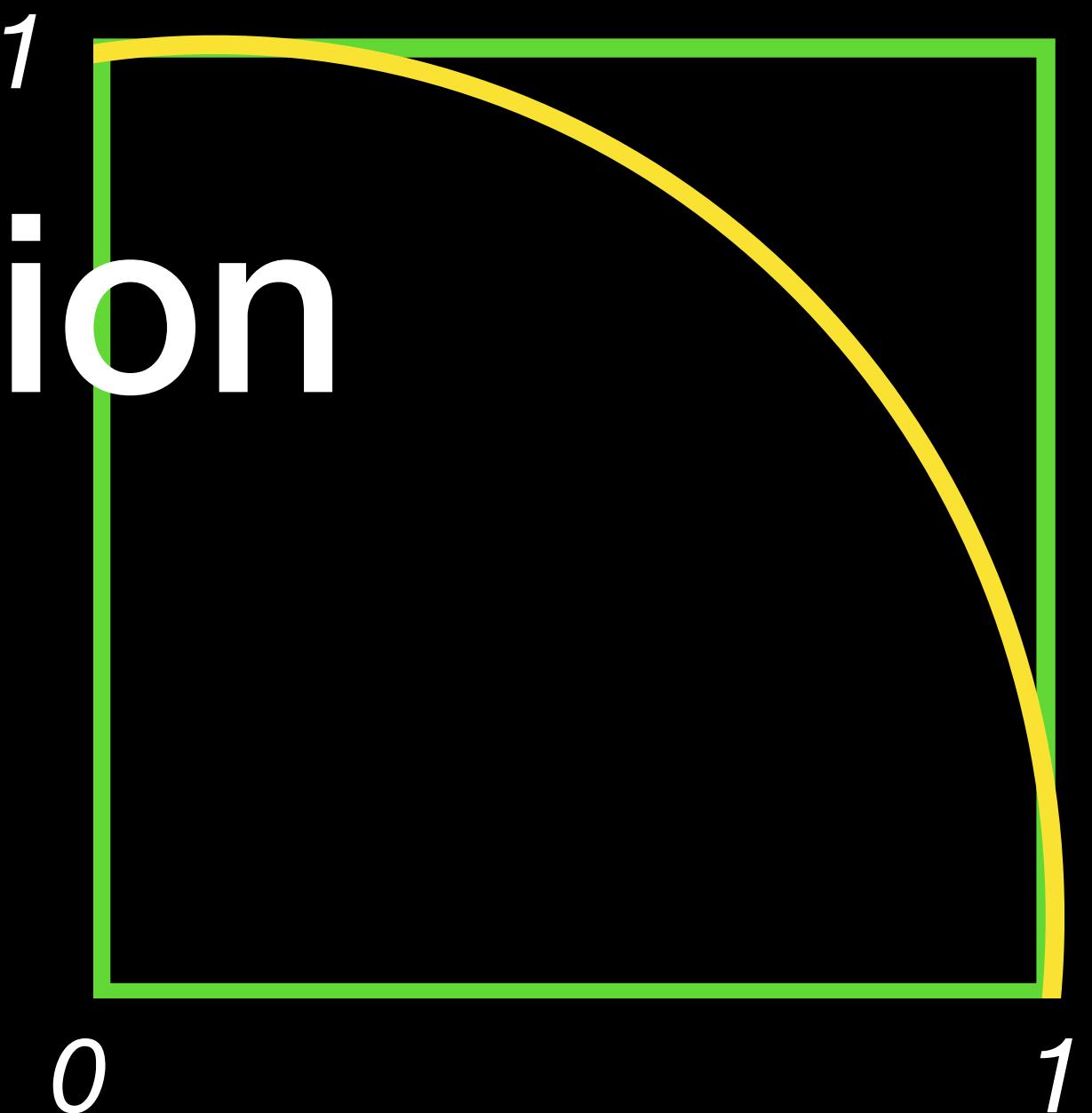
```
import math  
import random
```

```
hits = 0  
throws = 10
```

```
i = 0  
while i < throws:  
    i = i + 1
```

```
x = random.random()  
y = random.random()
```

```
rSquared = x**2 + y**2  
if rSquared < 1:  
    hits = hits + 1  
print(hits)
```



Pi Dartboard 5

- **Challenge:** Modify your program
- Put the code that throws the dart and sees if it hit inside a while loop, so that you throw 10 darts instead of 1 dart
- Your print statement should still be outside the while loop

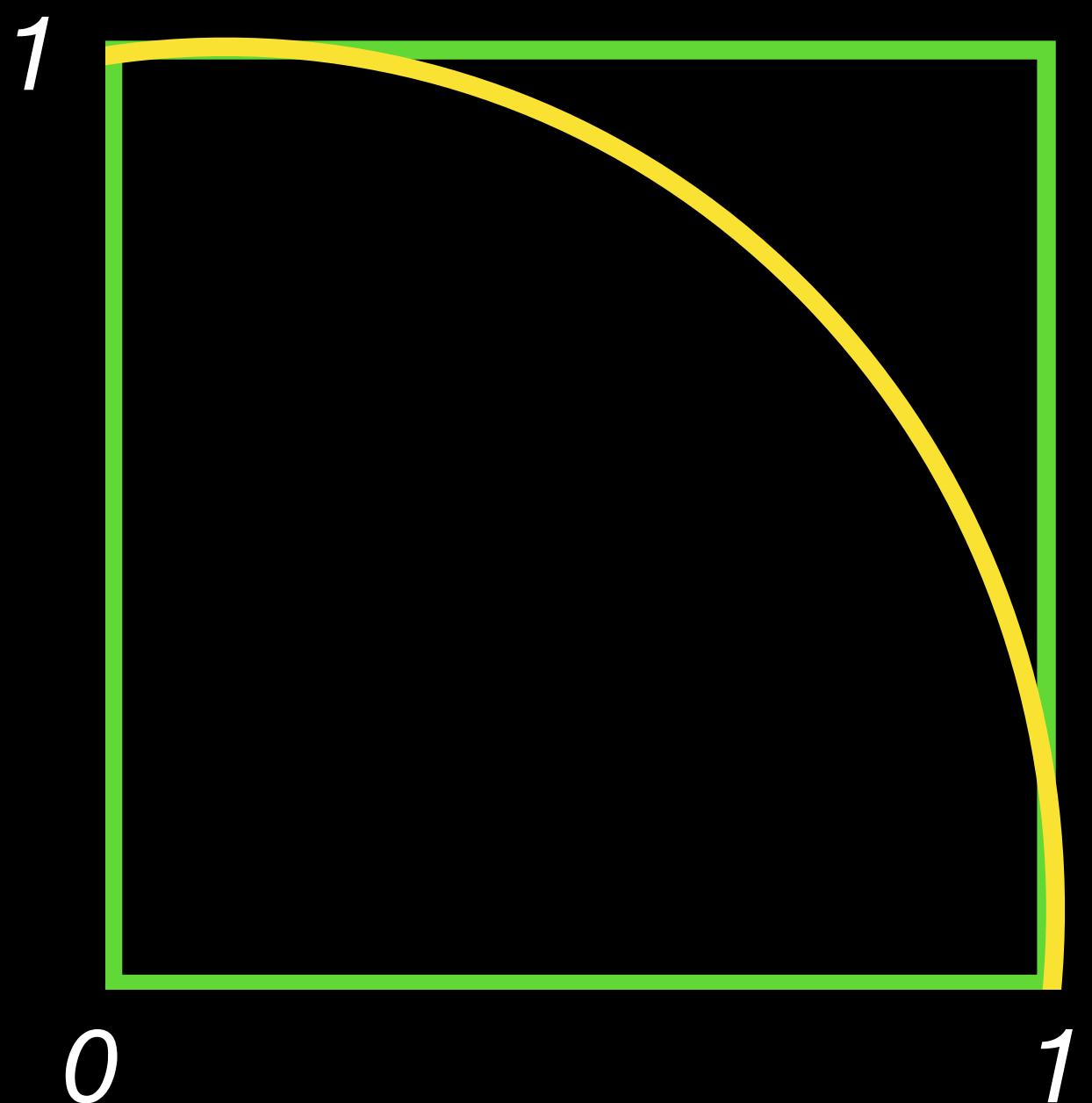
```
import math  
import random
```

```
hits = 0  
throws = 10
```

```
i = 0  
while i < throws:  
    i = i + 1
```

```
x = random.random()  
y = random.random()
```

```
rSquared = x**2 + y**2  
if rSquared < 1:  
    hits = hits + 1  
print(hits)
```



