

NeuralNet 101

2. Optimization based on gradients

What is the Optimization?

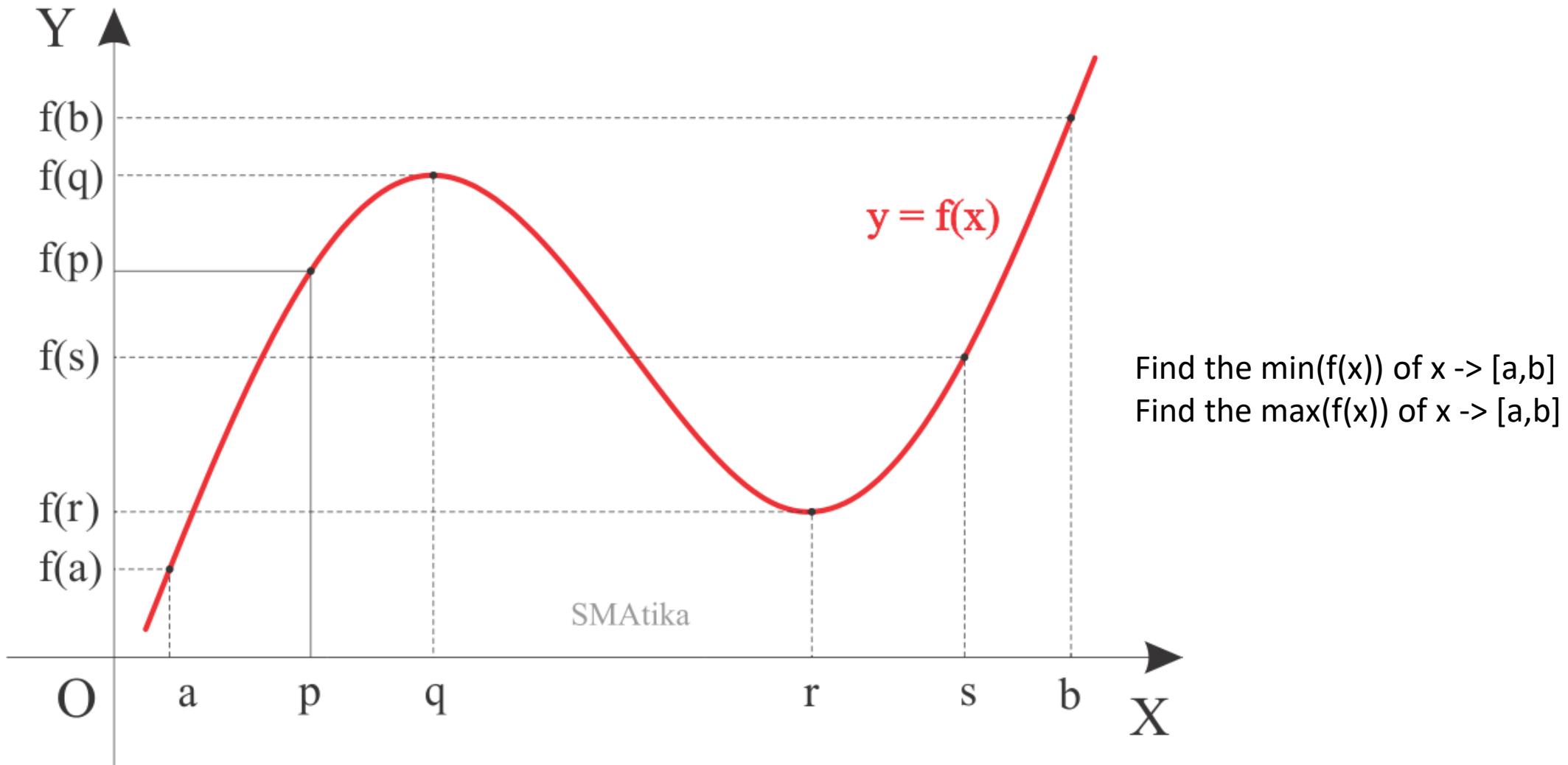
Usage of the word in real life, optimization

- We optimized the design of X to can reach the maximum performance.
- We optimized the recommendation algorithm to show the best individualized advertisement to each person
- We optimized the factory, so we can spend lesser about 21% than before.

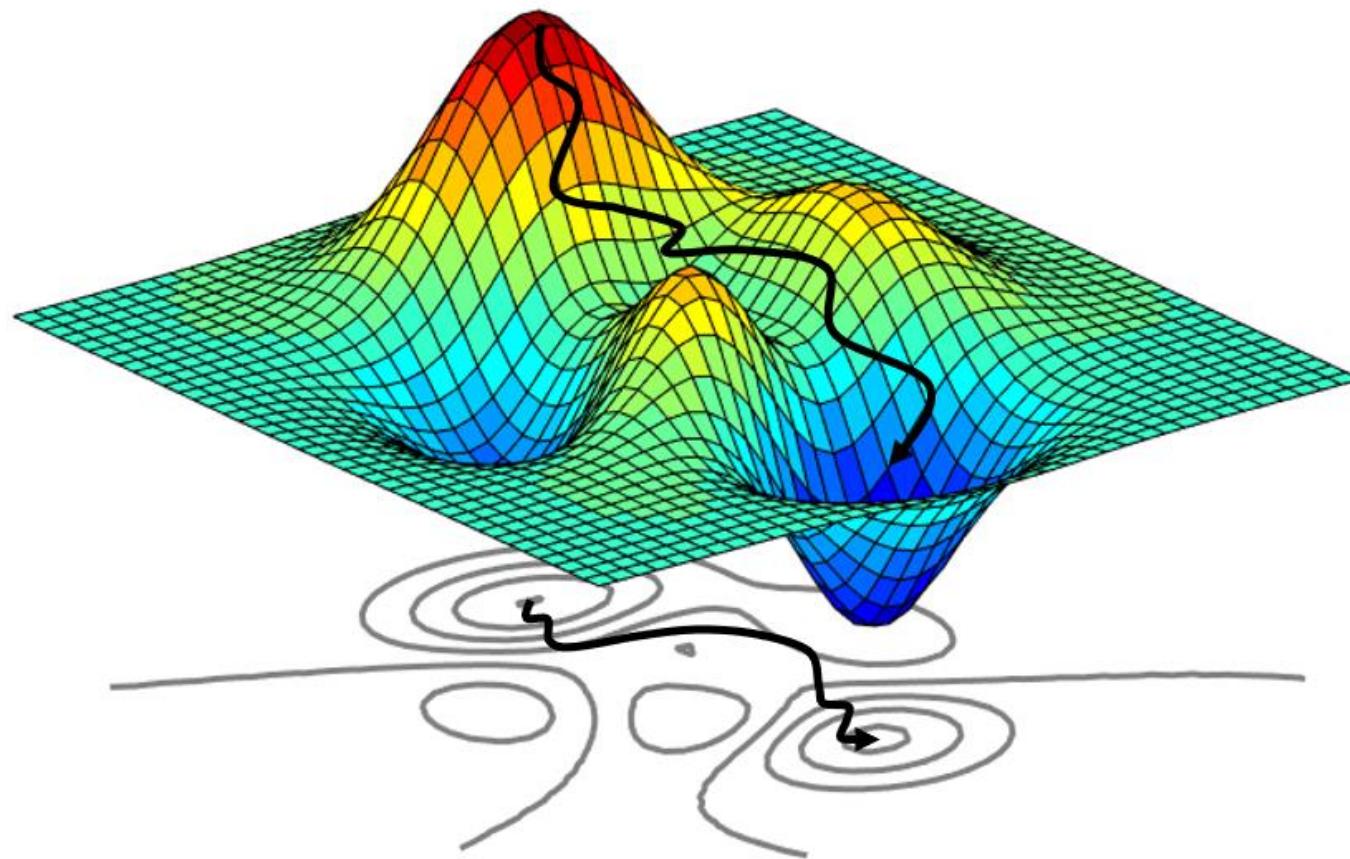
The optimization of NeuralNets : Mathematical Optimization

It's so simple, just find $\min(f(x))$ or $\max(f(x))$ in certain space.

Actually we did it on highschool, right?



But how can we do optimization this function f ?

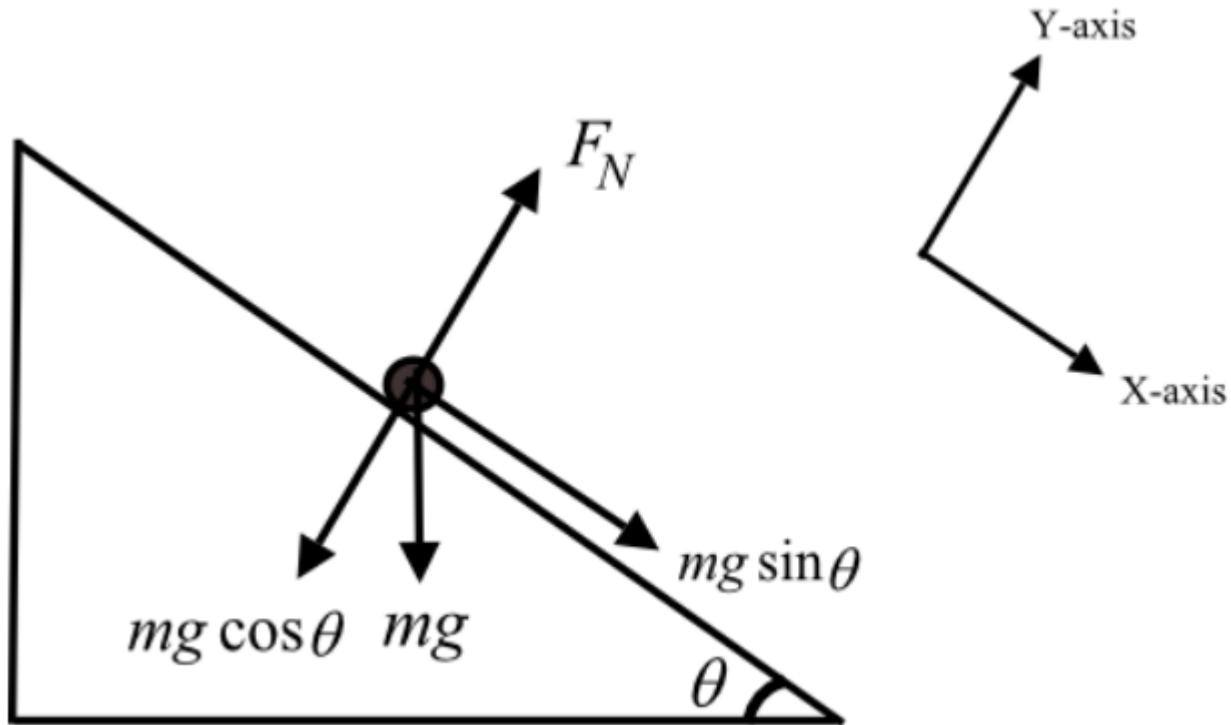


Understanding something based on physics view, it might help you to understand

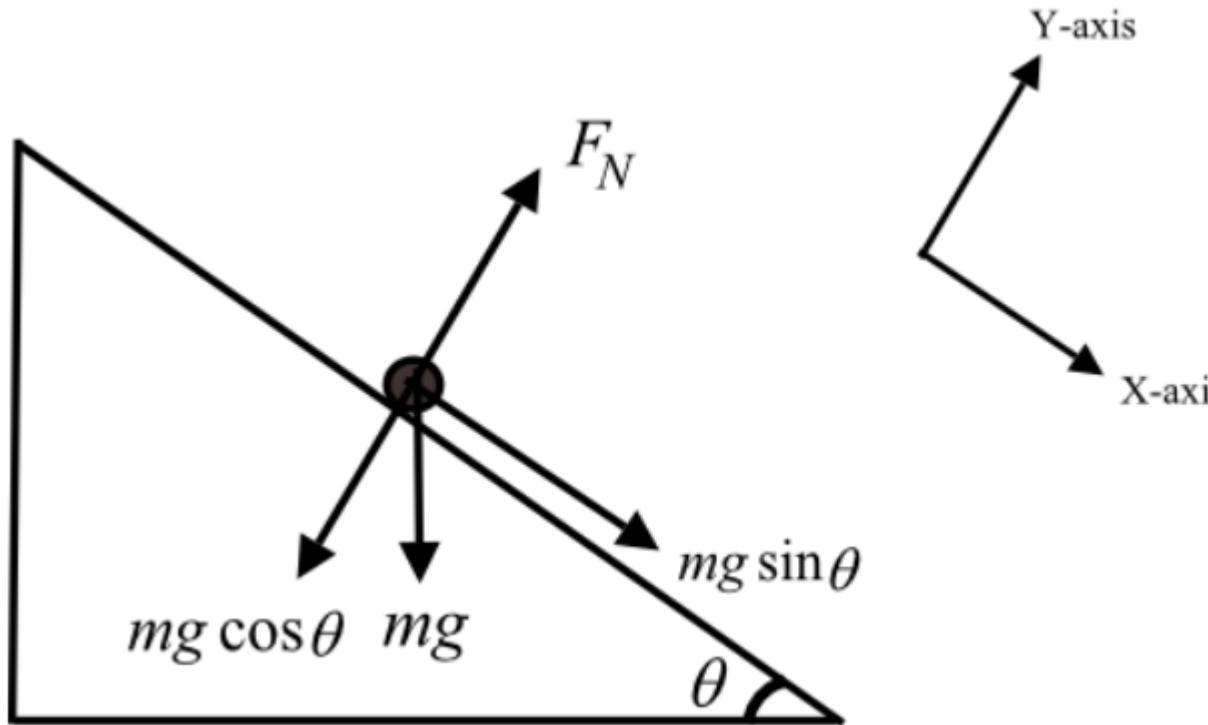
Looking gradient descent based on physics perspective

- Let's fall a ball on the top of mountain
- Then, how can we define the moving function of ball?

Let's look this plane in general physics...



Let's look this plane in general physics...

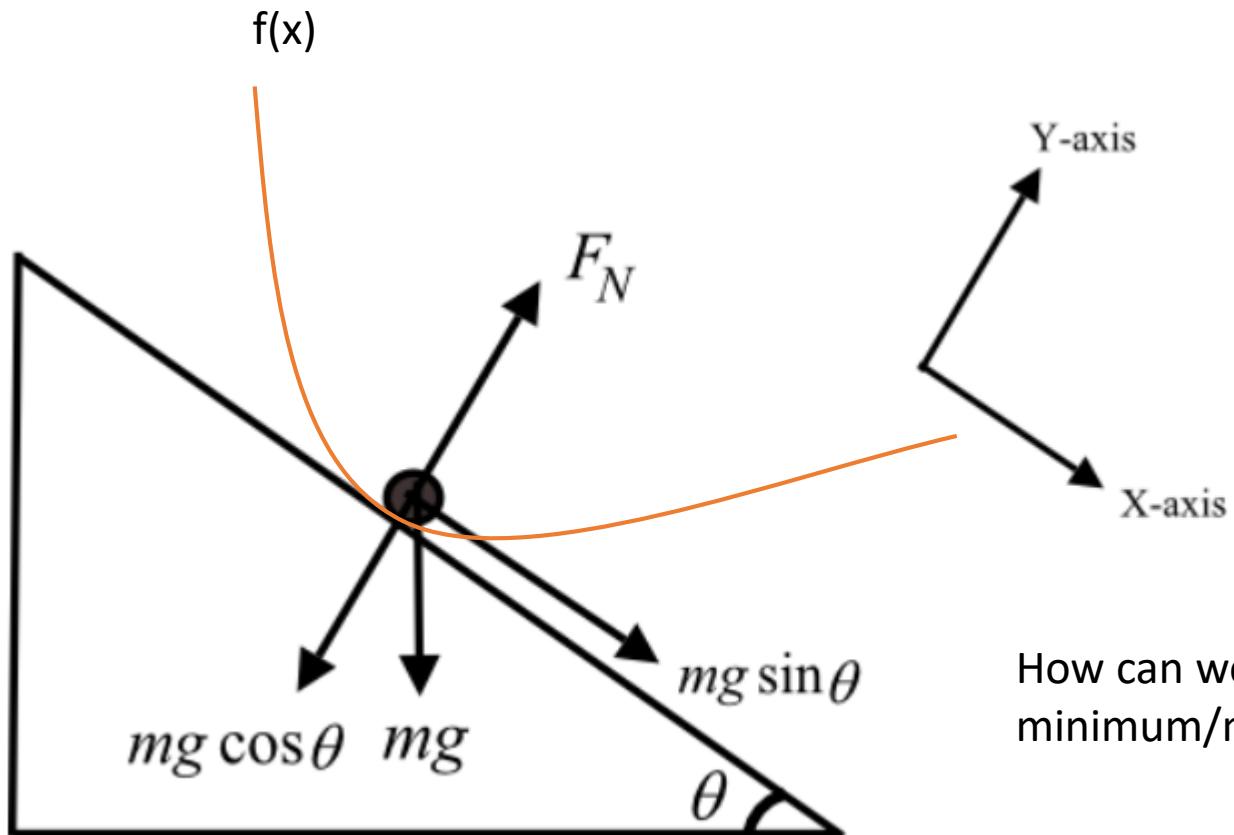


If the θ ($0 < \theta < \pi/2$) increases, then the F on the ball to X-axis will be larger

So we need to get θ , How can we do that?

Just get a gradient of $f(x)$ at the point of ball

Let's look this plane again...



How can we make the ball go to minimum/maximum points of $f(x)$?

What if the gradient is 0?

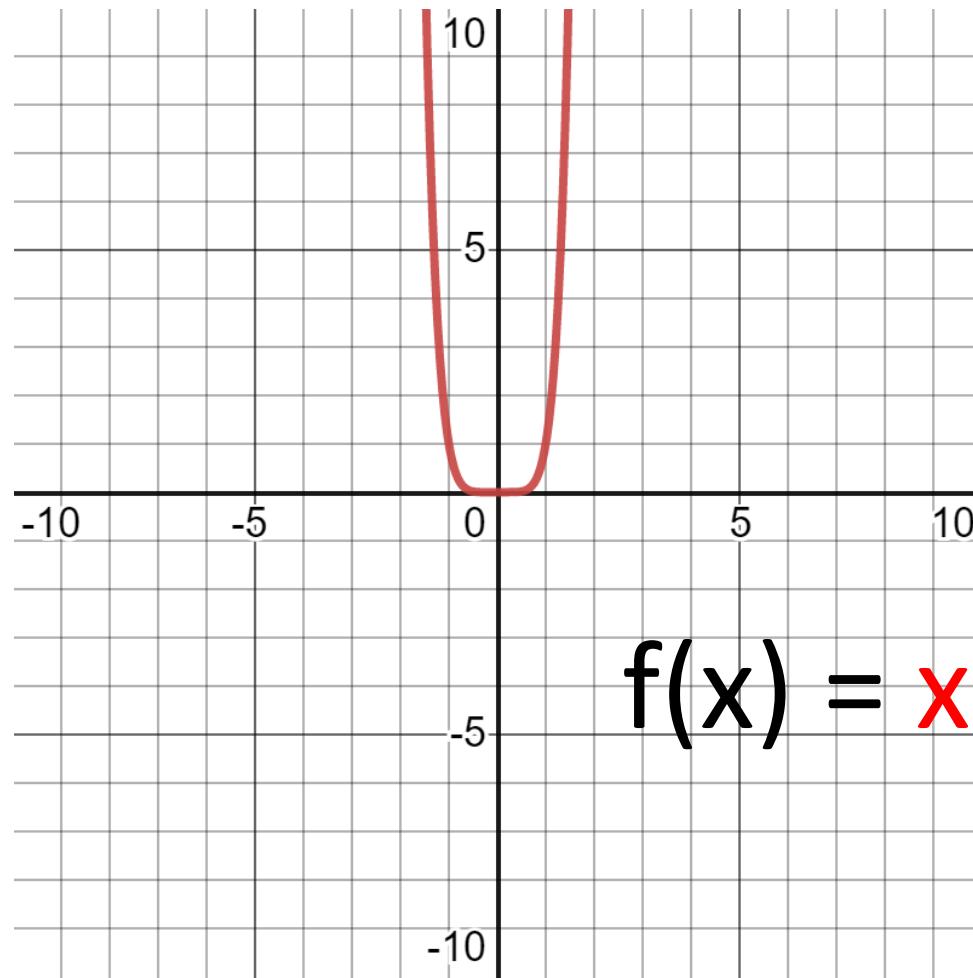
We can think the force to x-axis is 0
because $\sin(\theta)$ is 0

And the ball will stop because the force to x-axis is 0 and the mass of ball is almost 0

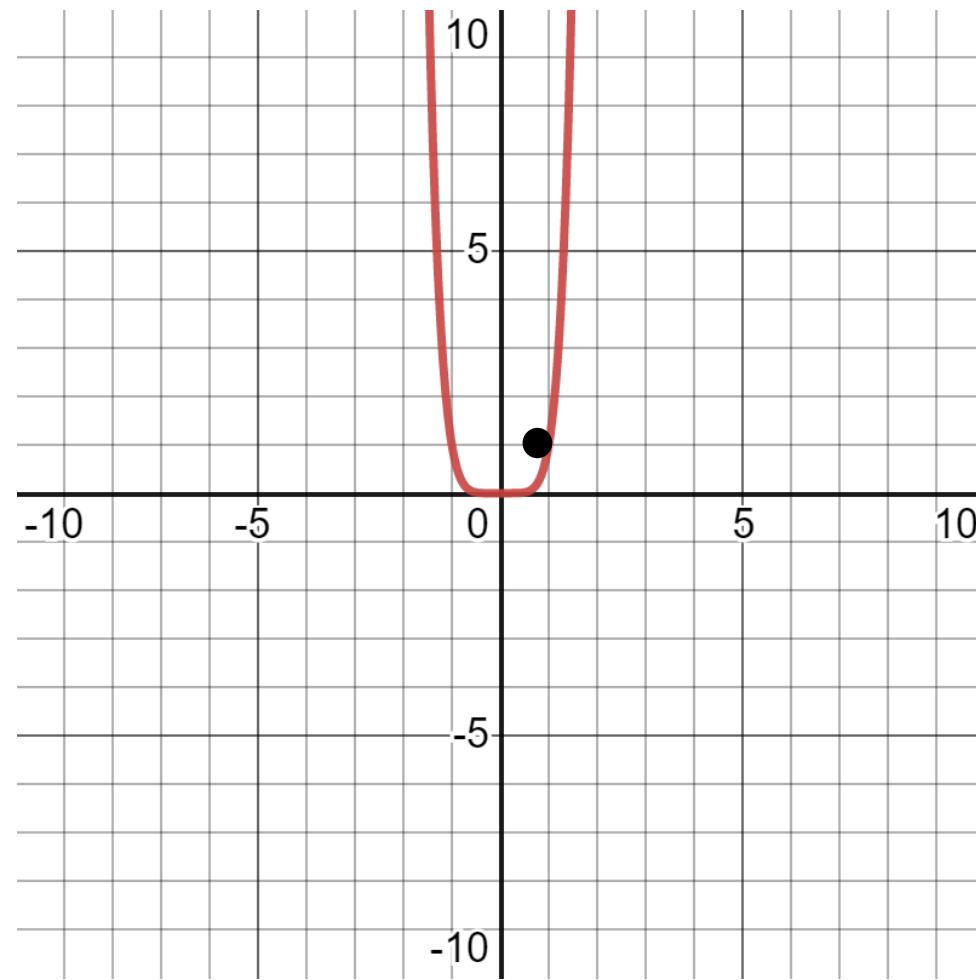
Then we can define the place of the ball by:

$$\text{New } X = \text{current } X - f'(x)$$

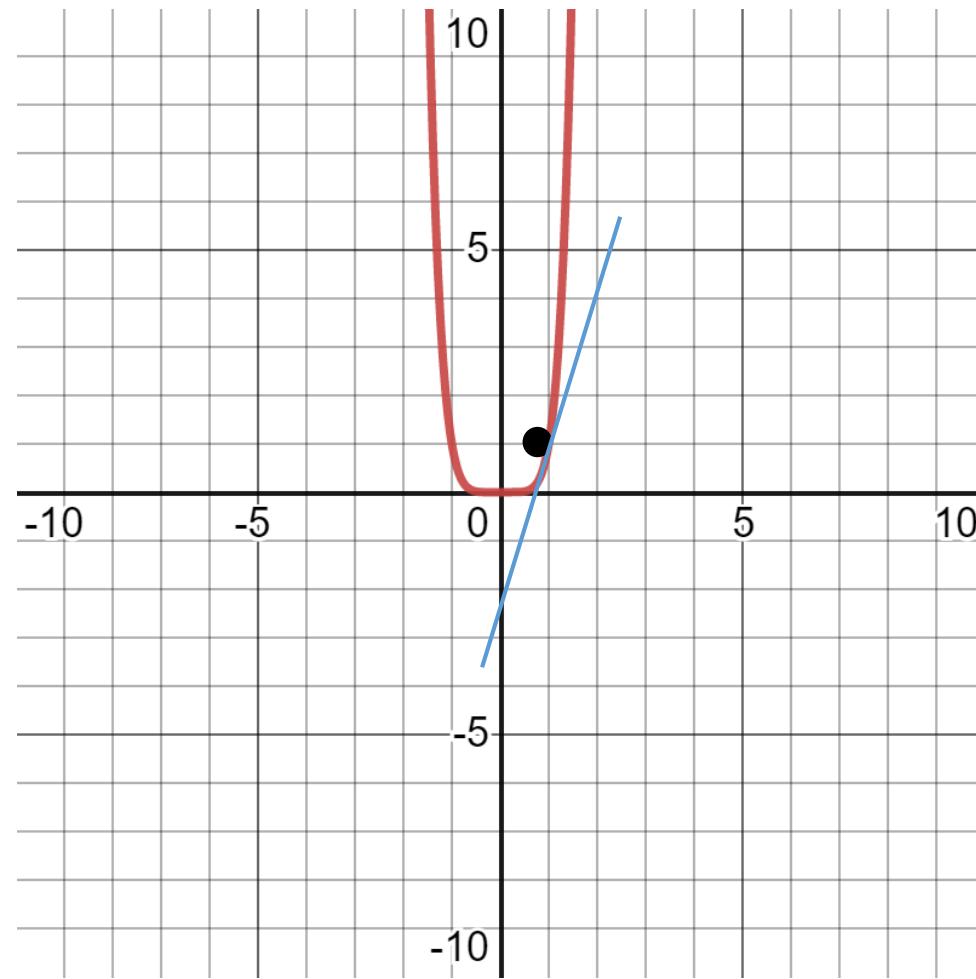
But what will happen in this function?



