機器學習於材料資訊的應用
Machine Learning on Material Informatics

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Build your own Development Environment

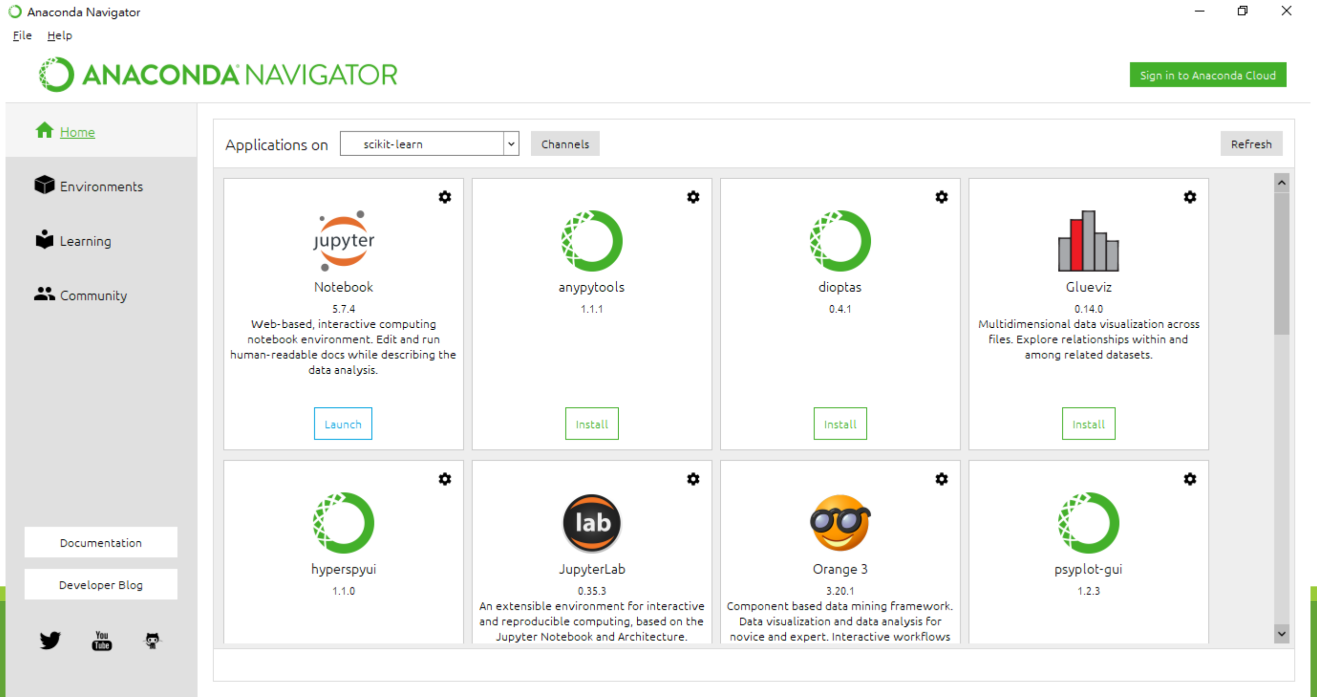
Use Miniconda/Anaconda

Conda is a package management system.

Miniconda/Anaconda is a distribution for python.

Anaconda is owned by Continuum Analytics™.

Packages in Conda are released by binary not source code. This means that if conda decide not to release certain package you will ...



Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.

Multidimensional data visualization across files. Explore relationships within and among related datasets.

An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Architecture.

Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows

Anaconda or Miniconda?

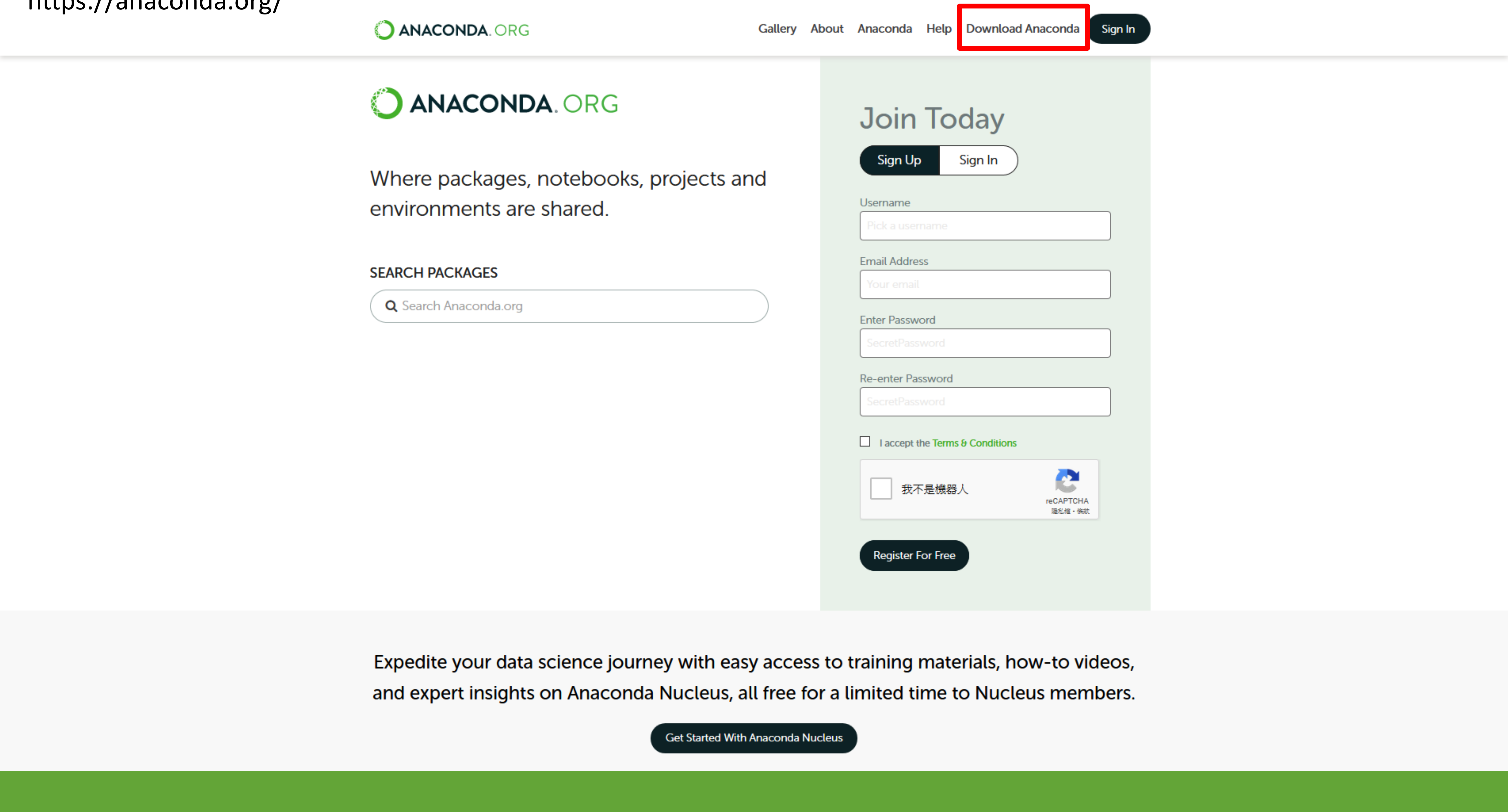
CHOOSE ANACONDA IF YOU:

- Are new to conda or Python.
- Like the convenience of having Python and over 1,500 scientific packages automatically installed at once.
- Have the time and disk space---a few minutes and 3 GB.
- Do not want to individually install each of the packages you want to use.
- Do not want to use command line interface.

CHOOSE MINICONDA IF YOU:

- Do not mind installing each of the packages you want to use individually.
- Do not have time or disk space to install over 1,500 packages at once.
- Want fast access to Python and the conda commands and you wish to sort out the other programs later.

https://anaconda.org/



ANACONDA.ORG

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ANACONDA.ORG

Where packages, notebooks, projects and environments are shared.

SEARCH PACKAGES

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Enter Password

SecretPassword

Re-enter Password

SecretPassword

□ I accept the Terms & Conditions

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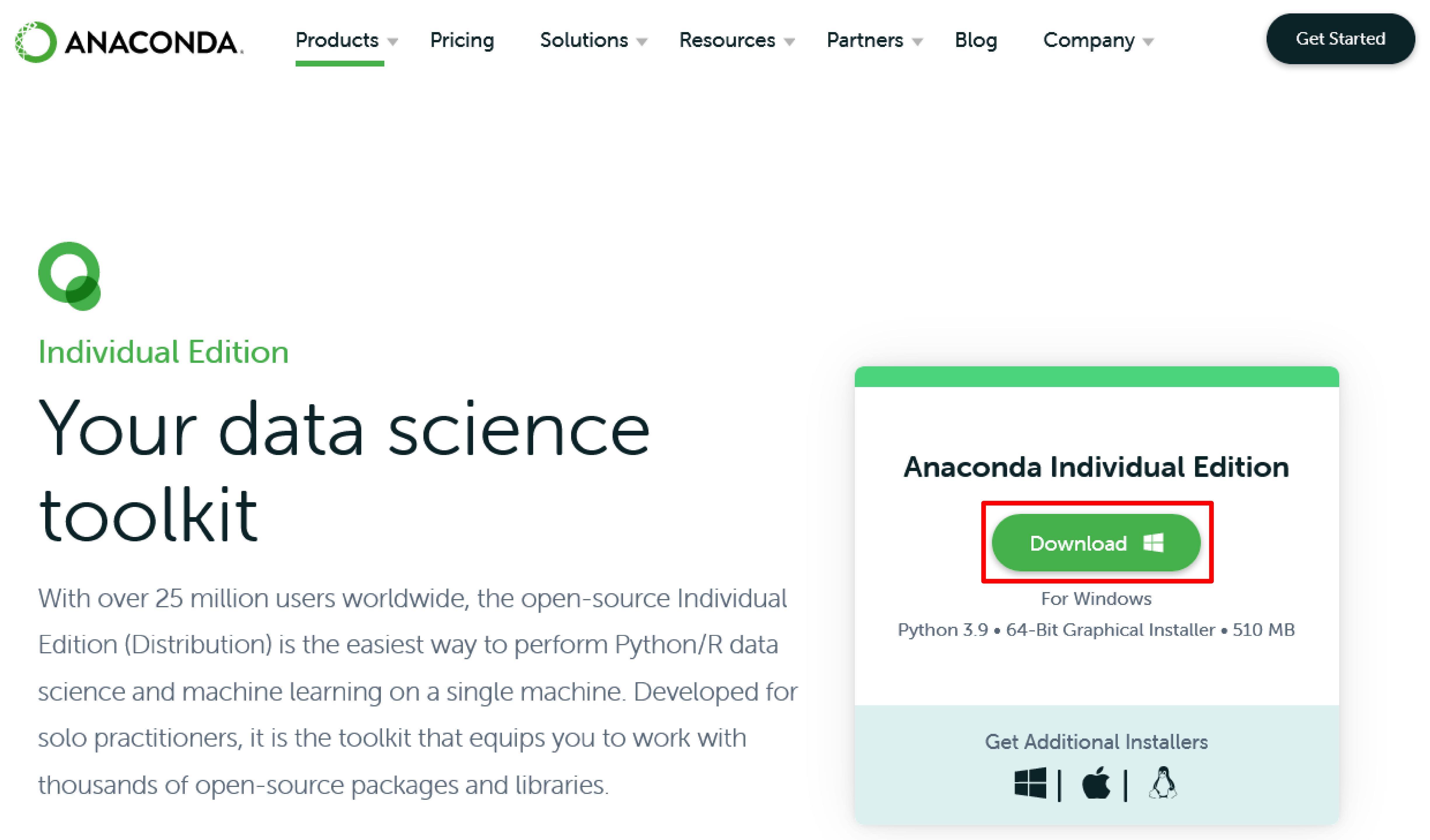
Register For Free

Expedite your data science journey with easy access to training materials, how-to videos, and expert insights on Anaconda Nucleus, all free for a limited time to Nucleus members.

Get Started With Anaconda Nucleus



Individual Edition

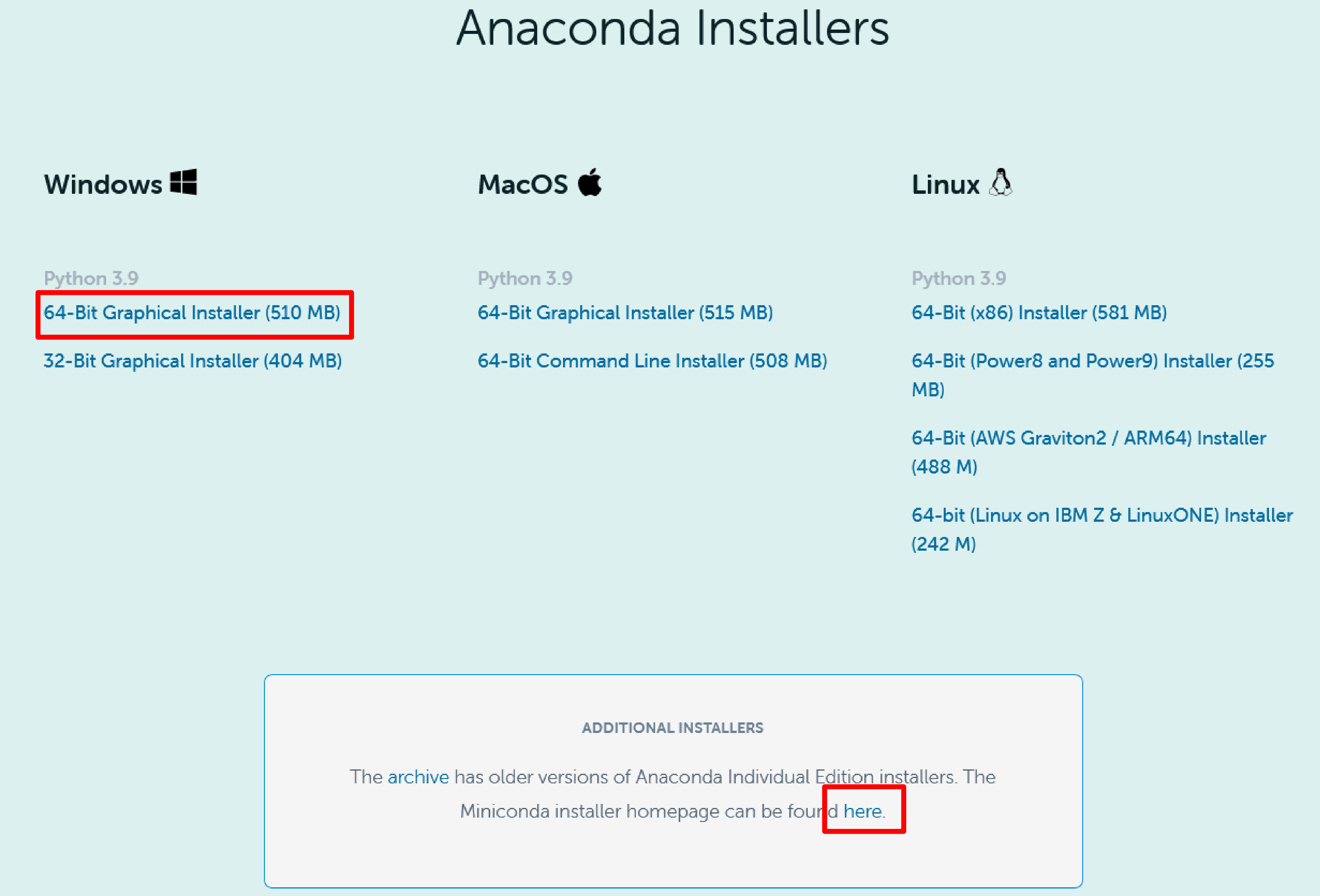
Your data science toolkit

With over 25 million users worldwide, the open-source Individual Edition (Distribution) is the easiest way to perform Python/R data science and machine learning on a single machine. Developed for solo practitioners, it is the toolkit that equips you to work with thousands of open-source packages and libraries.