Pi Dartboard 5 Solution

- **Challenge:** Modify your program
- Add a new variable, just below hits, called throws. Set it equal to 10.
- Put the code that throws the dart and sees if it hit inside a while loop, so that you throw 10 darts instead of 1 dart

```
import math
import random

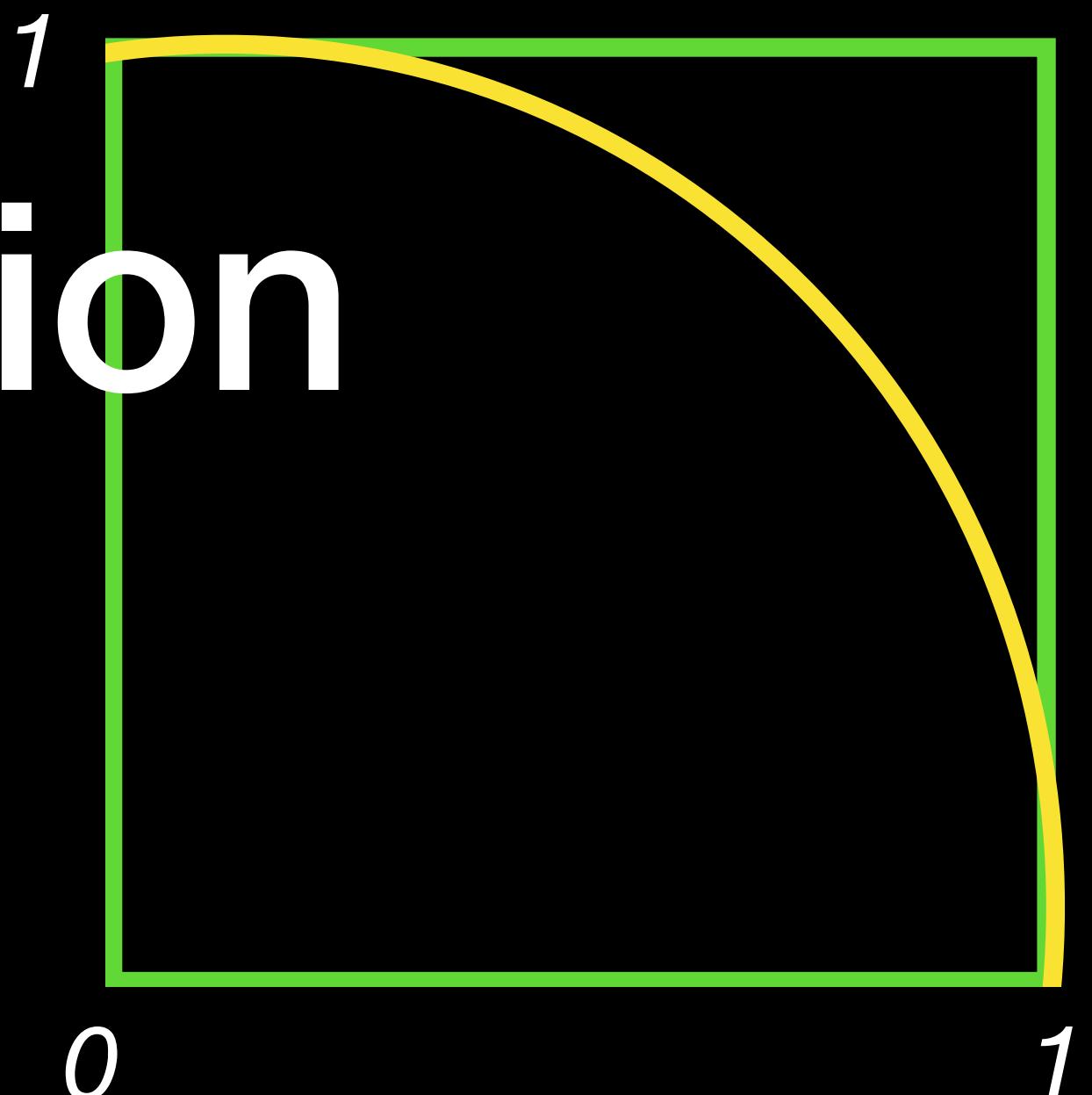
hits = 0
throws = 10

i = 0
while i < throws:
    x = random.random()
    y = random.random()

    rSquared = x**2 + y**2

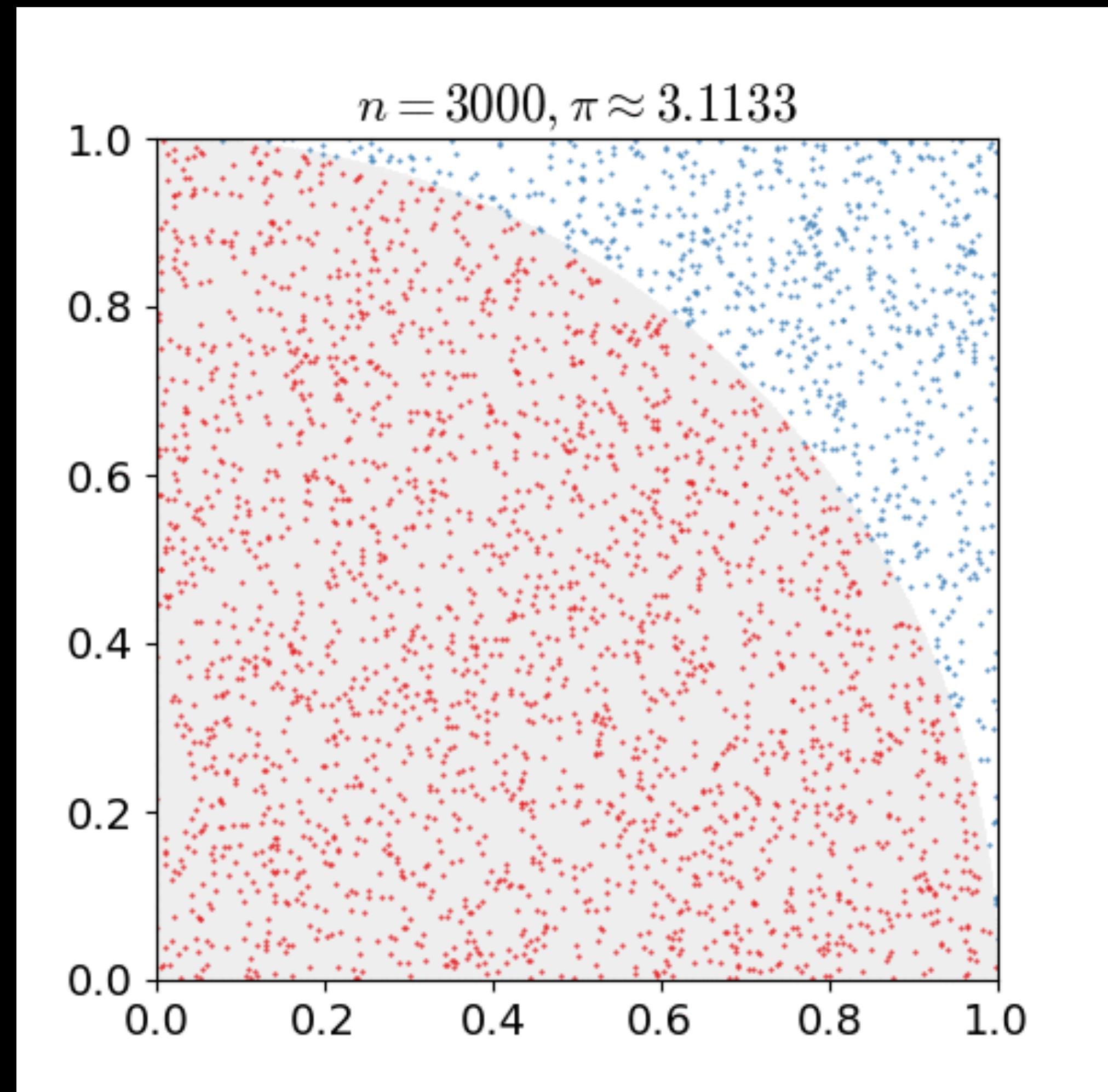
    if rSquared < 1:
        hits = hits + 1
    i = i + 1

print(hits)
```



A silly way to compute π

- Throw darts in square
 - $(\text{circle area}) \div (\text{square area}) \approx \text{hits} \div \text{throws} = \pi/4$
 - So $\pi \approx 4 * (\text{hits} \div \text{throws})$



Courtesy wikipedia

Pi Dartboard 6

- Finish the dartboard
 - Make a variable pi, set to $4.0 * \text{float(hits)} / \text{float(throws)}$
 - Should you do this inside or outside the while loop?
 - Print pi

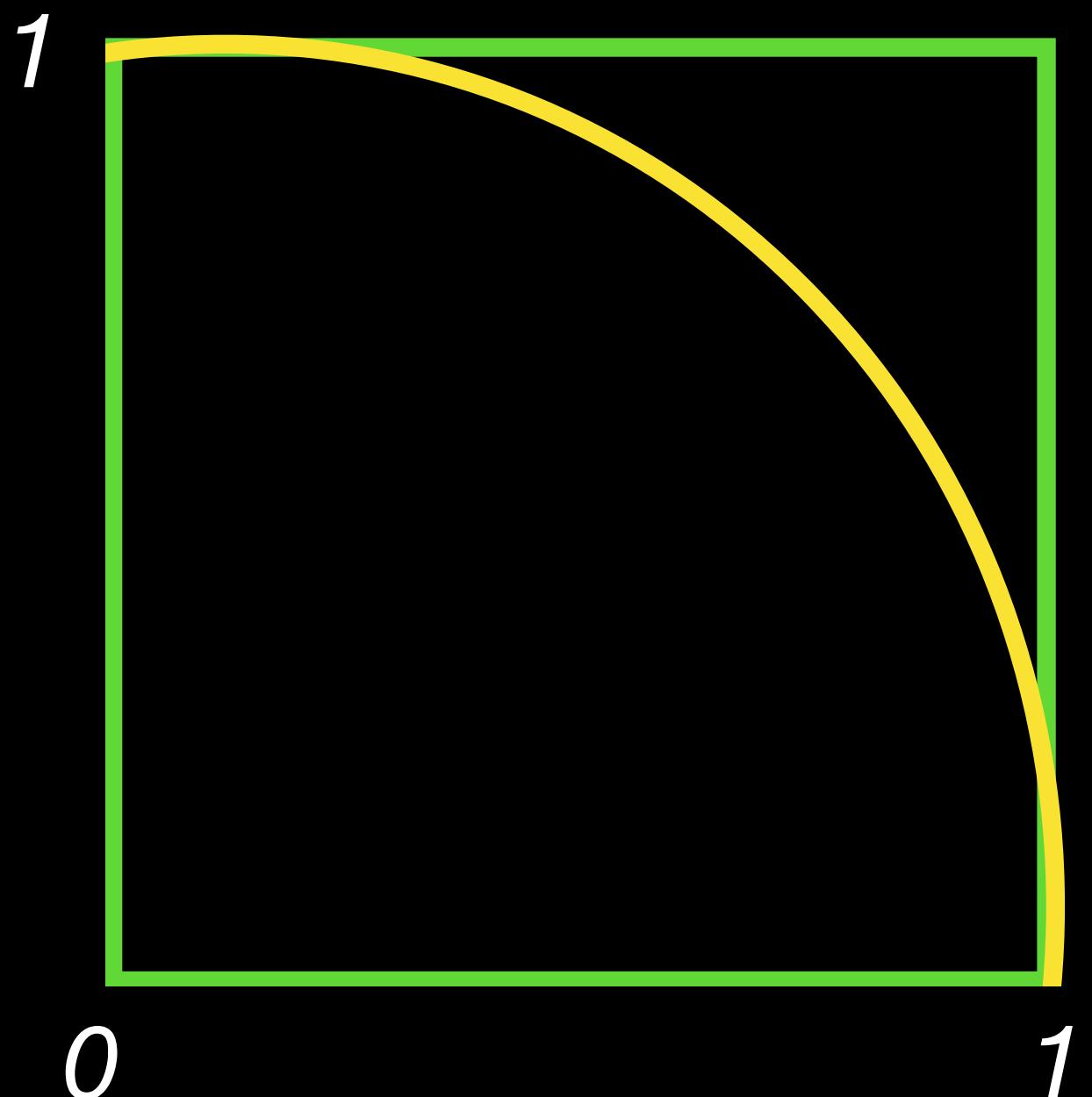
```
import math
import random

hits = 0
throws = 10

i = 0
while i < throws:
    x = random.random()
    y = random.random()

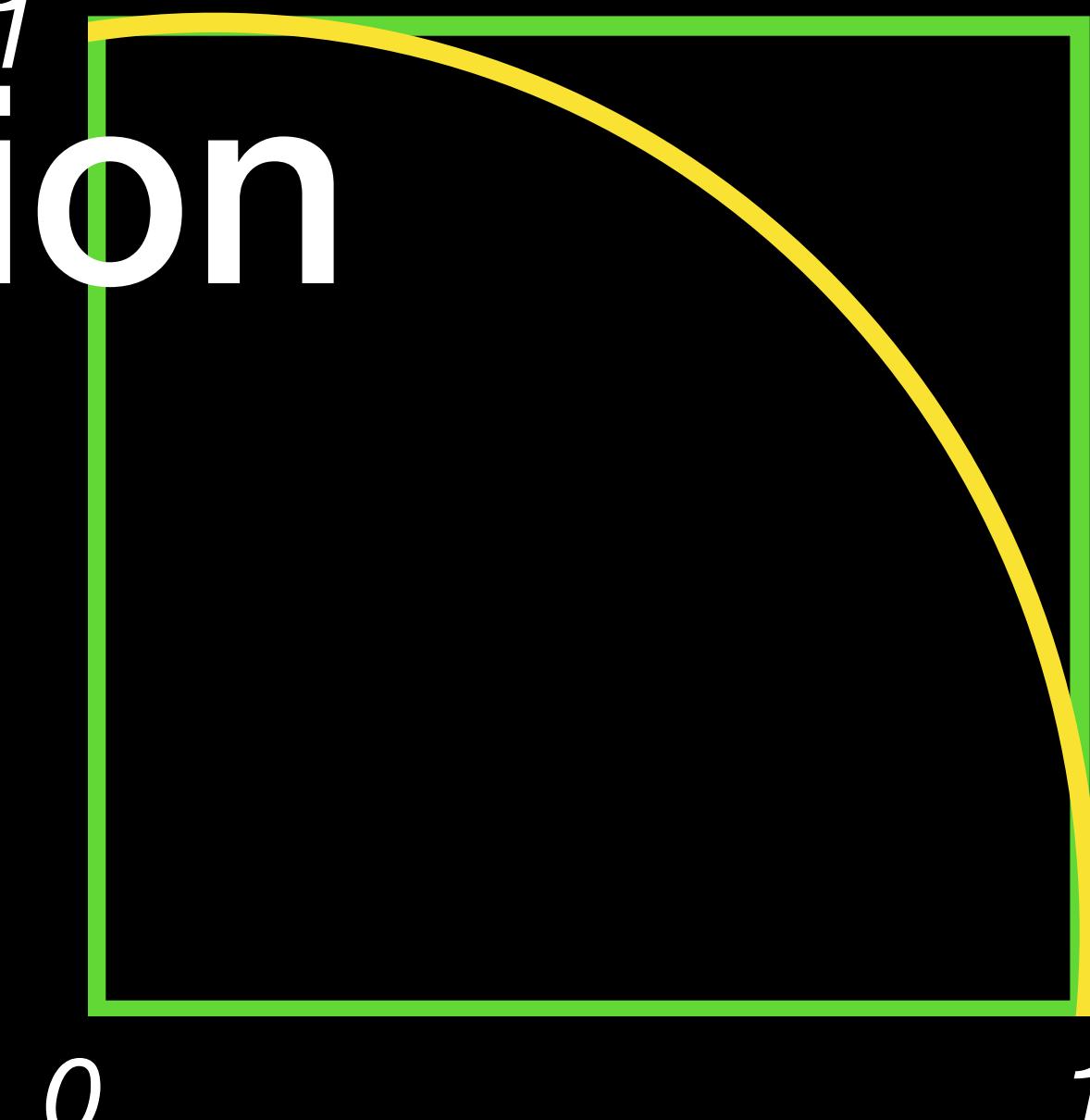
    rSquared = x**2 + y**2
    if rSquared < 1:
        hits = hits + 1
    i = i + 1

print(hits)
```