If the ball starts here, then...

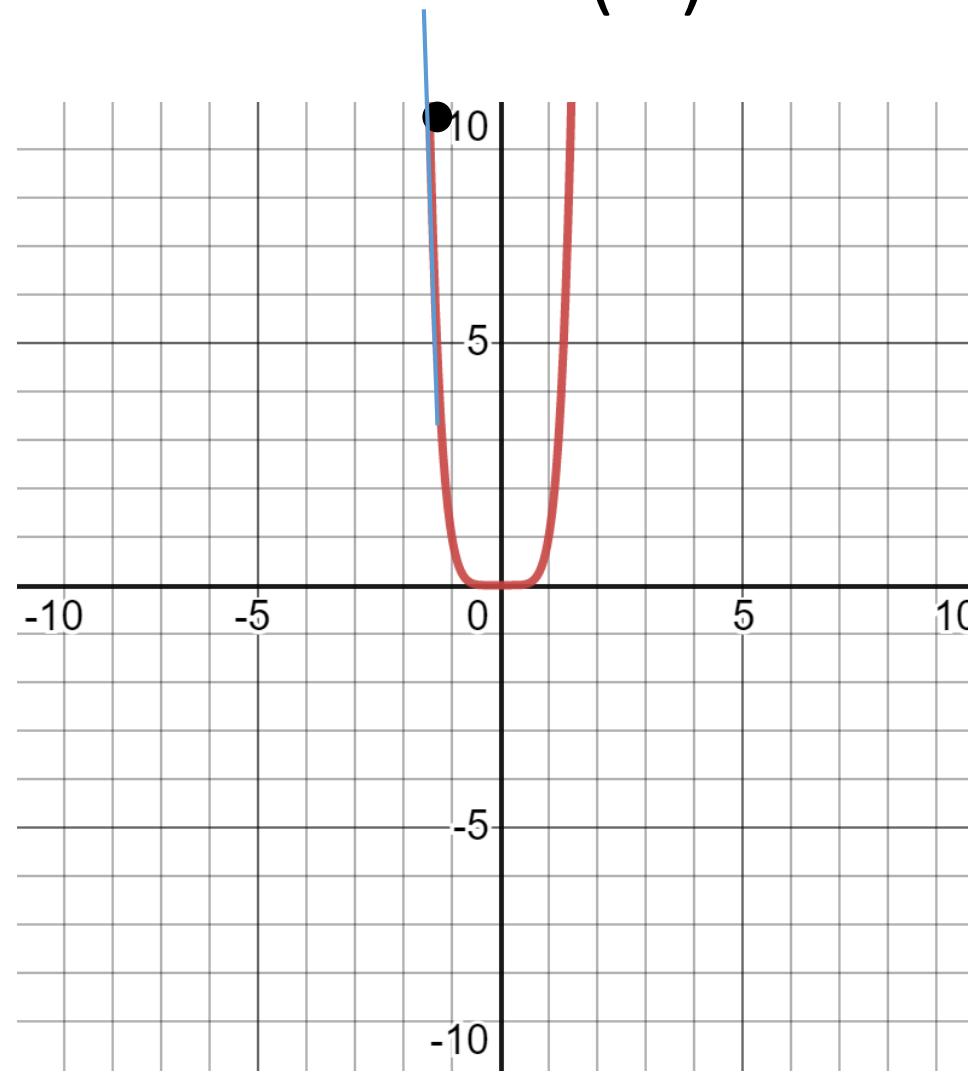


The gradient of ball is...



$f'(x)$ is about 2.5

The gradient of ball is(2)...



$f'(x)$ is about -10

If this process keeps going...

$f'(x) = \pm\infty$, it keeps moving so we cannot find the minimum of $f(x)$

So we adjust the defined equation...

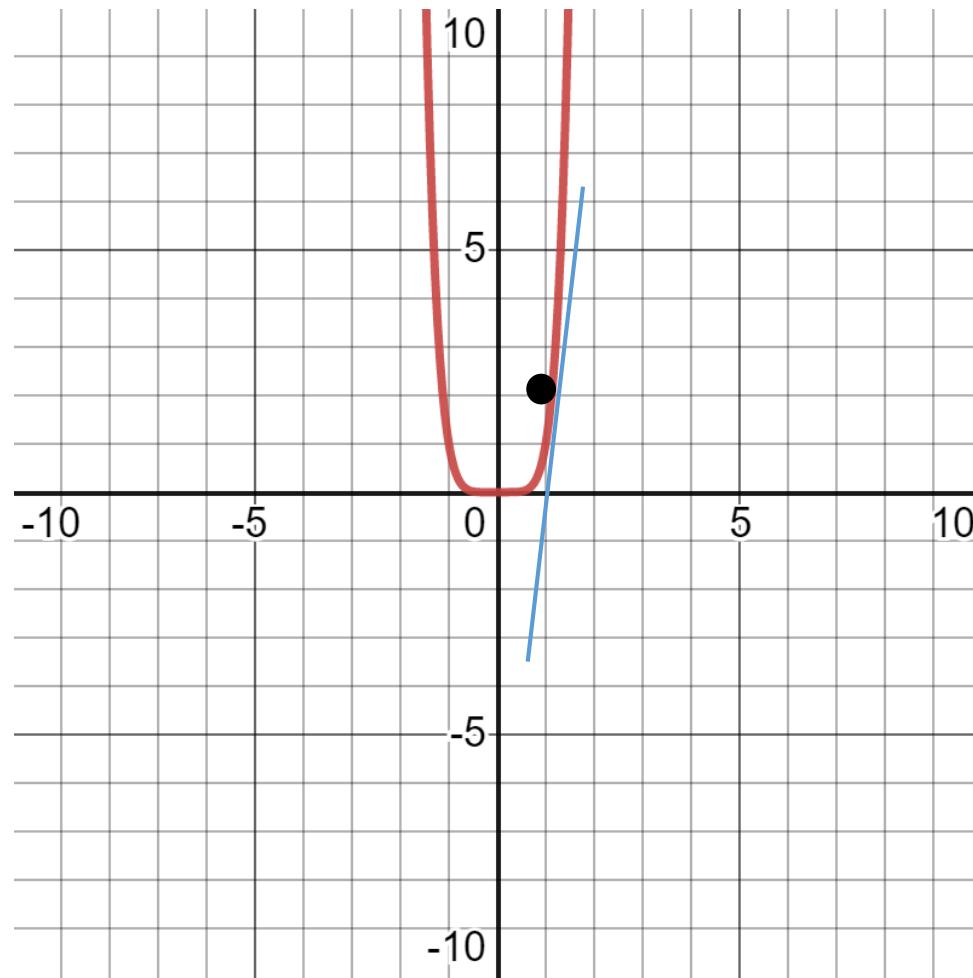
$$\text{New } X = \text{current } X - \alpha f'(x)$$

And set α as small number (like $1e -1$) ...

New $X = \text{current } X - \alpha f'(x)$

*Tip: $a e^{\pm b} <=> a * 10^{(\pm b)}$ <=> $a * 10^{\pm b}$

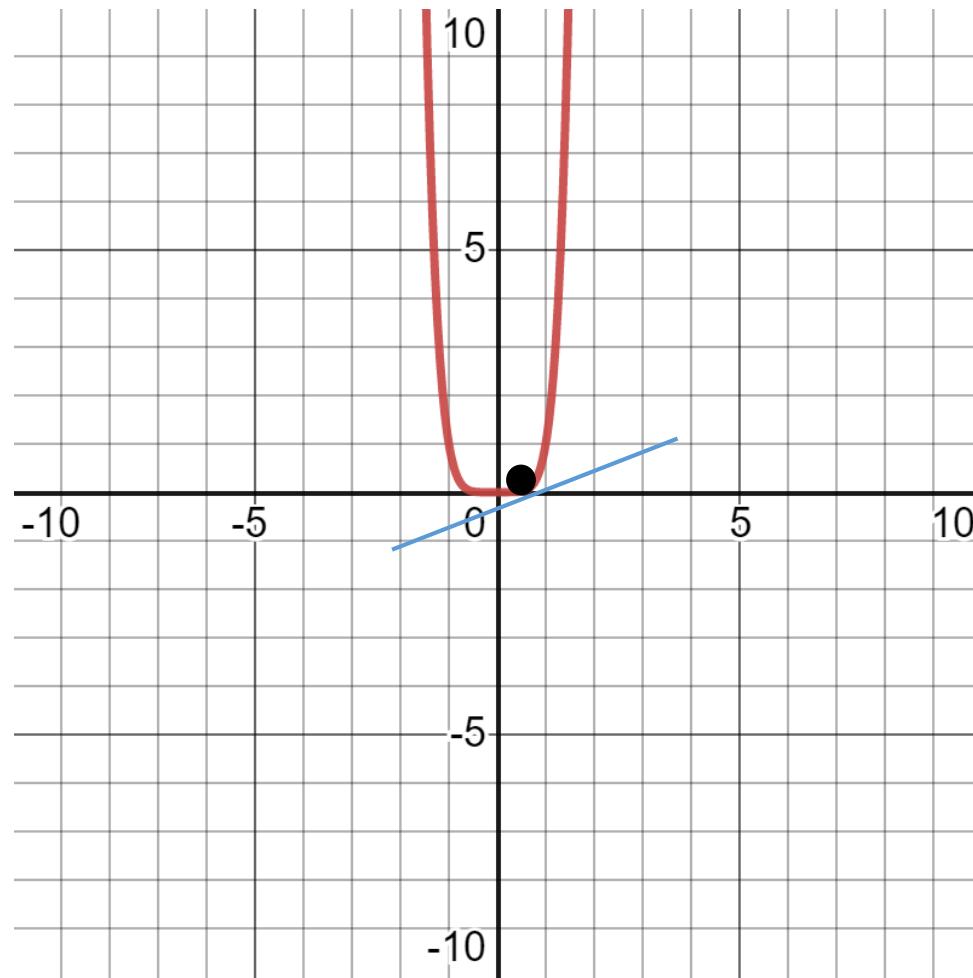
Then it will move like...



Real gradient: 7

Adjusted gradient($\alpha f'(x)$) : 0.7

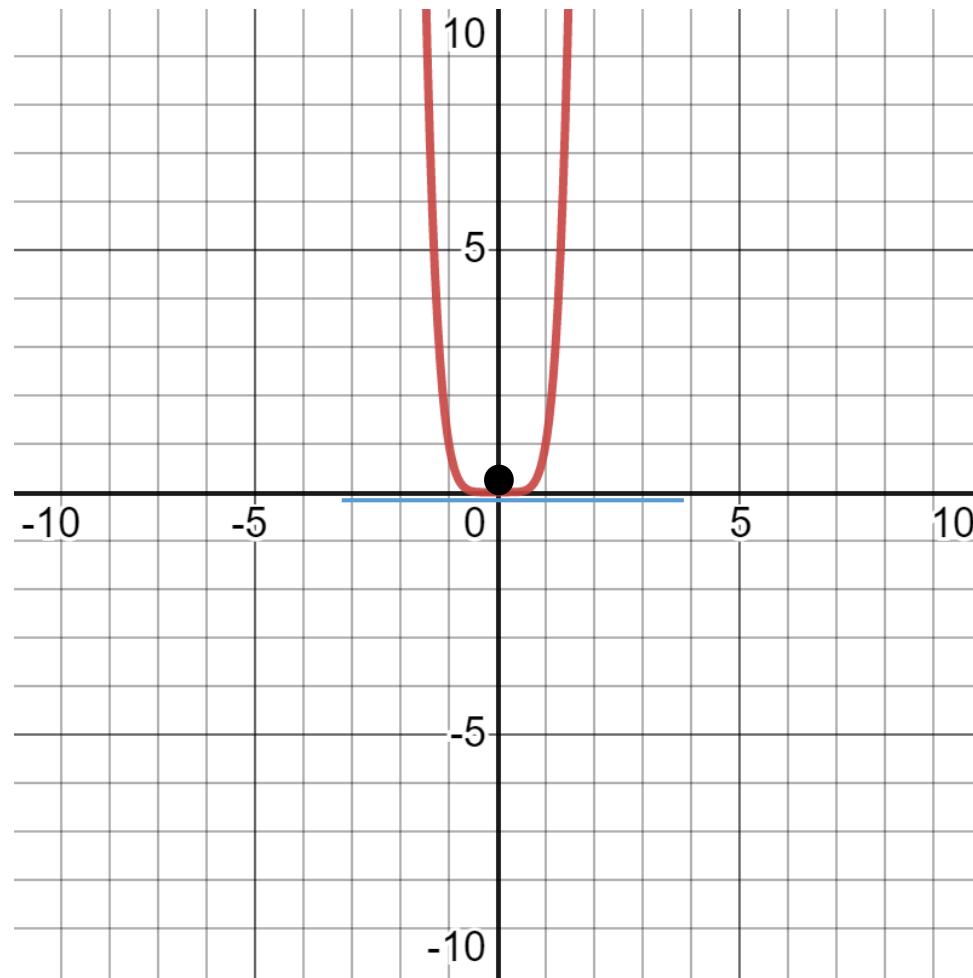
Then it will move like (2)...



Real gradient: 0.32

Adjusted gradient($\alpha f'(x)$) : 0.032

Then it will move like (1000+)...



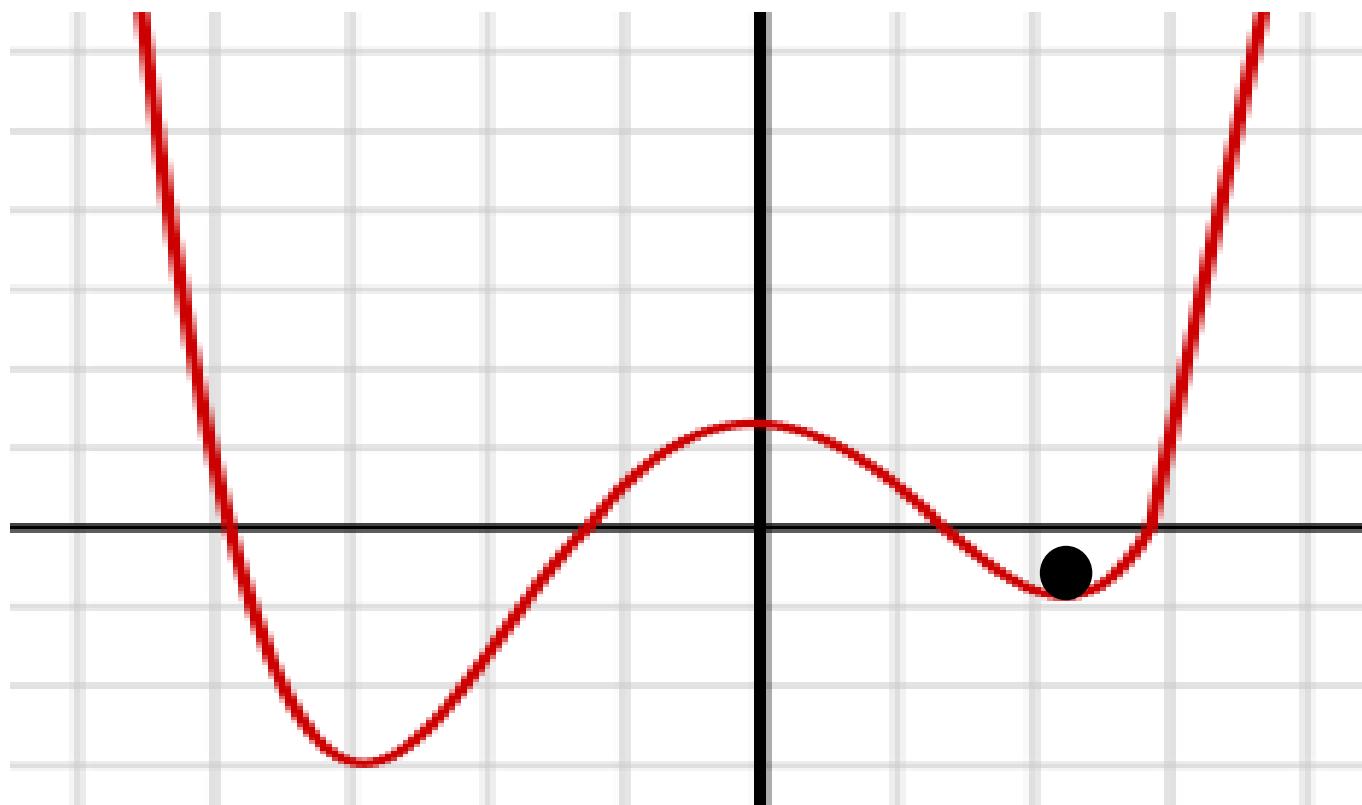
Real gradient: 0

Adjusted gradient($\alpha f'(x)$) : 0

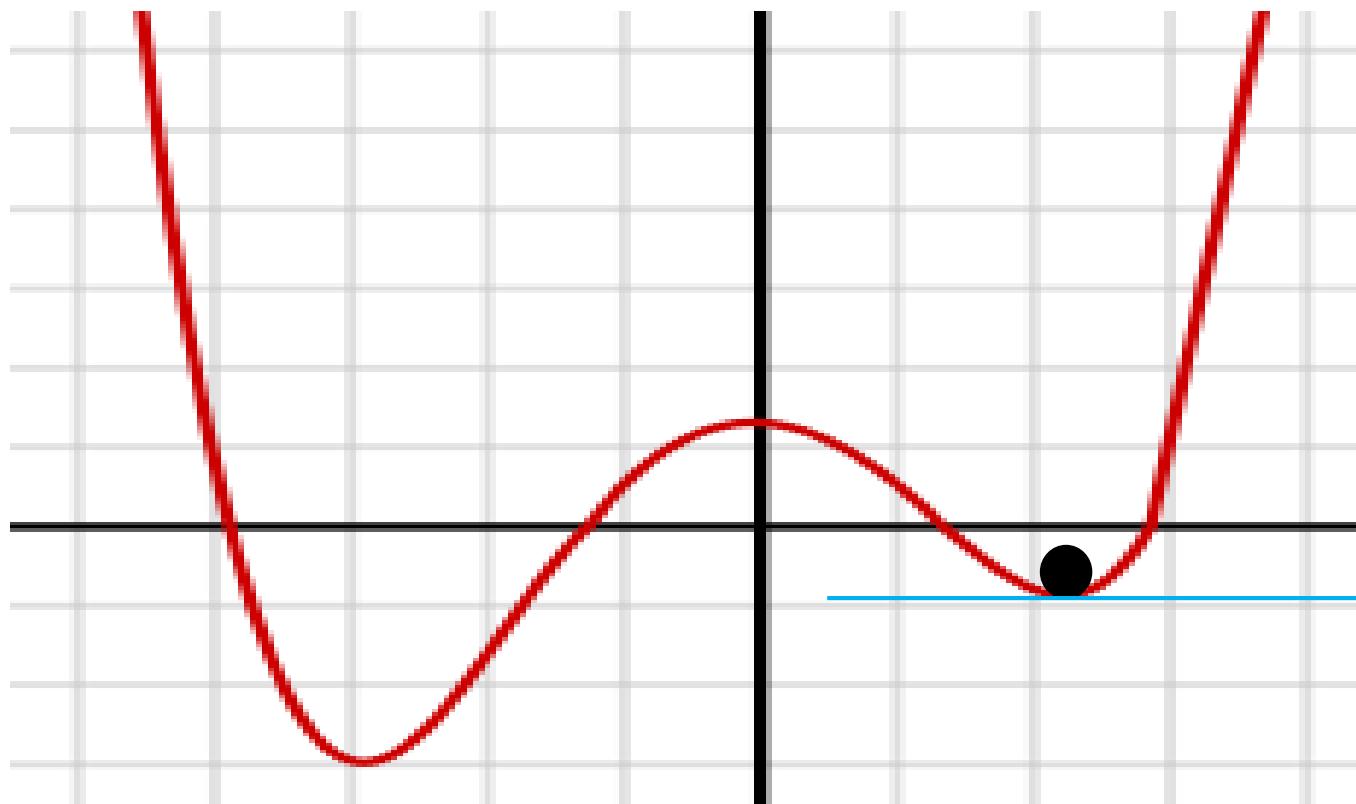
But what will happen in this function?



And the ball is placed on 2nd minimum point...



Which means the gradient is 0...