Anaconda Individual Edition

For Windows

Python 3.9 • 64-Bit Graphical Installer • 510 MB



Anaconda Installers

Windows

Python 3.9

64-Bit Graphical Installer (510 MB)

32-Bit Graphical Installer (404 MB)

MacOS

Python 3.9

64-Bit Graphical Installer (515 MB)

64-Bit Command Line Installer (508 MB)

Linux

Python 3.9

64-Bit (x86) Installer (581 MB)

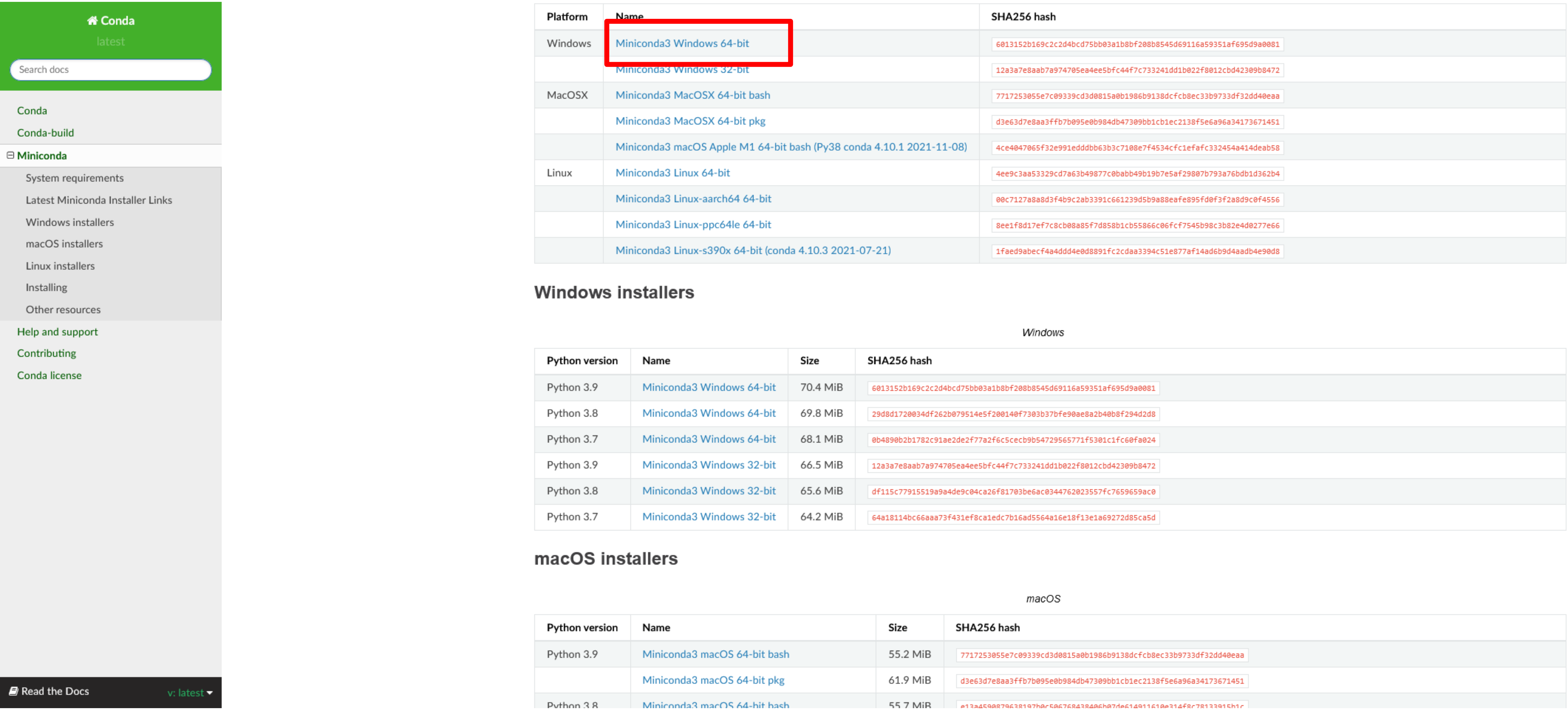
64-Bit (Power8 and Power9) Installer (255 MB)

64-Bit (AWS Graviton2 / ARM64) Installer (488 M)

64-bit (Linux on IBM Z & LinuxONE) Installer (242 M)

ADDITIONAL INSTALLERS

The archive has older versions of Anaconda Individual Edition installers. The Miniconda installer homepage can be found here.



Conda
latest

Search docs

- Conda
- Conda-build
- ⊟ Miniconda
  - System requirements
  - Latest Miniconda Installer Links
  - Windows installers
  - macOS installers
  - Linux installers
  - Installing
  - Other resources
- Help and support
- Contributing
- Conda license

Read the Docs   v: latest ▾

Platform	Name	SHA256 hash
Windows	Miniconda3 Windows 64-bit	6013152b169c2c2d4bcd75bb03a1b8bf208b8545d69116a59351af695d9a0081
	Miniconda3 Windows 32-bit	12a3a7e8aab7a974705ea4ee5bfc44f7c733241dd1b022f8012cbd42309b8472
MacOSX	Miniconda3 MacOSX 64-bit bash	7717253055e7c09339cd3d0815a0b1986b9138dcfcb8ec33b9733df32dd40eaa
	Miniconda3 MacOSX 64-bit pkg	d3e63d7e8aa3ffb7b095e0b984db47309bb1cb1ec2138f5e6a96a34173671451
	Miniconda3 macOS Apple M1 64-bit bash (Py38 conda 4.10.1 2021-11-08)	4ce4047065f32e991edddbb63b3c7108e7f4534cfc1efafc332454a414deab58
Linux	Miniconda3 Linux 64-bit	4ee9c3aa53329cd7a63b49877c0babb49b19b7e5af29807b793a76bdb1d362b4
	Miniconda3 Linux-aarch64 64-bit	00c7127a8a8d3f4b9c2ab3391c661239d5b9a88eafe895fd0f3f2a8d9c0f4556
	Miniconda3 Linux-ppc64le 64-bit	8ee1f8d17ef7c8cb08a85f7d858b1cb55866c06fcf7545b98c3b82e4d0277e66
	Miniconda3 Linux-s390x 64-bit (conda 4.10.3 2021-07-21)	1faed9abecf4a4ddd4e0d8891fc2cdaa3394c51e877af14ad6b9d4aadb4e90d8

Windows installers

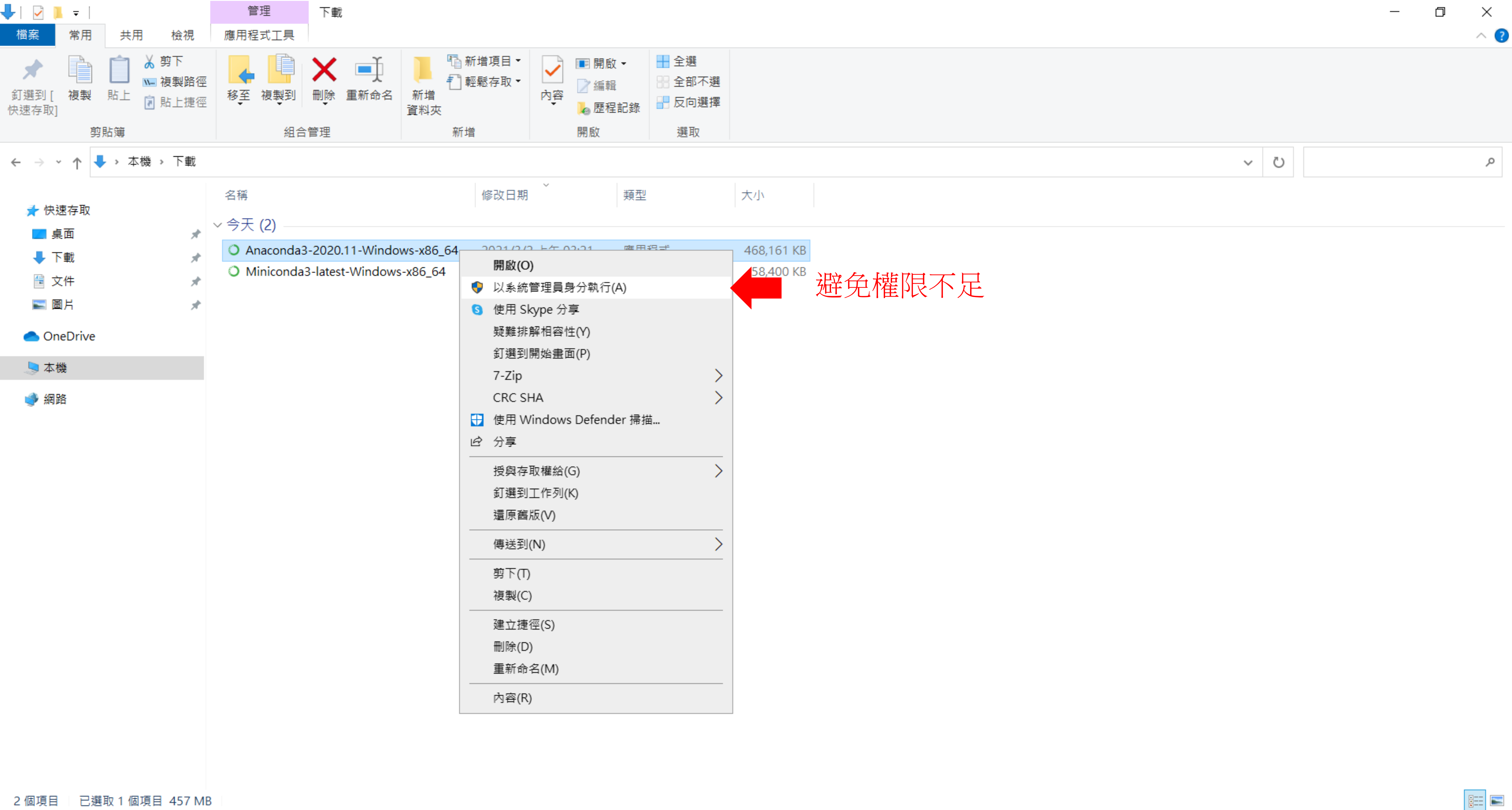
Windows

Python version	Name	Size	SHA256 hash
Python 3.9	Miniconda3 Windows 64-bit	70.4 MiB	6013152b169c2c2d4bcd75bb03a1b8bf208b8545d69116a59351af695d9a0081
Python 3.8	Miniconda3 Windows 64-bit	69.8 MiB	29d8d1720034df262b079514e5f200140f7303b37bfe90ae8a2b40b8f294d2d8
Python 3.7	Miniconda3 Windows 64-bit	68.1 MiB	0b4890b2b1782c91ae2de2f77a2f6c5cecb9b54729565771f5301c1fc60fa024
Python 3.9	Miniconda3 Windows 32-bit	66.5 MiB	12a3a7e8aab7a974705ea4ee5bfc44f7c733241dd1b022f8012cbd42309b8472
Python 3.8	Miniconda3 Windows 32-bit	65.6 MiB	df115c77915519a9a4de9c04ca26f81703be6ac0344762023557fc7659659ac0
Python 3.7	Miniconda3 Windows 32-bit	64.2 MiB	64a18114bc66aaa73f431ef8ca1edc7b16ad5564a16e18f13e1a69272d85ca5d

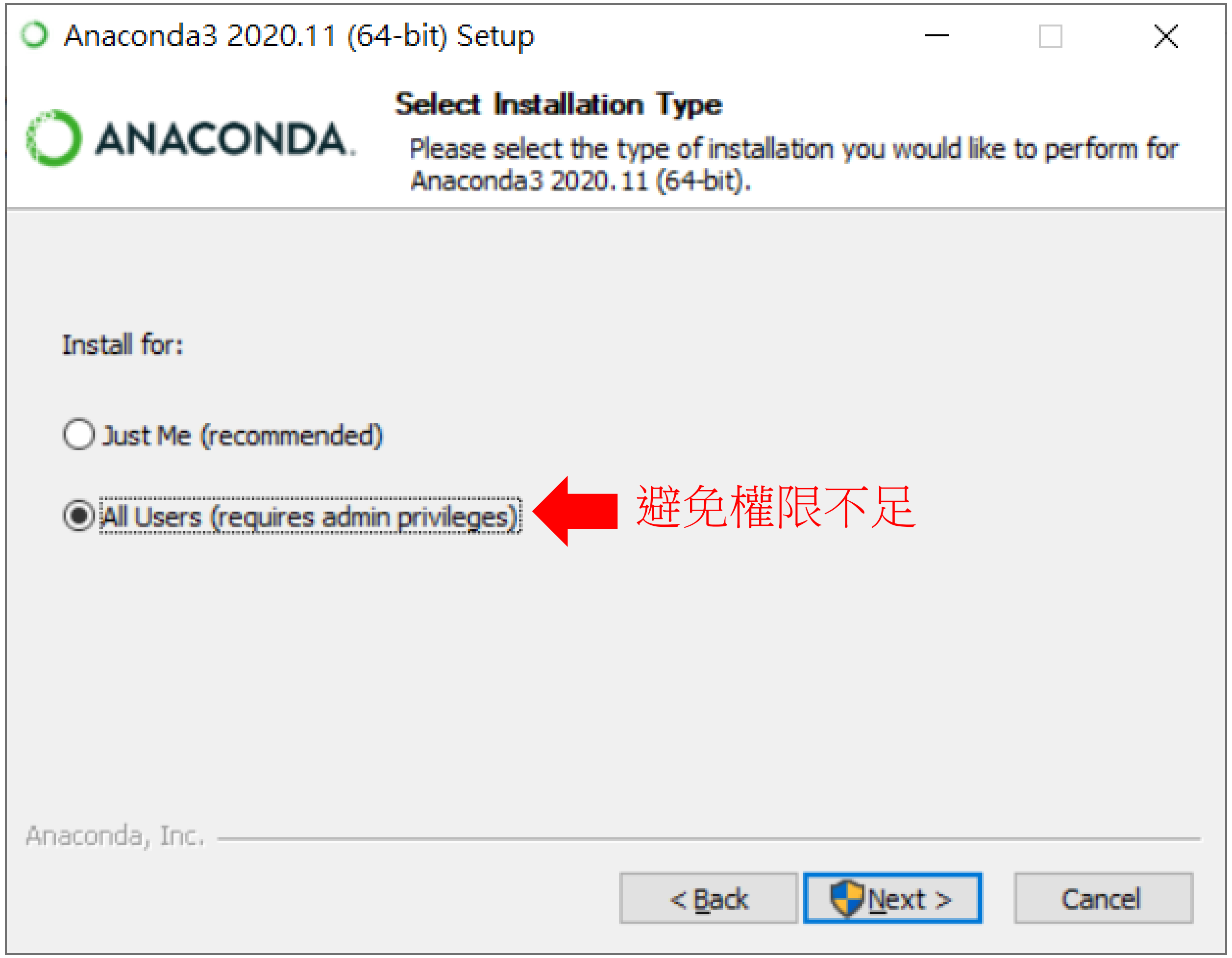
macOS installers

macOS

Python version	Name	Size	SHA256 hash
Python 3.9	Miniconda3 macOS 64-bit bash	55.2 MiB	7717253055e7c09339cd3d0815a0b1986b9138dcfcb8ec33b9733df32dd40eaa
	Miniconda3 macOS 64-bit pkg	61.9 MiB	d3e63d7e8aa3ffb7b095e0b984db47309bb1cb1ec2138f5e6a96a34173671451
Python 3.8	Miniconda3 macOS 64-bit bash	55.7 MiB	e13a4590879638197b0c506768438406b07de614911610e314f8c78133915b1c


管理
下載
檔案
常用
共用
檢視
應用程式工具
釘選到 [快速存取]
複製
貼上
剪下
複製路徑
貼上捷徑
剪貼簿
移至
複製到
刪除
重新命名
組合管理
新增資料夾
新增項目
輕鬆存取
新增
內容
開啟
編輯
歷程記錄
開啟
全選
全部不選
反向選擇
選取
本機 › 下載
名稱
修改日期
類型
大小
快速存取
桌面
下載
文件
圖片
OneDrive
本機
網路
今天 (2)
Anaconda3-2020.11-Windows-x86_64
468,161 KB
Miniconda3-latest-Windows-x86_64
58,400 KB
開啟(O)
以系統管理員身分執行(A)
使用 Skype 分享
疑難排解相容性(Y)
釘選到開始畫面(P)
7-Zip
CRC SHA
使用 Windows Defender 掃描...
分享
授與存取權給(G)
釘選到工作列(K)
還原舊版(V)
傳送到(N)
剪下(T)
複製(C)
建立捷徑(S)
刪除(D)
重新命名(M)
內容(R)
2 個項目
已選取 1 個項目 457 MB

避免權限不足



Anaconda3 2020.11 (64-bit) Setup

ANACONDA.

