Lecture A4. Simulation 1

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I. Motivation - estimation of π

What is π?

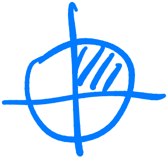
- π is defined as
$$\pi = \frac{\text{a circle's circumference}}{\text{a circle's diameter}}$$
- To list a few reasons why π is such an important quantity:
  - In Architecture
  - In Construction
  - In Art
  - In Military operation
  - so many $\cdots$

How to estimate?

- In your elemetary school

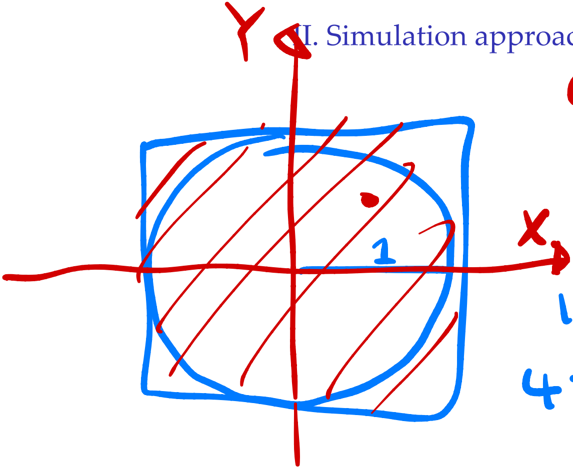
- From your high school, you learned that

$$
\begin{aligned}
(\text{quarter size of a unit circle}) &= \int_0^1 \sqrt{1-x^2}\,dx \\
&= \pi/4
\end{aligned}
$$



- In ancient days, people used $\pi/4 = \int_0^1 \sqrt{1-x^2}dx$ to estimate π.

II. Simulation approach



$X \sim U(-1,1)$
$(x, y) \sim$ $Y \sim U(-1,1)$

4 vs π

1000 vs 800

$4 : \pi = 1000 : 800$

$\pi = 3.2$

Design

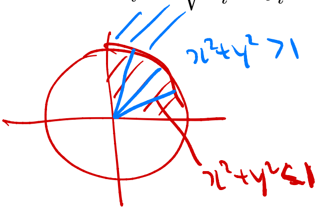
MC-N

$\mathbf{x} = \begin{bmatrix} \vdots \end{bmatrix}$ $\mathbf{y} = \begin{bmatrix} \vdots \end{bmatrix}$

- Step 1.
  - Let $X \sim U(-1, 1)$ and $Y \sim U(-1, 1)$.
  - Generate two vectors length of N, i.e. $\mathbf{x} = (x_1, x_2, \dots, x_N)$ and $\mathbf{y} = (y_1, y_2, \dots, y_N)$, where x_i is a sample of X and y_i is a sample of Y for all i.

$\mathbf{x}$: vector
x_i : element

- Step 2.
  - Let $t_i := \sqrt{x_i^2 + y_i^2}$ for all i, that is,



$$
\begin{aligned}
t_1 &:= \sqrt{x_1^2 + y_1^2} \\
t_2 &:= \sqrt{x_2^2 + y_2^2} \\
\cdots & \quad\ \cdots \\
t_N &:= \sqrt{x_N^2 + y_N^2}
\end{aligned}
\qquad
\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ \vdots \\ 1 \\ 0 \\ 0 \end{bmatrix}
$$

binary fn
indicator.

$\mathbb{1}_{\{t_i \le 1\}} = \begin{cases} 1 & \text{true} \\ 0 & \text{false} \end{cases}$

- Step 3.

$$\hat{\pi} = 4 \times \frac{\text{number of } \{t_i \le 1\}}{N} = 4 \times \frac{\sum_{i=1}^{N} I_{\{t_i \le 1\}}}{N}$$

1000

Remark 1

The function $I_{\{\cdot\}}$ is called an *indicator function* that returns 1 if the statement is true and 0 if false.

- $\frac{\sum_{i=1}^{N} I_{\{t_i \leq 1\}}}{N}$ counts the number of t_i that is less than or equal to 1, among all i.

A statistical software, R

- I am a firm believer of that you should comfortably interchange between R and python.