Let's think...

- We only discuss about the momentum of the ball is 0
- In this case, there always has no kinetic energy in physics perspective (because there has no momentum – quite weird but it is true)
- If we set the momentum, then we can use the stored kinetic energy in physics perspective

What is the momentum?

- In physics, we define the momentum as $p = mv$
- And the $F = dp/dt$, the general definition by newton.
- If we define an iteration(step) as unit time, then we can think the momentum resists immediate moving by gradient

An intuition of momentum in gradient descent based on physics...

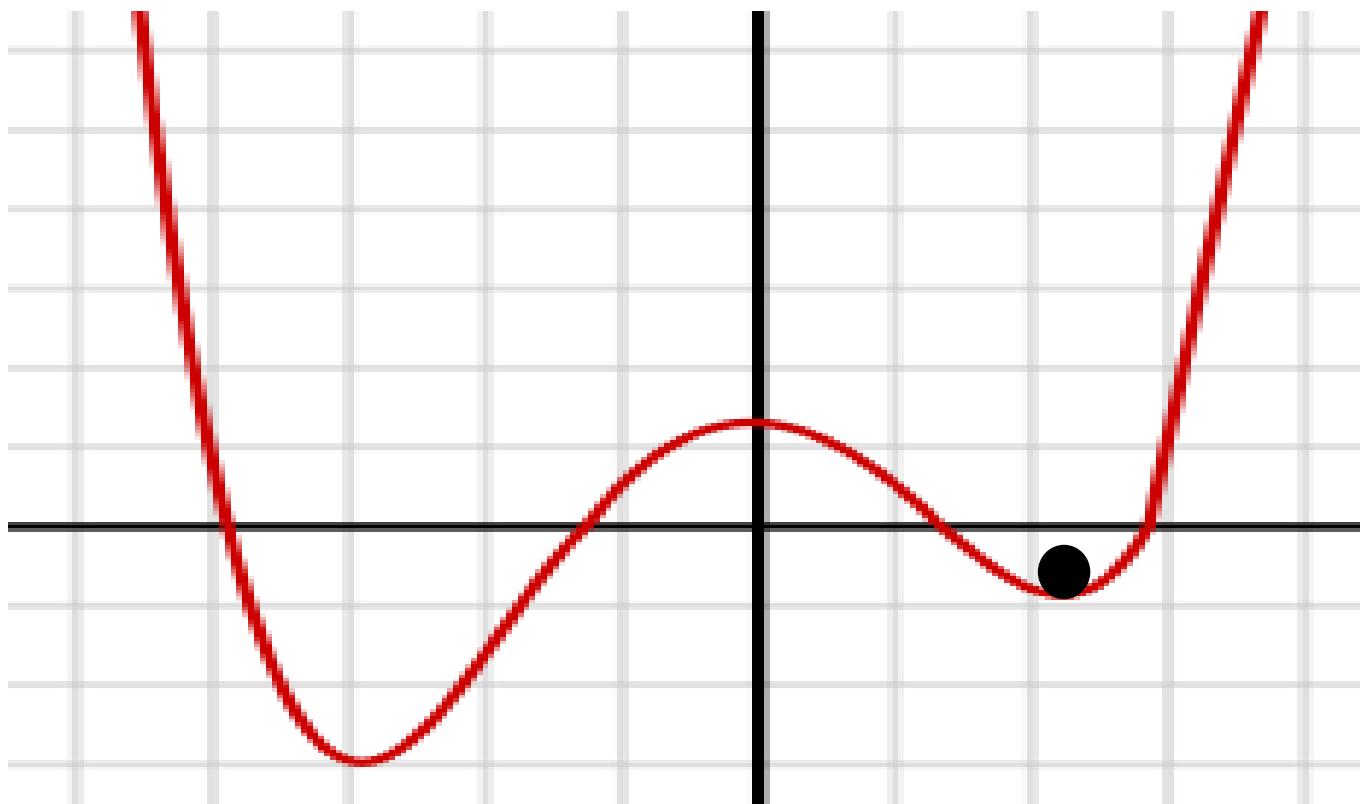
- Gravitaional force = mg
 - momentum = mv
 - Mechanical Energy = $\int(mg+mv)$
 - $v \sim mv - d/dt (\int(mg+mv))$
-
- New $X \sim$ current $X +$ current v

Changing into mathematical equation:

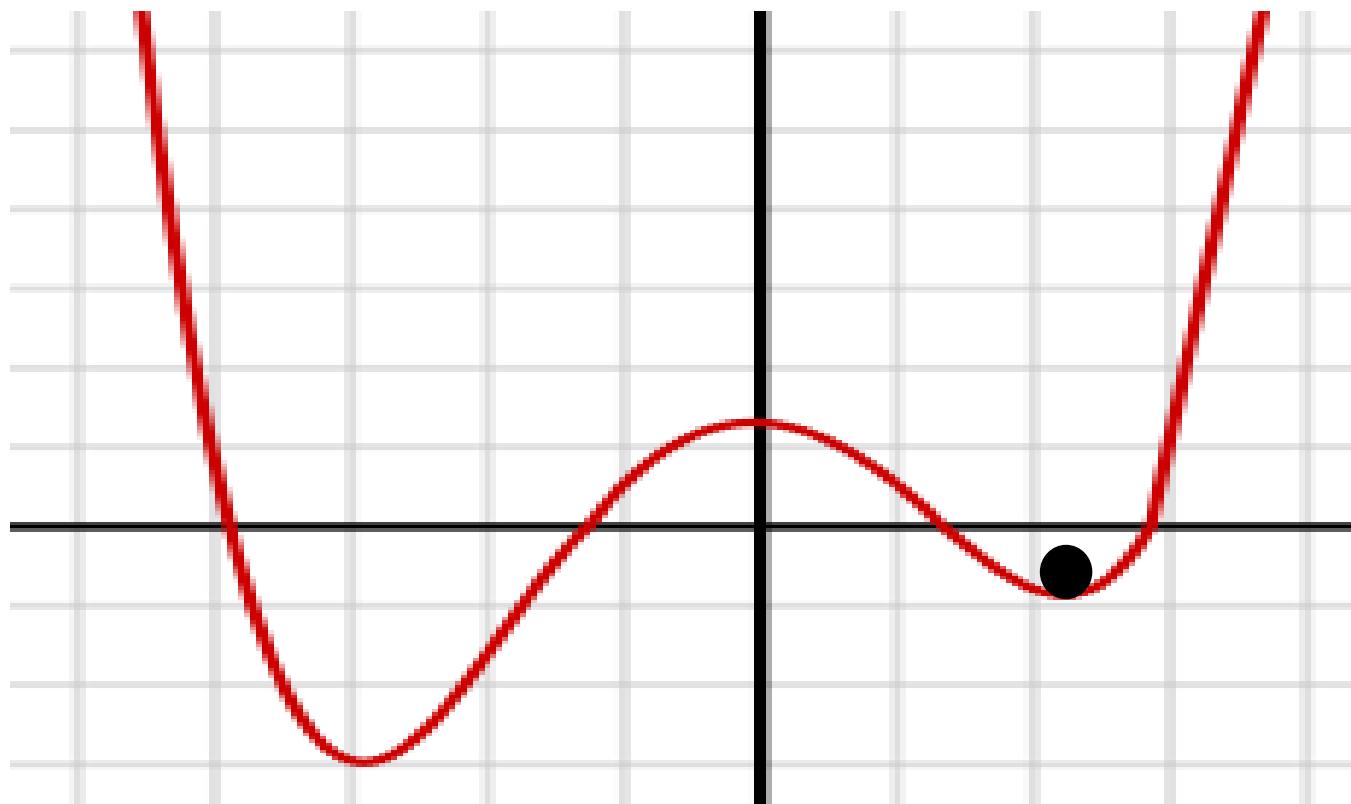
$$v^{k+1} = \beta v^k - \alpha \nabla f(x^k + \beta v^k)$$

$$x^{k+1} = x^k + v^{k+1}$$

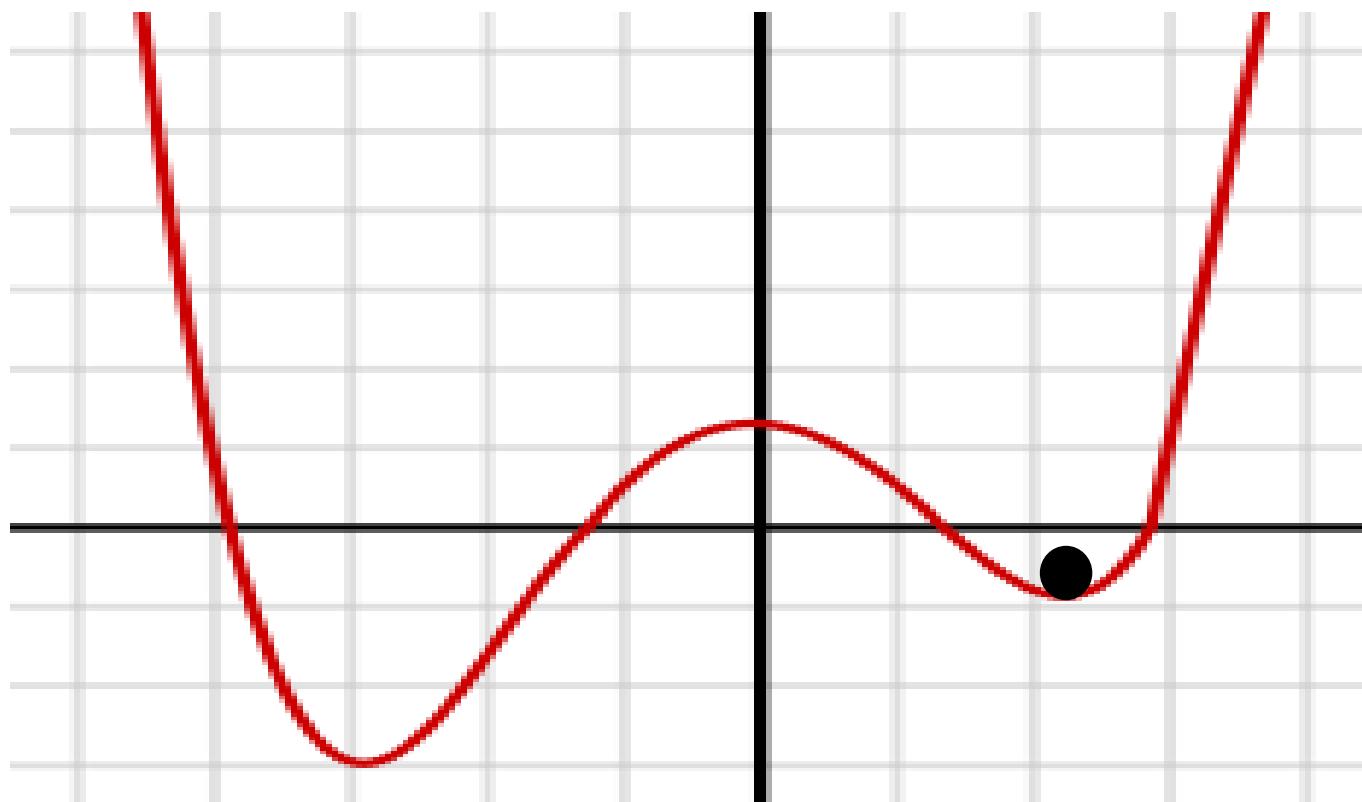
Now back on this problem with momentum based gradient...



with initial v^0 as -2...

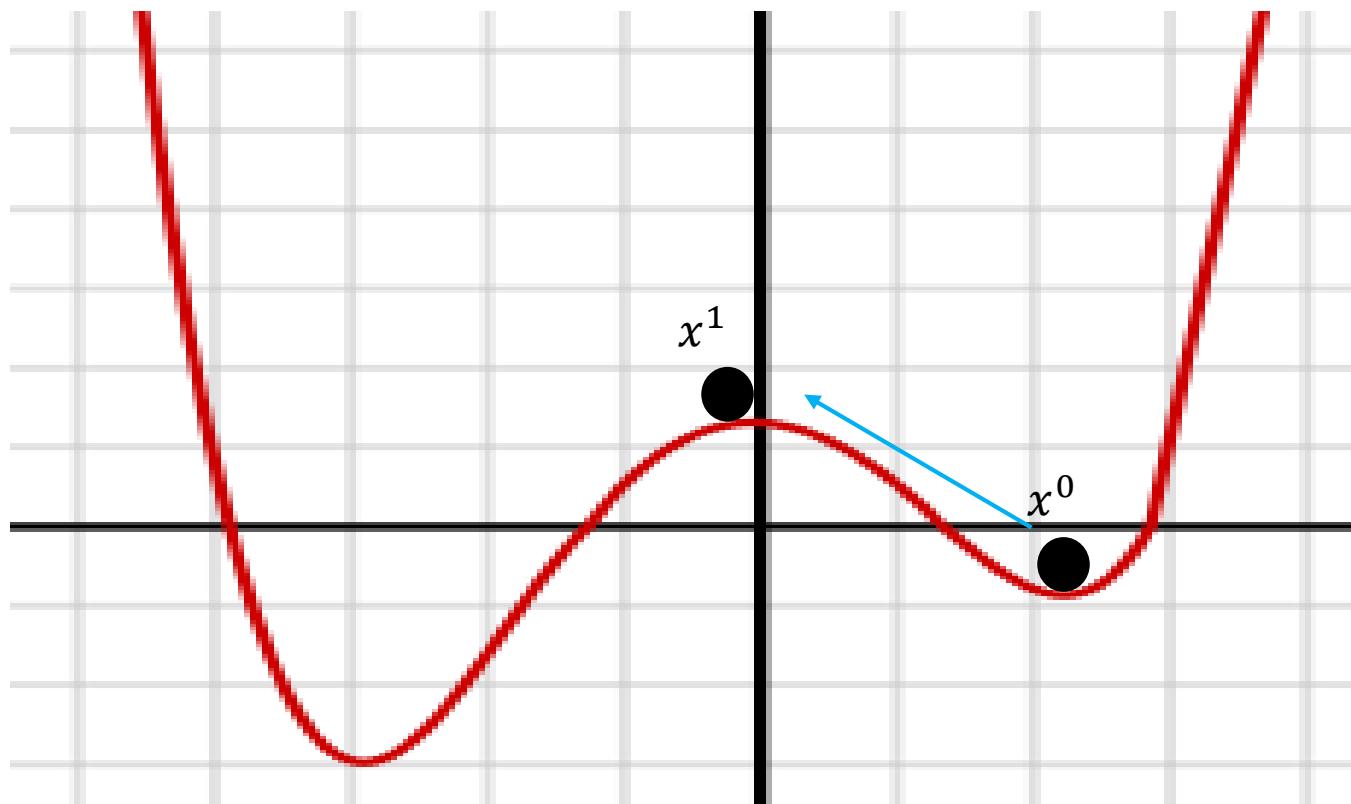


If $\beta = 1$, then v^1 is -2, so the position will be changed as...

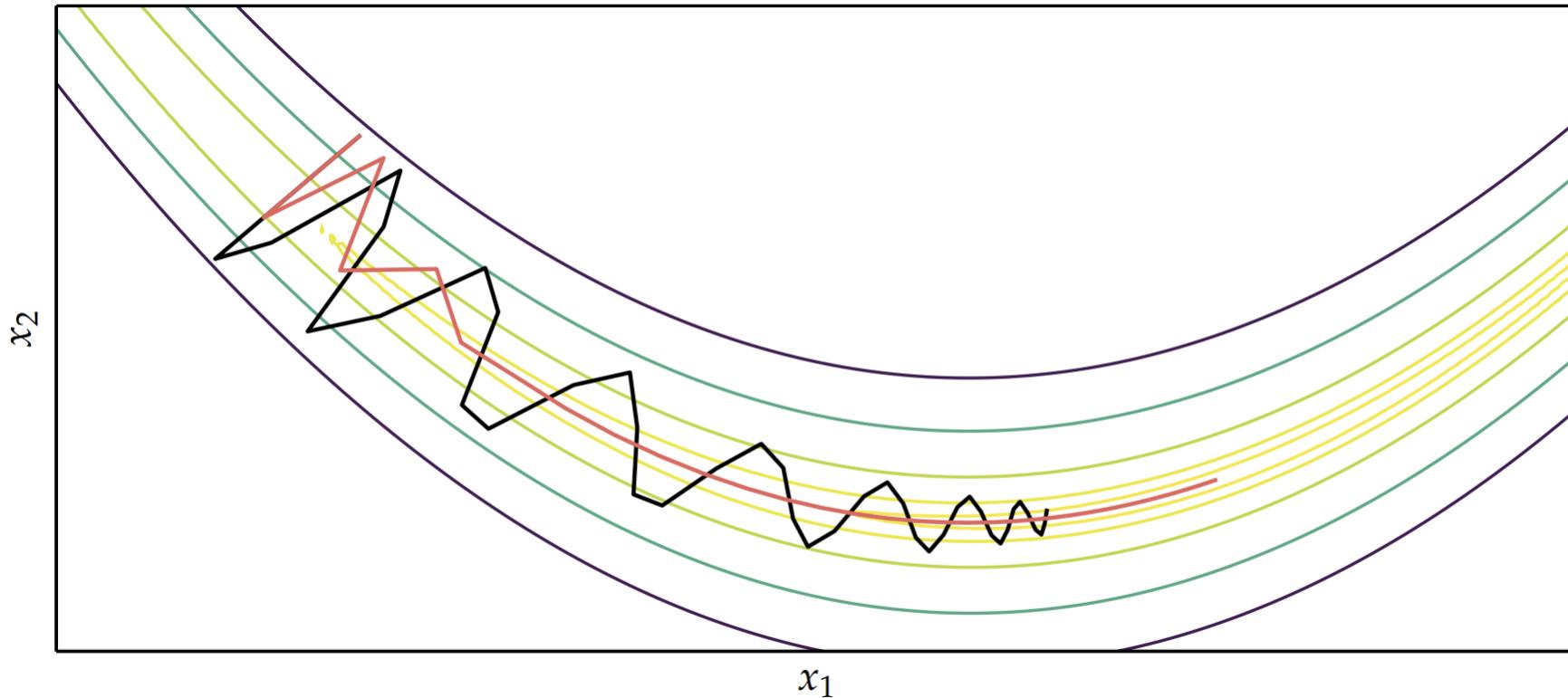


Real gradient: 0
Adjusted gradient($\alpha f'(x)$) : 0
But Adjusted position by
momentum: $x^1 = x^0 - 2$

So the ball can escape from the valley(local minimum)



The comparison of normal gradient descent vs. momentum based gradient descent



Black one: normal gradient descent

Red one: momentum based gradient descent

And this momentum based gradient descent is made by Nesterov, so it is called as “Nesterov momentum”

And researchers have been making more detailed momentum and applied to their optimizers like adagrad, adadelta, adam... etc

References

- [Mykel J. Kochenderfer](#) and [Tim A. Wheeler](#), Algorithms for optimization,
MIT press

Lab session

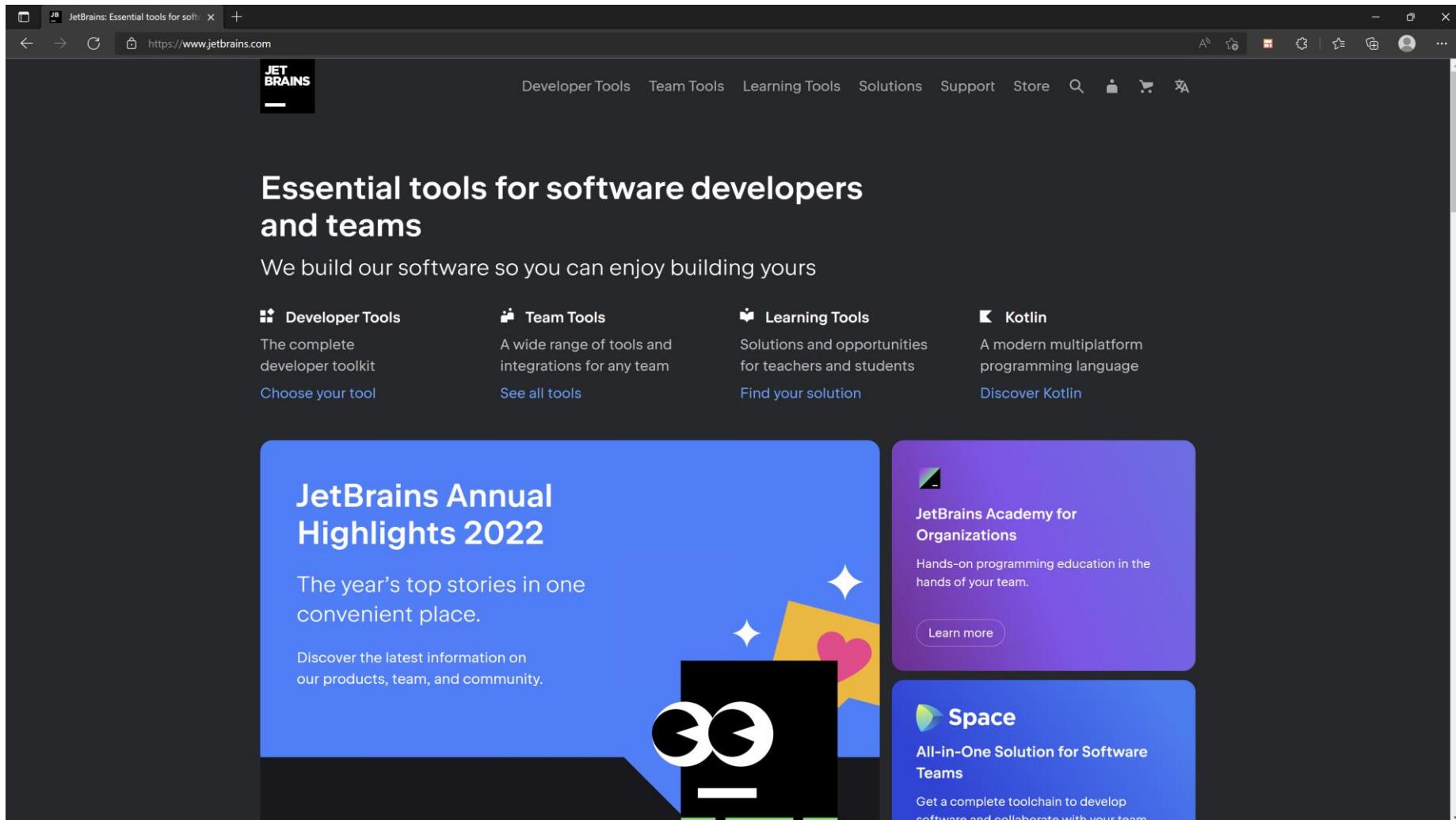
Welcome to lab session!