Select Installation Type

Please select the type of installation you would like to perform for Anaconda3 2020.11 (64-bit).

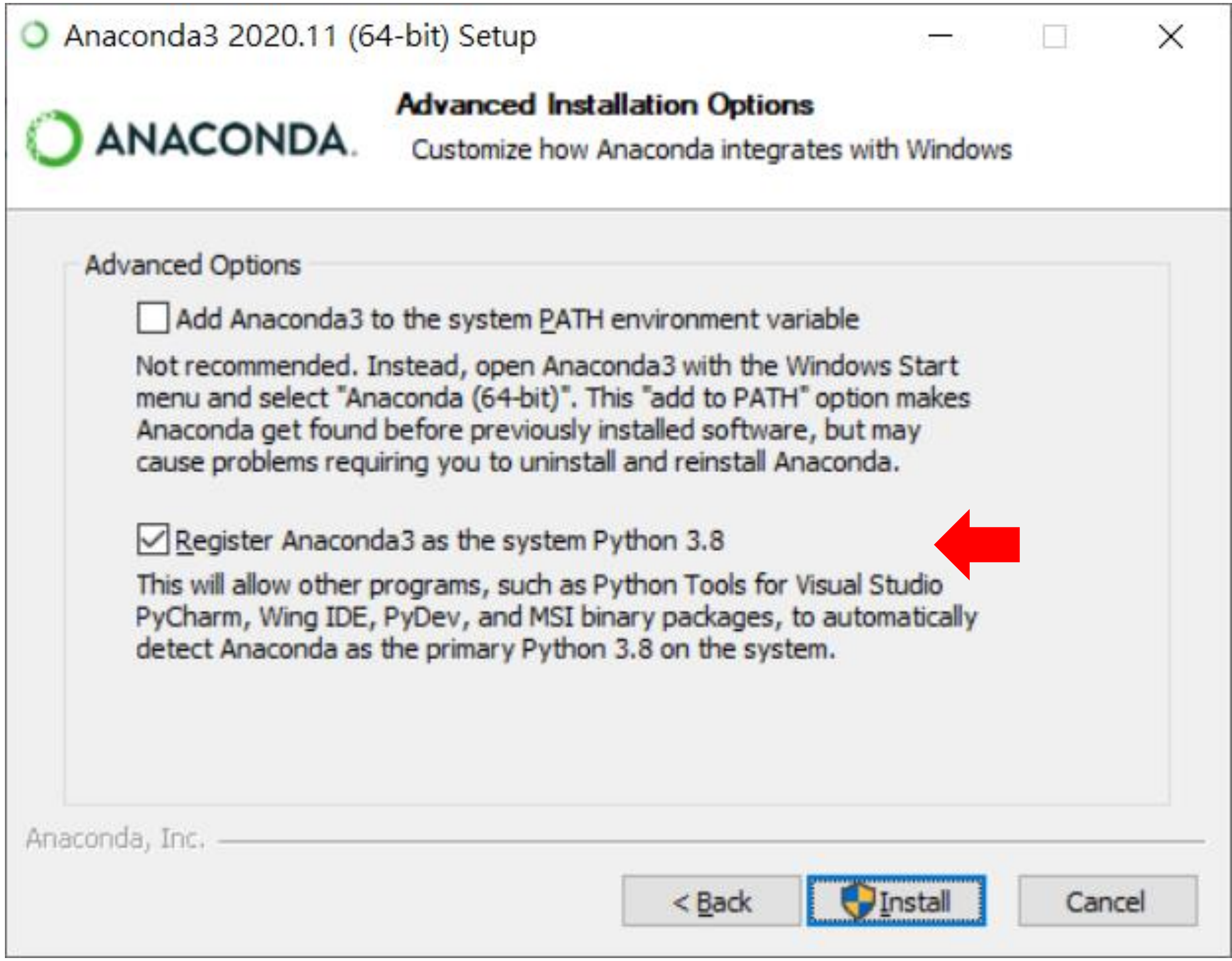
Install for:

○ Just Me (recommended)

● All Users (requires admin privileges)

避免權限不足

Anaconda, Inc.



Anaconda3 2020.11 (64-bit) Setup

ANACONDA.

Advanced Installation Options

Customize how Anaconda integrates with Windows

Advanced Options

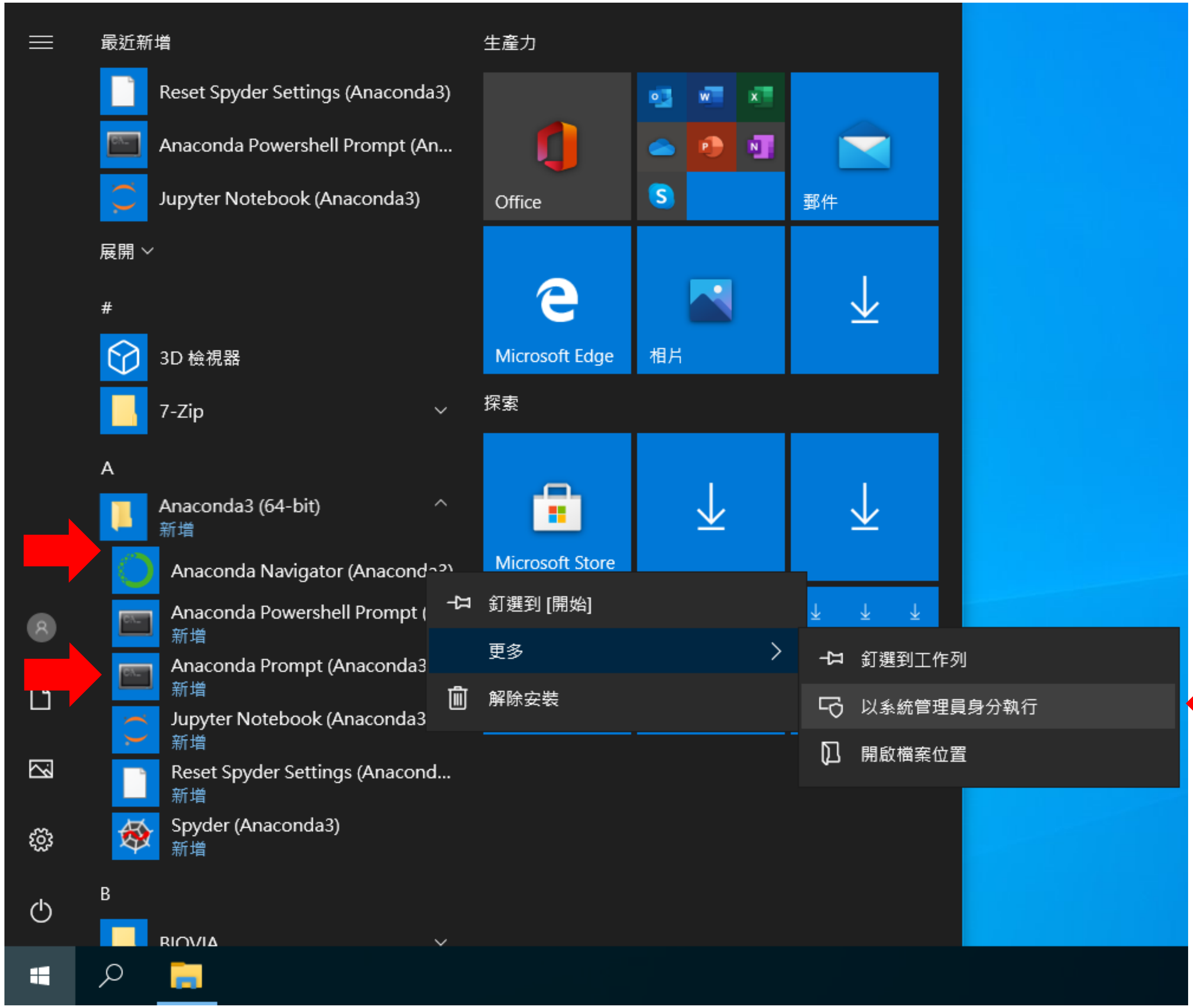
□ Add Anaconda3 to the system PATH environment variable

Not recommended. Instead, open Anaconda3 with the Windows Start menu and select "Anaconda (64-bit)". This "add to PATH" option makes Anaconda get found before previously installed software, but may cause problems requiring you to uninstall and reinstall Anaconda.

☑ Register Anaconda3 as the system Python 3.8

This will allow other programs, such as Python Tools for Visual Studio PyCharm, Wing IDE, PyDev, and MSI binary packages, to automatically detect Anaconda as the primary Python 3.8 on the system.

Anaconda, Inc.


最近新增
Reset Spyder Settings (Anaconda3)
Anaconda Powershell Prompt (An...
Jupyter Notebook (Anaconda3)
展開
#
3D 檢視器
7-Zip
A
Anaconda3 (64-bit)
新增
Anaconda Navigator (Anaconda3)
Anaconda Powershell Prompt (
新增
Anaconda Prompt (Anaconda3
新增
Jupyter Notebook (Anaconda3
新增
Reset Spyder Settings (Anacond...
新增
Spyder (Anaconda3)
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B
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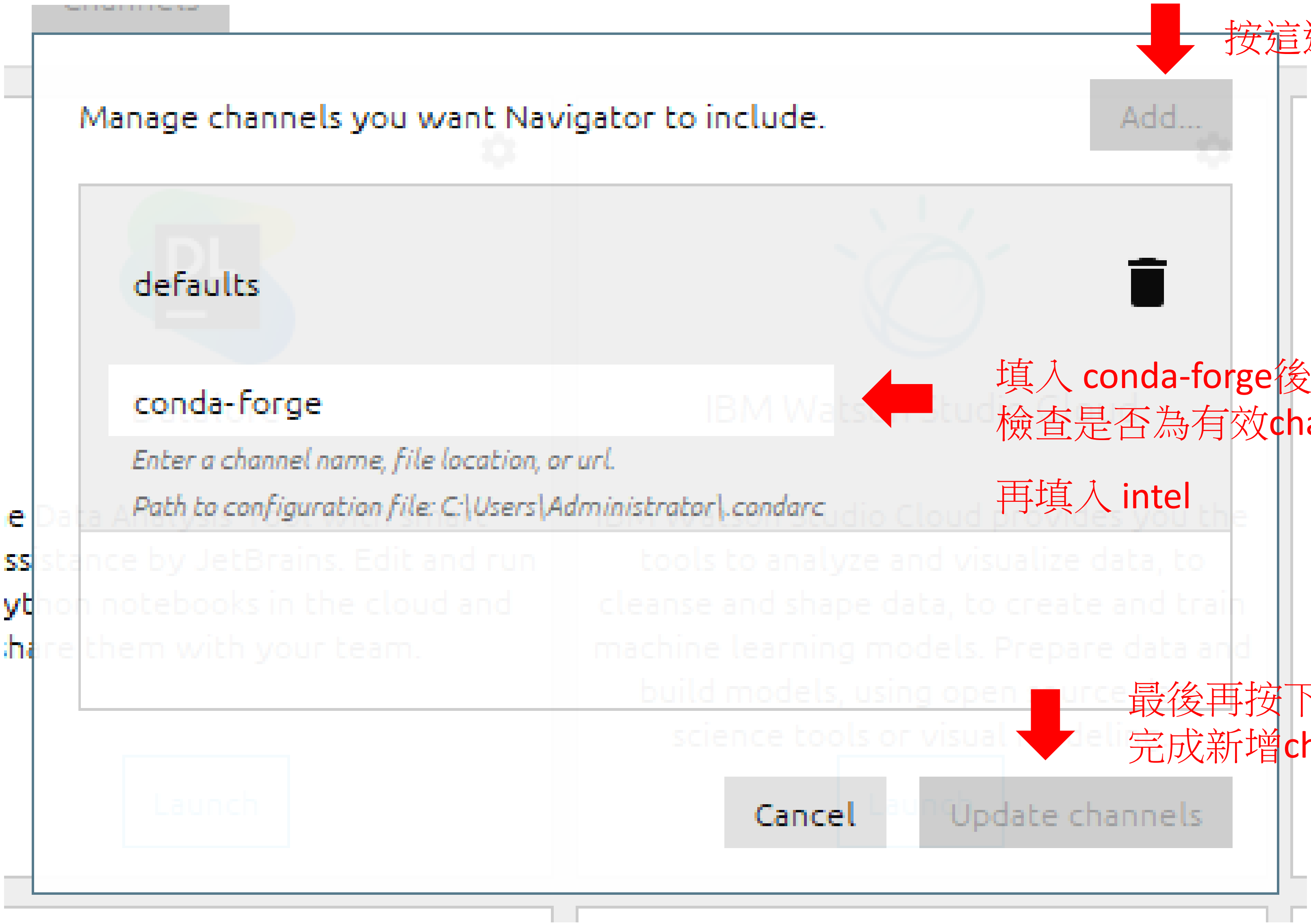
郵件
Microsoft Edge
相片
探索
Microsoft Store
釘選到 [開始]
更多
解除安裝
釘選到工作列
以系統管理員身分執行
開啟檔案位置

GUI

CLI

避免權限不足



Manage channels you want Navigator to include.

defaults

conda-forge

Enter a channel name, file location, or url.

Path to configuration file: C:\Users\Administrator\.condarc

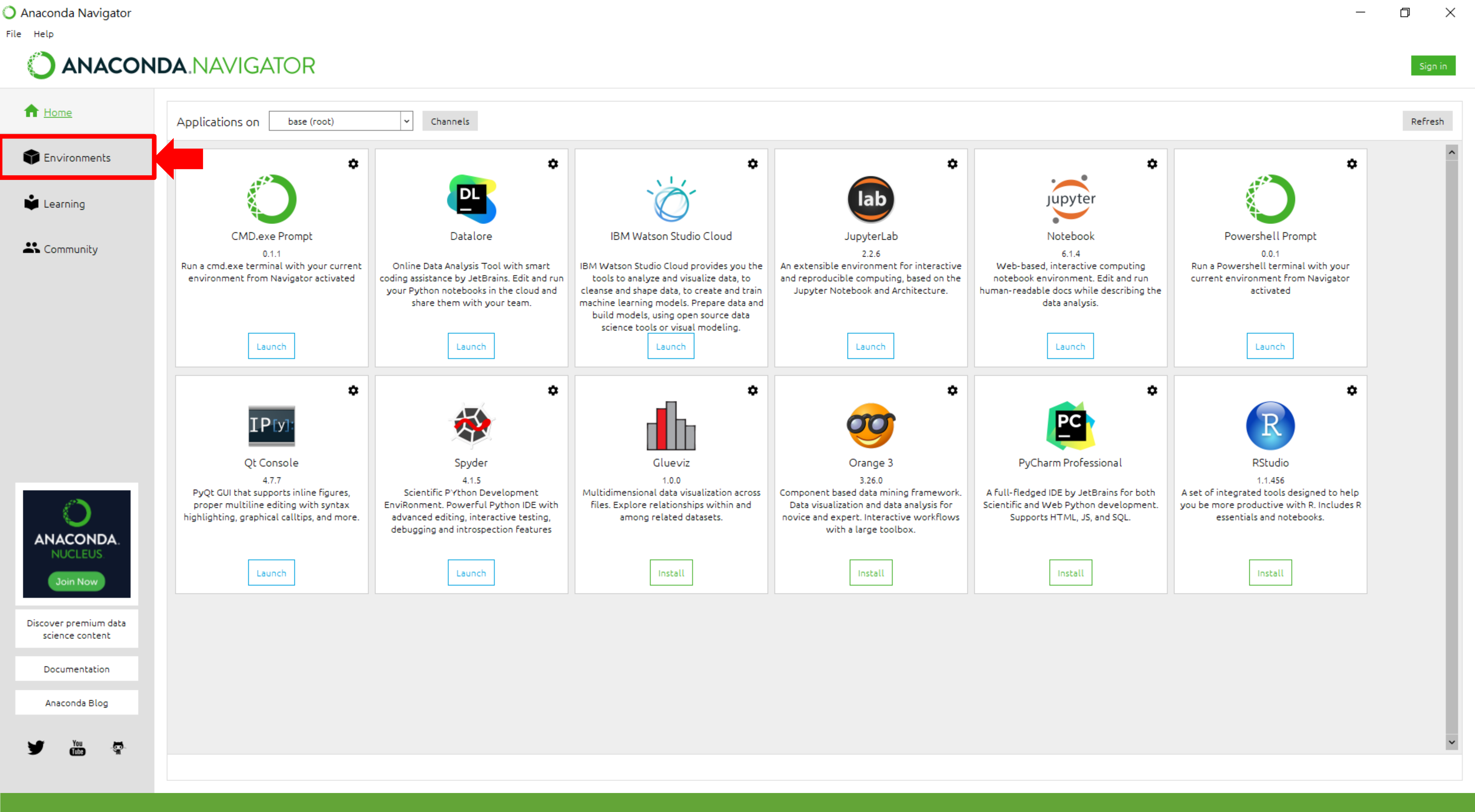
按這邊新增channel

填入 conda-forge後，按下ENTER會執行檢查是否為有效channel

再填入 intel

最後再按下Update channels，完成新增channel

```
conda config --add channels conda-forge
```



CMD.exe Prompt
0.1.1
Run a cmd.exe terminal with your current environment from Navigator activated

Datalore
Online Data Analysis Tool with smart coding assistance by JetBrains. Edit and run your Python notebooks in the cloud and share them with your team.