Pi Dartboard 6 Solution

- Finish the dartboard
- Compute pi as $4.0 * \text{float(hits)} / \text{float(throws)}$
- Print your pi estimate



```
import math
import random

hits = 0
throws = 10

i = 0
while i < throws:
    x = random.random()
    y = random.random()

    rSquared = x**2 + y**2

    if rSquared < 1:
        hits = hits + 1
        i = i + 1

pi = 4.0 * float(hits) / float(throws)
print(pi)
```

Pi Dartboard 7

- The tutor won't let us run lots of darts
- So paste this into a cell in Jupyter on colab.google.com and run it
- See what happens as you make throws 10^{**n} , $n=1,2,3,4,5,6,7$

```
import math
import random

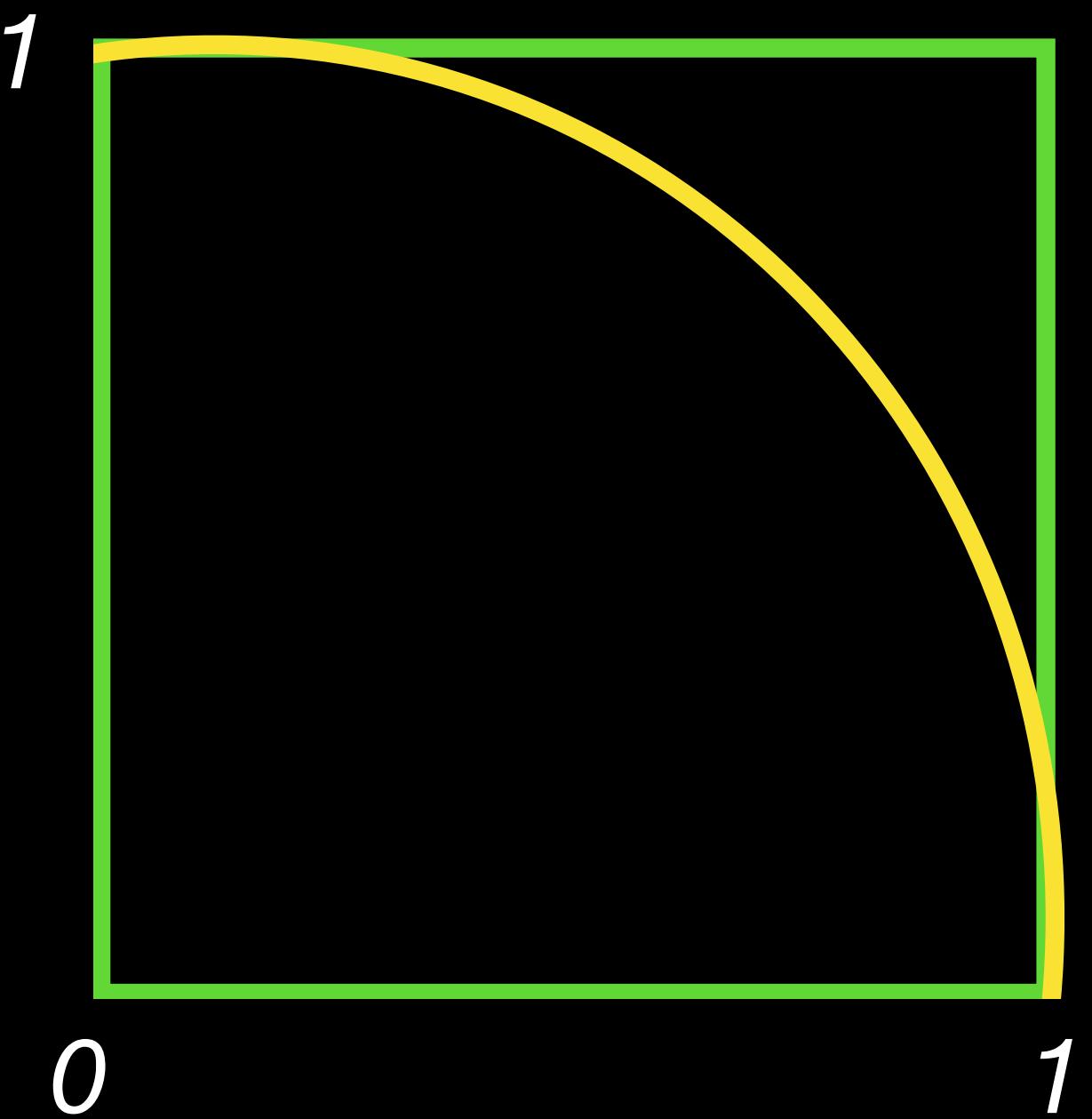
hits = 0
throws = 10

i = 0
while i < throws:
    x = random.random()
    y = random.random()

    rSquared = x**2 + y**2

    if rSquared < 1:
        hits = hits + 1
    i = i + 1

pi = 4.0 * float(hits) / float(throws)
print(pi)
```



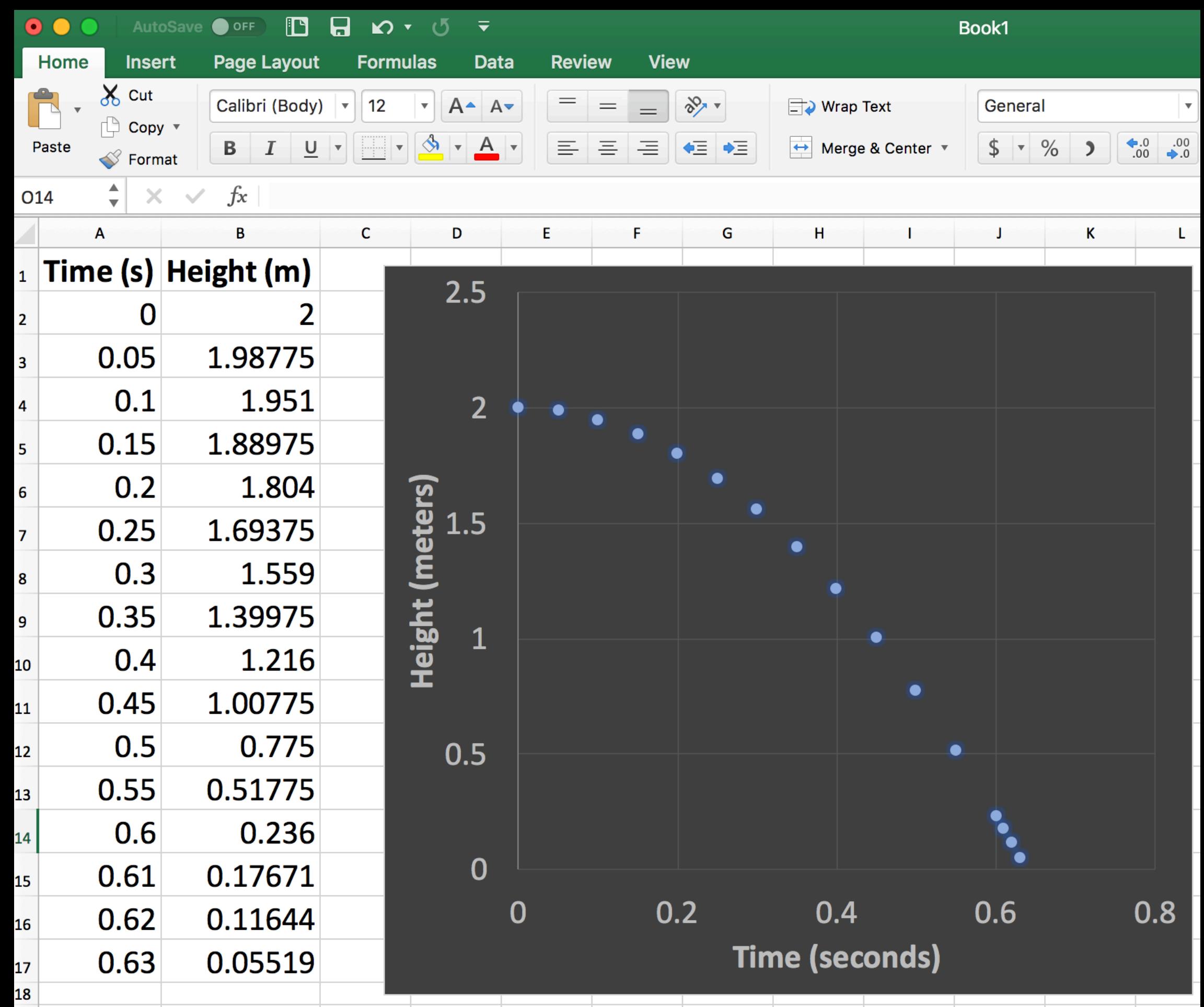
- [https://mybinder.org/v2/gh/geoffrey4444/
NRDataExample/master](https://mybinder.org/v2/gh/geoffrey4444/NRDataExample/master)

Plotting your results

- Scatter plots
- Lists and numpy arrays
- Pyplot plotting

Scatter plots

- Data: result or output given some input
 - Example: dropped marker height vs. time
 - Tools to make scatter plots
 - Excel
 - Python
 - Lists of numbers
 - Computations on lists of numbers: numpy arrays
 - pyplot: makes scatter plots



Lists

- **Values** - ordered sets of objects, all the same type (like floats or ints)

```
x = [-2.0, -1.0, 0.0, 1.0, 2.0]
y = ["Hello", "world"]
z = [1, 4, 9, 16]
```

- **Operators** -
[], .append()

```
z.append(25) == [1, 4, 9, 16, 25]
```

- **Easily add on elements in loops** with .append()

```
x[0] == -2.0
x[1] == -1.0
x[4] == 2.0
y[0] == "Hello"
y[-1] == "world"
z[-1] == 16
z[0] == 1
```

Loop over lists

```
for i in [1,2,3,4]:  
    print(i*i)
```

0
1
4
9

```
import numpy as np  
print(np.arange(1,5,1))  
[1,2,3,4]
```

```
import numpy as np  
myCountArray = np.arange(1,5)  
myList = []  
for i in myCountArray:  
    myList.append(i*i)  
print(myCountArray)  
print(myList)
```

[1,2,3,4]
[1,4,9,16]

Clicker question #2.6

- What value does the program print?

```
x = [1.0, 4.0, 9.0]  
print(x[1])
```

- A 1.0
- B 4.0
- C 9.0
- D The entire list

Numpy arrays

- **Values** - ordered sets of objects, all the same type (like floats or ints)

- **Operators** - `[]`, `+`, `-`, `*`, `/`,
`np.sqrt()`, `np.sin()`, `np.cos()`,
...