- We will learn how to use PyTorch & NumPy
- You do not have to consider installing the gpu version of PyTorch. I will not give examples & assignments which needs extreme matrix calculation.
- I will do examples & assignments based on PyCharm virtual environment, so you do not have to care about the environmental differences
- If you have any questions on examples & assignments, please contact me with dongyeongkim33@kaist.ac.kr or kakaotalk

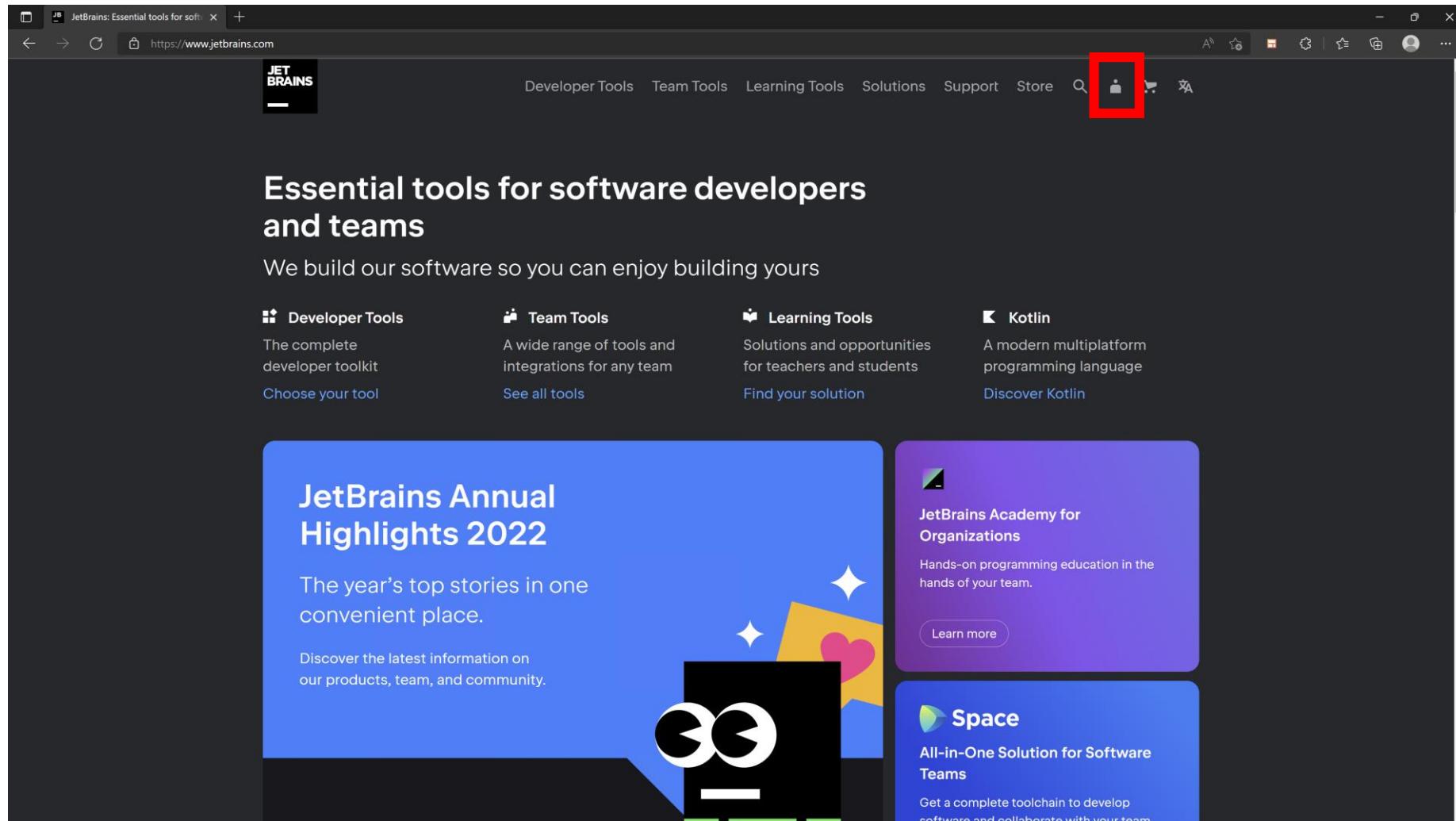
Then, let's start to code!

First step: you need to make Jetbrains account

Go to www.jetbrains.com



And click here to make an account



Fill the blank with your KAIST email & press sign up button

The screenshot shows a web browser window for the JetBrains Account login page at <https://account.jetbrains.com/login>. The page has a dark header with the JetBrains logo. Below the header, there's a section titled "Welcome to JetBrains Account" with three items: "Access your purchases", "Identify expired and outdated licenses", and "Manage your company licenses". To the right is a "Sign in with existing account" form with fields for "Email address or Username" and "Password", and a "Sign In" button. Below that is a "Or sign in with:" section with icons for Google, GitHub, LinkedIn, and others. At the bottom, there's a "Create JetBrains Account" section with a red box around the "Your email address" input field and a red box around the "Sign Up" button.

Welcome to JetBrains Account

Access your purchases and view your order history

Identify expired and outdated licenses, order new licenses and upgrades

Manage your company licenses and distribute them to end users

Sign in with existing account

Email address or Username

Password

Sign In [Forgot password?](#)

Or sign in with:

Google GitHub LinkedIn

Not registered yet?
Create JetBrains Account

Your email address

Sign Up

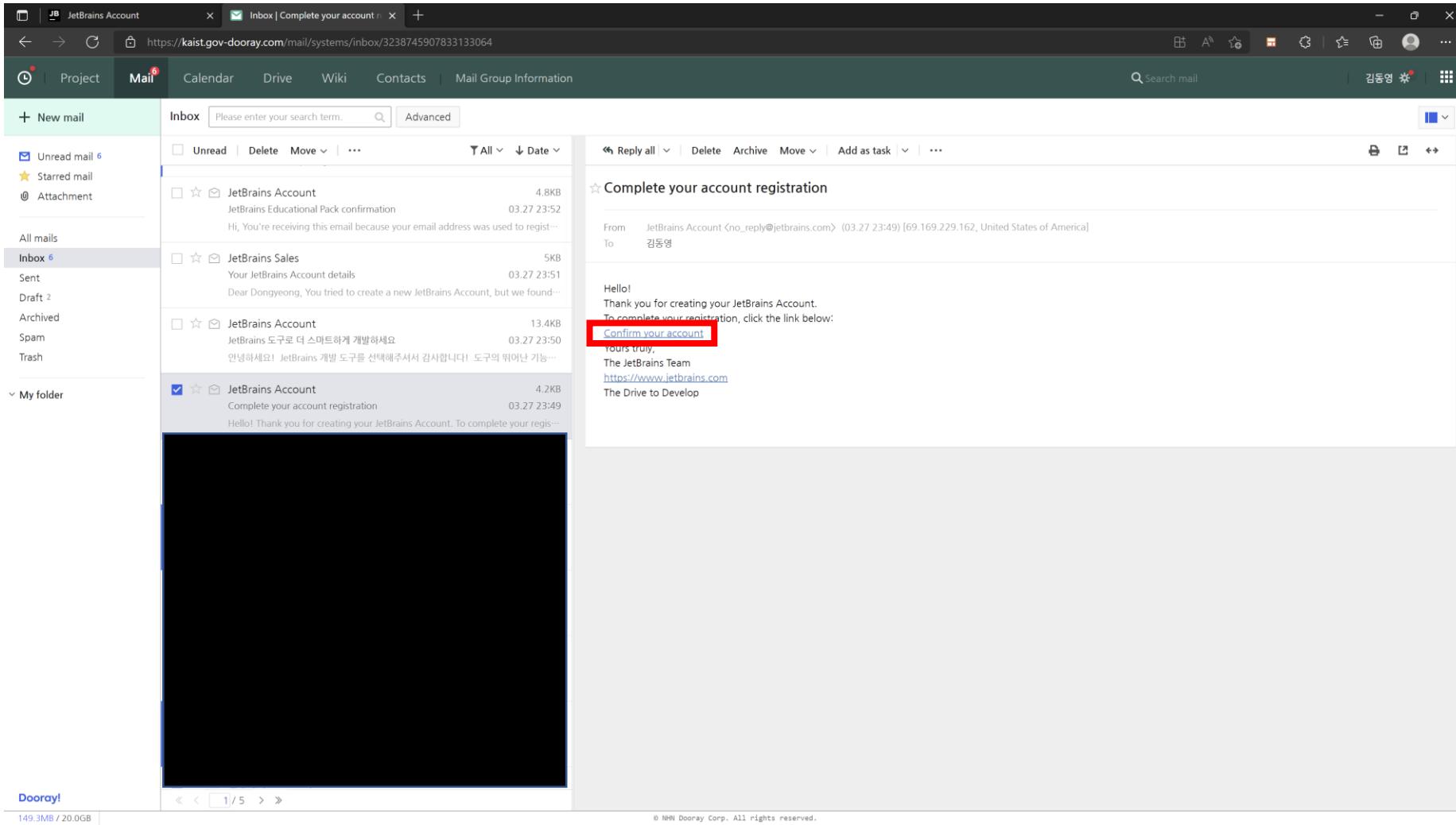
By using the JetBrains Account website, you agree to the JetBrains Account Agreement. [Review now](#) [Remind me later](#)

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Support

You will get verify email to dooray, go to kaist.gov-dooray.com

Click this link to complete the registration



Fill out this registration form and press submit

The screenshot shows a web browser window with the title "JB JetBrains Account". The URL in the address bar is <https://account.jetbrains.com/signup-complete>. The page content is as follows:

Welcome to JetBrains Account!

Please complete the registration form below

Email Address

First Name

Last Name

Username

Latin symbols (A-z), digits (0-9) or a valid email address 5 to 100 characters long.

Please make sure you choose a strong password, as your account will have access to your purchases.

Password

Repeat Password

I have read and I accept the [JetBrains Account Agreement](#)

I consent to the use of my name, email address, and location data in email communication concerning JetBrains products held or services used by me or my organization. [More](#)

Submit

You will receive emails from us in **한국어**. [Change](#)
You can set preferred language anytime in JetBrains Account.

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Support

Second step: get student license

Go to www.jetbrains.com/community/education/#students/

The screenshot shows a web browser window displaying the JetBrains website at <https://www.jetbrains.com/community/education/#students/>. The page has a dark header with the JetBrain logo and navigation links for Developer Tools, Team Tools, Learning Tools, Solutions, Support, Store, and more. Below the header, there's a main navigation bar with links for Free License Programs, Academic Licensing, Open Source, User Groups, Events Partnership, and Developer Recognition. The main content area features a large section titled "Free Educational Licenses" with a sub-section for "Individual licenses for students and teachers". It includes a callout for free access to JetBrains IDEs for personal use at school or home, and a link to "Who can get free individual licenses for education". At the bottom, there's a note about students and faculty from accredited educational institutions.

Free Educational Licenses

Learn or teach coding with best-in-class development tools from JetBrains!

For students and teachers For schools and universities For training courses and bootcamps

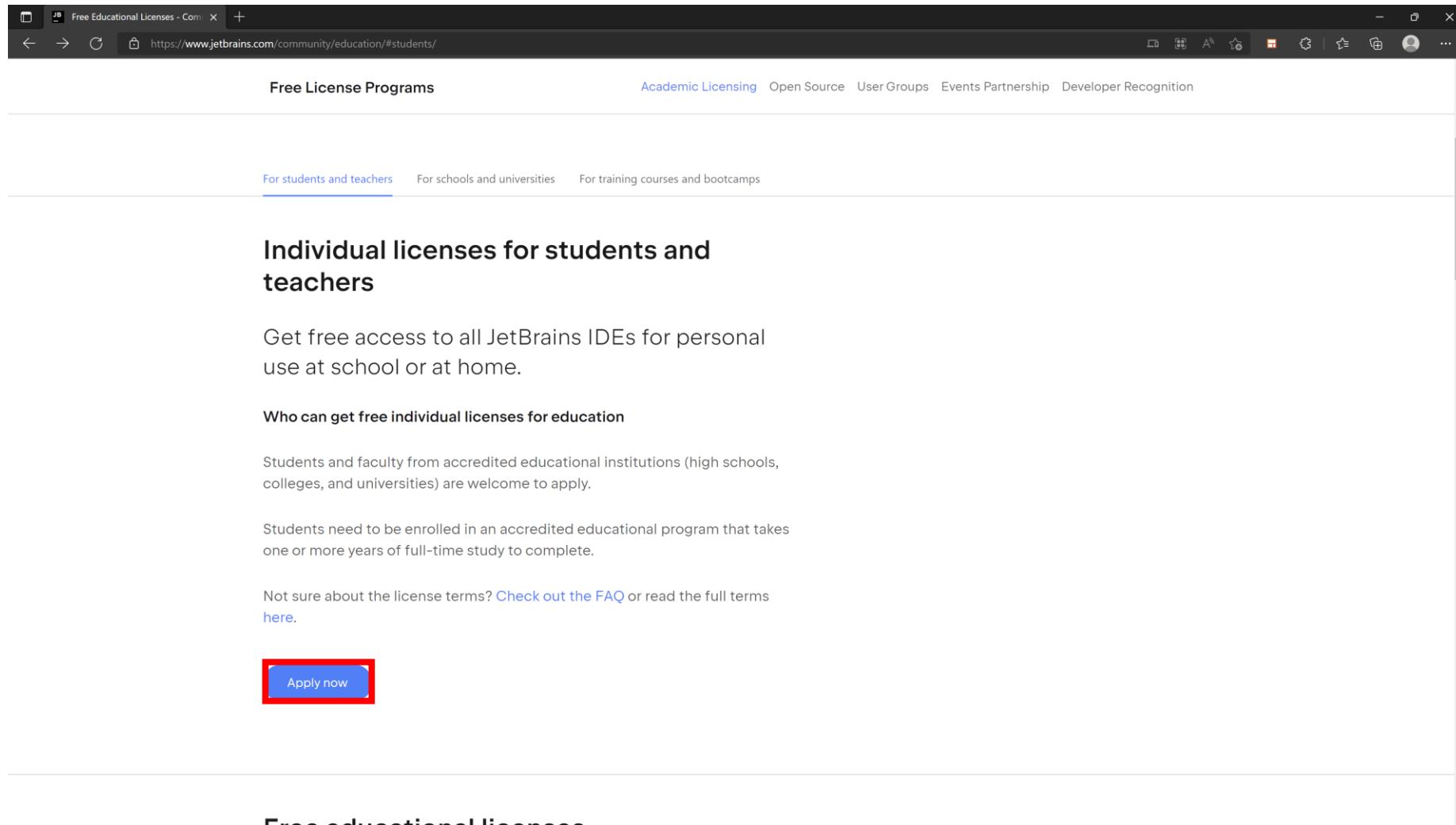
Individual licenses for students and teachers

Get free access to all JetBrains IDEs for personal use at school or at home.

[Who can get free individual licenses for education](#)

Students and faculty from accredited educational institutions (high schools,

Scroll down and click Apply now



The screenshot shows a web browser window with the URL <https://www.jetbrains.com/community/education/#students/>. The page is titled "Free License Programs" and features a navigation bar with links to "Academic Licensing", "Open Source", "User Groups", "Events Partnership", and "Developer Recognition". Below the navigation bar, there are three categories: "For students and teachers" (which is underlined in blue), "For schools and universities", and "For training courses and bootcamps". The main section is titled "Individual licenses for students and teachers" and contains the text: "Get free access to all JetBrains IDEs for personal use at school or at home." It also includes sections for "Who can get free individual licenses for education" (mentioning accredited educational institutions) and "Students need to be enrolled in an accredited educational program that takes one or more years of full-time study to complete." At the bottom, there is a link to "Check out the FAQ or read the full terms here." A prominent blue button labeled "Apply now" is located at the bottom left, with a red box drawn around it to indicate where the user should click.

Fill out the form and click apply for free products

The screenshot shows a web browser window with the title "JB JetBrains Products for Learning". The URL in the address bar is <https://www.jetbrains.com/shop/eform/students>. A red rectangular box highlights the main form area, which includes fields for "Apply with:" (University email address selected), "Status" (I'm a student selected), "Level of study" (Undergraduate), "Is Computer Science or Engineering your major field of study?" (Yes selected), "Email address" (University email address, e.g. js@mit.edu), "Name" (First Name and Last Name fields), "Country / region" (Republic of Korea), and three consent checkboxes. At the bottom, a large red button highlights the "APPLY FOR FREE PRODUCTS" button.

Apply with:

- University email address
- ISIC/ITIC membership
- Official document
- GitHub

Status:

I'm a student

I'm a teacher

Level of study:

Undergraduate

Is Computer Science or Engineering your major field of study?

Yes

No

Email address:

University email address, e.g. js@mit.edu

I certify that the university email address provided above is valid and belongs to me.

Name:

Your **real name** as it appears in your passport, driver's license, or other legal documents.

First Name Last Name

Country / region:

Republic of Korea

I am under 13 years old

I have read and I accept the [JetBrains Account Agreement](#)

I consent to the use of my name, email address, and location data in email communication concerning JetBrains products held or services used by me or my organization. [More](#)

APPLY FOR FREE PRODUCTS

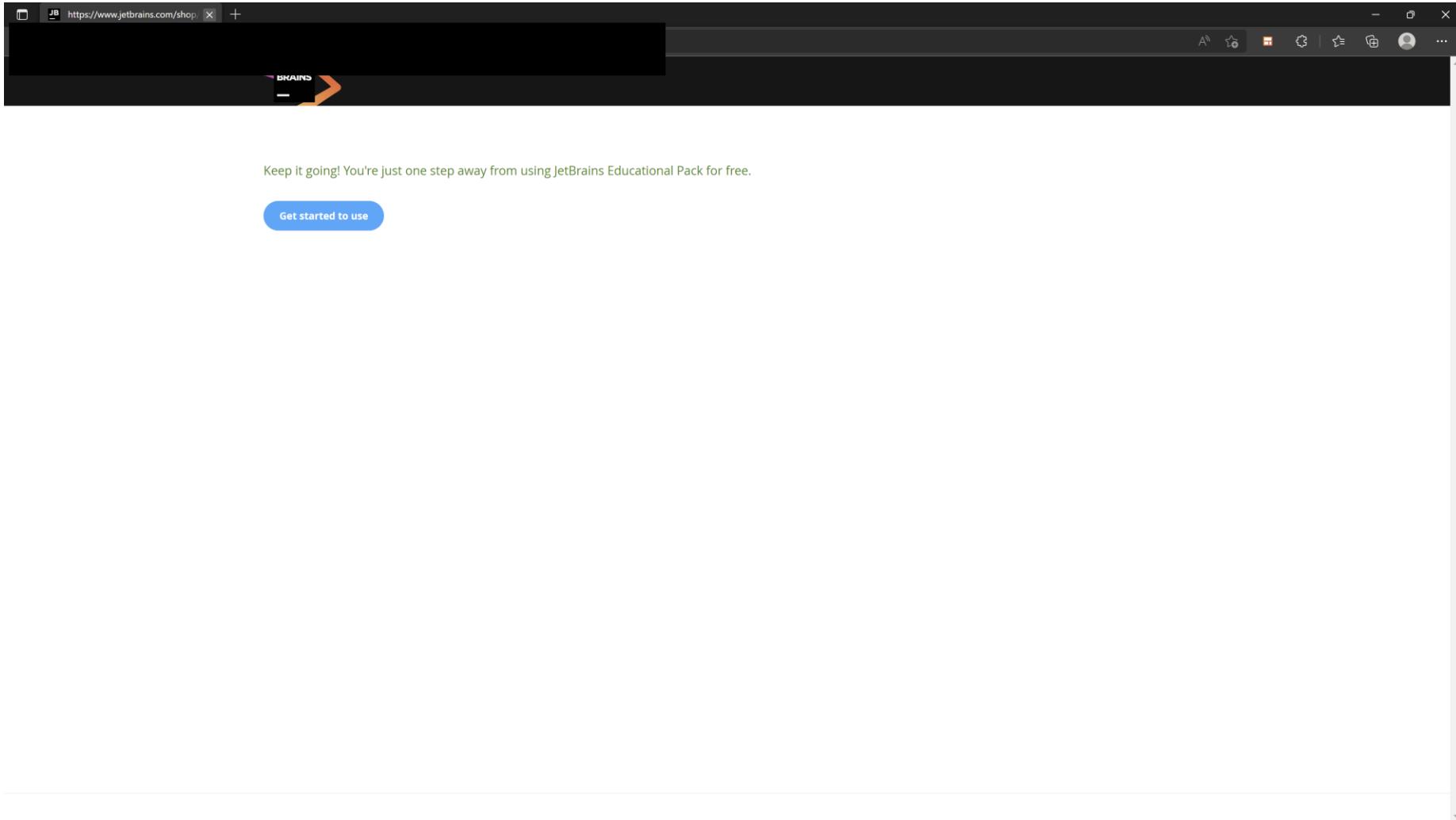
You will get this email and click the link to get the license

The screenshot shows an email inbox interface from 'Inbox | JetBrains Educational Pack'. The left sidebar lists categories like 'Project', 'Mail' (selected), 'Calendar', 'Drive', 'Wiki', 'Contacts', and 'Mail Group Information'. Under 'Inbox', there are 5 unread emails:

- JetBrains Sales**: License Certificate for your JetBrains Educational Pack / Order...
- JetBrains Account**: JetBrains Educational Pack confirmation. The message body starts with "Hi, You're receiving this email because your email address was used to register or update a JetBrains Educational Pack." A red box highlights the URL [https://www.jetbrains.com/shop/eform/students/request?code=\[REDACTED\]](https://www.jetbrains.com/shop/eform/students/request?code=[REDACTED]).
- JetBrains Sales**: Your JetBrains Account details. It says "Dear Dongyeong, You tried to create a new JetBrains Account, but we found..."
- JetBrains Account**: JetBrains 도구로 더 스마트하게 개발하세요. It says "안녕하세요! JetBrains 개발 도구를 선택해주시셔서 감사합니다! 도구의 뛰어난 기능..."
- JetBrains Account**: Complete your account registration. It says "Hello! Thank you for creating your JetBrains Account. To complete your regis..."