R for python user

- Resources 1 - `datacamp.com`
  - `datacamp.com` allows access for >100 courses for R and python.
  - I suggest you at least do ‘Introduction to R’ and ‘Intermediate R’.
  - You can subscribe for free using your `@seoultech.ac.kr` email with the following link.
  - https://www.datacamp.com/groups/shared_links/b3b5fc6f798aaf54ada0c03cee875c0099c34e300f5be6b8375e4850646b0b59
  - The above link expires at March 2021, but I always renew it.
  - You can always request me for an invitation link if yours is expired.
- Resources 2 - lecture material for data visualization
  - From the following repository, study L01-L03 for installation and basic usage.
  - https://github.com/aceMKSim/teaching/tree/master/Data%20Visualization/Lecture%20Notes

Implementation - basic

- Implementation with 1000 repetitions.

MC-N

```
set.seed(1234) # fix the random seed
N <- 10^3
x <- runif(N)*2-1 # runif() generates U(0,1)
y <- runif(N)*2-1   # this code gen. U(-1,1)
t <- sqrt(x^2+y^2)
head(cbind(x,y,t)) # always display and check!
```

```
##               x          y         t
## [1,] -0.7725932  0.6752678 1.0261028
## [2,]  0.2445988 -0.0250675 0.2458800
## [3,]  0.2185495 -0.7793260 0.8093904
## [4,]  0.2467589 -0.2972740 0.3863441
## [5,]  0.7218308  0.5221261 0.8908733
## [6,]  0.2806212 -0.2206703 0.3569925
```

```
pi_hat <- 4*sum(t<=1)/N
pi_hat
```

```
## [1] 3.188
```

1. `set.seed()` fixes randomization, which is often convenient to get consistent outcome.
2. `runif(N)` generates a vector of length N, where each element follows $U(0,1)$.
3. `runif(N)*2` follows $U(0,2)$, and `runif(N)*2-1` follows $U(-1,1)$.
4. `t<=1` returns the 0-1 vector of length same as `t`, where an element is 1 if corresponding element in `t` is less than or equal to 1, and 0 otherwise.
5. `cbind()` combines (column) vectors into a matrix.
6. `head()` displays the first six observations.

Vectorized programming

- From the previous slide

```
beg_time <- Sys.time()
set.seed(1234)
N <- 10^6
x <- runif(N)*2-1
y <- runif(N)*2-1
t <- sqrt(x^2+y^2)
pi_hat <- 4*sum(t<=1)/N
end_time <- Sys.time()
print(end_time-beg_time)
```

```
## Time difference of 0.1457582 secs
```

- What first-timer would write.

```
beg_time <- Sys.time()
set.seed(1234)
N <- 10^6
count <- 0
for (i in 1:N) {
  x_i <- runif(1)*2-1
  y_i <- runif(1)*2-1
  t_i <- sqrt(x_i^2+y_i^2)
  if (t_i <= 1) count <- count + 1
}
pi_hat <- 4*count/N
end_time <- Sys.time()
print(end_time-beg_time)
```

```
## Time difference of 6.264948 secs
```

- The style of the code on the left is called *vectorized programming*.
- It is elegant, economic, and efficient.
- You must be able to *write as the left* side and *communicate as the right* side (to non-expert).

Implementation - varying number of trials

p.13 code
python

- Approach with a custom function

```r
pi_simulator <- function(N) {
  set.seed(1234)
  x <- runif(N)*2-1
  y <- runif(N)*2-1
  t <- sqrt(x^2+y^2)
  pi_hat <- 4*sum(t<=1)/N
  return(pi_hat)
}
```


```r
pi_simulator(100)
```

```
## [1] 3.04
```

```r
pi_simulator(1000)
```

```
## [1] 3.188
```

```r
pi_simulator(10000)
```

```
## [1] 3.1876
```

```r
pi_simulator(100000)
```

```
## [1] 3.13432
```