IBM Watson Studio Cloud
IBM Watson Studio Cloud provides you the tools to analyze and visualize data, to cleanse and shape data, to create and train machine learning models. Prepare data and build models, using open source data science tools or visual modeling.

JupyterLab
2.2.6
An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Architecture.

Notebook
6.1.4
Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.

Powershell Prompt
0.0.1
Run a Powershell terminal with your current environment from Navigator activated

Qt Console
4.7.7
PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.

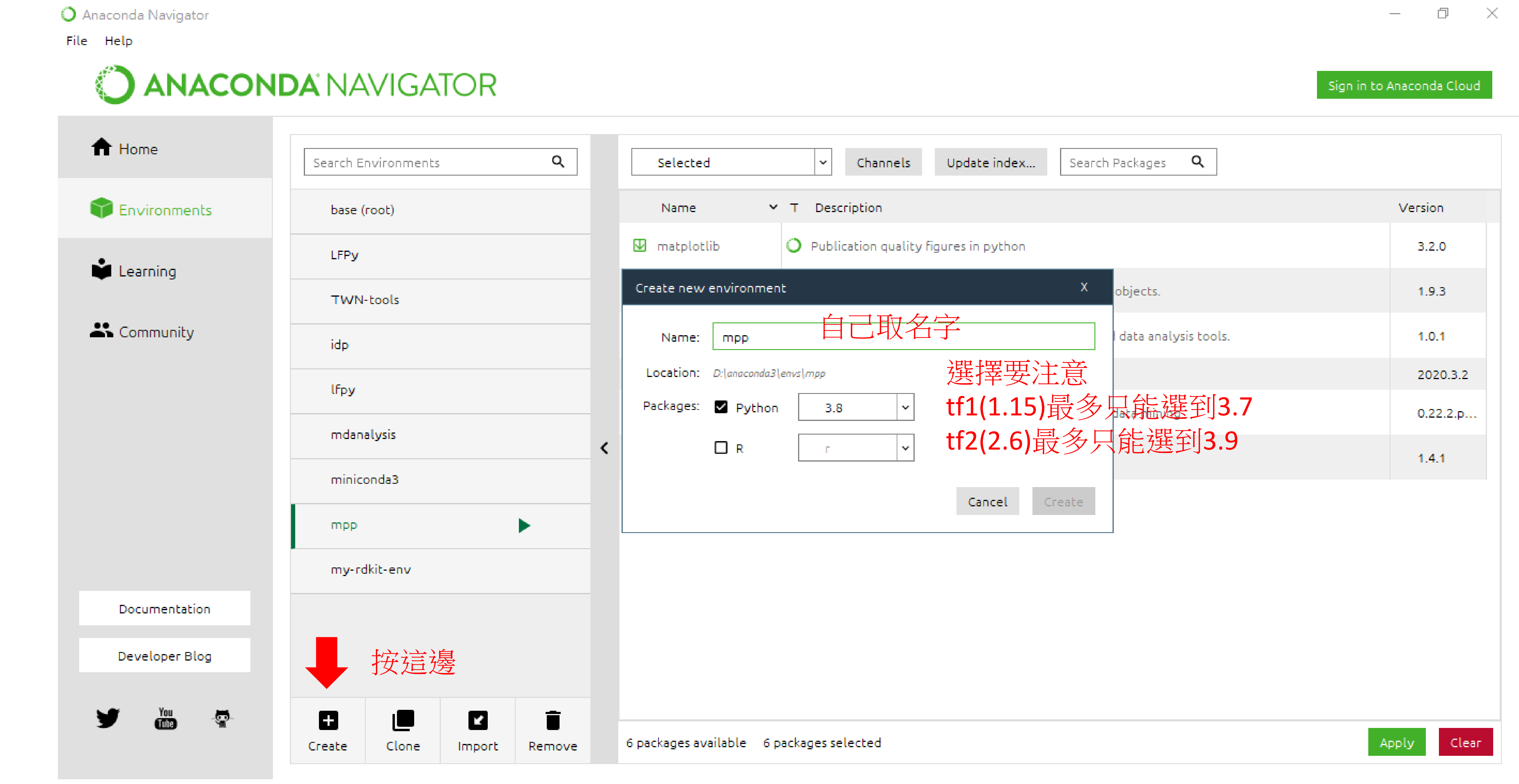
Spyder
4.1.5
Scientific PYthon Development EnviRonment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features

Glueviz
1.0.0
Multidimensional data visualization across files. Explore relationships within and among related datasets.

Orange 3
3.26.0
Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.

PyCharm Professional
A full-fledged IDE by JetBrains for both Scientific and Web Python development. Supports HTML, JS, and SQL.

RStudio
1.1.456
A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.



Create new environment

Name: mpp

Location: D:\anaconda3\envs\mpp

Packages: ☑ Python 3.8

□ R r

Cancel Create

自己取名字

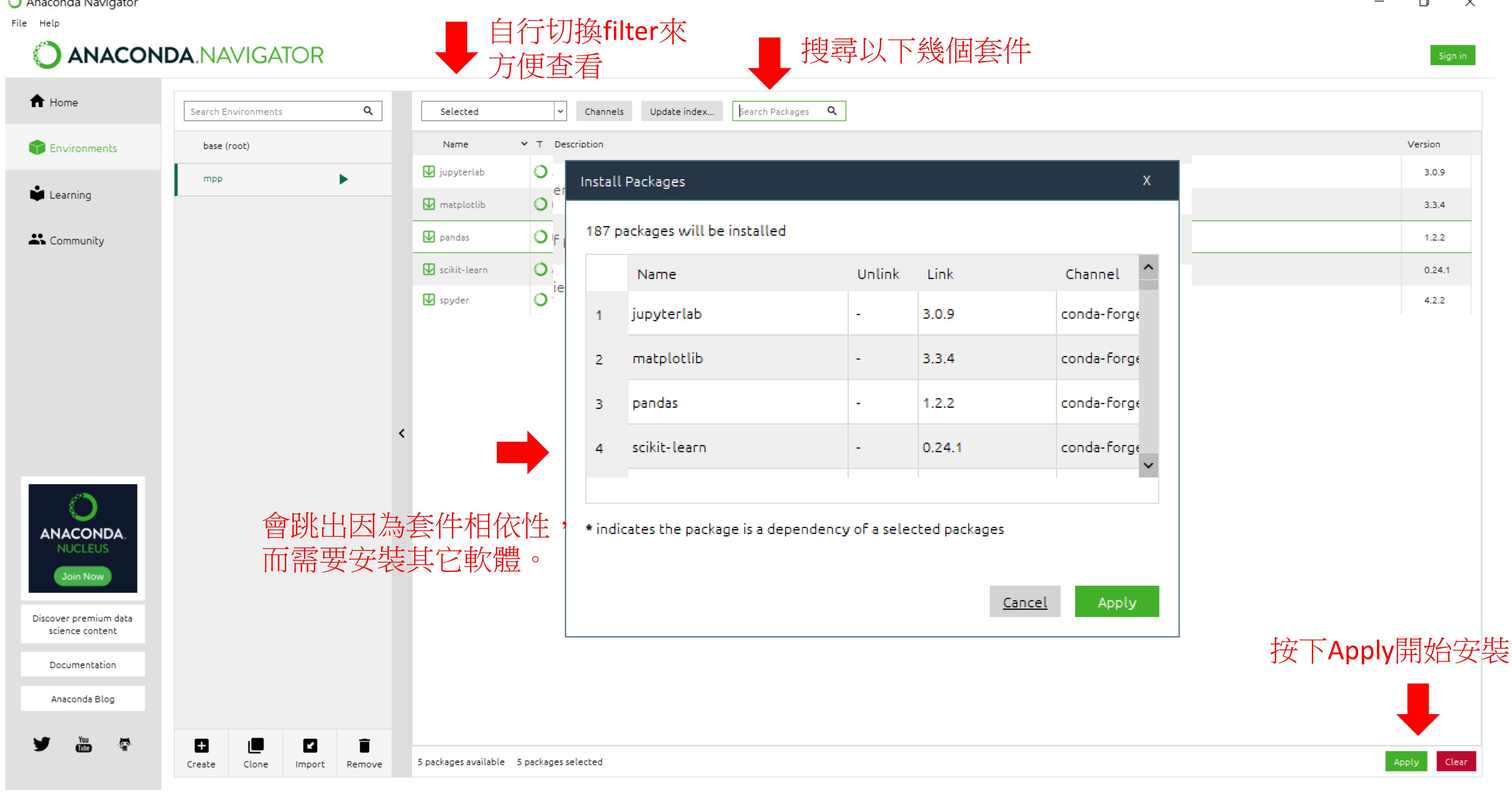
選擇要注意

tf1(1.15)最多只能選到3.7

tf2(2.6)最多只能選到3.9

按這邊

```
conda create --name mpp python=3.8
```



自行切換filter來方便查看

搜尋以下幾個套件

Name	Version
☑ jupyterlab	3.0.9
☑ matplotlib	3.3.4
☑ pandas	1.2.2
☑ scikit-learn	0.24.1
☑ spyder	4.2.2

Install Packages X

187 packages will be installed

	Name	Unlink	Link	Channel
1	jupyterlab	-	3.0.9	conda-forge
2	matplotlib	-	3.3.4	conda-forge
3	pandas	-	1.2.2	conda-forge
4	scikit-learn	-	0.24.1	conda-forge

* indicates the package is a dependency of a selected packages

Cancel Apply

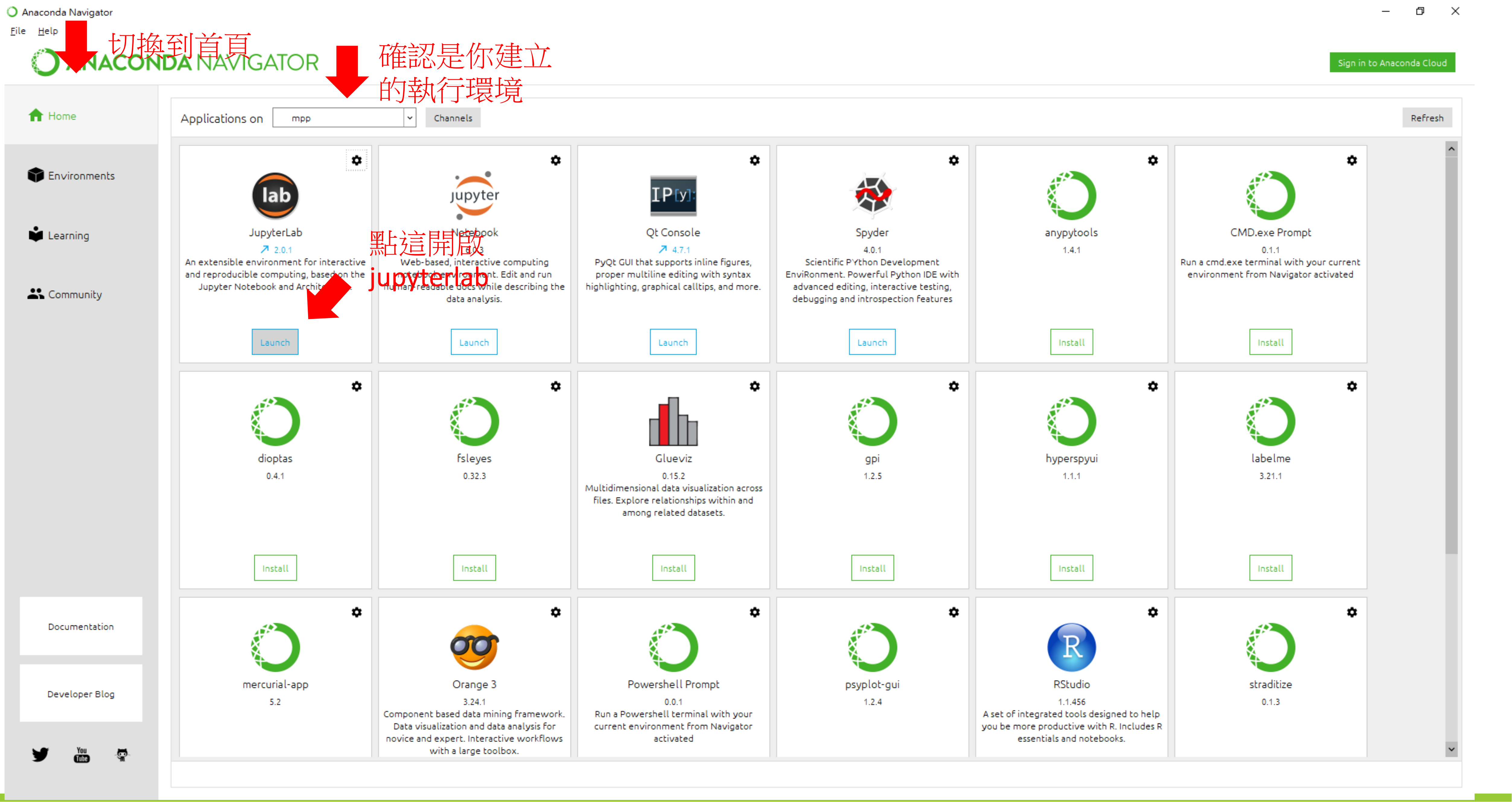
會跳出因為套件相依性，而需要安裝其它軟體。

按下Apply開始安裝

5 packages available 5 packages selected

Apply Clear

```
conda run -n mpp conda install jupyterlab matplotlib pandas scikit-learn spyder tensorflow
```



切換到首頁

確認是你建立的執行環境

點這開啟jupyterlab

Applications on mpp

JupyterLab
2.0.1
An extensible environment for interactive and reproducible computing, based on the Jupyter Notebook and Archit

Notebook
Web-based, interactive computing notebook environment. Edit and run human-readable docs while describing the data analysis.

Qt Console
4.7.1
PyQt GUI that supports inline figures, proper multiline editing with syntax highlighting, graphical calltips, and more.