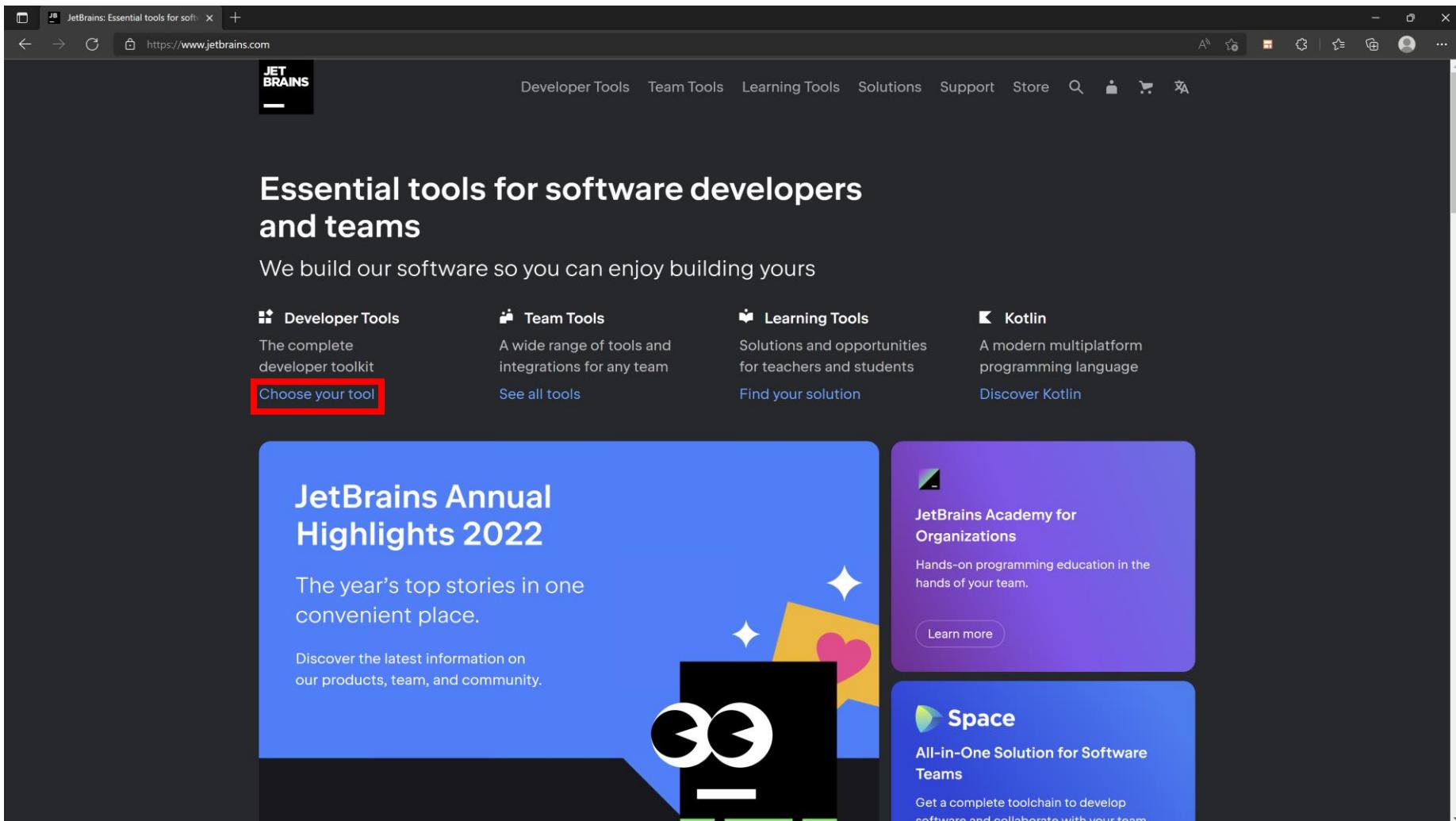
The right pane displays the selected email's content. The subject is 'JetBrains Educational Pack confirmation'. The 'From' field is 'JetBrains Account <no_reply@jetbrains.com> (03.27 23:52) [69.169.229.161, United States of America]' and the 'To' field is '김동영'. The message body continues with instructions and a link.

Now we are done!

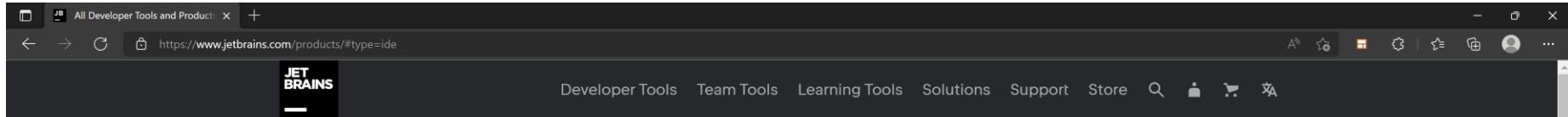


Third step: Download PyCharm

Click choose your tool



Click Download the PyCharm section



Find the right tool

Whichever technologies you use, there's a JetBrains tool to match

A screenshot of the JetBrains website showing the "Find the right tool" section. It displays cards for IntelliJ IDEA, PyCharm, WebStorm, PhpStorm, Rider, and CLion. The PyCharm card is highlighted with a red box around its "Download" button. To the right, a sidebar titled "Filters" allows users to refine their search by language, with checkboxes for C/C++, C#, Dart, DSL, F#, Go, Groovy, HTML, and Java.

In Windows: click download

The screenshot shows a web browser window displaying the PyCharm download page on the JetBrains website. The URL in the address bar is <https://www.jetbrains.com/pycharm/download/#section=windows>. The page has a dark header with the JetBrain logo and navigation links for Developer Tools, Team Tools, Learning Tools, Solutions, Support, Store, a search icon, and user account options.

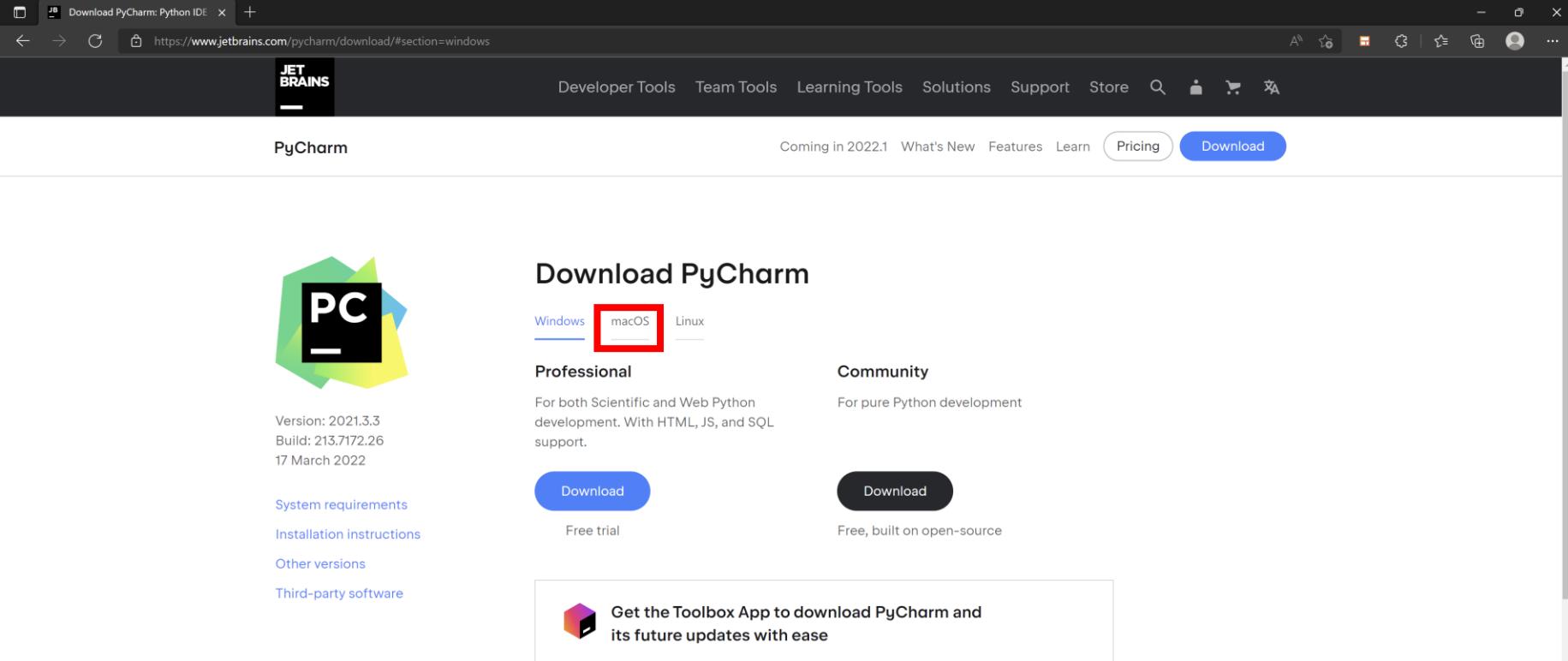
The main content area is titled "Download PyCharm". It features three download options:

- Professional**: For both Scientific and Web Python development. With HTML, JS, and SQL support. Includes a "Download" button (which is highlighted with a red box) and a "Free trial" link.
- Community**: For pure Python development. Includes a "Download" button and a note that it is "Free, built on open-source".
- A call-to-action box at the bottom encourages users to "Get the Toolbox App to download PyCharm and its future updates with ease".

On the left side, there is a large PyCharm logo icon and a sidebar with links for System requirements, Installation instructions, Other versions, and Third-party software. The sidebar also displays the version information: Version: 2021.3.3, Build: 213.7172.26, and Date: 17 March 2022.

The footer contains a navigation menu with sections: Products, Solutions, Initiatives, Community, Resources, and Company. Each section lists various tools and services offered by JetBrains.

In macOS: click macOS



A screenshot of a web browser window showing the PyCharm download page on the JetBrains website. The browser's title bar reads "Download PyCharm: Python IDE". The address bar shows the URL <https://www.jetbrains.com/pycharm/download/#section=windows>. The page features the Jet Brains logo and navigation links for Developer Tools, Team Tools, Learning Tools, Solutions, Support, Store, and a search bar. Below this is a main navigation bar with "PyCharm" on the left, "Coming in 2022.1 What's New Features Learn Pricing Download" on the right, and a "macOS" tab highlighted with a red box. The central content area displays the PyCharm logo, version information (Version: 2021.3.3, Build: 213.7172.26, 17 March 2022), and download links for Windows, macOS, and Linux. It also includes sections for Professional and Community editions, system requirements, installation instructions, other versions, and third-party software. A callout box at the bottom encourages users to get the Toolbox App for ease of download.

Download PyCharm

Windows macOS Linux

Professional

For both Scientific and Web Python development. With HTML, JS, and SQL support.

Community

For pure Python development

Download

Download

Free trial

Free, built on open-source

Get the Toolbox App to download PyCharm and its future updates with ease

Products

- IDEs
- .NET & Visual Studio
- Team Tools

Solutions

- C++ Tools
- Data Tools
- DevOps

Initiatives

- Kotlin
- JetBrains Mono
- JetBrains Research

Community

- Academic Licensing
- Open Source Support
- User Groups

Resources

- Sales Support
- Product Support
- Licensing FAQ

Company

- About
- Contacts
- Careers

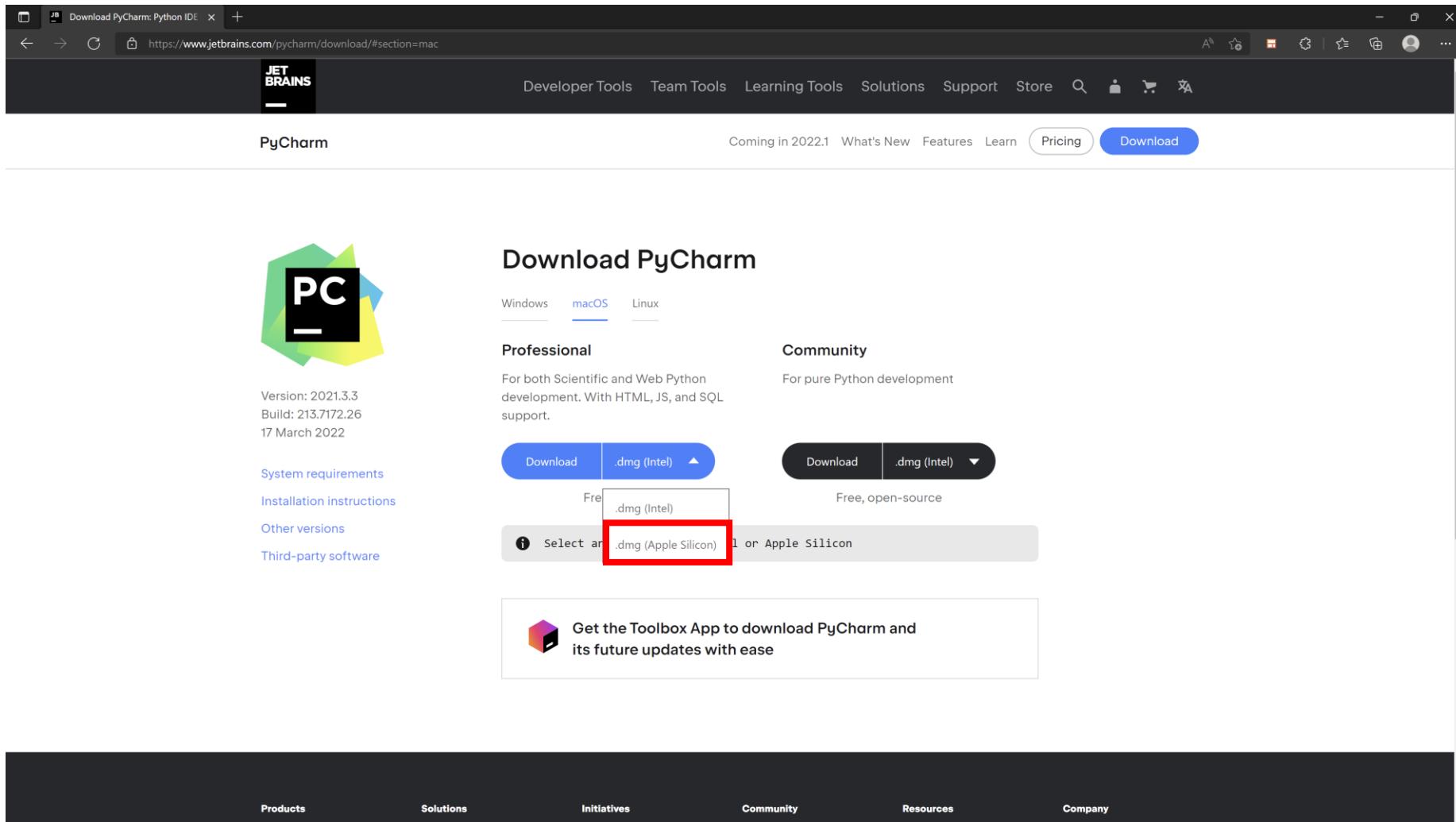
If you use intel CPU, click here

The screenshot shows the 'Download PyCharm' page on the JetBrains website. The URL in the browser is <https://www.jetbrains.com/pycharm/download/#section=mac>. The page features a dark header with the Jet Brains logo and navigation links for Developer Tools, Team Tools, Learning Tools, Solutions, Support, Store, and a search bar. Below the header, there's a navigation bar with links for Coming in 2022.1, What's New, Features, Learn, Pricing, and a prominent blue 'Download' button. The main content area is titled 'Download PyCharm' and includes tabs for Windows, macOS (which is selected), and Linux. It shows two download options: 'Professional' and 'Community'. The 'Professional' section is described as 'For both Scientific and Web Python development. With HTML, JS, and SQL support.' and includes a 'Download' button with a red box around it. The 'Community' section is described as 'For pure Python development' and includes a 'Download' button. A note below the download buttons says 'Select an installer for Intel or Apple Silicon'. At the bottom of the page is a footer with links for Products, Solutions, Initiatives, Community, Resources, and Company.

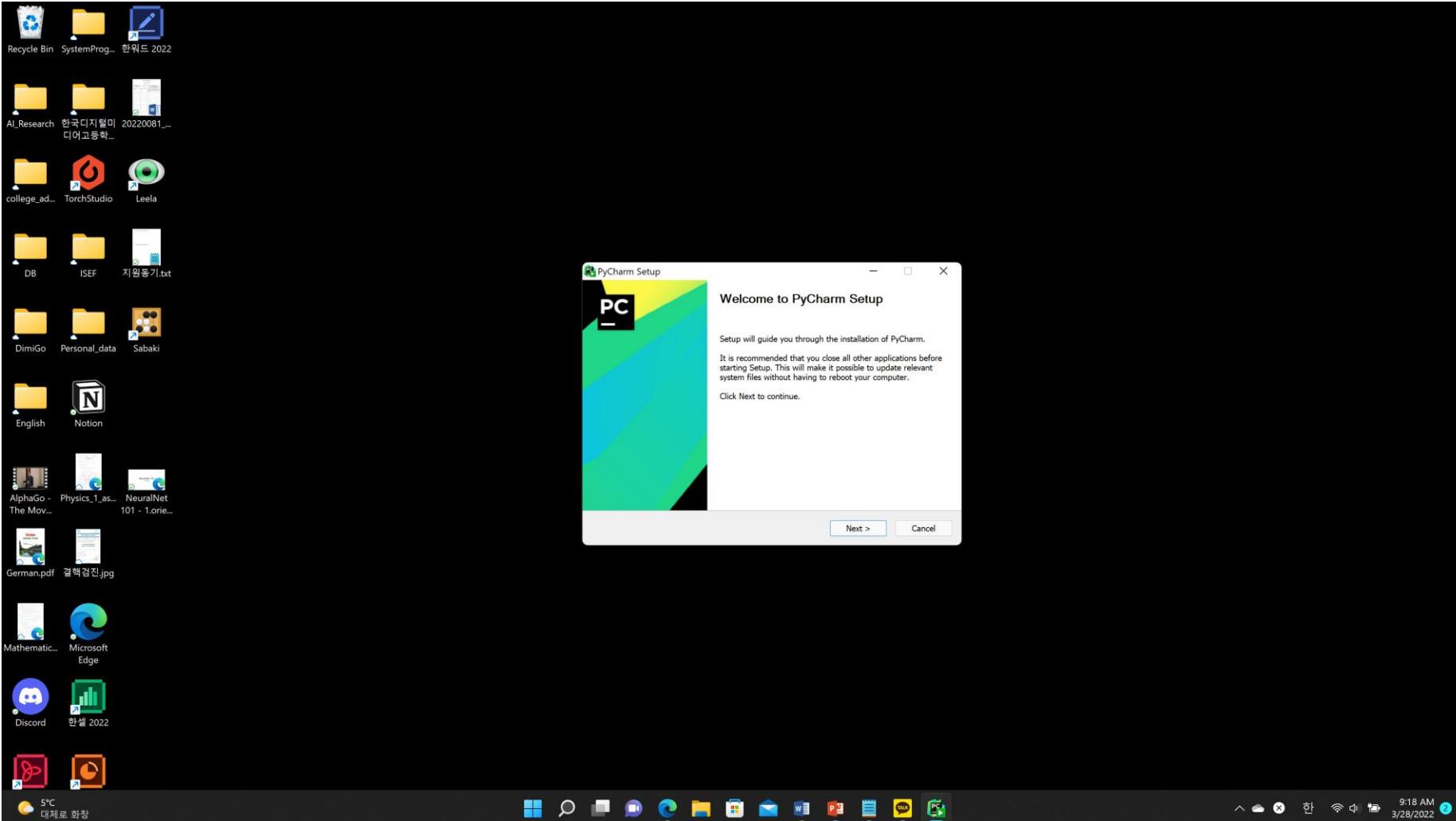
If you use ARM based processor, click here

The screenshot shows a web browser window displaying the PyCharm download page on the JetBrains website. The URL in the address bar is <https://www.jetbrains.com/pycharm/download/#section=mac>. The page has a dark header with the Jet Brains logo and navigation links for Developer Tools, Team Tools, Learning Tools, Solutions, Support, Store, and a search bar. Below the header, there are links for Coming in 2022.1, What's New, Features, Learn, Pricing, and Download. The main content area is titled "Download PyCharm" and features tabs for Windows, macOS, and Linux. Under the macOS tab, there are two download options: "Professional" and "Community". Each option has a "Download" button and a ".dmg (Intel)" dropdown menu. The "Professional" section is described as "For both Scientific and Web Python development. With HTML, JS, and SQL support." and is labeled "Free trial". The "Community" section is described as "For pure Python development" and is labeled "Free, open-source". A note at the bottom of the Professional section says "Select an installer for Intel or Apple Silicon". At the bottom of the page, there is a call-to-action for the "Toolbox App" with a "Get the Toolbox App to download PyCharm and its future updates with ease" button.

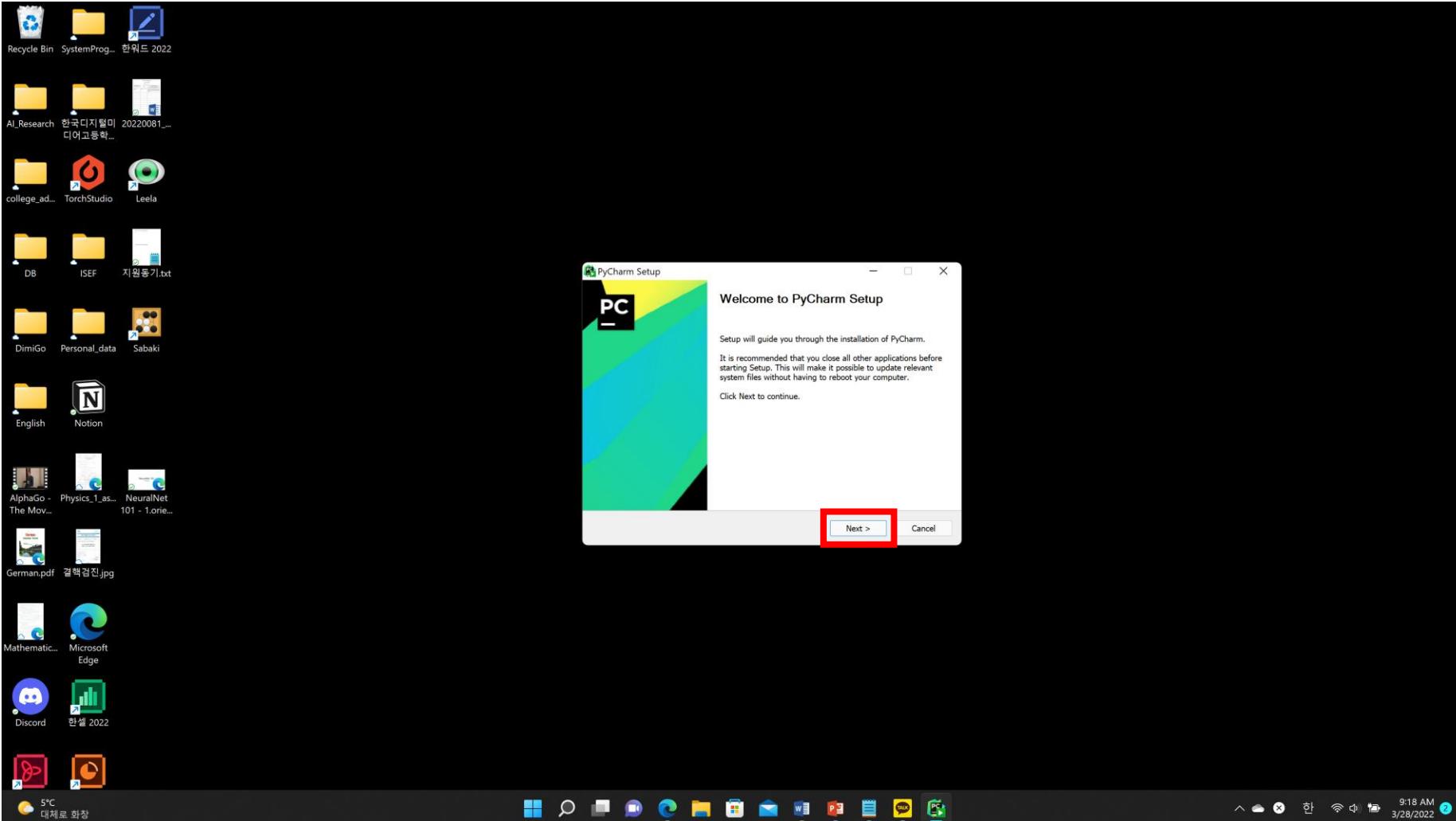
And select “.dmg (Apple Silicon)”