- **Easily do math on whole lists at once** (like formulas in Excel)

```
x = np.array([-2.0, -1.0, 0.0, 1.0, 2.0])
y = np.array(["Hello", "world"])
q = np.array([1, 2, 3, 4])
r = q * 2
s = q + r
z = q * q
```

```
r == np.array([2, 4, 6, 8])
s == np.array([3, 6, 9, 12])
z == np.array([1, 4, 9, 16])
```

```
x[0] == -2.0
x[1] == -1.0
x[4] == 2.0
y[0] == "Hello"
y[-1] == "world"
z[-1] == 16
z[0] == 1
```

Making sample data

- Annoying to type [1,2,3,4,...] all the time
- Instead: np.arange(start, stop, step)
- What do all these numbers mean??
- Make a plot to visualize them

Try in colab!

```
import numpy as np
x = np.arange(-4.0, 4.0, 0.01)
y = np.sin(x)**3
print(x)
print(y)
```

```
-9.99825171e-01 -9.99351433e-01 -9.98578166e-01 -9.97505912e-01
-9.96135421e-01 -9.94467651e-01 -9.92503769e-01 -9.90245148e-01
-9.87693366e-01 -9.84850205e-01 -9.81717651e-01 -9.78297888e-01
-9.74593301e-01 -9.70606471e-01 -9.66340175e-01 -9.61797379e-01
-9.56981241e-01 -9.51895105e-01 -9.46542499e-01 -9.40927131e-01
-9.35052889e-01 -9.28923832e-01 -9.22544191e-01 -9.15918365e-01
-9.09050915e-01 -9.01946561e-01 -8.94610179e-01 -8.87046794e-01
-8.79261581e-01 -8.71259853e-01 -8.63047062e-01 -8.54628794e-01
-8.46010761e-01 -8.37198799e-01 -8.28198860e-01 -8.19017011e-01
-8.09659425e-01 -8.00132377e-01 -7.90442239e-01 -7.80595473e-01
-7.70598629e-01 -7.60458333e-01 -7.50181290e-01 -7.39774268e-01
-7.29244102e-01 -7.18597680e-01 -7.07841944e-01 -6.96983877e-01
-6.86030504e-01 -6.74988880e-01 -6.63866088e-01 -6.52669231e-01
-6.41405427e-01 -6.30081800e-01 -6.18705479e-01 -6.07283586e-01
-5.95823237e-01 -5.84331527e-01 -5.72815532e-01 -5.61282298e-01
-5.49738839e-01 -5.38192126e-01 -5.26649084e-01 -5.15116589e-01
-5.03601455e-01 -4.92110435e-01 -4.80650212e-01 -4.69227393e-01
-4.57848505e-01 -4.46519990e-01 -4.35248195e-01 -4.24039375e-01
-4.12899678e-01 -4.01835147e-01 -3.90851715e-01 -3.79955193e-01
-3.69151273e-01 -3.58445520e-01 -3.47843366e-01 -3.37350109e-01
-3.26970907e-01 -3.16710771e-01 -3.06574566e-01 -2.96567003e-01
-2.86692639e-01 -2.76955868e-01 -2.67360924e-01 -2.57911871e-01
```

Plotting sample data

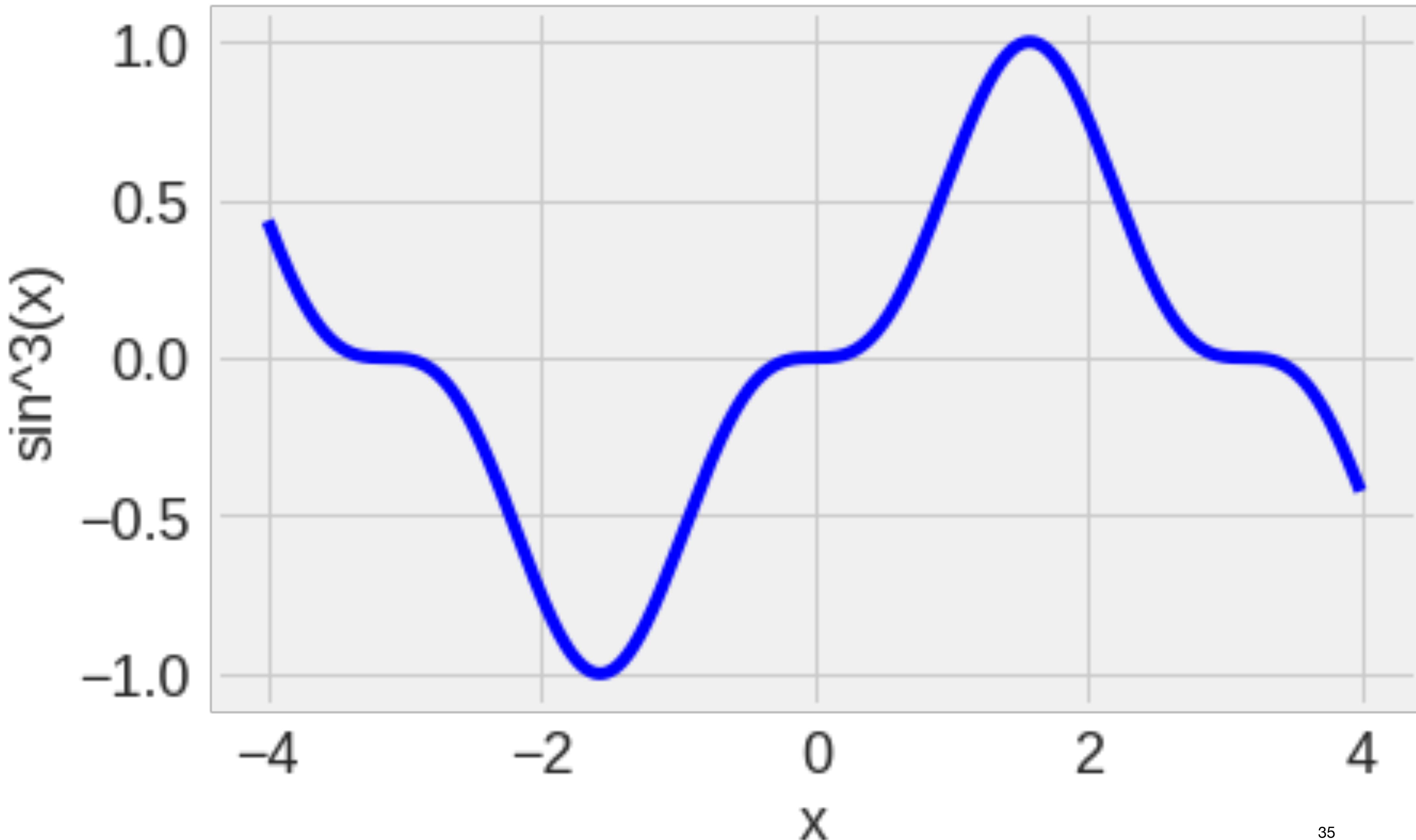
Try in colab!

```
import numpy as np
import matplotlib
from matplotlib import pyplot as plt
matplotlib.rcParams['axes', labelsize=18]
matplotlib.rcParams['xtick', labelsize = 18]
matplotlib.rcParams['ytick', labelsize = 18]
```

- Make plots with pyplot

```
x = np.arange(-4.0, 4.0, 0.01)
y = np.sin(x)**3
```

```
plt.clf() #clear figure
plt.plot(x,y, color='b')
plt.xlabel('x')
plt.ylabel('sin^3(x)')
plt.show()
```



Functions

Try in tutor!

```
def square(x):  
    return x*x
```

```
square(4)  
16
```

- Input(s) ("arguments")
- Returns output
- Functions can call other functions

Plotting π 1

- **Activity: edit your code**

- Make everything but the first two lines and last two lines inside a function that takes one input, throws
- Instead of setting throws = 10, throws in an input to the function
- Return the pi estimate
- Have your print statement just use your function

```
import math
import random

hits = 0
throws = 10

i = 0
while i < throws:
    x = random.random()
    y = random.random()

    rSquared = x**2 + y**2
    if rSquared < 1:
        hits = hits + 1
    i = i + 1

pi = 4.0 * float(hits) / float(throws)
print(pi)
```

Solution 1

- Activity: edit your code
- Make everything but the last two lines inside a function that takes one input, n
- Instead of setting throws = 10, set throws=n
- Return the pi estimate

```
import math
import random

def estimatePi(throws):
    hits = 0
    i = 0
    while i < throws:
        x = random.random()
        y = random.random()

        rSquared = x**2 + y**2
        if rSquared < 1:
            hits = hits + 1
        i = i + 1

    pi = 4.0 * float(hits) / float(throws)
    return pi

print(estimatePi(1e4))
```

Plotting π^2

- **Activity: edit your code**
 - Make a list of different numbers of throws: 10, 100, 1000, ... up to 1e7
 - Make an empty list called piEstimates
 - Loop over the list you made, estimating π for different numbers of throws

```
import math
import random

def estimatePi(throws):
    # (same definition of estimatePi function here)
    return pi

print(estimatePi(1e4))
```

Plotting π solution 2

- **Activity: edit your code**

- Make a list of different numbers of throws: 10, 100, 1000, ... up to 1e7
- Make an empty list called piEstimates
- Loop over the list you made, estimating π for different numbers of throws

```
import math
import random

def estimatePi(throws):
    # (same definition of estimatePi function here)
    return pi

throwsList = [1e1, 1e2, 1e3, 1e4, 1e5, 1e6, 1e7]
piEstimatesList = []
for throws in throwsList:
    piEstimatesList.append(estimatePi(throws))
print(piEstimatesList)
```

Plotting π 3

- **Activity:** edit your code

- Don't print
piEstimatesList
- Instead, make a
scatter plot of
throwsList vs.
piEstimatesList

- Use a log scale on the
x axis: plt.xscale('log')

```
import math
import random

def estimatePi(throws):
    # (same definition of estimatePi function here)
    return pi

throwsList = [1e1, 1e2, 1e3, 1e4, 1e5, 1e6, 1e7]
piEstimatesList = []
for throws in throwsList:
    piEstimatesList.append(estimatePi(throws))
print(piEstimatesList)
```

Solution 3

- **Activity: edit your code**

- Don't print
piEstimatesList
- Instead, make a
scatter plot of
throwsList vs.
piEstimatesList

- Use a log scale on the
x axis: plt.xscale('log')

```
import math
import random
import numpy as np
import matplotlib
from matplotlib import pyplot as plt
matplotlib.rc('axes', labelsize=18)
matplotlib.rc('xtick', labelsize = 18)
matplotlib.rc('ytick', labelsize = 18)
```