Spyder
4.0.1
Scientific PYthon Development EnviRonment. Powerful Python IDE with advanced editing, interactive testing, debugging and introspection features

anypytools
1.4.1

CMD.exe Prompt
0.1.1
Run a cmd.exe terminal with your current environment from Navigator activated

dioptas
0.4.1

fsleyes
0.32.3

Glueviz
0.15.2
Multidimensional data visualization across files. Explore relationships within and among related datasets.

gpi
1.2.5

hyperspyui
1.1.1

labelme
3.21.1

mercurial-app
5.2

Orange 3
3.24.1
Component based data mining framework. Data visualization and data analysis for novice and expert. Interactive workflows with a large toolbox.

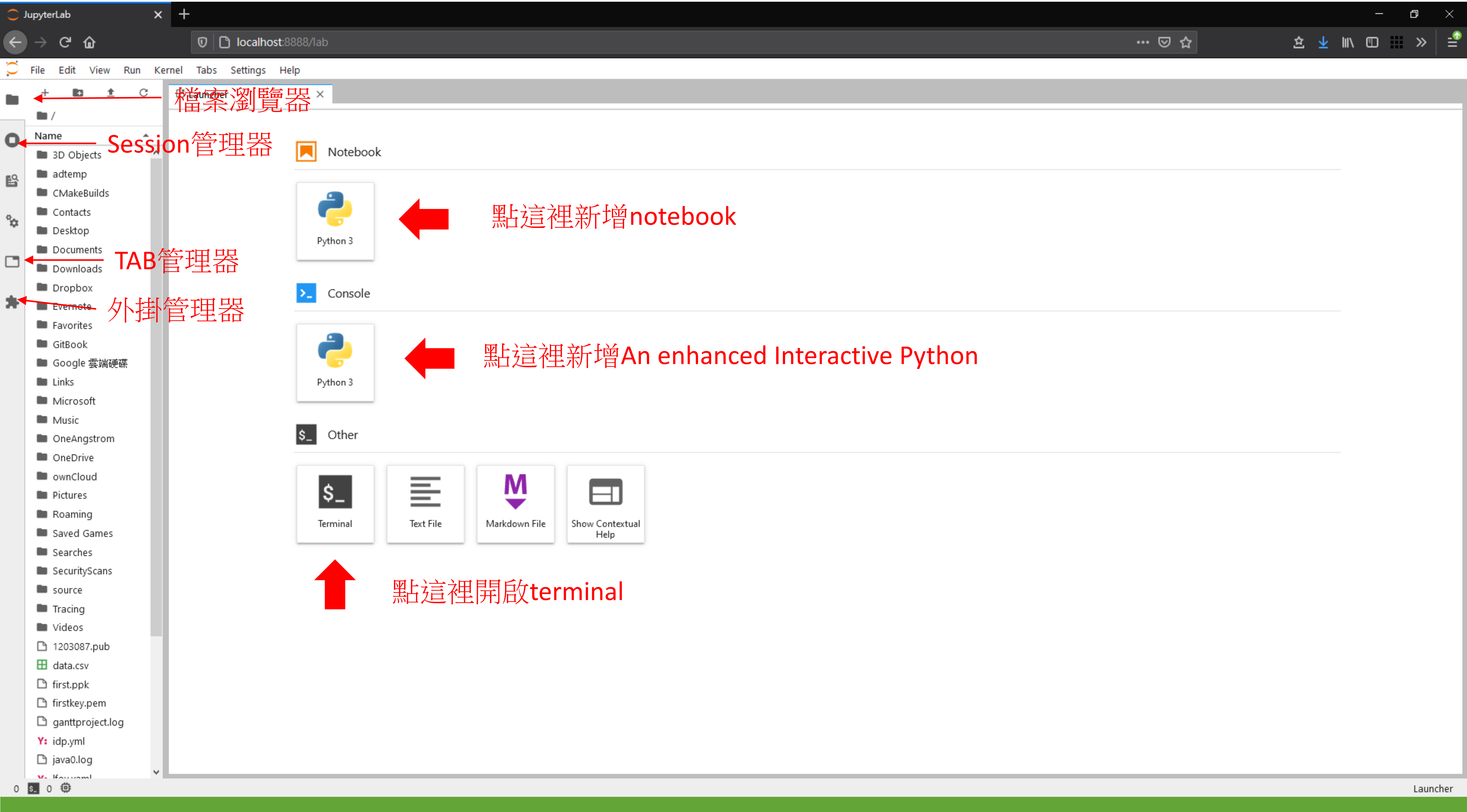
Powershell Prompt
0.0.1
Run a Powershell terminal with your current environment from Navigator activated

psyplot-gui
1.2.4

RStudio
1.1.456
A set of integrated tools designed to help you be more productive with R. Includes R essentials and notebooks.

straditize
0.1.3

```
conda run -n mpp jupyter lab
```



檔案瀏覽器

Session管理器

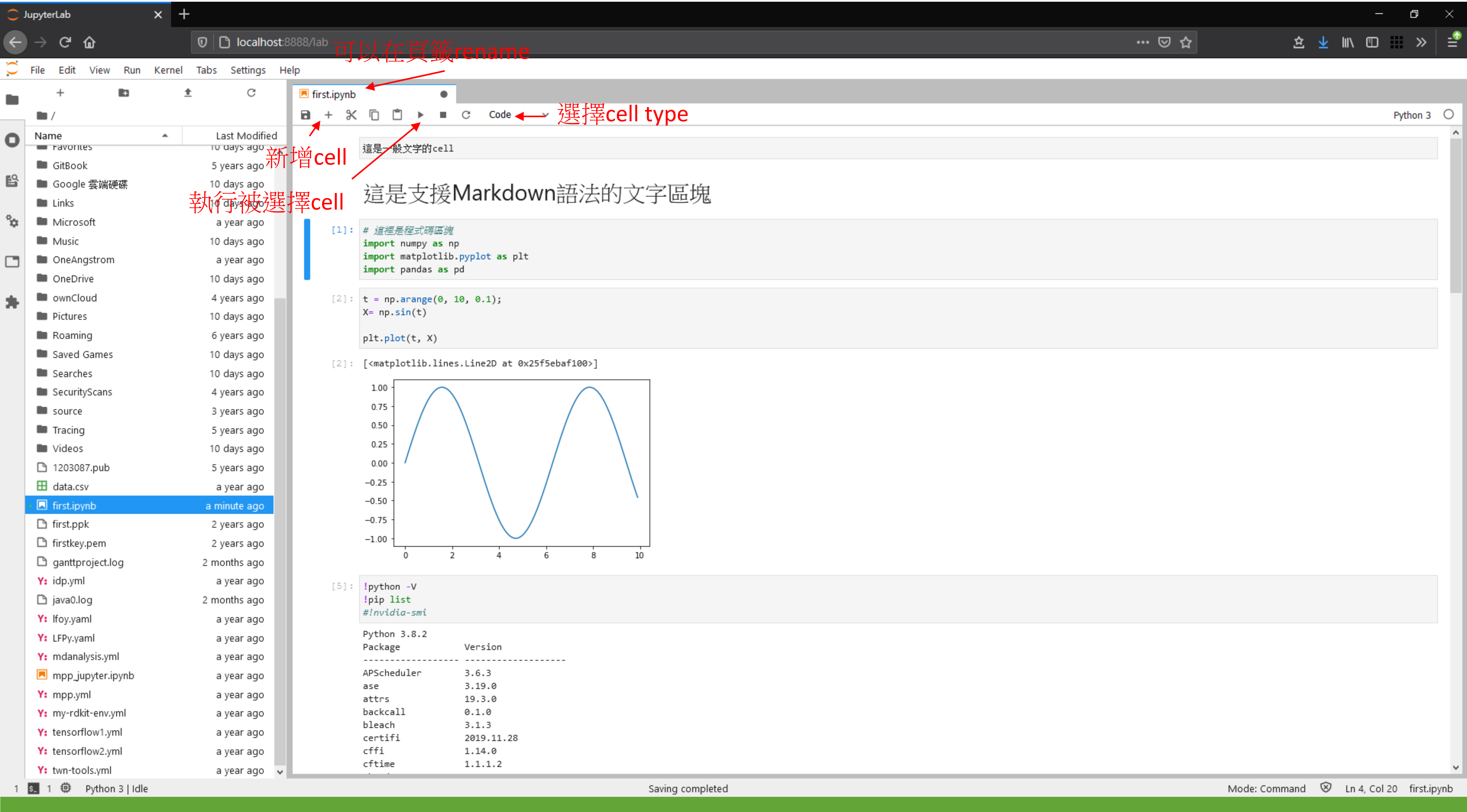
TAB管理器

外掛管理器

點這裡新增notebook

點這裡新增An enhanced Interactive Python

點這裡開啟terminal



可以在頁籤rename

選擇cell type

新增cell

執行被選擇cell

Name	Last Modified
Favorites	10 days ago
GitBook	5 years ago
Google 雲端硬碟	10 days ago
Links	10 days ago
Microsoft	a year ago
Music	10 days ago
OneAngstrom	a year ago
OneDrive	10 days ago
ownCloud	4 years ago
Pictures	10 days ago
Roaming	6 years ago
Saved Games	10 days ago
Searches	10 days ago
SecurityScans	4 years ago
source	3 years ago
Tracing	5 years ago
Videos	10 days ago
1203087.pub	5 years ago
data.csv	a year ago
first.ipynb	a minute ago
first.ppk	2 years ago
firstkey.pem	2 years ago
ganttproject.log	2 months ago
idp.yml	a year ago
java0.log	2 months ago
lfoy.yaml	a year ago
LFPy.yaml	a year ago
mdanalysis.yml	a year ago
mpp_jupyter.ipynb	a year ago
mpp.yml	a year ago
my-rdkit-env.yml	a year ago
tensorflow1.yml	a year ago
tensorflow2.yml	a year ago
twn-tools.yml	a year ago

```
這是一般文字的cell
```

這是支援Markdown語法的文字區塊

```
[1]: # 這裡是程式碼區塊
     import numpy as np
     import matplotlib.pyplot as plt
     import pandas as pd
```

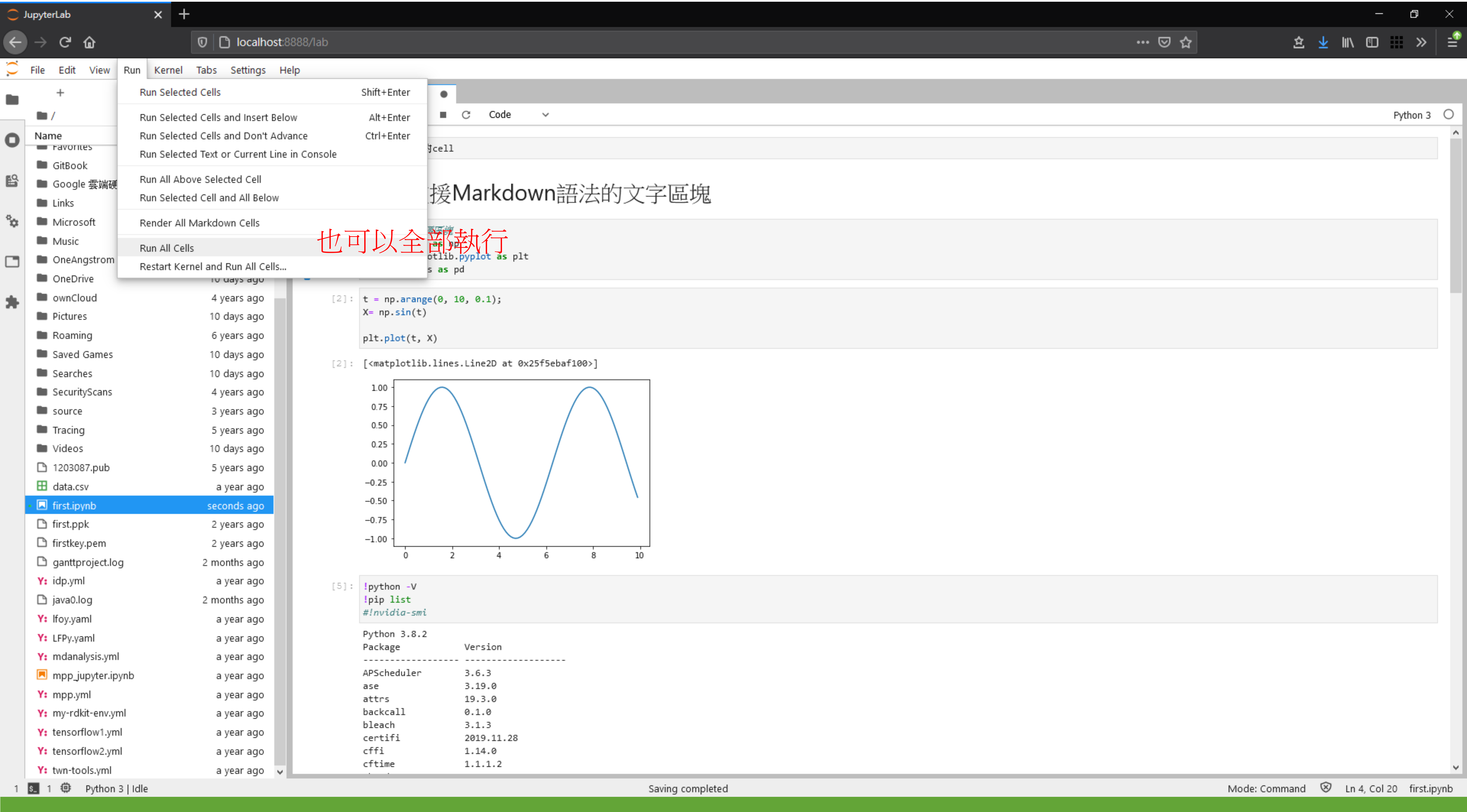
```
[2]: t = np.arange(0, 10, 0.1);
     X= np.sin(t)

     plt.plot(t, X)
```

```
[2]: [<matplotlib.lines.Line2D at 0x25f5ebaf100>]
```

```
[5]: !python -V
     !pip list
     #!nvidia-smi
```

```
Python 3.8.2
Package            Version
------------------ -------------------
APScheduler        3.6.3
ase                3.19.0
attrs              19.3.0
backcall           0.1.0
bleach             3.1.3
certifi            2019.11.28
cffi               1.14.0
cftime             1.1.1.2
```


JupyterLab
localhost:8888/lab
File
Edit
View
Run
Kernel
Tabs
Settings
Help
Run Selected Cells Shift+Enter
Run Selected Cells and Insert Below Alt+Enter
Run Selected Cells and Don't Advance Ctrl+Enter
Run Selected Text or Current Line in Console
Run All Above Selected Cell
Run Selected Cell and All Below
Render All Markdown Cells
Run All Cells
Restart Kernel and Run All Cells...
Code
Python 3

也可以全部執行

Name	
Favorites	
GitBook	
Google 雲端硬	
Links	
Microsoft	
Music	
OneAngstrom	
OneDrive	10 days ago
ownCloud	4 years ago
Pictures	10 days ago
Roaming	6 years ago
Saved Games	10 days ago
Searches	10 days ago
SecurityScans	4 years ago
source	3 years ago
Tracing	5 years ago
Videos	10 days ago
1203087.pub	5 years ago
data.csv	a year ago
first.ipynb	seconds ago
first.ppk	2 years ago
firstkey.pem	2 years ago
ganttproject.log	2 months ago
idp.yml	a year ago
java0.log	2 months ago
lfoy.yaml	a year ago
LFPy.yaml	a year ago
mdanalysis.yml	a year ago
mpp_jupyter.ipynb	a year ago
mpp.yml	a year ago
my-rdkit-env.yml	a year ago
tensorflow1.yml	a year ago
tensorflow2.yml	a year ago
twn-tools.yml	a year ago

```
cell
```

援Markdown語法的文字區塊

```
 as np
otlib.pyplot as plt
s as pd
```

```
[2]: t = np.arange(0, 10, 0.1);
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```