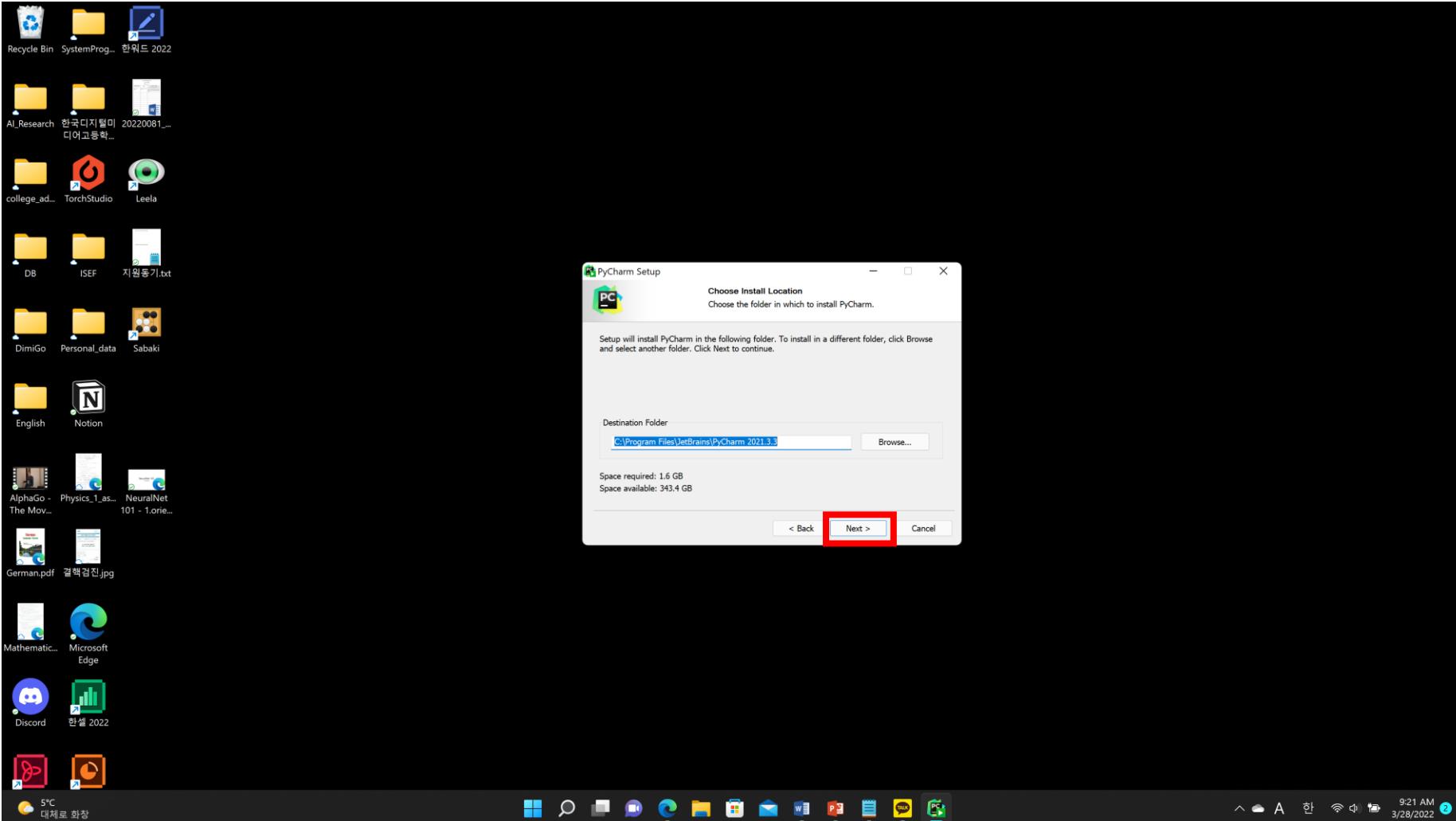
Open PyCharm installer to install



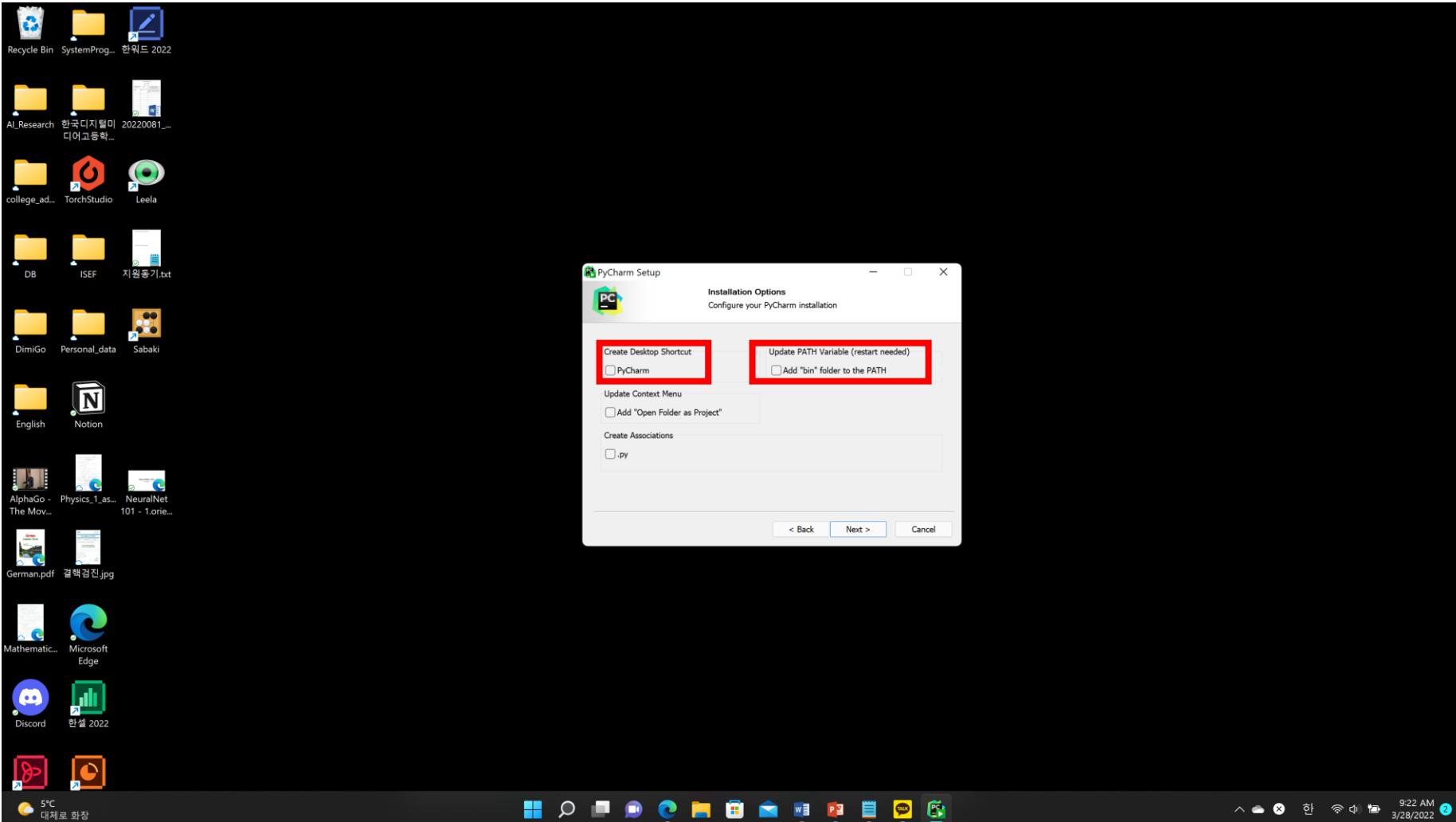
Click Next



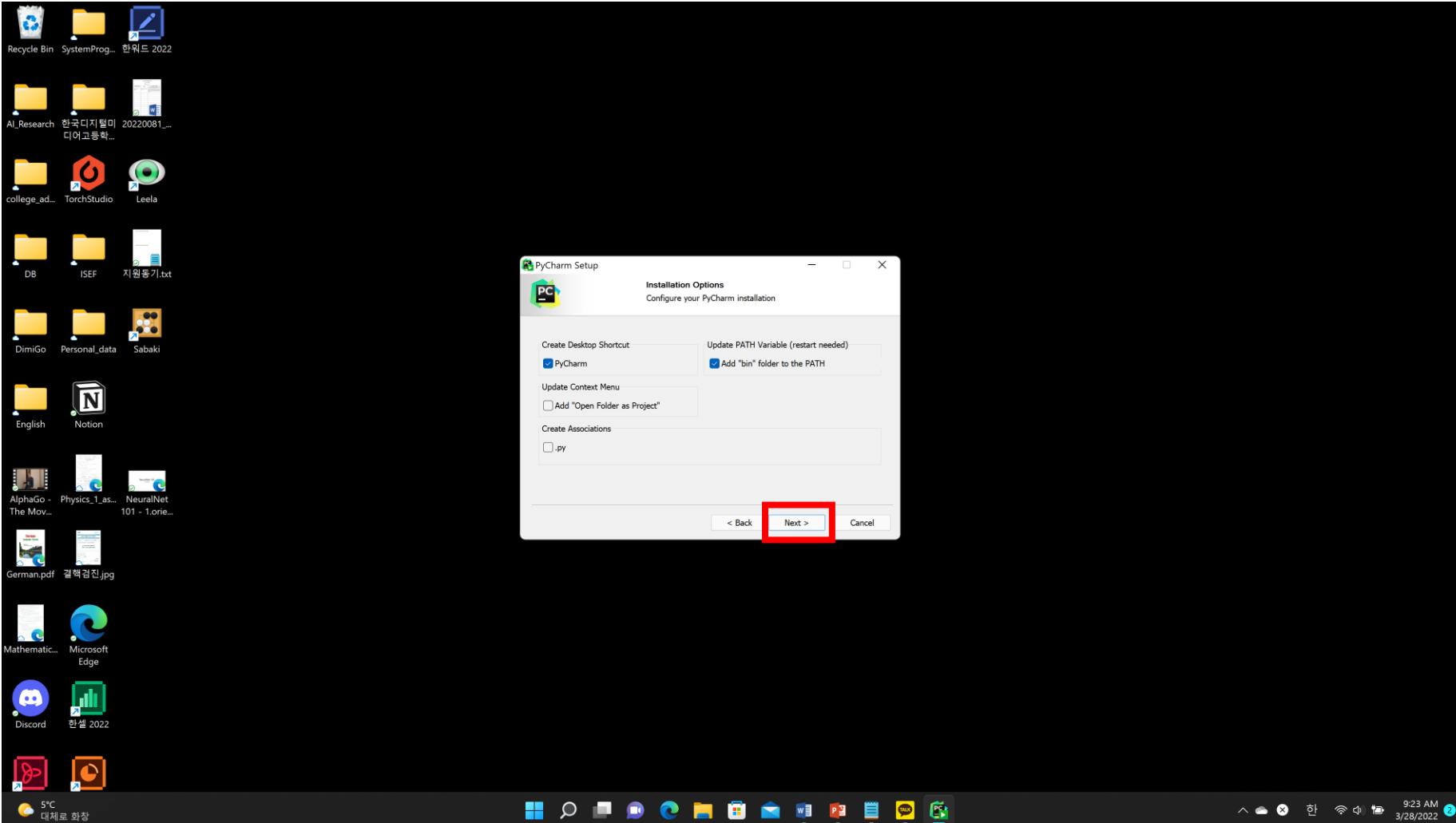
Click Next



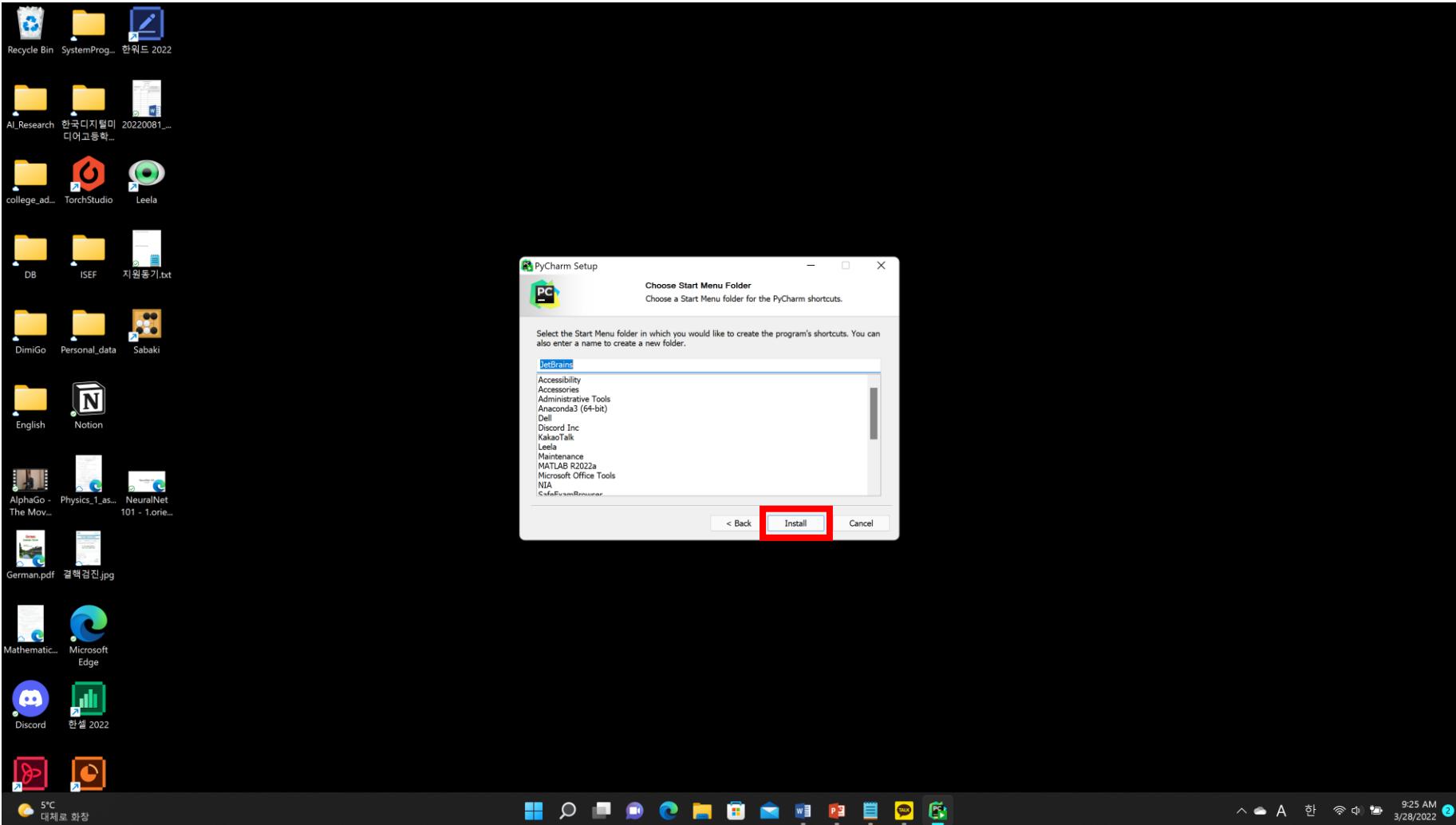
Check “create Desktop Shortcut” & “update PATH variable”



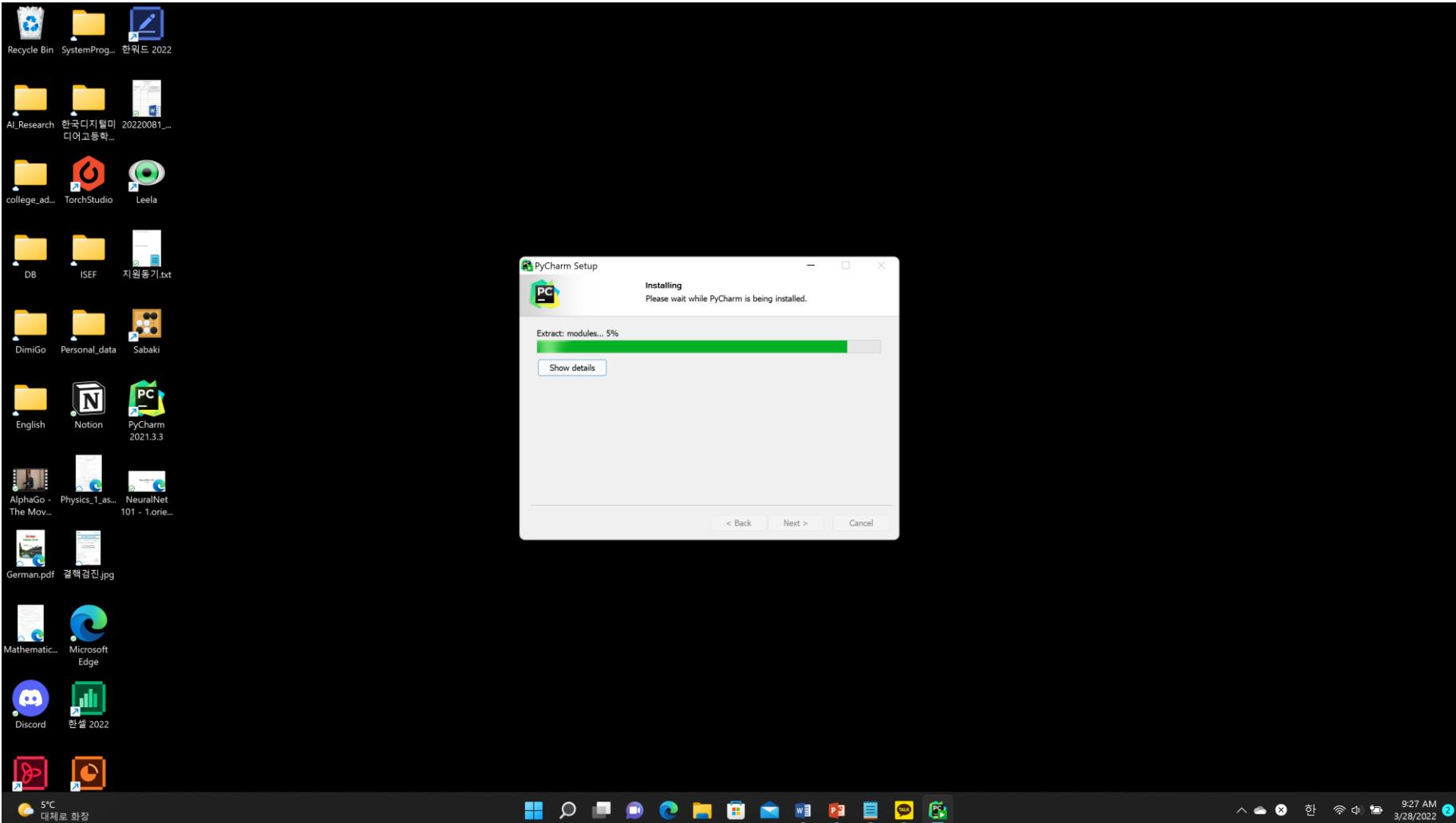
Click Next



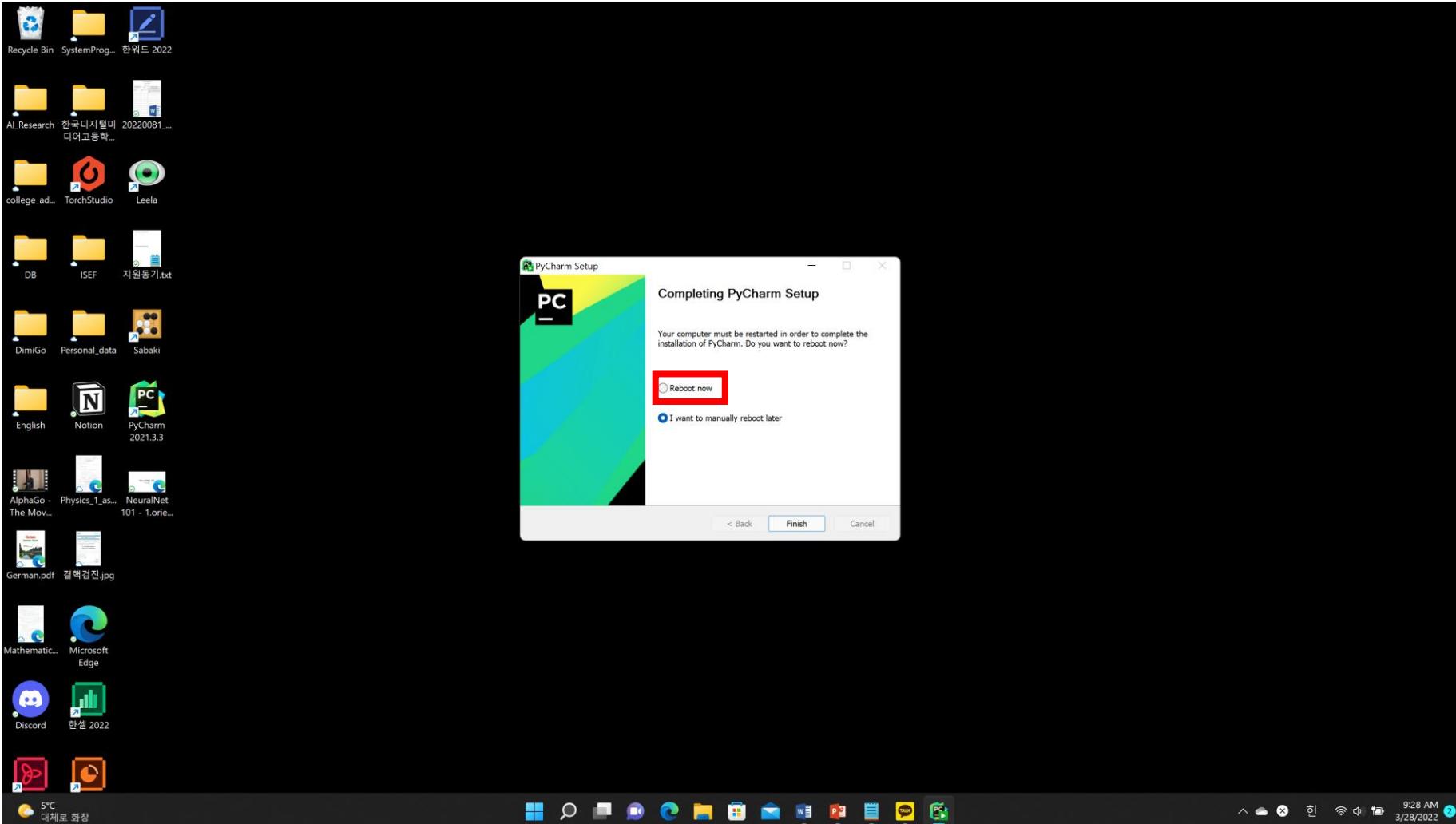
Click Install



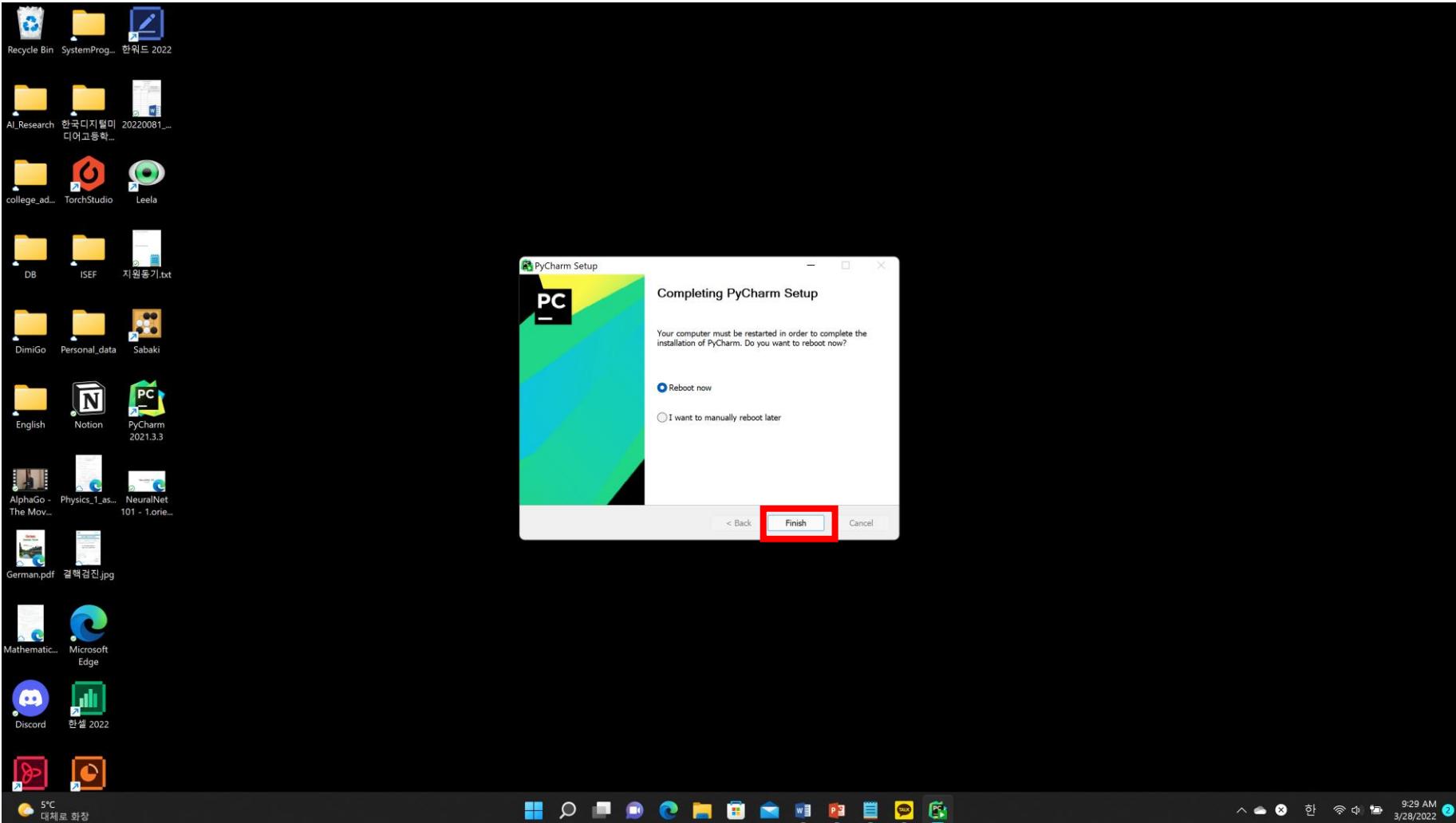
Installing...