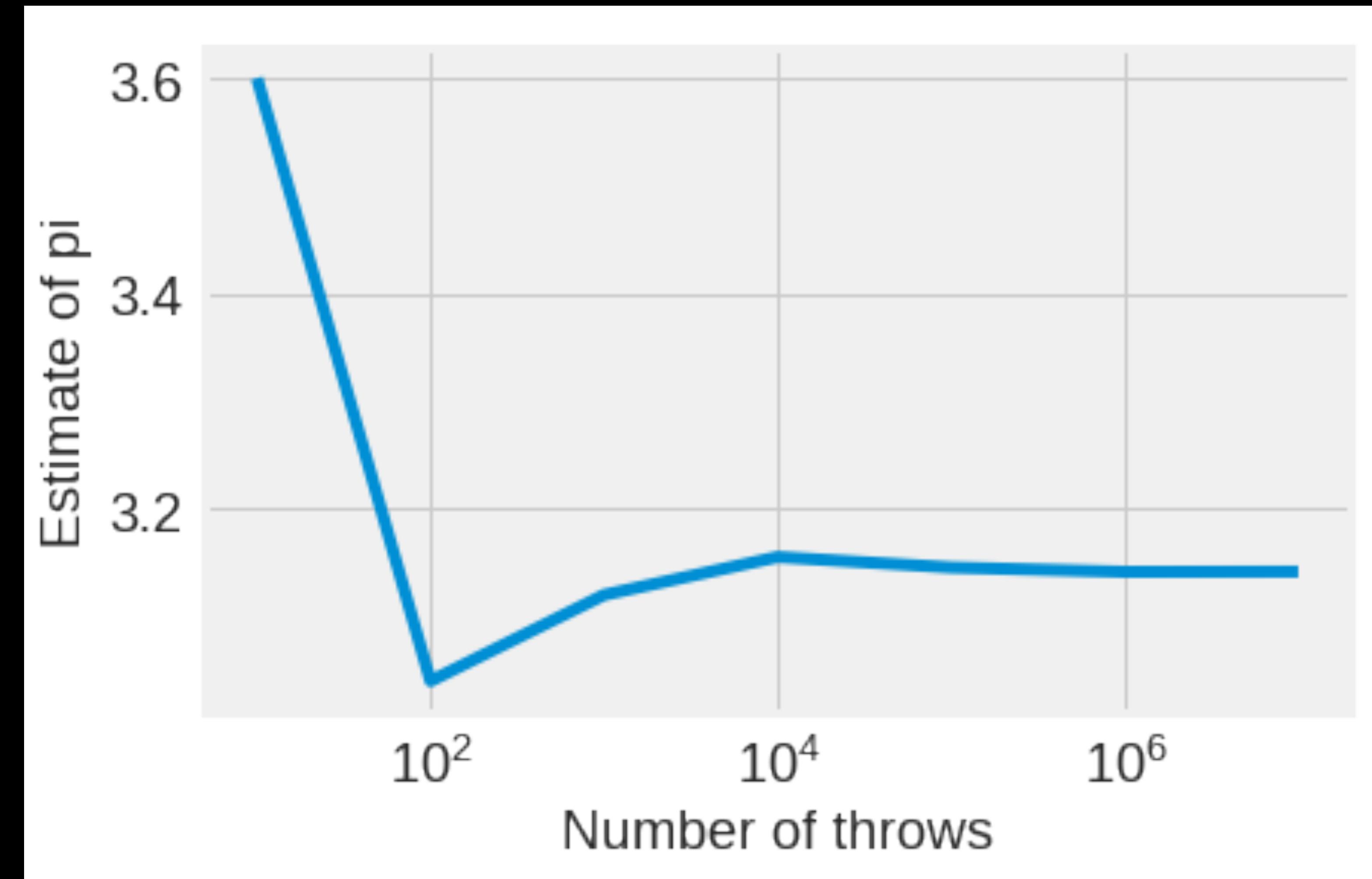
```
def estimatePi(throws):
    # (same definition of estimatePi function here)
    return pi
```

```
throwsList = [1e1, 1e2, 1e3, 1e4, 1e5, 1e6, 1e7]
piEstimatesList = []
for throws in throwsList:
    piEstimatesList.append(estimatePi(throws))
```

```
plt.clf()
plt.plot(throwsList, piEstimatesList)
plt.xlabel('Number of throws')
plt.xscale('log')
plt.ylabel('Estimate of pi')
plt.show()
```

Accuracy of the π dart board

- As throws goes up, answer gets closer to pi
- But it's hard to see how close it is later on
- So instead, plot the difference between the estimate and the real answer



Plotting π 4

- Challenge: edit your code
 - import numpy as np
 - piEstimates = np.array(piEstimatesList)
 - Plot throwsList vs. abs(piEstimates - math.pi)
 - Put y axis on a log scale
 - Update y axis label to be abs(estimate of pi - pi)

```
# ... code that computes pi
```

```
throwsList = [1e1, 1e2, 1e3, 1e4, 1e5, 1e6, 1e7]
piEstimatesList = []
for throws in throwsList:
    piEstimatesList.append(estimatePi(throws))

plt.clf()
plt.plot(throwsList, piEstimatesList)
plt.xlabel('Number of throws')
plt.xscale('log')
plt.ylabel('Estimate of pi')
plt.show()
```

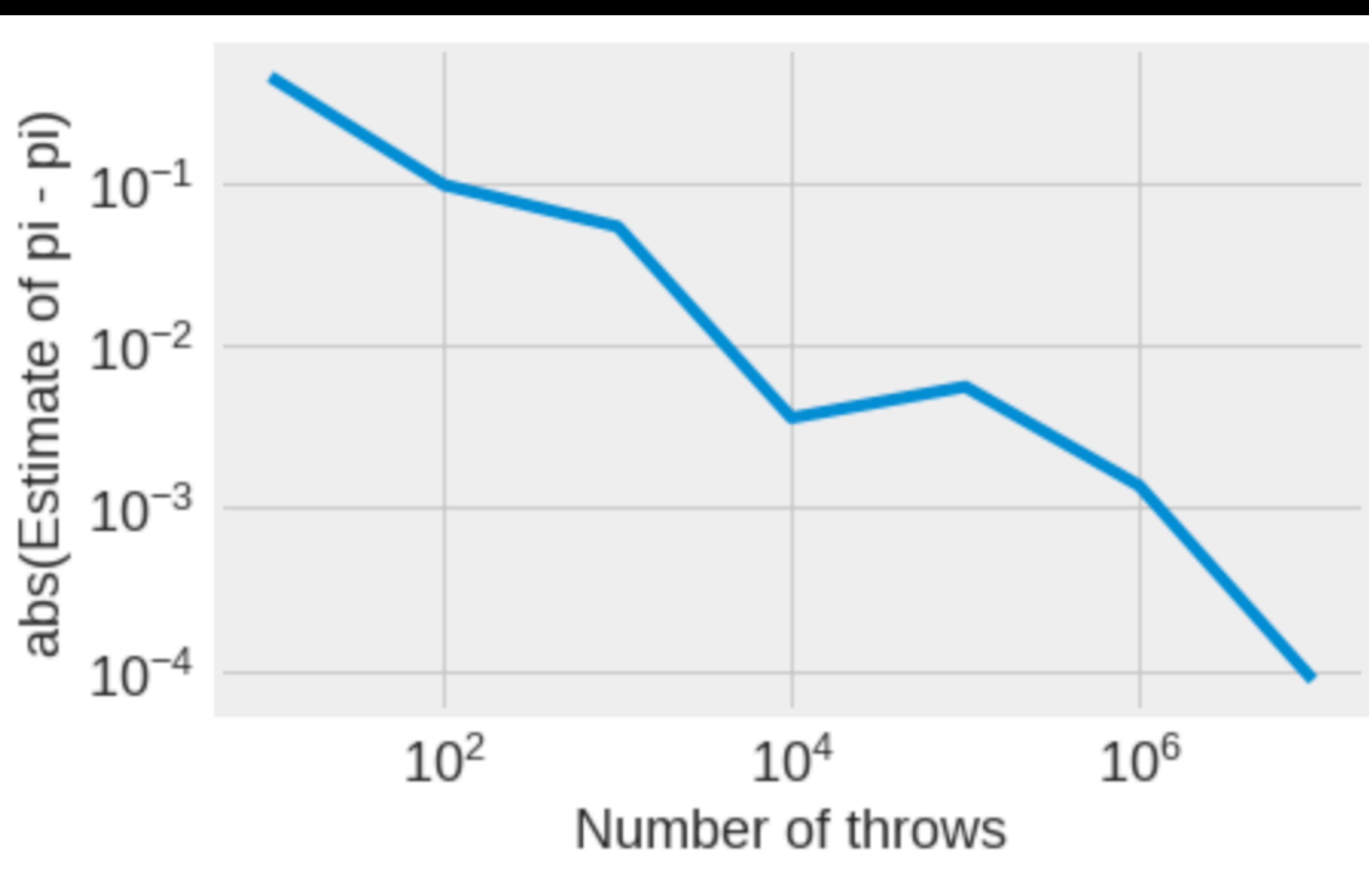
Solution 4

- Challenge: edit your code
 - import numpy as np
 - piEstimates = np.array(piEstimatesList)
- Plot throwsList vs. abs(piEstimates - math.pi)
- Put y axis on a log scale
- Update y axis label to be abs(estimate of pi - pi)

```
# ... code that computes pi
```

```
throwsList = [1e1, 1e2, 1e3, 1e4, 1e5, 1e6, 1e7]
piEstimatesList = []
for throws in throwsList:
    piEstimatesList.append(estimatePi(throws))
```

```
plt.clf()
piEstimates = np.array(piEstimatesList)
plt.plot(throwsList, abs(piEstimates - math.pi))
plt.xlabel('Number of throws')
plt.xscale('log')
plt.yscale('log')
plt.ylabel('abs(Estimate of pi - pi)')
plt.show()
```



Concepts in numerical programming

- Resolution
- Accuracy
- Precision



Low resolution

Entire image: 227KB

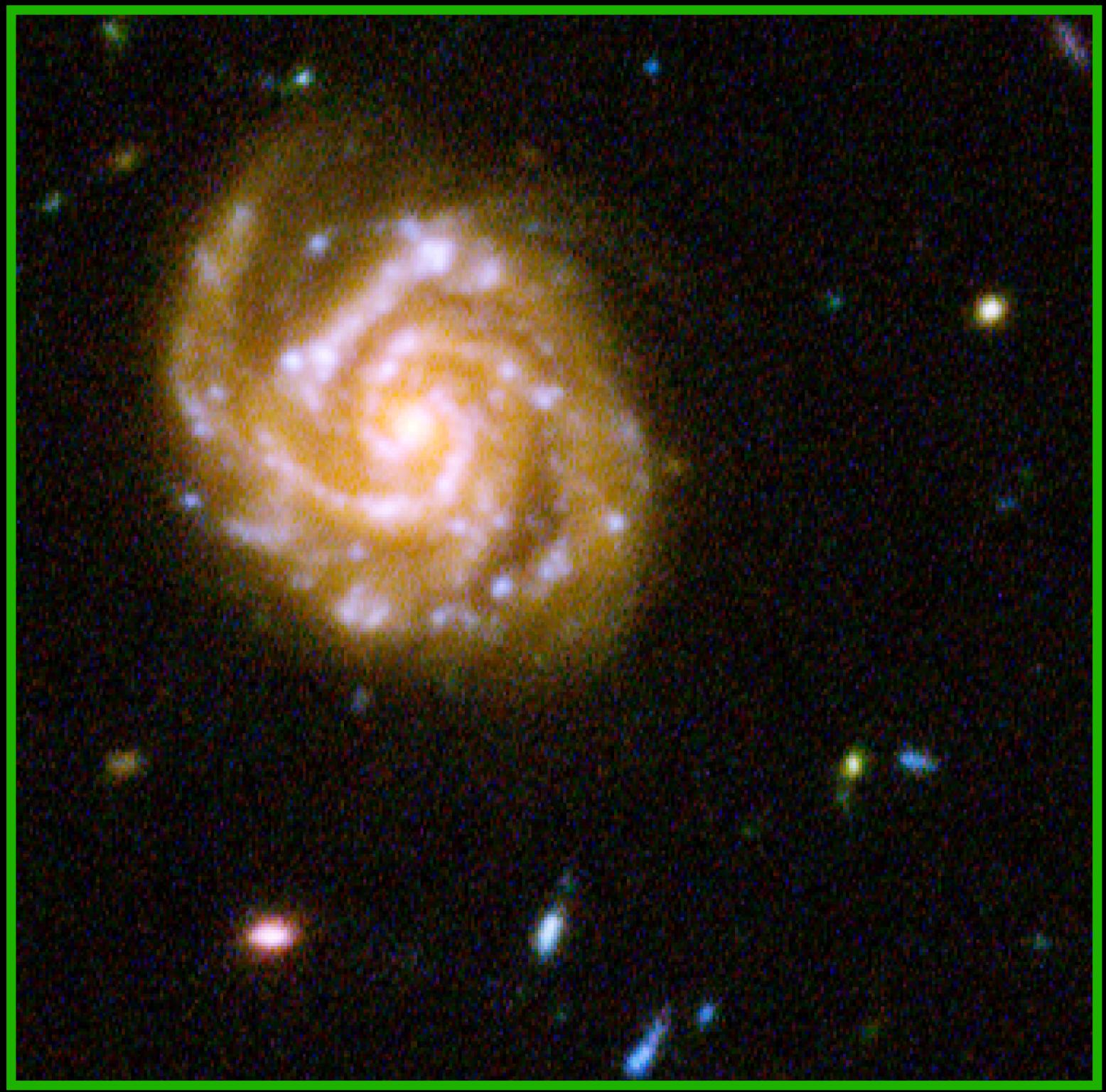
*Large galaxies
1 billion light years away*