```
[2]: [<matplotlib.lines.Line2D at 0x25f5ebaf100>]
```

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[5]: !python -V
     !pip list
     #!nvidia-smi
```

```
Python 3.8.2
Package            Version
------------------ -------------------
APScheduler        3.6.3
ase                3.19.0
attrs              19.3.0
backcall           0.1.0
bleach             3.1.3
certifi            2019.11.28
cffi               1.14.0
cftime             1.1.1.2
```

動手試做一下

下載google tensorflow 2官網教學檔案，實際在jupyterlab執行一遍。

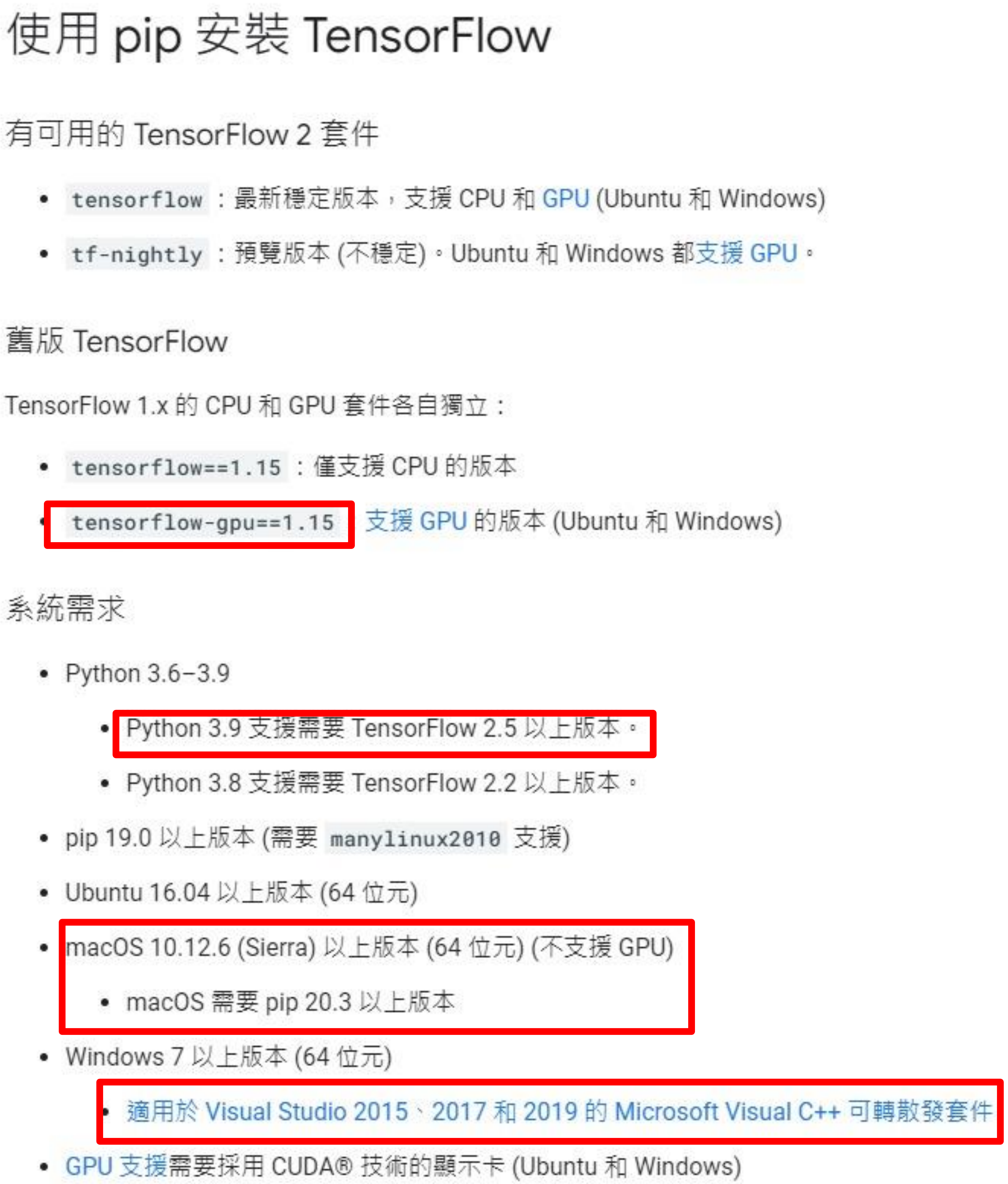
https://storage.googleapis.com/tensorflow_docs/docs/site/en/tutorials/quickstart/beginner.ipynb

可能問題解法

1. jupyterlab不支援舊版EDGE、IE。

2. tensorflow2 WINDOWS版需要Visual Studio 2015、2017 和 2019 最新支援的 Visual C++ 可轉散發套件，但是Anaconda無法提供(這是微軟的授權軟體)。

https://support.microsoft.com/zh-tw/topic/%E6%9C%80%E6%96%B0%E6%94%AF%E6%8F%B4%E7%9A%84-visual-c-%E4%B8%8B%E8%BC%89-2647da03-1eea-4433-9aff-95f26a218cc0



使用 pip 安裝 TensorFlow

有可用的 TensorFlow 2 套件

- `tensorflow`：最新穩定版本，支援 CPU 和 GPU (Ubuntu 和 Windows)
- `tf-nightly`：預覽版本 (不穩定)。Ubuntu 和 Windows 都支援 GPU。

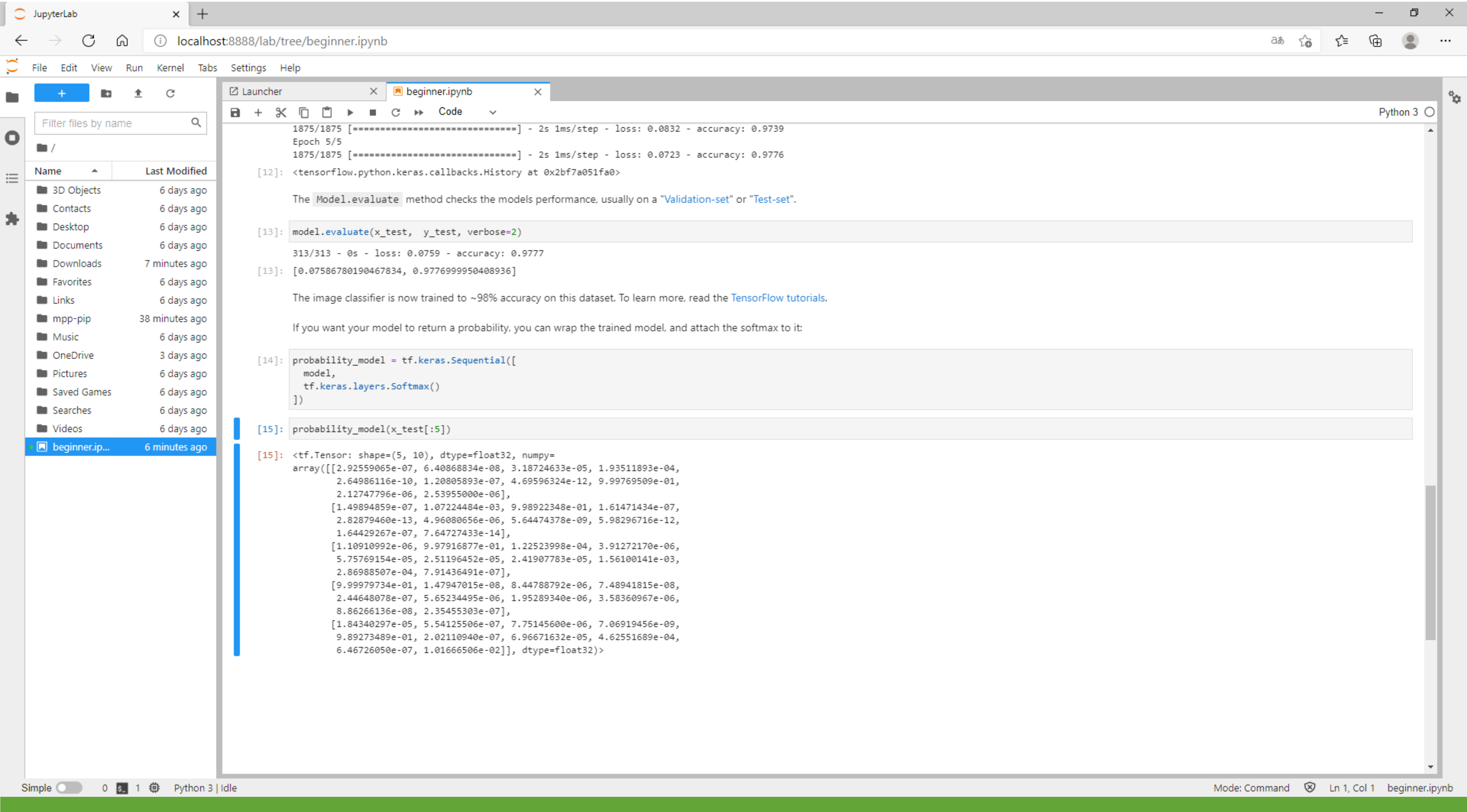
舊版 TensorFlow

TensorFlow 1.x 的 CPU 和 GPU 套件各自獨立：

- `tensorflow==1.15`：僅支援 CPU 的版本
- `tensorflow-gpu==1.15` 支援 GPU 的版本 (Ubuntu 和 Windows)

系統需求

- Python 3.6–3.9
  - Python 3.9 支援需要 TensorFlow 2.5 以上版本。
  - Python 3.8 支援需要 TensorFlow 2.2 以上版本。
- pip 19.0 以上版本 (需要 `manylinux2010` 支援)
- Ubuntu 16.04 以上版本 (64 位元)
- macOS 10.12.6 (Sierra) 以上版本 (64 位元) (不支援 GPU)
  - macOS 需要 pip 20.3 以上版本
- Windows 7 以上版本 (64 位元)
  - 適用於 Visual Studio 2015、2017 和 2019 的 Microsoft Visual C++ 可轉散發套件
- GPU 支援需要採用 CUDA® 技術的顯示卡 (Ubuntu 和 Windows)



Name	Last Modified
3D Objects	6 days ago
Contacts	6 days ago
Desktop	6 days ago
Documents	6 days ago
Downloads	7 minutes ago
Favorites	6 days ago
Links	6 days ago
mpp-pip	38 minutes ago
Music	6 days ago
OneDrive	3 days ago
Pictures	6 days ago
Saved Games	6 days ago
Searches	6 days ago
Videos	6 days ago
beginner.ip...	6 minutes ago

```
1875/1875 [==============================] - 2s 1ms/step - loss: 0.0832 - accuracy: 0.9739
Epoch 5/5
1875/1875 [==============================] - 2s 1ms/step - loss: 0.0723 - accuracy: 0.9776
```

```
[12]: <tensorflow.python.keras.callbacks.History at 0x2bf7a051fa0>
```

The `Model.evaluate` method checks the models performance, usually on a "Validation-set" or "Test-set".

```
[13]: model.evaluate(x_test,  y_test, verbose=2)
```

```
313/313 - 0s - loss: 0.0759 - accuracy: 0.9777
```

```
[13]: [0.07586780190467834, 0.9776999950408936]
```

The image classifier is now trained to ~98% accuracy on this dataset. To learn more, read the TensorFlow tutorials.

If you want your model to return a probability, you can wrap the trained model, and attach the softmax to it:

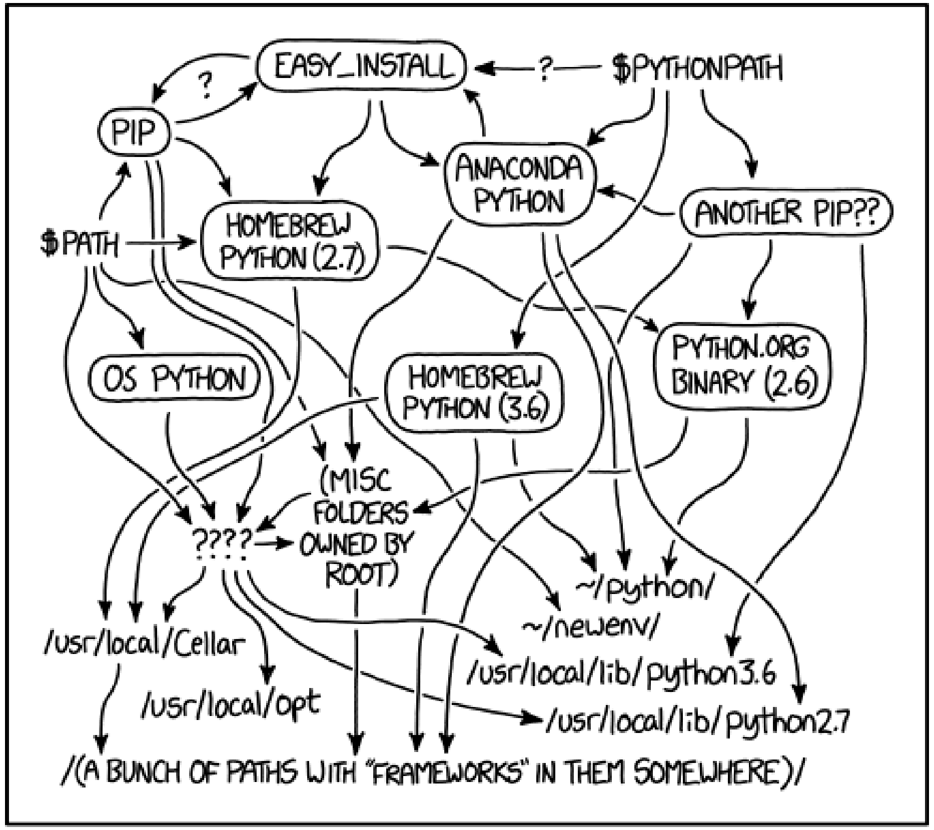
```
[14]: probability_model = tf.keras.Sequential([
        model,
        tf.keras.layers.Softmax()
      ])
```

```
[15]: probability_model(x_test[:5])
```

```
[15]: <tf.Tensor: shape=(5, 10), dtype=float32, numpy=
      array([[2.92559065e-07, 6.40868834e-08, 3.18724633e-05, 1.93511893e-04,
              2.64986116e-10, 1.20805893e-07, 4.69596324e-12, 9.99769509e-01,
              2.12747796e-06, 2.53955000e-06],
             [1.49894859e-07, 1.07224484e-03, 9.98922348e-01, 1.61471434e-07,
              2.82879460e-13, 4.96080656e-06, 5.64474378e-09, 5.98296716e-12,
              1.64429267e-07, 7.64727433e-14],
             [1.10910992e-06, 9.97916877e-01, 1.22523998e-04, 3.91272170e-06,
              5.75769154e-05, 2.51196452e-05, 2.41907783e-05, 1.56100141e-03,
              2.86988507e-04, 7.91436491e-07],
             [9.99979734e-01, 1.47947015e-08, 8.44788792e-06, 7.48941815e-08,
              2.44648078e-07, 5.65234495e-06, 1.95289340e-06, 3.58360967e-06,
              8.86266136e-08, 2.35455303e-07],
             [1.84340297e-05, 5.54125506e-07, 7.75145600e-06, 7.06919456e-09,
              9.89273489e-01, 2.02110940e-07, 6.96671632e-05, 4.62551689e-04,
              6.46726050e-07, 1.01666506e-02]], dtype=float32)>
```