Click “reboot now”



Click Finish (caution: you need to end your task before rebooting)

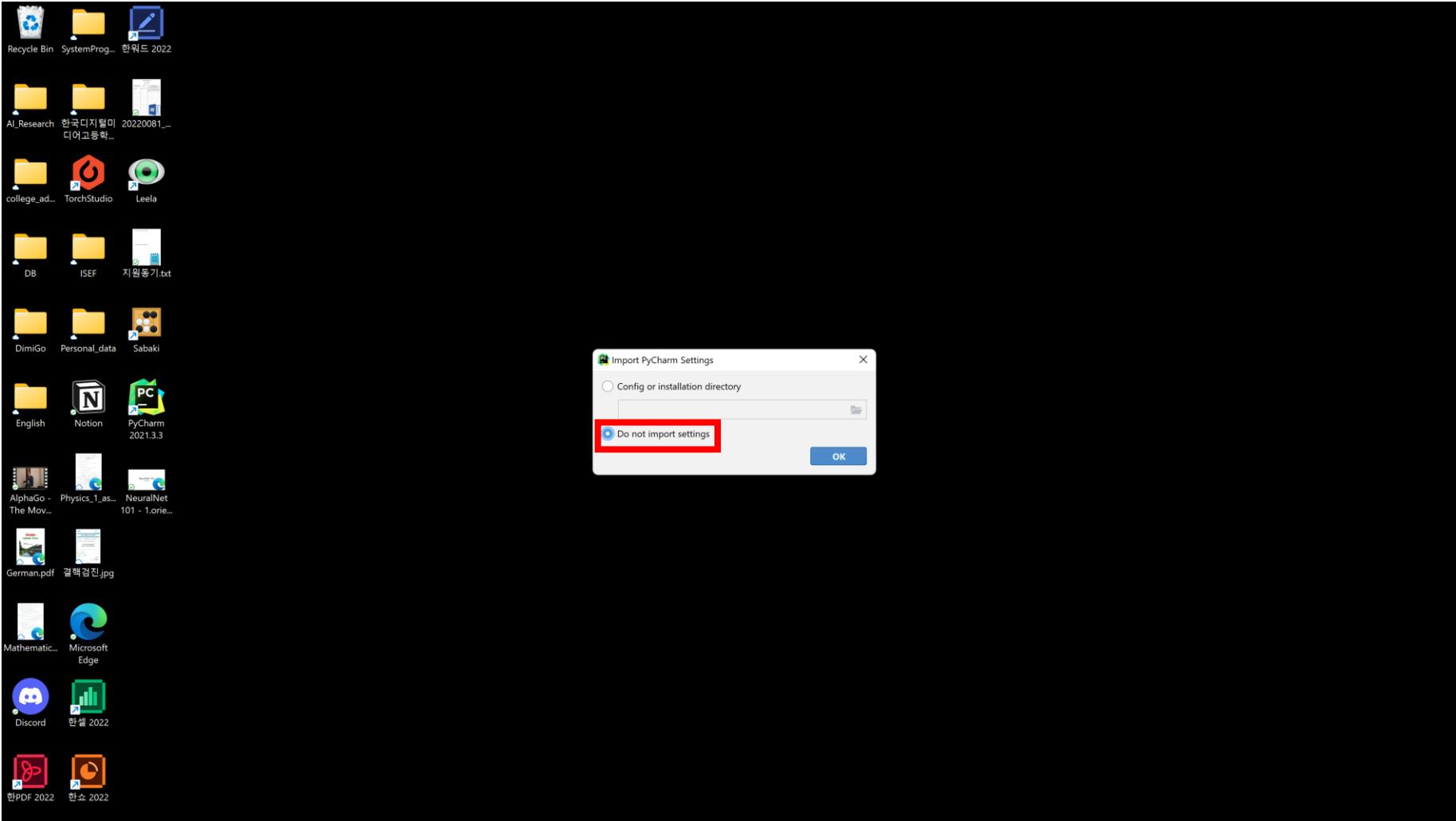


4th step: Install PyTorch and Numpy on PyCharm

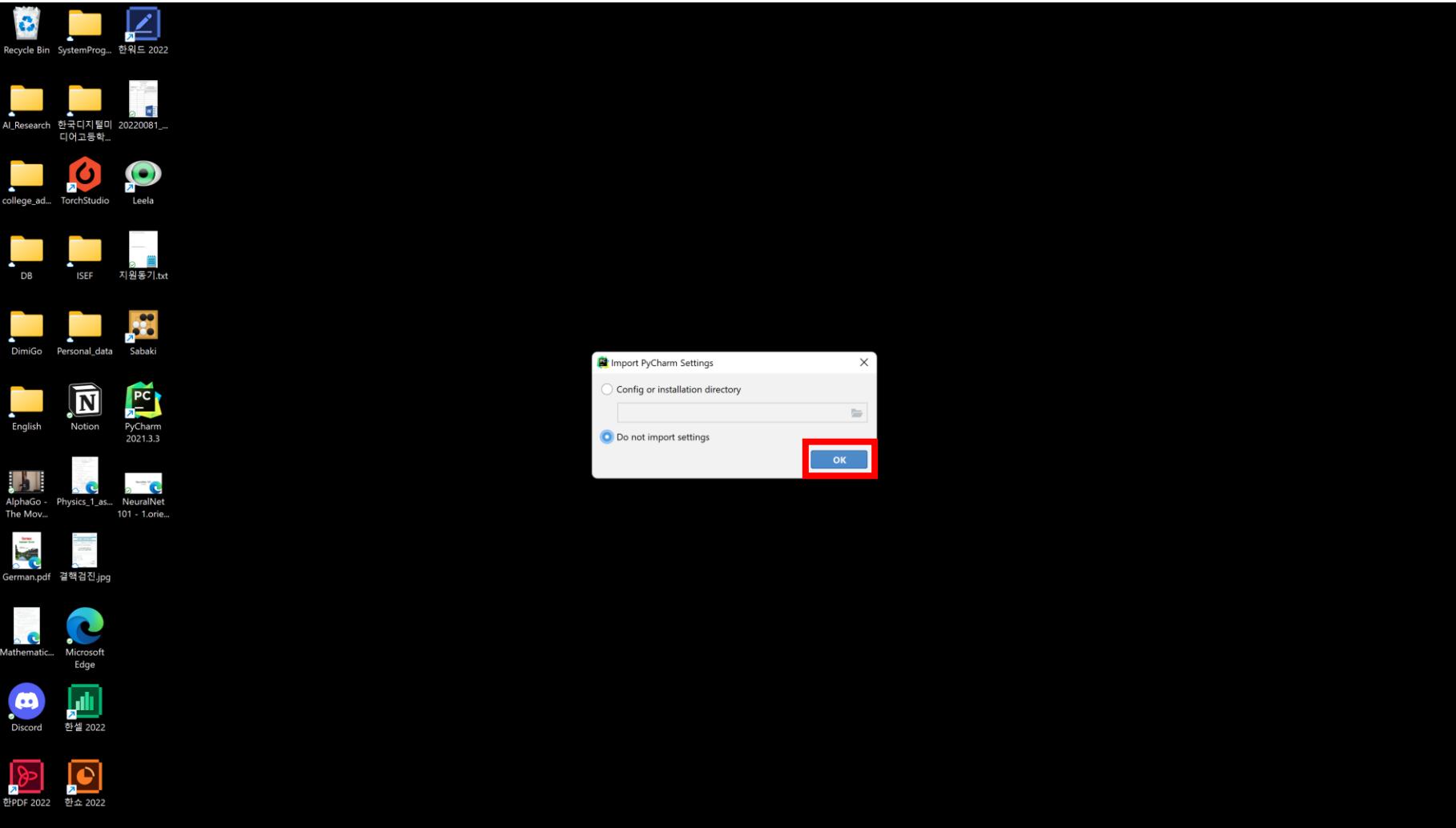
Open PyCharm...



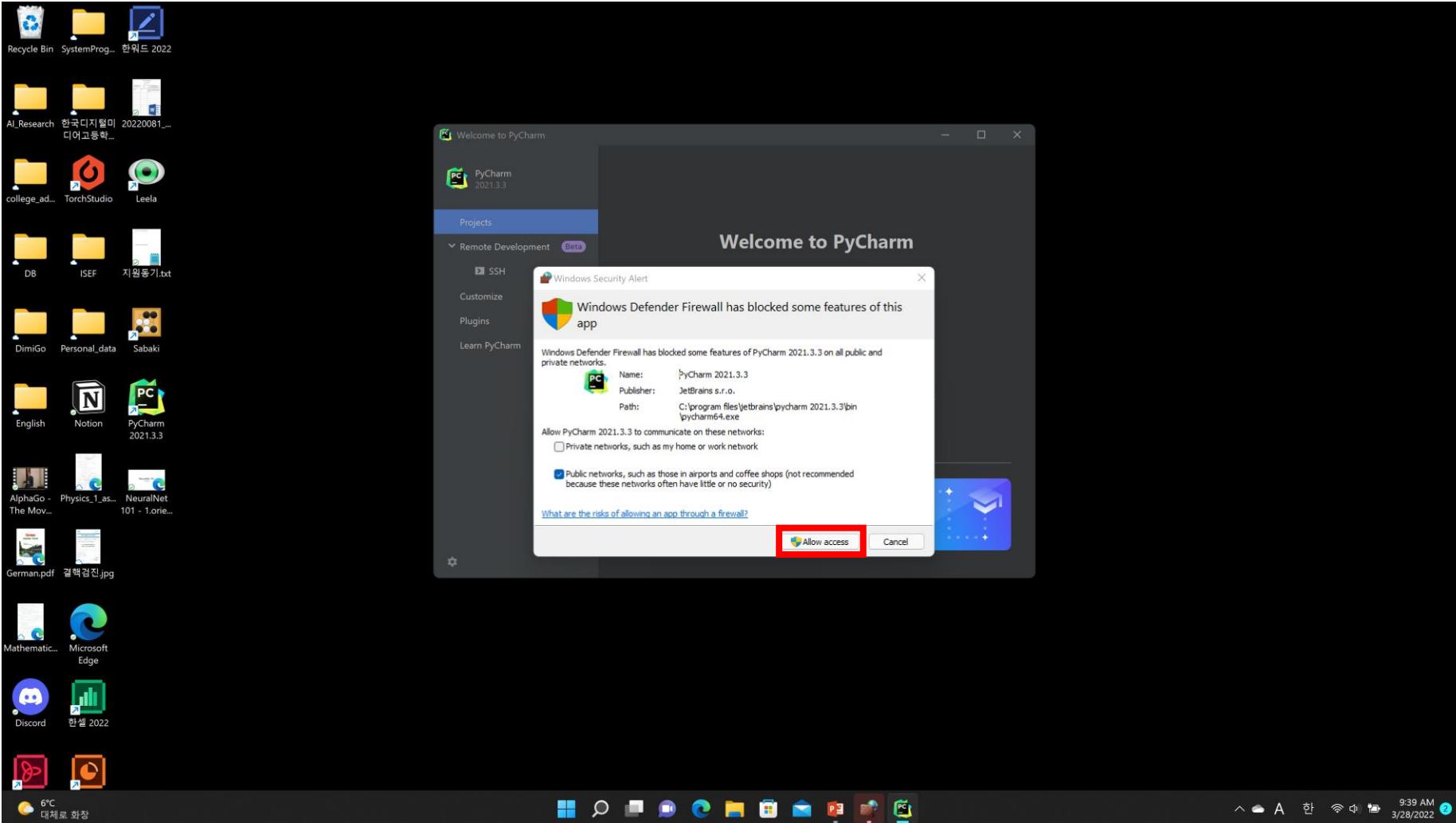
Check “Do not import settings”



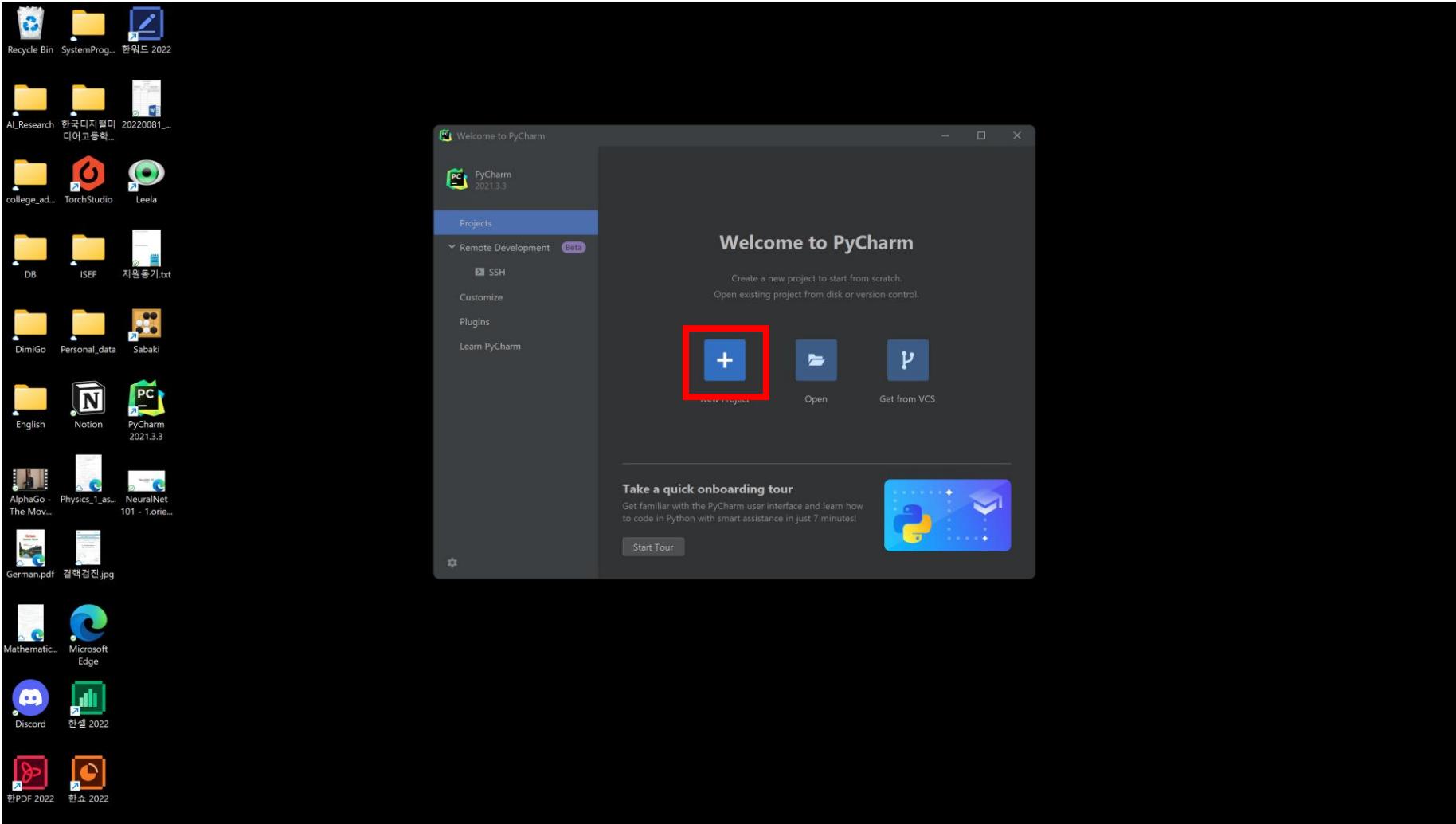
Click “OK”



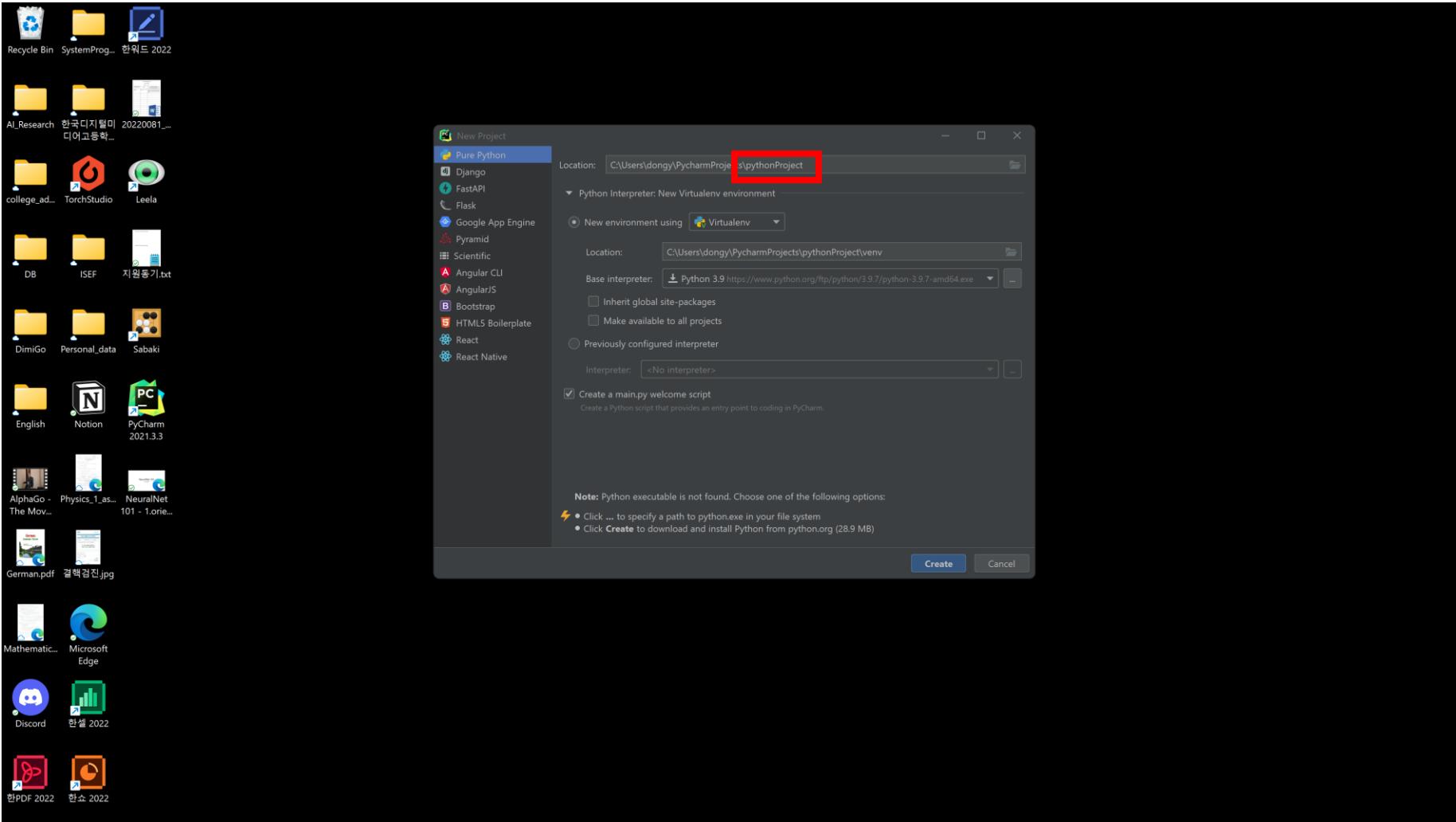
Click “Allow Access”