*Small galaxies up to
13 billion light years away*

Image courtesy NASA

Resolution





Resolution

High resolution
Entire image: 110MB

*Large galaxies
1 billion light years away*

*Small galaxies up to
13 billion light years away*

Image courtesy NASA

Resolution

- **Low resolution**

- Smaller data
- Faster computation
- Less precise

- **High resolution**

- Bigger data
- Slower computation
- More precise

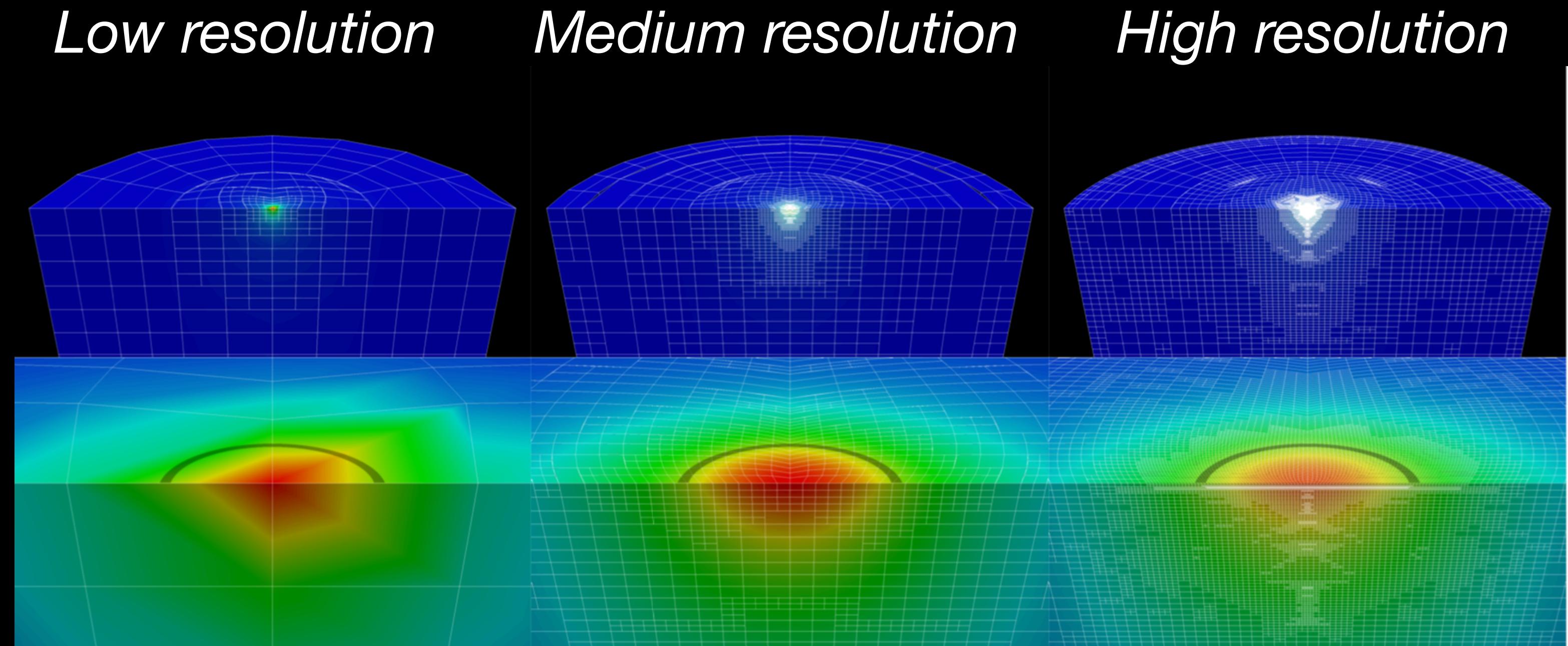


Precision & accuracy

- Precision
 - How much result changes when you add more resolution
 - "How many digits"
- Accuracy
 - How close result is to the correct result

Example: thermal noise

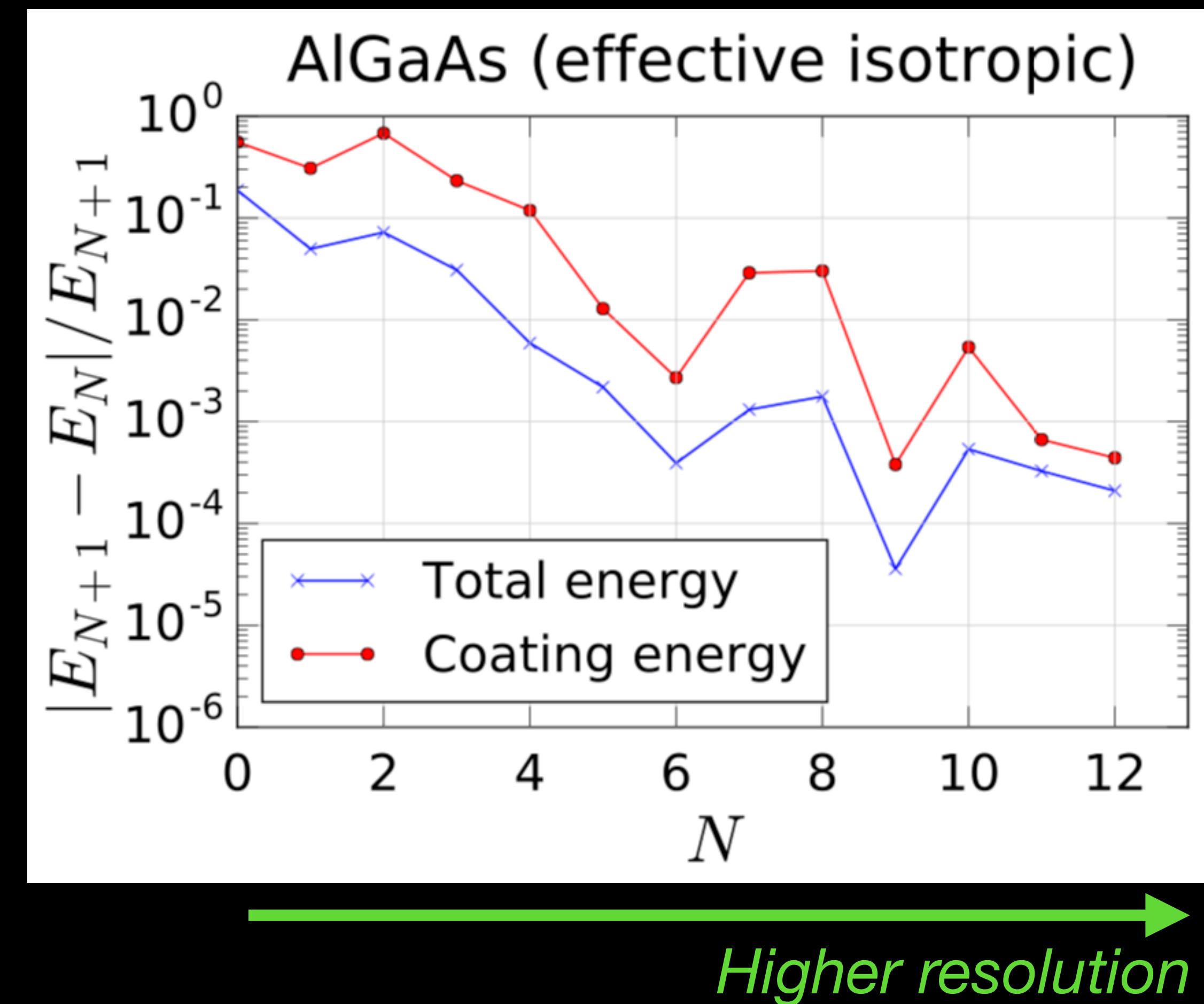
- Thermal noise of a mirror in LIGO depends on how much potential energy it gets when you push on the face



Color = how much mirror deforms

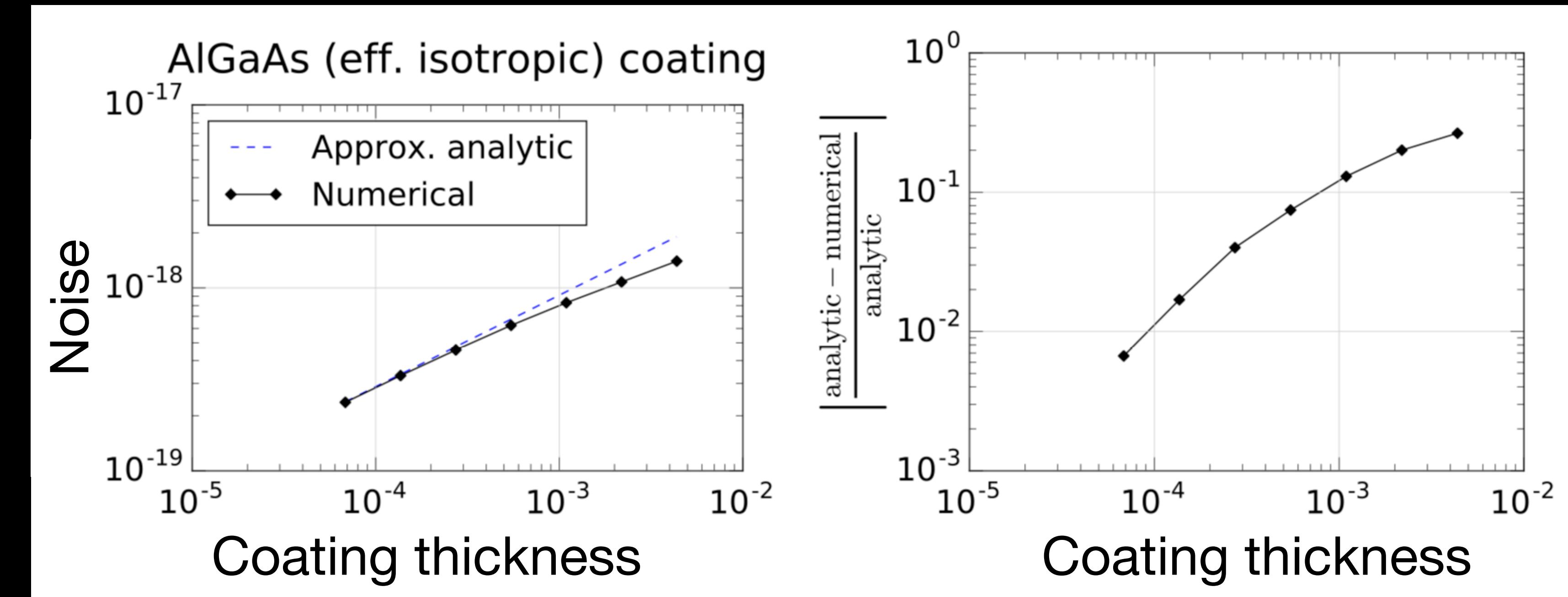
Example: thermal noise

- Potential energy E in deformed mirror
- Precision of energy as resolution increases
 - Label resolution by integer N



Example: thermal noise

- Thermal noise of thin coating
- Accuracy: compare code to known "analytic" solution