Build your own Development Environment

Use python + pip + virtualenv



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

Windows

1. Download and install python.
2. Install virtualenv via pip
3. Activate virtualenv
4. Install package in virtualenv

Mac & Linux

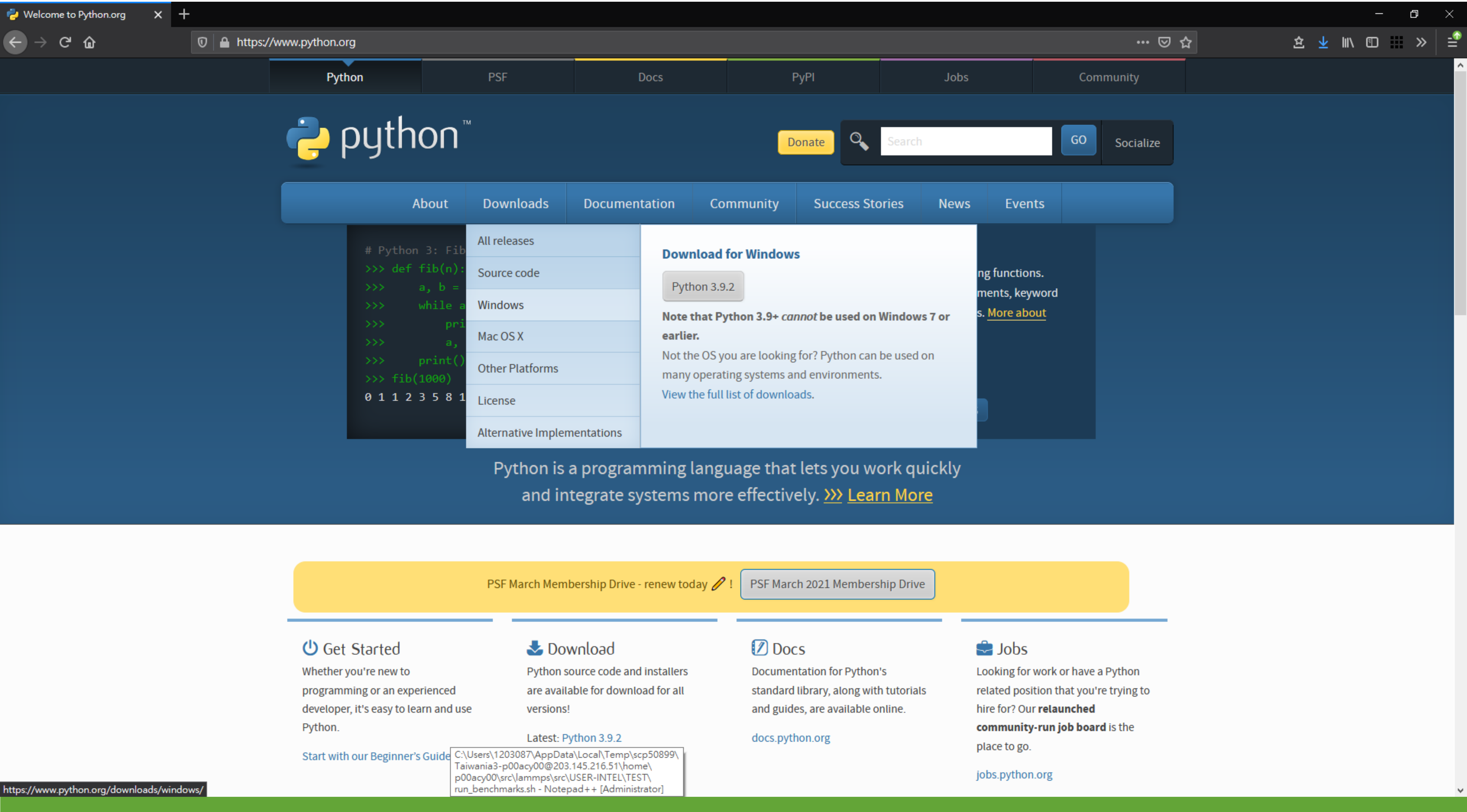
Don’t use system python

Don’t use system python

Don’t use system python

1. Download and compiler python.
2. Install virtualenv via pip
3. Activate virtualenv
4. Install package in virtualenv

courtesy of https://xkcd.com/1987/



```
# Python 3: Fib
>>> def fib(n):
>>>     a, b =
>>>     while a
>>>         pri
>>>         a,
>>>     print()
>>> fib(1000)
0 1 1 2 3 5 8 1
```

ng functions.
ments, keyword
s. More about

Download for Windows

Note that Python 3.9+ *cannot* be used on Windows 7 or earlier.

Not the OS you are looking for? Python can be used on many operating systems and environments.

View the full list of downloads.

Python is a programming language that lets you work quickly and integrate systems more effectively. >>> Learn More

PSF March Membership Drive - renew today ✎ !

Get Started

Whether you're new to programming or an experienced developer, it's easy to learn and use Python.

Start with our Beginner's Guide

Download

Python source code and installers are available for download for all versions!

Latest: Python 3.9.2

Docs

Documentation for Python's standard library, along with tutorials and guides, are available online.

docs.python.org

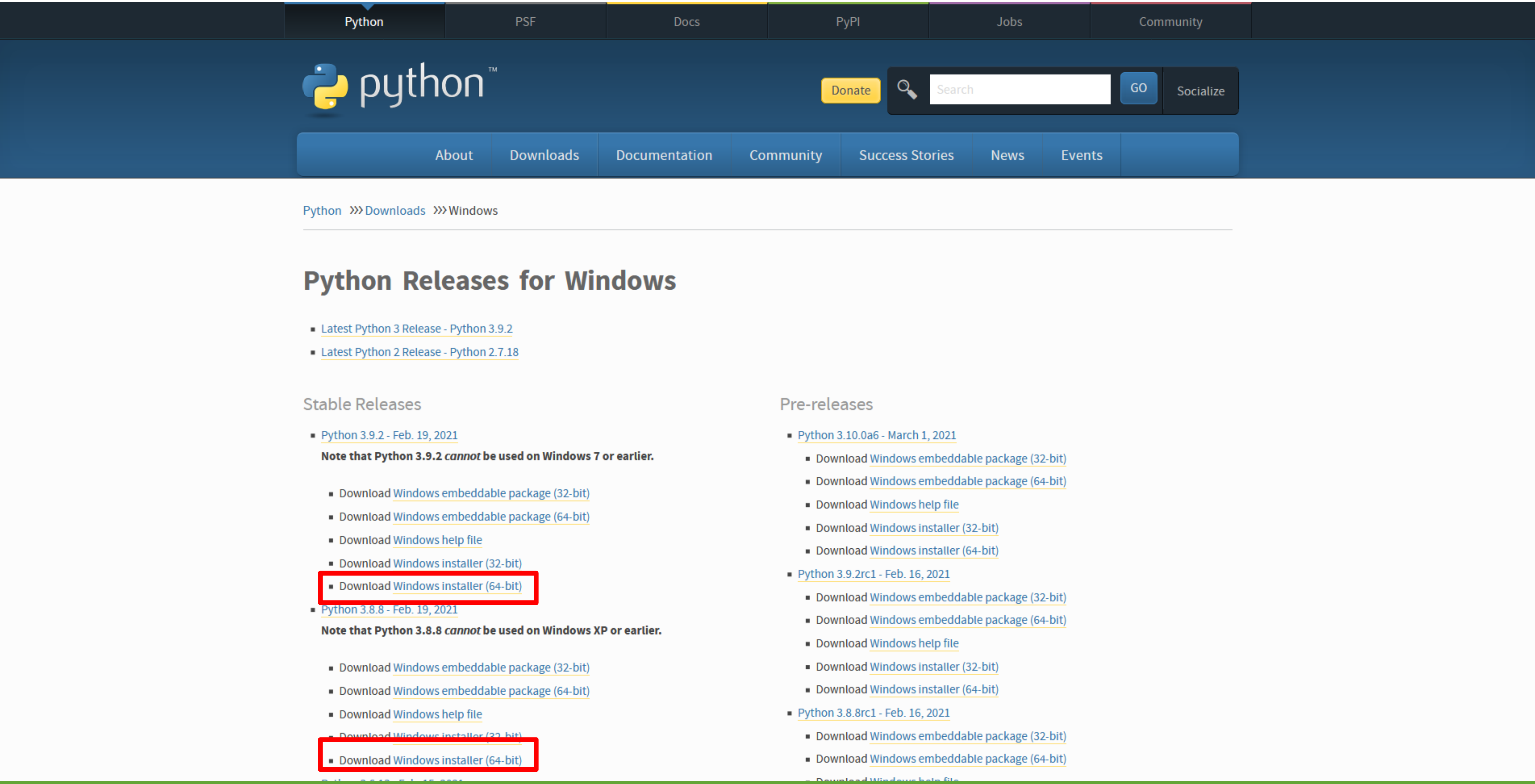
Jobs

Looking for work or have a Python related position that you're trying to hire for? Our **relaunched community-run job board** is the place to go.

jobs.python.org

C:\Users\1203087\AppData\Local\Temp\scp50899\Taiwania3-p00acy00@203.145.216.51\home\p00acy00\src\lammps\src\USER-INTEL\TEST\run_benchmarks.sh - Notepad++ [Administrator]

https://www.python.org/downloads/windows/



Python »» Downloads »» Windows

Python Releases for Windows

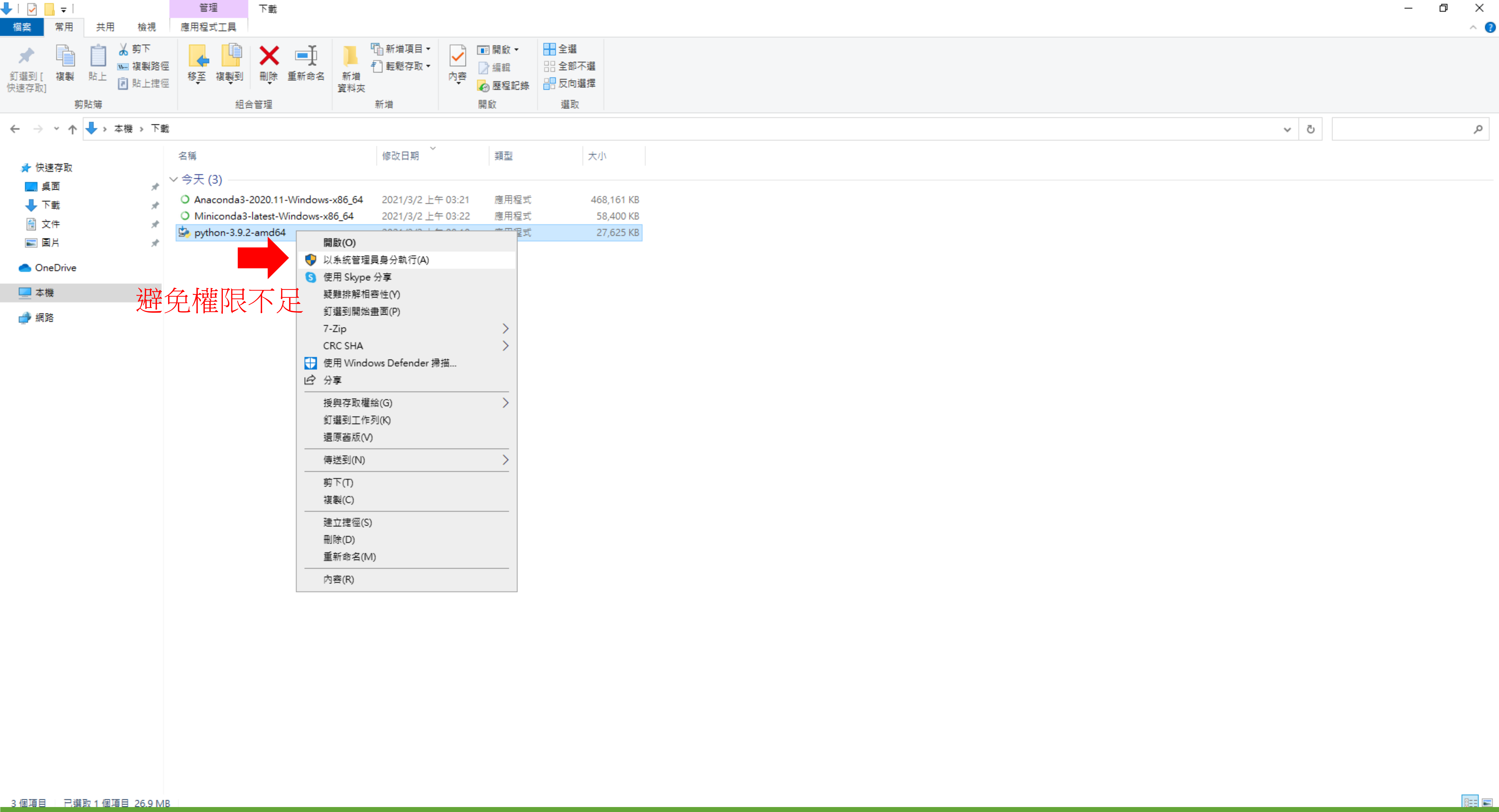
- Latest Python 3 Release - Python 3.9.2
- Latest Python 2 Release - Python 2.7.18

Stable Releases

- Python 3.9.2 - Feb. 19, 2021
  Note that Python 3.9.2 *cannot* be used on Windows 7 or earlier.
  - Download Windows embeddable package (32-bit)
  - Download Windows embeddable package (64-bit)
  - Download Windows help file
  - Download Windows installer (32-bit)
  - Download Windows installer (64-bit)
- Python 3.8.8 - Feb. 19, 2021
  Note that Python 3.8.8 *cannot* be used on Windows XP or earlier.
  - Download Windows embeddable package (32-bit)
  - Download Windows embeddable package (64-bit)
  - Download Windows help file
  - Download Windows installer (32-bit)
  - Download Windows installer (64-bit)
- Python 3.6.13 - Feb. 15, 2021

Pre-releases

- Python 3.10.0a6 - March 1, 2021
  - Download Windows embeddable package (32-bit)
  - Download Windows embeddable package (64-bit)
  - Download Windows help file
  - Download Windows installer (32-bit)
  - Download Windows installer (64-bit)
- Python 3.9.2rc1 - Feb. 16, 2021
  - Download Windows embeddable package (32-bit)
  - Download Windows embeddable package (64-bit)
  - Download Windows help file
  - Download Windows installer (32-bit)
  - Download Windows installer (64-bit)
- Python 3.8.8rc1 - Feb. 16, 2021
  - Download Windows embeddable package (32-bit)
  - Download Windows embeddable package (64-bit)
  - Download Windows help file

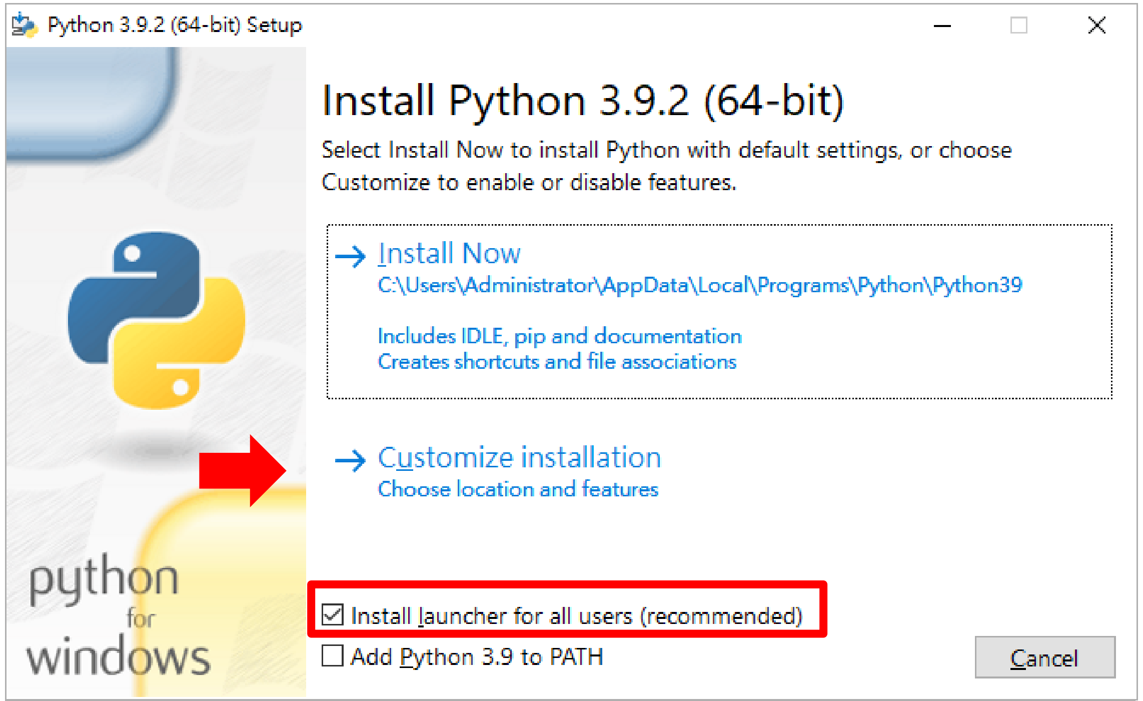


本機 › 下載

名稱	修改日期	類型	大小
Anaconda3-2020.11-Windows-x86_64	2021/3/2 上午 03:21	應用程式	468,161 KB
Miniconda3-latest-Windows-x86_64	2021/3/2 上午 03:22	應用程式	58,400 KB
python-3.9.2-amd64	[illegible]	應用程式	27,625 KB