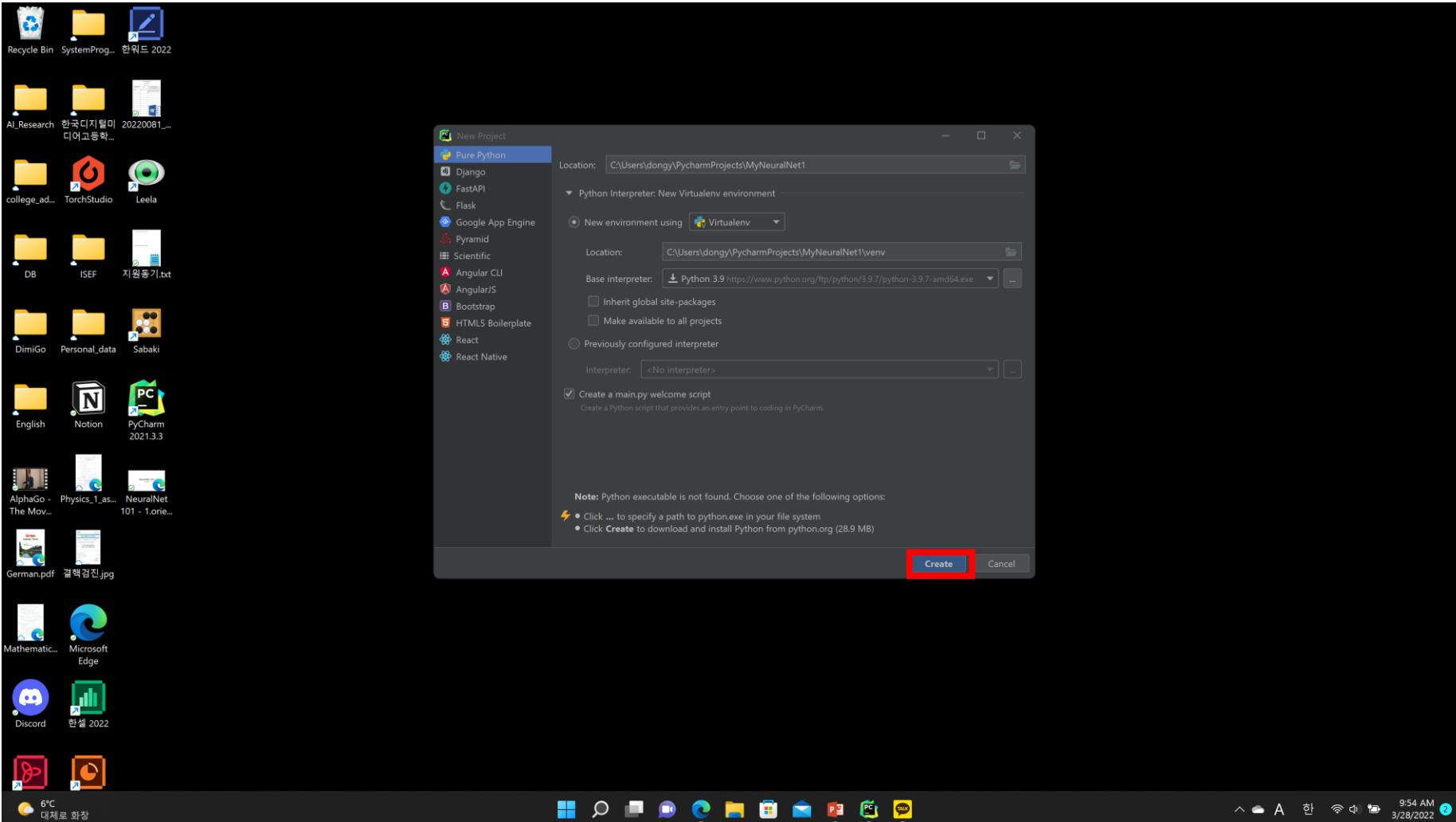
Click “New project”



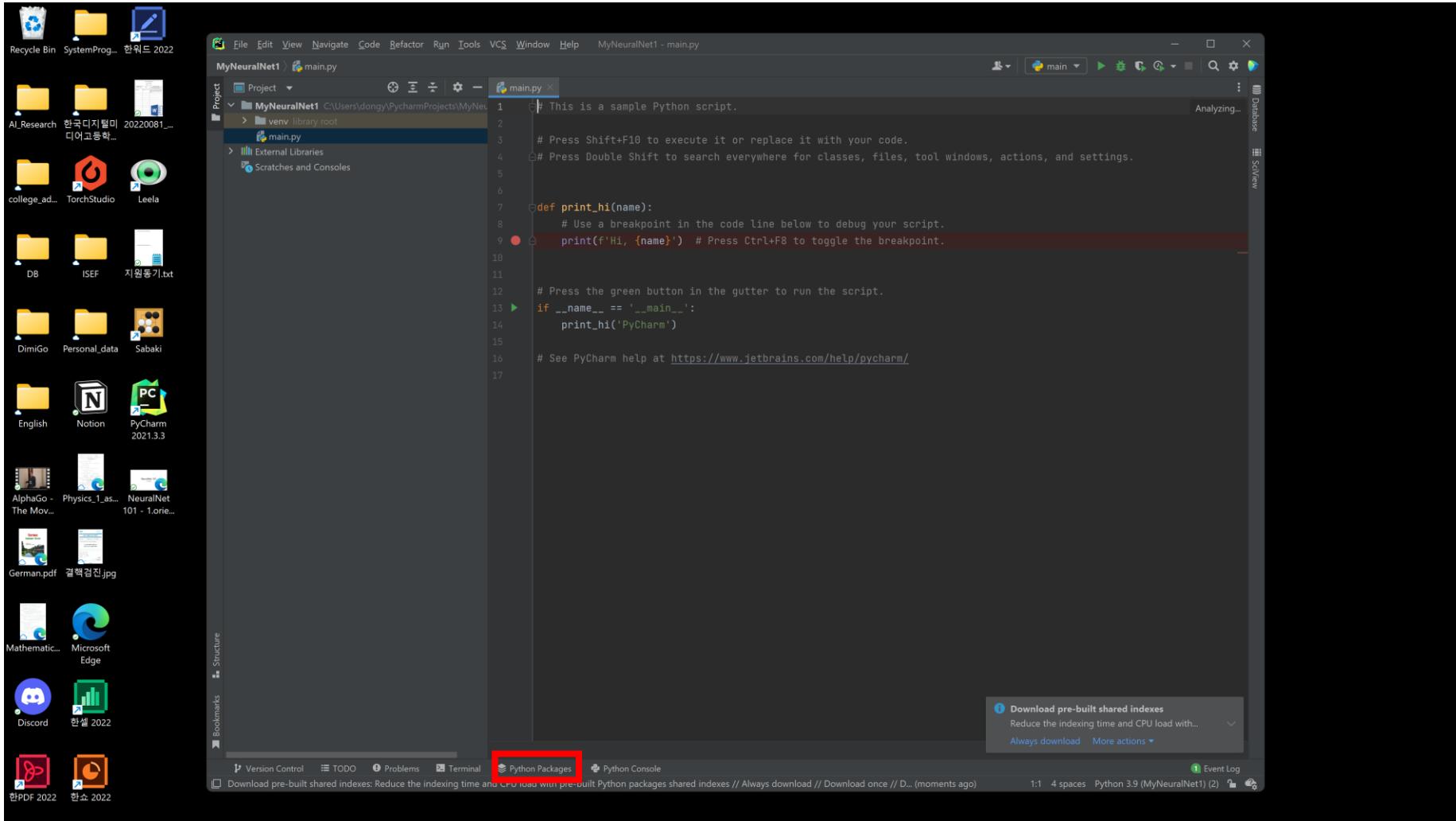
Change project name “pythonproject” to “MyNeuralNet101”



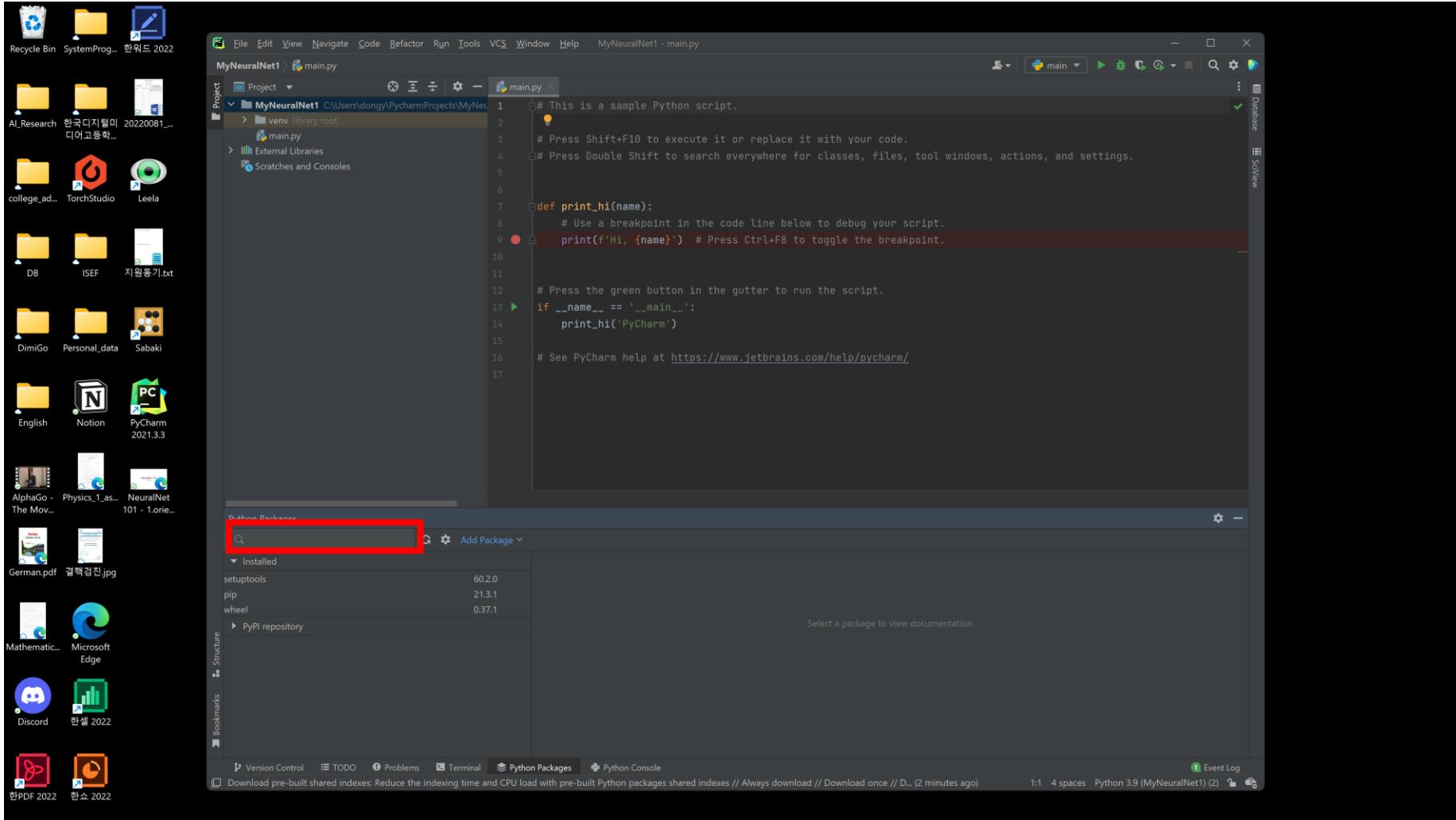
Click “Create”



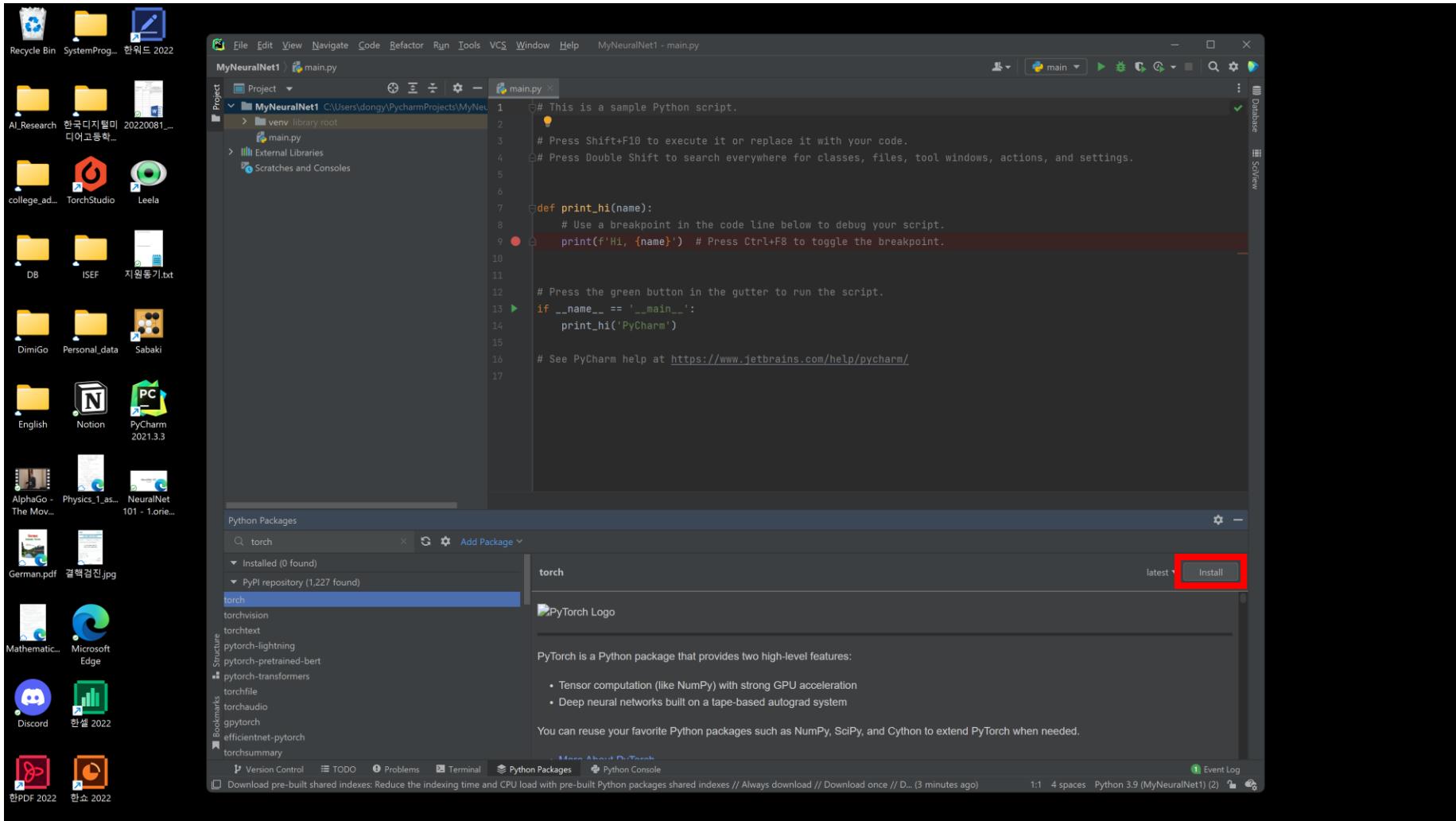
Click “python packages”



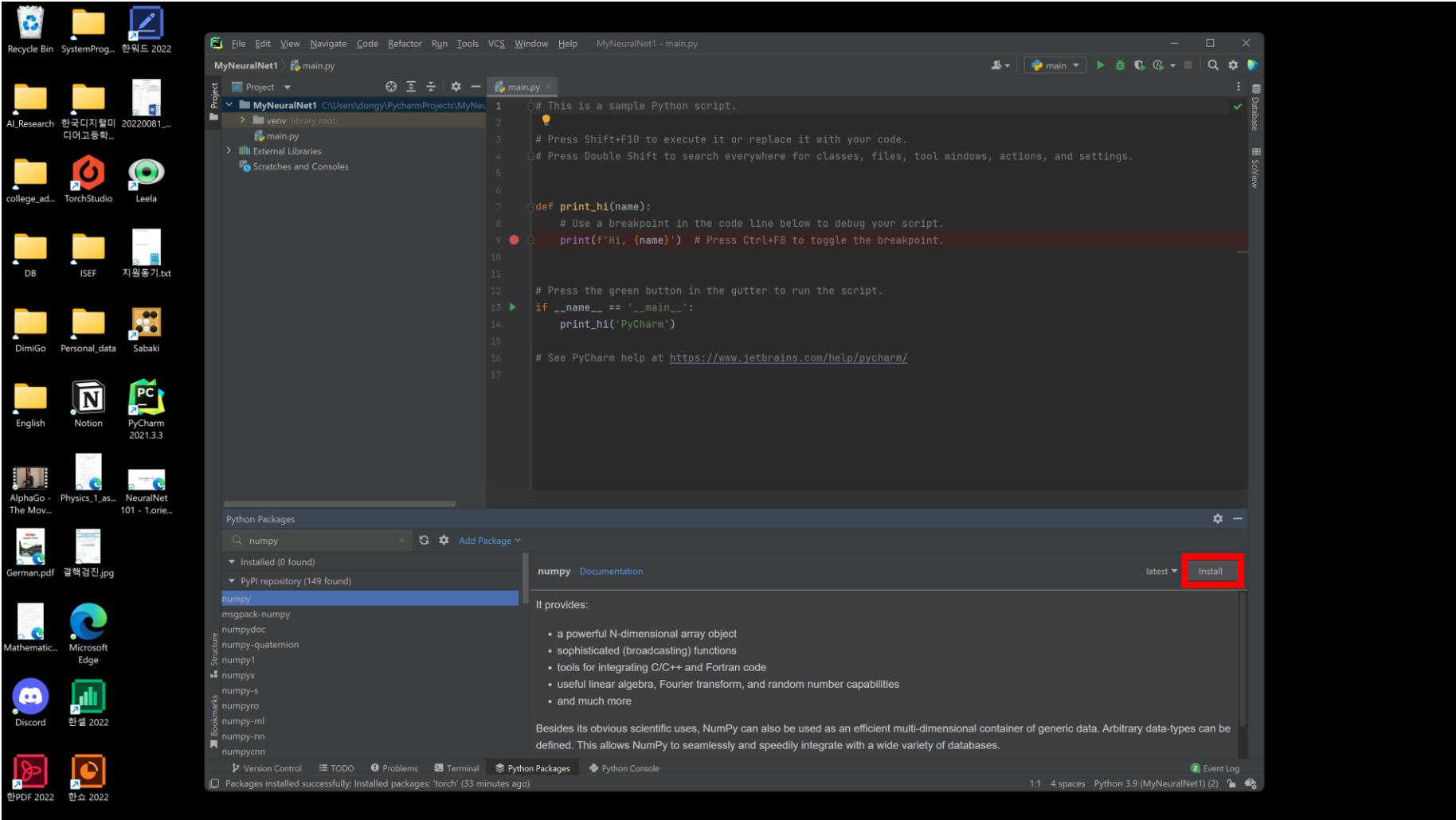
Type “torch” on searchbox



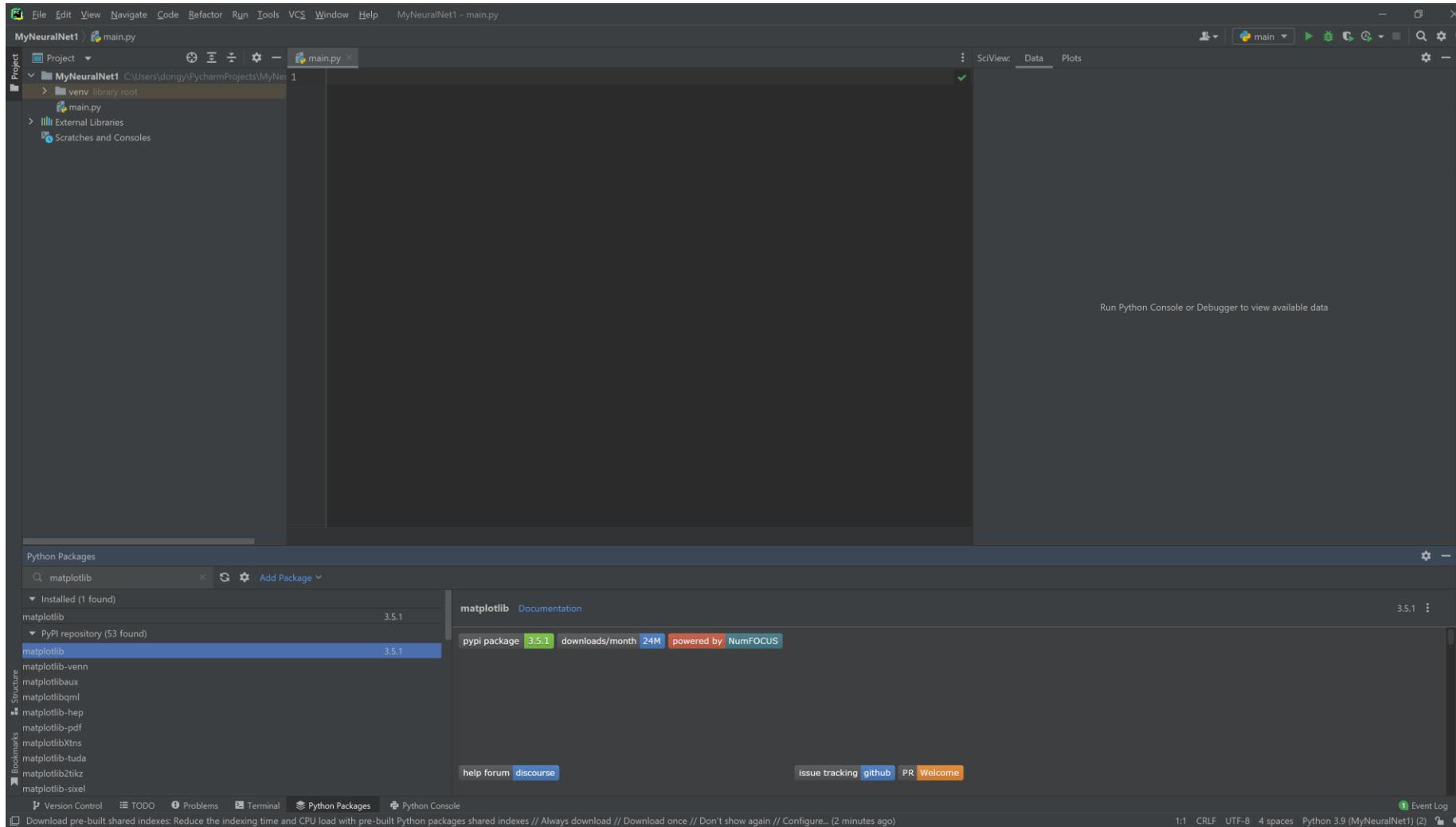
Click “install”



Also type “numpy” in searchbox & install it



Also type “matplotlib” in searchbox & install it



Now we are done to setup the environment!

How to use NumPy:

Quick note:

`numpy.array -> ex) a = np.array([1,2,3])`

`numpy.zeros() -> ex) a = numpy.zeros(2) => [0. 0]`

`numpy.ones() -> ex) a = numpy.ones(2) => [1. 1]`

And there has data type='float' or 'int'

You also can make an operation `+, -, *, /, **, //, %` like python

Try to use with documentation in here:
numpy.org

How to use PyTorch:

Quick note:

`torch.tensor()` -> it is like the `numpy.array` object

Define a function `g` with tensor `a` and tensor `b`, like $g = 6*a^{**}5 - b^{**}2$

We can assign the function has 1 outside from the error, then

```
External_grad = torch.tensor([1,1])
g.backward(gradient=external_grad)
Print(a.grad, b.grad) for checking the gradient values
```

You also can make an operation `+, -, *, /, **, //, %` between tensors like python object

Try to use with documentation in here:
pytorch.org/docs/stable/index.html

Lab 1: find the optimal point of quadratic function in iteration 1000

$$f(x) = 0.0001x^2$$

When x starts at
x = 50000

Lab 2: find the optimal point of quaternary function

$$f(x) = x^4 - 3x^3 + 3x$$

When x starts at
x = -0.5

Lab 3: find the which optimizing equation can do fastest convergence on below function. Just try to find the small $f(x,y)$ as possible than your friend

$$f(x,y) = \frac{x^2 + (y - 3)^2(y + 2)^2(y - 1)(y + 1)}{20}$$

When (x,y) starts at
 $(x,y) = (0, 1.948)$

Post your codes and results on github:
<https://github.com/vlab-kaist/NeuralNet101> by
making issue with the name (your class A or
B)_(your name)_lab_(number of the week)week

Ex) A_김동영_lab_1week

In next learning, we will learn about linear regression. Thank you for listening!