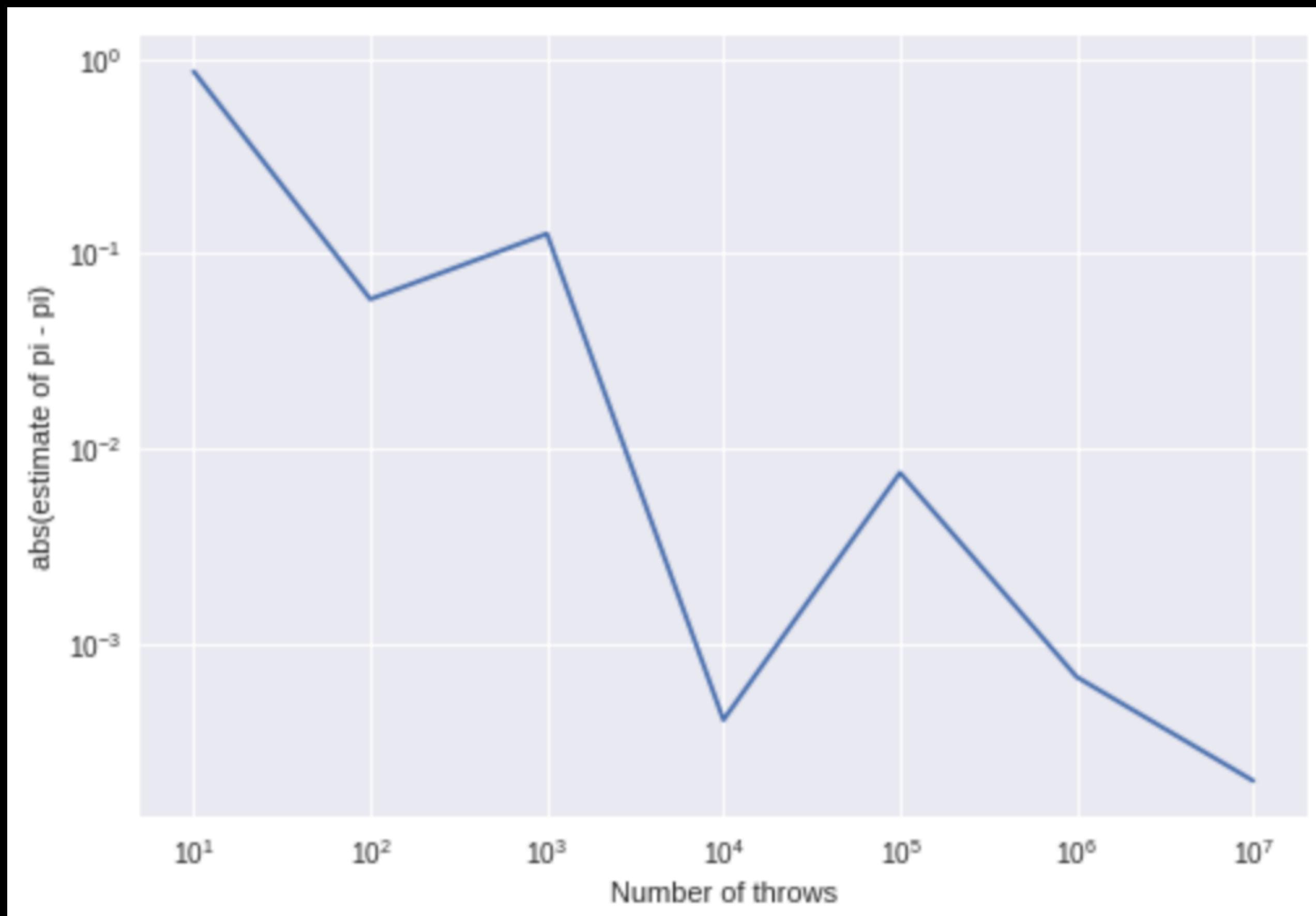


Unix terminal on the web

- Go to [https://mybinder.org/v2/gh/geoffrey4444/
NRDataExample/master](https://mybinder.org/v2/gh/geoffrey4444/NRDataExample/master)
- Choose "New Terminal"

Clicker question #2.7a

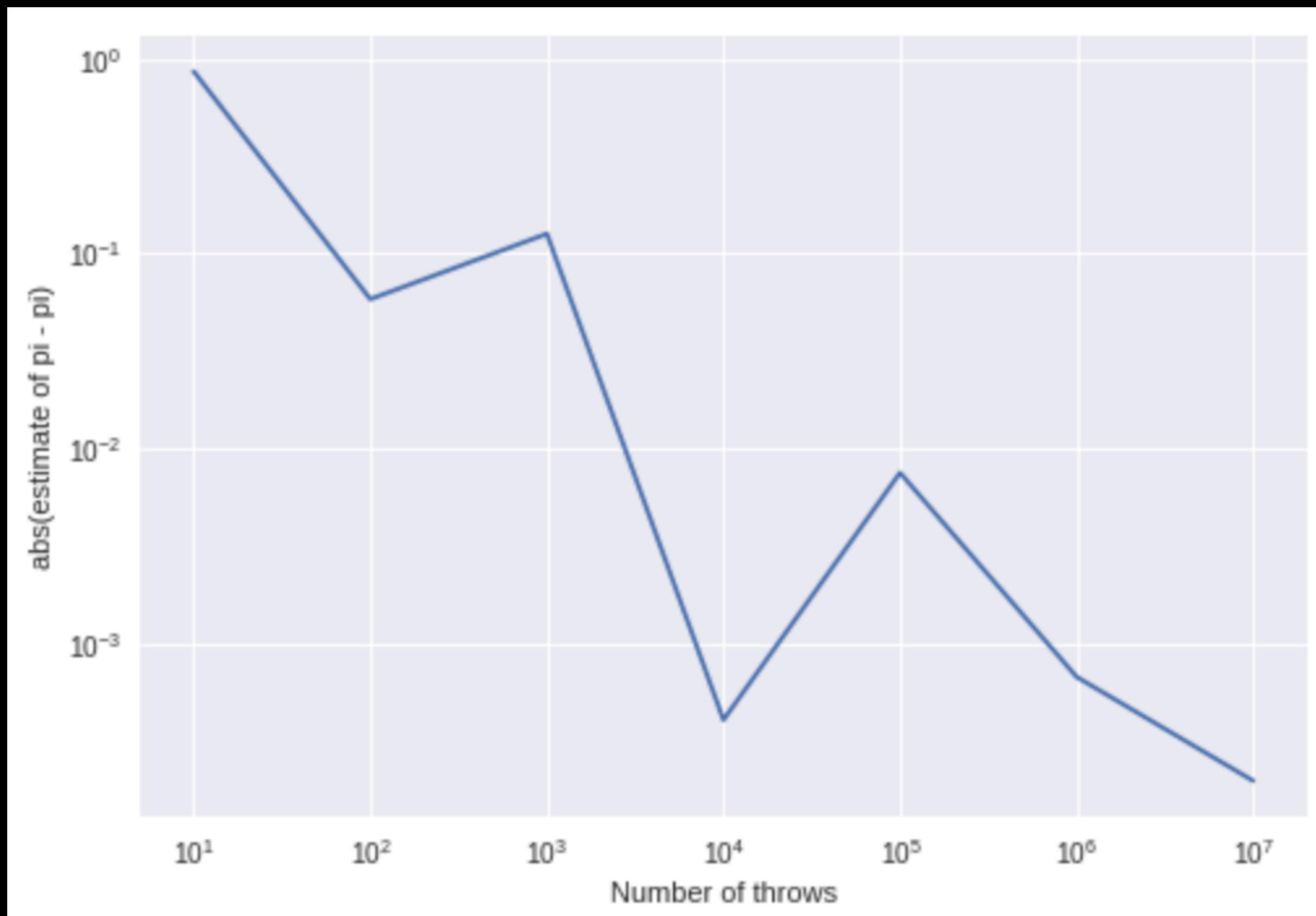
- Your graph plots $\text{abs}(\text{estimate of } \pi - \pi)$ vs number of throws. The **horizontal axis** shows



- A A Precision
- B B Accuracy
- C C Resolution
- D D None of ABC

Clicker question #2.7b

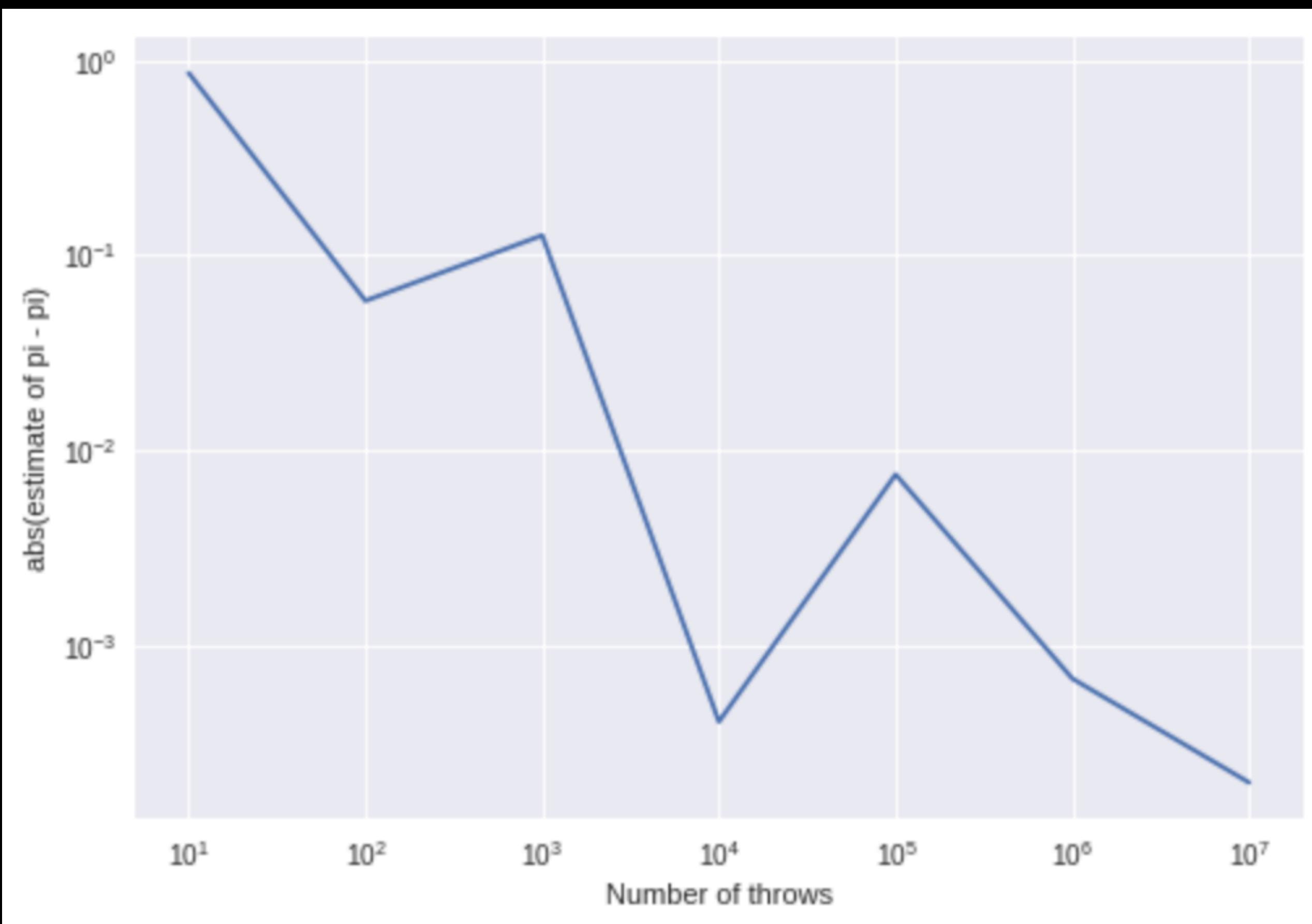
- Your graph plots $\text{abs}(\text{estimate of } \pi - \pi)$ vs number of throws. The **vertical axis** shows