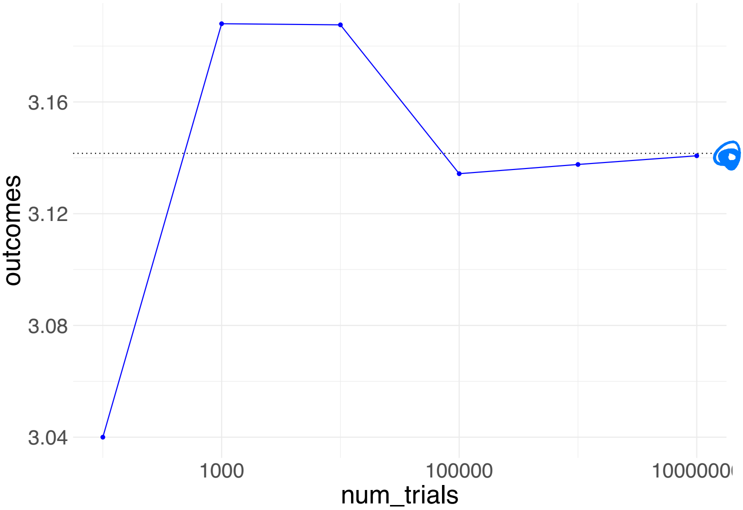
- How many repetition is necessary to get closer?

```r
num_trials <- 10^(2:7)
outcomes <- sapply(num_trials, pi_simulator)
results <- cbind(num_trials, outcomes)
results
```

```
##      num_trials outcomes
## [1,]        100 3.040000
## [2,]       1000 3.188000
## [3,]      10000 3.187600
## [4,]     100000 3.134320
## [5,]    1000000 3.137616
## [6,]   10000000 3.140733
```

- `sapply(num_trials, pi_simulator)` *applies* the function `pi_simulator()` to *each element* of `num_trials`.

- How many repetition is necessary to get closer?



The previous figure was plotted by the following code.

```
results <- data.frame(results)
library(tidyverse)
ggplot(results, aes(x=num_trials, y=outcomes)) +
  geom_point(color = "blue") + geom_path(color = "blue") +
  geom_abline(slope = 0, intercept = 3.14159, linetype = "dotted") +
  scale_x_log10() +
  theme_minimal() + theme(text = element_text(size=25))
```

III. Discussion

Computation time

- In this implementation, number of trials were increased from 10^2 to 10^7. No wonder that this increases the computational time.
- Following modified function displays the elapsed time.

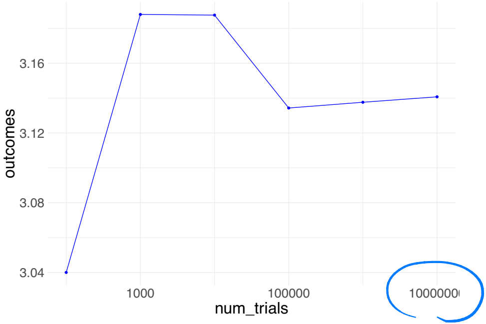
```r
pi_simulator2 <- function(N) { # name change
  beg_time <- Sys.time() # newly added
  set.seed(1234)
  x <- runif(N)*2-1
  y <- runif(N)*2-1
  t <- sqrt(x^2+y^2)
  pi_hat <- 4*sum(t<=1)/N
  end_time <- Sys.time() # newly added
  print(N)
  print(end_time-beg_time) # newly added
  return(pi_hat)
}
```

```r
sapply(num_trials, pi_simulator2)
```

```
## [1] 100
## Time difference of 0 secs
## [1] 1000
## Time difference of 0.0007610321 secs
## [1] 10000
## Time difference of 0.002549887 secs
## [1] 100000
## Time difference of 0.01874018 secs
## [1] 1000000
## Time difference of 0.202595 secs
## [1] 10000000
## Time difference of 1.864766 secs
## [1] 3.040000 3.188000 3.187600 3.134320 3.137616 3
```

Confidence on the result

- In estimation of π example, we were in the luxurious situation because we already knew the correct value of π, 3.14159.
- In reality, this situation is rare. Rather, you shouldn't be in need of doing simulation after all if you already know the exact value.
- In reality, following figure is what you would normally face. Notice that the correct value indicating line is gone.



- One legimate way to have some confidence is to observe the plot and say ‘It seems converging with good degree’. Then, present a number that seems to be within the tolerance.
- Are there any way to present a confidence interval, just as good statistical estimations should present?

IV. Confidence interval

Motivation

여기서 넣어 MC-N.

- Building a confidence interval from experiment generally involves repetitive experiments. But in the simulation approach, we already do have the repetitive simulation experiments? Isn't this enough?
- Not really so. In order to build a confidence interval, we should treat *one entire simulation experiment* as *one observation*. For example, we treat the result from a $N = 1000$ simulation experiment as a single observation on the true value. Then repeat this simulation experiment, say, n times, to build a confidence interval.
- Let's set $N = 1,000$ for a simulation experiment and do this for $n = 100$ times.