- A Precision
- B Accuracy
- C Resolution
- D None of ABC

Clicker question #2.7c

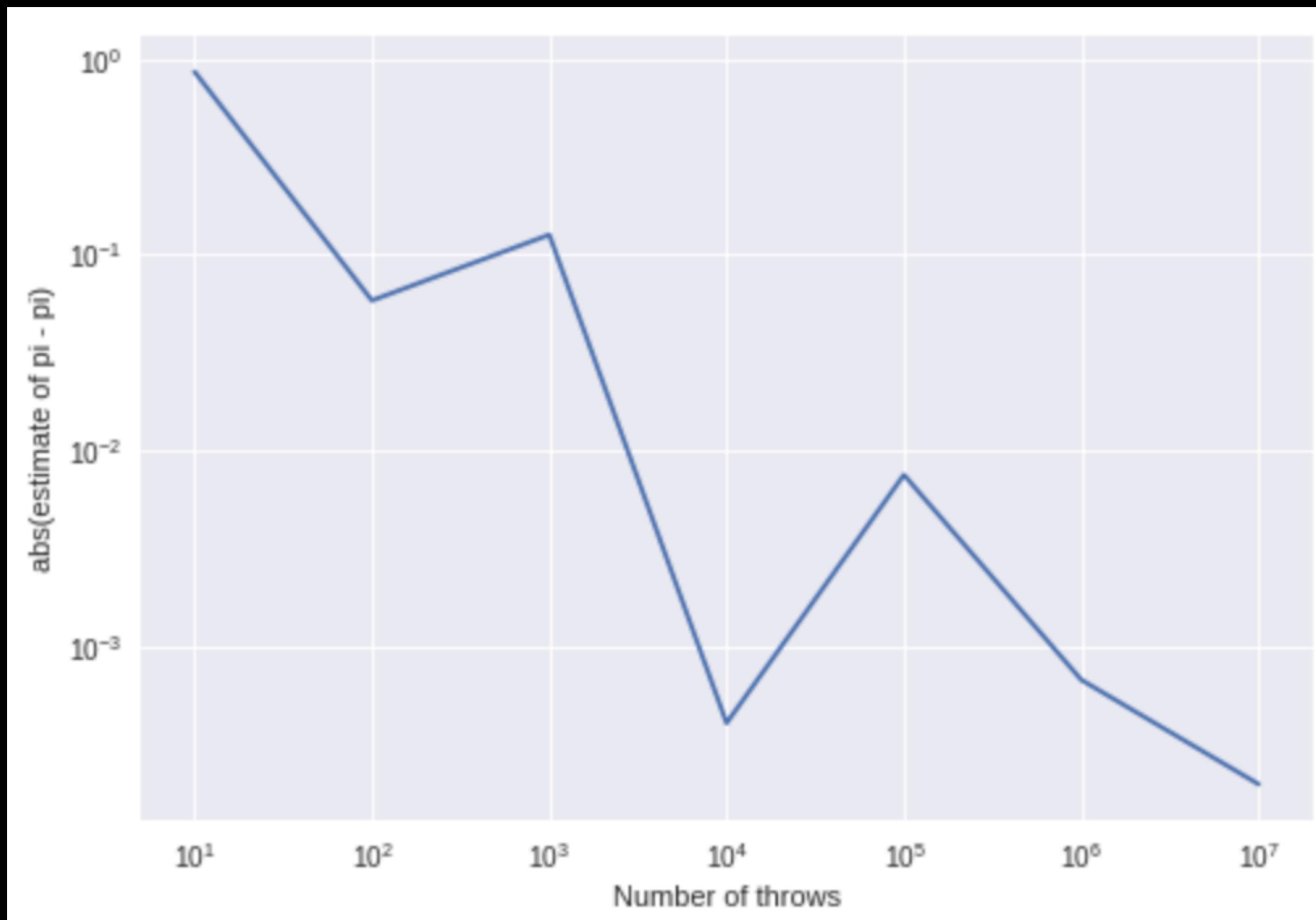
- As the number of throws increases, the **resolution**



- A Increases
- B Decreases
- C Stays the same

Clicker question #2.7d

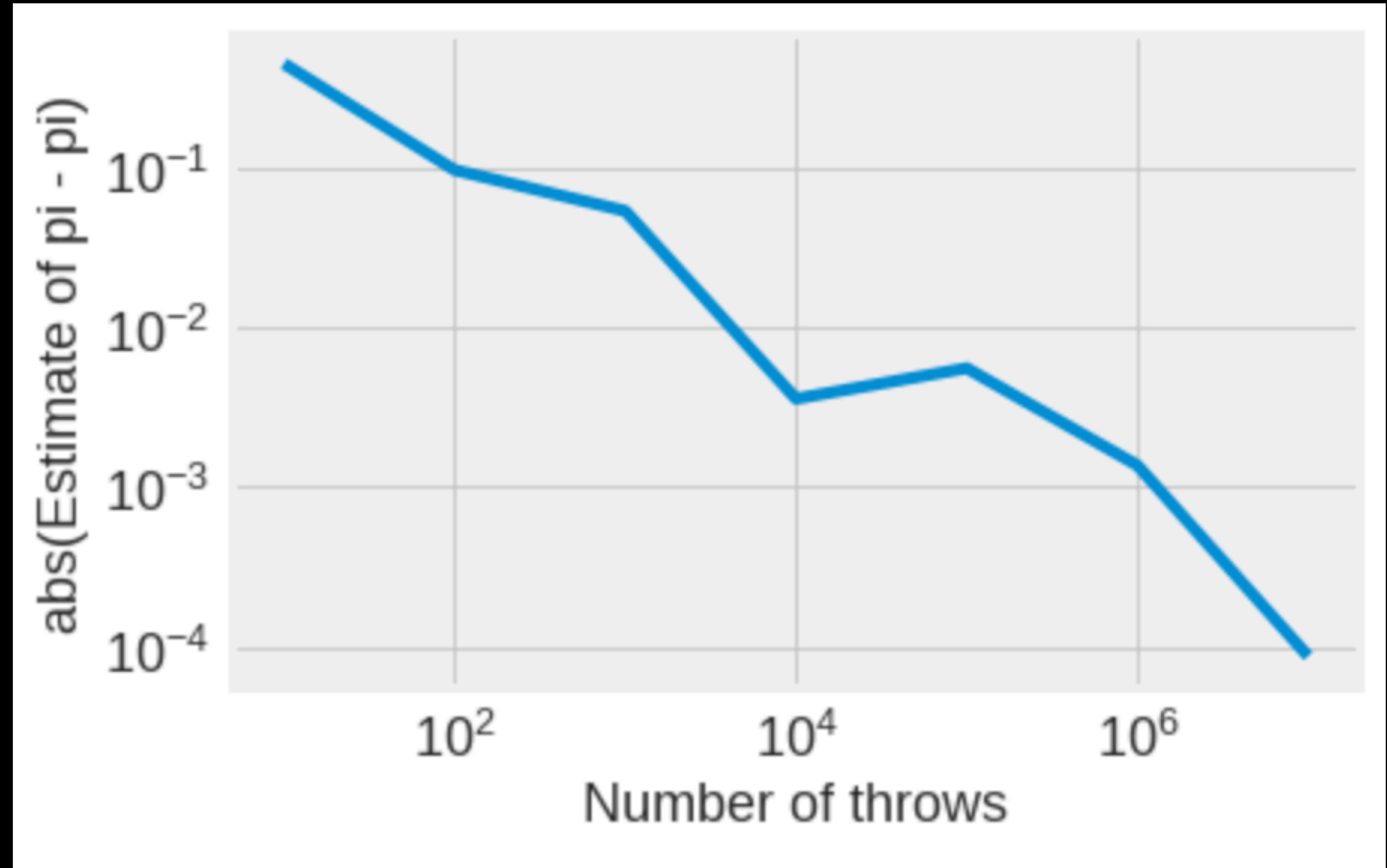
- As the number of throws increases, the **accuracy**



- A** Increases
- B** Decreases
- C** Stays the same

Example: π dart board

- Need roughly 100x more darts to get 10x more accuracy
- That is, 100x darts gives you 10x more accuracy
- This gets slow fast!
- Can we do better?



Connect to ocean (use our laptops)

- Open "PuTTY 64-bit" on the desktop
- Under "saved sessions" select "ocean"
- Click "Open"
- Username: workshopStudents2019
- Passphrase
 - Some computers: workshop2019!!
- squeue
- `srun -p orca-1 --nodes=1 --tasks-per-node=20 --pty /bin/bash`

UNIX command line crash course activity

- **Commands to know**
 - ls, pwd, cd, mkdir
 - ./, ../, paths
 - cp, mv, rm, rmdir
 - cat, less
 - nano
 - whoami, date, ...
- **Play along with me...**
 - mkdir YOURNAME and cd into it
 - Navigate file system: ls, pwd, cd, ./ and ../
 - Use nano to write a text file
 - Copy, rename, remove a file
 - Cat, less, more, head, tail
 - > to redirect output
 - Grab bag: whoami, date, grep, sed, zip...

Unix commands to know

- **Commands to know**
 - ls, pwd, cd, mkdir
 - ./, ../, paths
 - cp, mv, rm, rmdir
 - cat, less
 - nano
 - whoami, date, ...
- **Play along with me...**
 - mkdir YOURNAME and cd into it
 - Navigate file system: ls, pwd, cd, ./ and ../
 - Use nano to write a text file
 - Copy, rename, remove a file
 - Cat, less, more, head, tail
 - > to redirect output
 - Grab bag: whoami, date, grep, sed, man, ...

Clicker question #1.8

- I want to list the files in the directory I'm in. Which command would I use?

A

ls

C

pwd

B

cd

D

nano

Clicker question #1.9

- Which command edits the file “Hello.txt” in the directory I am currently in?

A

`nano ./Hello.txt`

B

`cat ./Hello.txt`

C

`nano ../Hello.txt`

D

`cat ../Hello.txt`

Clicker question #1.9

- Which command makes a new directory called “TestFolder”?

A

ls TestFolder

B

cd TestFolder

C

mkdir TestFolder

D

cp TestFolder

Clicker question #1.9

- Which command removes everything in the current directory, which is not empty?

A

`rmdir .`

B

`rm -r ./*`

C

`rm -r . /*`

D

More than one of these will work

Unix activity

- **Commands to know**
 - ls, pwd, cd, mkdir
 - ./, ../, paths
 - cp, mv, rm, rmdir
 - cat, less
 - nano
 - whoami, date, ...
- Use nano to write a bash script (each line is a command like you would enter on the command line)
 - The script should...
 - Print the current date and time
 - Print the current directory
 - Copy /proc/cpuinfo into the current directory
 - Get the first line of the copied file, and save it to a file called FirstLineOfProc.txt
 - Bonus: Use grep to only show the line with "cpu cores"
 - Bonus: use sed to remove all but the core number
 - Bonus: instead of copying the /proc/cpuinfo file, copy whatever file users specify as an argument (google bash arguments)

Parallel computing

- Supercomputers have lots of cores
- But each core is not much faster than a PC
- To take full advantage, you have to write code that can run on more than one core at the same time
- That is, code that runs in parallel



Image courtesy Blue Waters

Connect to ocean

- Open "PuTTY 64-bit" on the desktop
- Under "saved sessions" select "ocean"
- Click "Open"
- Username: workshopStudents2019
- Passphrase
 - Some computers: workshop2019!!
- squeue
- `srun -p orca-1 --nodes=1 --tasks-per-node=20 --pty /bin/bash`

Parallel computing 1

- Log into ocean
- Do this

```
#Replace GeoffreyLovelace with YourName  
cd student_folders  
mkdir YOUR_NAME #replace with your lastName(firstName  
cd YOUR_NAME
```

```
mkdir PiDart  
cd PiDart  
source /opt/ohpc/pub/apps/anaconda2/bin/activate root
```

Parallel computing 2

- nano Hello.py

```
print("Hello")
```

- mpirun -np 8 python Hello.py
- What happens? What happens if you change 8 to another number less than 8?

What happened?

- mpirun ran many copies of “Hello.py”
- Each copy printed “Hello”
 - But the processors are not working together yet, or even doing anything different
- Next: make different processors do different things

Parallel computing 3

- cp Hello.py MpiHello.py
- nano MpiHello.py

```
from mpi4py import MPI
comm = MPI.COMM_WORLD
rank = comm.Get_rank()
size = comm.Get_size()

print("Hello from processor "+str(rank)+" out of
"+str(size))
```

- mpirun -np 4 python MpiHello.py
- mpirun -np 8 python MpiHello.py