MC-N

Repetitive simulation experiments

MC

- Let's set $N = 1,000$ for a simulation experiment and do this for $n = 100$ times.
- For each experiment, record the result to collect $n = 100$ samples.

```
pi_simulator3 <- function(N) { # name change
  # set.seed(1234) # seed must not be fixed
  x <- runif(N)*2-1
  y <- runif(N)*2-1
  t <- sqrt(x^2+y^2)
  pi_hat <- 4*sum(t<=1)/N
  return(pi_hat)
}
```

```
n <- 100 # number of experiments to repeat
N <- 1000 # number of simulation repetition in a single experiment
set.seed(1234)
samples <- rep(0, n) # create an empty zero vector
for (i in 1:n) { # do this for n times
  samples[i] <- pi_simulator3(N)
}
head(samples)
```

```
## [1] 3.188 3.144 3.060 3.240 3.148 3.172
```

- From LN.A4.p13,

1.96
2

$$\mathbb{P}[\overline{X} - t_{0.975,n-1} \cdot s/\sqrt{n} \le \mu \le \overline{X} + t_{0.975,n-1} \cdot s/\sqrt{n}] = 0.95$$

- Obtain the numbers as follows:

```
X_bar <- mean(samples)
s <- sqrt(sum((X_bar-samples)^2)/(n-1))
t <- qt(p=0.975, df = n-1)
```

```
X_bar

## [1] 3.137

s

## [1] 0.05186579

t

## [1] 1.984217
```

Thus,

$$\mathbb{P}[3.137 - 1.984 \cdot 0.0519/\sqrt{100} \ \le \ \mu \ \le \ 3.137 + 1.984 \cdot 0.0519/\sqrt{100}] = 0.95$$

$$\Downarrow$$

$$\boxed{\mathbb{P}[3.127 \ \le \ \mu \ \le \ 3.147] = 0.95}$$

0.02

- Note that the length of interval was 0.020 (=3.147-3.127)
- Obviously, increasing $\cancel{N}$ and/or increasing n should narrow the confidence interval.

MC-N

Exercise 1

MC-N

Do the above experiment with $\cancel{N}$ increased by the factor of ten, and present the confidence interval. (Use `set.seed(1234)`*)*

```
n <- 100 # number of exp. to rep.
N <- 10000 # number of sim. rep. in a single exp.
set.seed(1234)
samples <- rep(0, n)
for (i in 1:n) {
  samples[i] <- pi_simulator3(N)
}
X_bar <- mean(samples)
s <- sqrt(sum((X_bar-samples)^2)/(n-1))
t <- qt(p=0.975, df = n-1)
lb <- X_bar-t*s/sqrt(n) # lower bound
ub <- X_bar+t*s/sqrt(n) # upper bound
```

```
lb
## [1] 3.137164
ub
## [1] 3.143788
ub-lb
## [1] 0.006624215
```

Exercise 2

Do the Exercise 1 above with n increased by the factor of ten, and present the confidence interval. (Use `set.seed(1234)`*)*

```
n <- 1000 # number of exp. to rep.
N <- 10000 # number of sim. rep. in a single exp.
set.seed(1234)
samples <- rep(0, n)
for (i in 1:n) {
  samples[i] <- pi_simulator3(N)
}
X_bar <- mean(samples)
s <- sqrt(sum((X_bar-samples)^2)/(n-1))
t <- qt(p=0.975, df = n-1)
lb <- X_bar-t*s/sqrt(n) # lower bound
ub <- X_bar+t*s/sqrt(n) # upper bound
```

```
lb
## [1] 3.139777
ub
## [1] 3.141834
ub-lb
## [1] 0.002057237
```

1/3 $1/\sqrt{10}$

Computation cost and The accuracy

N	n	length of CI
1,000	100	0.020
1,0000	100	0.0066
1,0000	1000	0.00205

$1/\sqrt{10}$

$1/\sqrt{10}$

- Increasing N or n gives the same effect.
  - When N was increased by the factor of 10, the length of CI was decreased by the factor of $\sqrt{10}$.
  - When n was increased by the factor of 10, the length of CI was decreased by the factor of $\sqrt{10}$.
- Repetitive simulation experiments is beneficial if $\cdots$
  - when you need confidence interval.
  - when you face memory issue that prevents increasing N any more.

```
## If I only had an hour to chop down a tree, I would spend the first 45 minutes sharpening my axe. -
A. Lincoln
```