避免權限不足

3 個項目　已選取 1 個項目 26.9 MB



Python 3.9.2 (64-bit) Setup

Install Python 3.9.2 (64-bit)

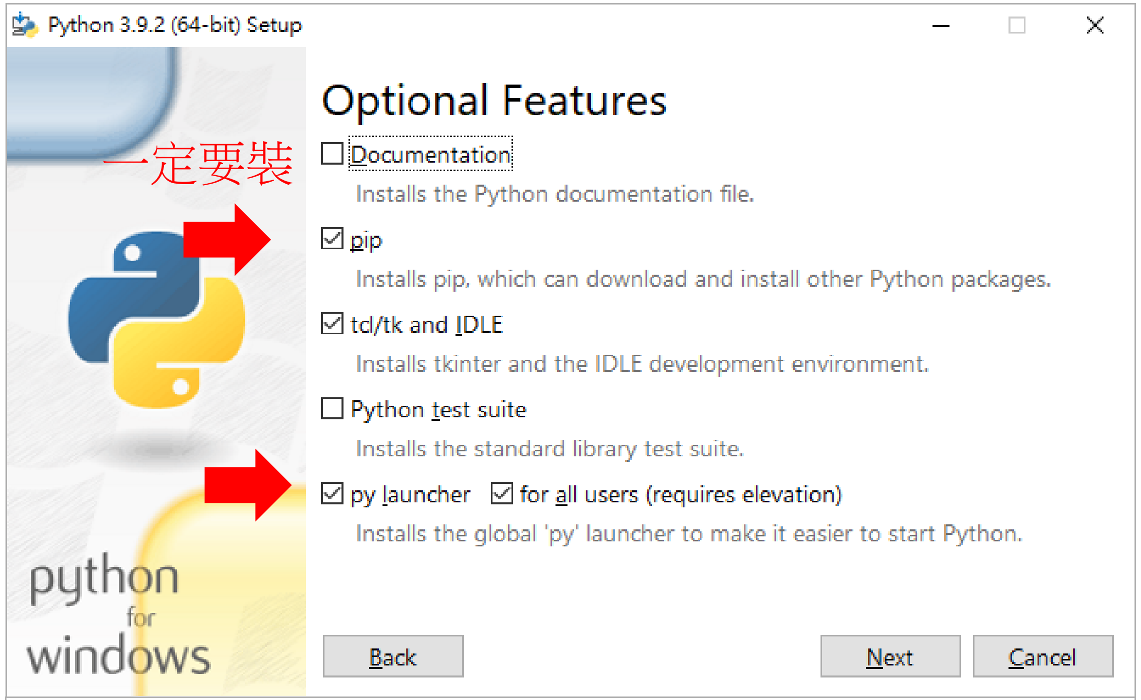
Select Install Now to install Python with default settings, or choose Customize to enable or disable features.

→ Install Now
C:\Users\Administrator\AppData\Local\Programs\Python\Python39

Includes IDLE, pip and documentation
Creates shortcuts and file associations

→ Customize installation
Choose location and features

☑ Install launcher for all users (recommended)
☐ Add Python 3.9 to PATH



Python 3.9.2 (64-bit) Setup

Optional Features

一定要裝

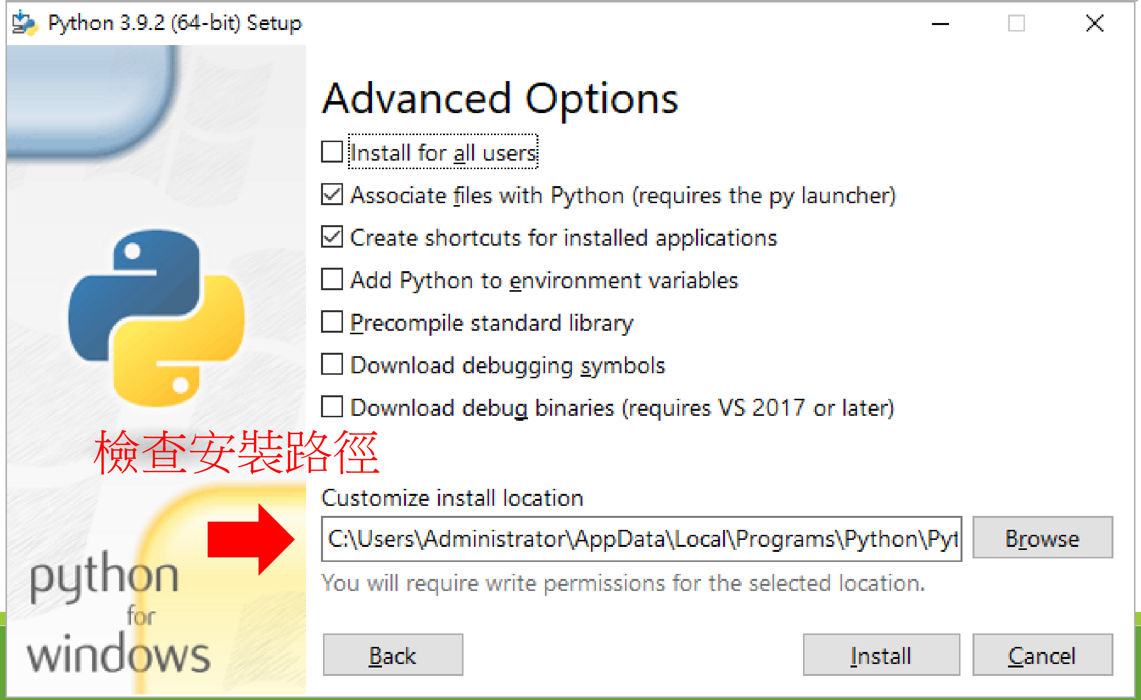
☐ Documentation
Installs the Python documentation file.

☑ pip
Installs pip, which can download and install other Python packages.

☑ tcl/tk and IDLE
Installs tkinter and the IDLE development environment.

☐ Python test suite
Installs the standard library test suite.

☑ py launcher ☑ for all users (requires elevation)
Installs the global 'py' launcher to make it easier to start Python.



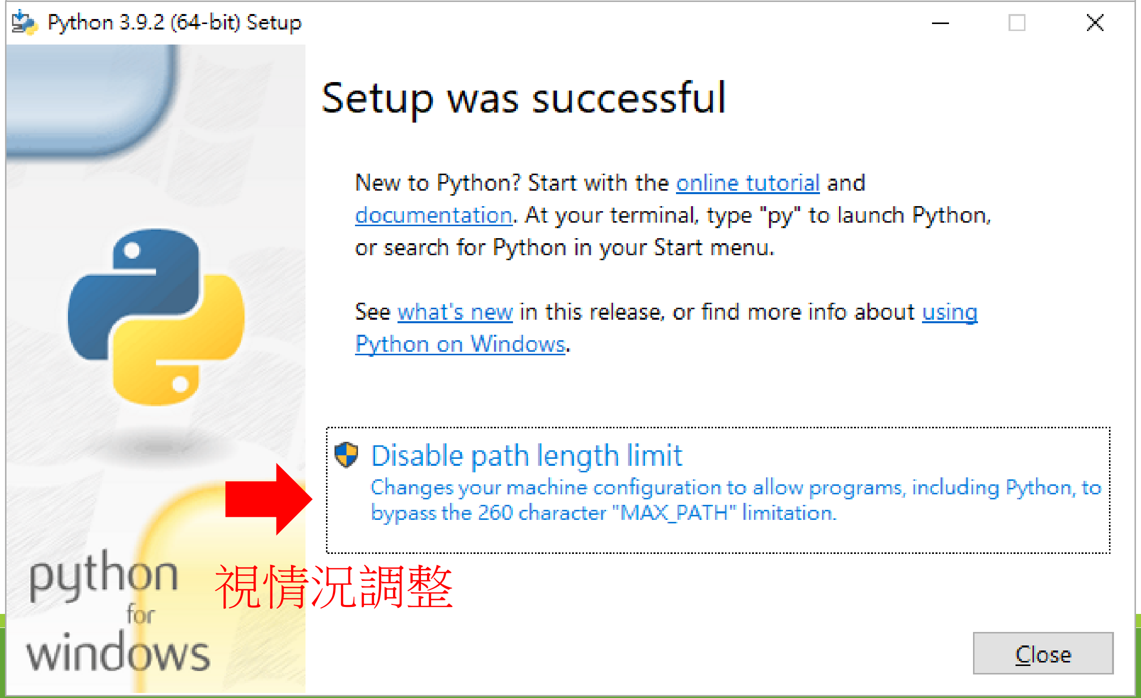
Python 3.9.2 (64-bit) Setup

Advanced Options

☐ Install for all users
☑ Associate files with Python (requires the py launcher)
☑ Create shortcuts for installed applications
☐ Add Python to environment variables
☐ Precompile standard library
☐ Download debugging symbols
☐ Download debug binaries (requires VS 2017 or later)

檢查安裝路徑

Customize install location
C:\Users\Administrator\AppData\Local\Programs\Python\Pyt
You will require write permissions for the selected location.



Python 3.9.2 (64-bit) Setup

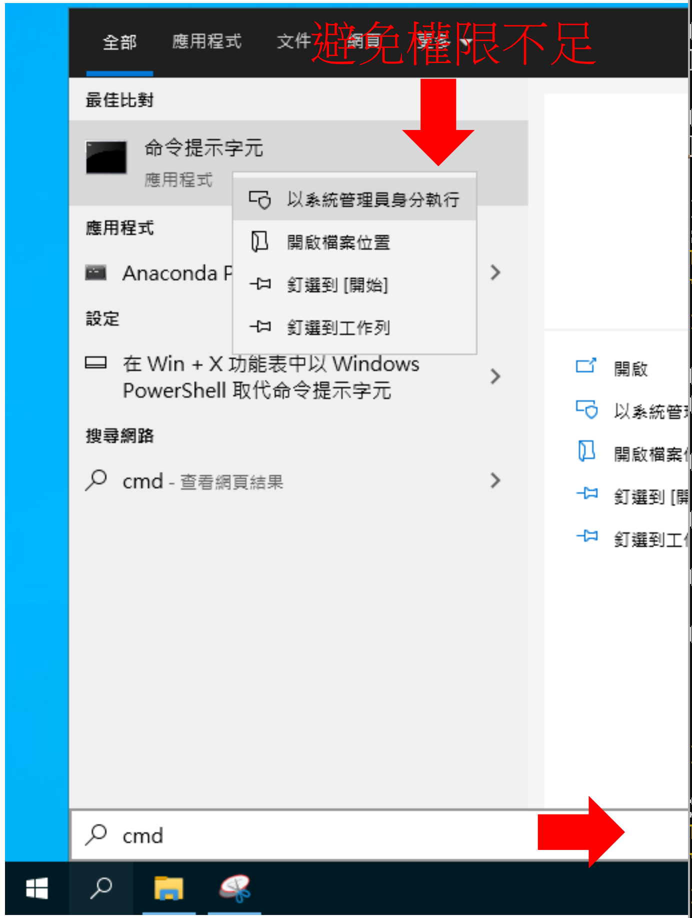
Setup was successful

New to Python? Start with the online tutorial and documentation. At your terminal, type "py" to launch Python, or search for Python in your Start menu.

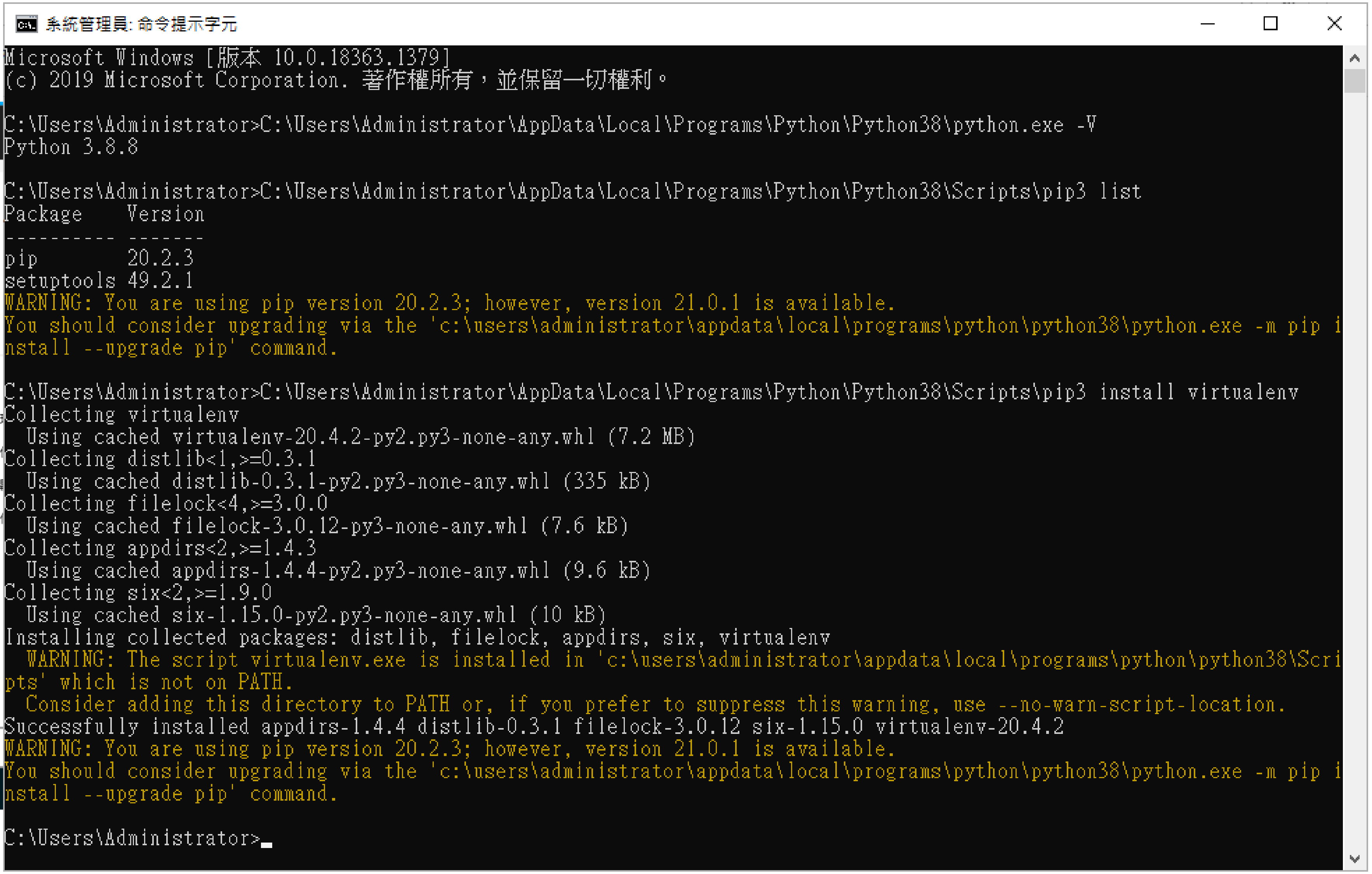
See what's new in this release, or find more info about using Python on Windows.

Disable path length limit
Changes your machine configuration to allow programs, including Python, to bypass the 260 character "MAX_PATH" limitation.

視情況調整



避免權限不足



```
Microsoft Windows [版本 10.0.18363.1379]
(c) 2019 Microsoft Corporation. 著作權所有，並保留一切權利。

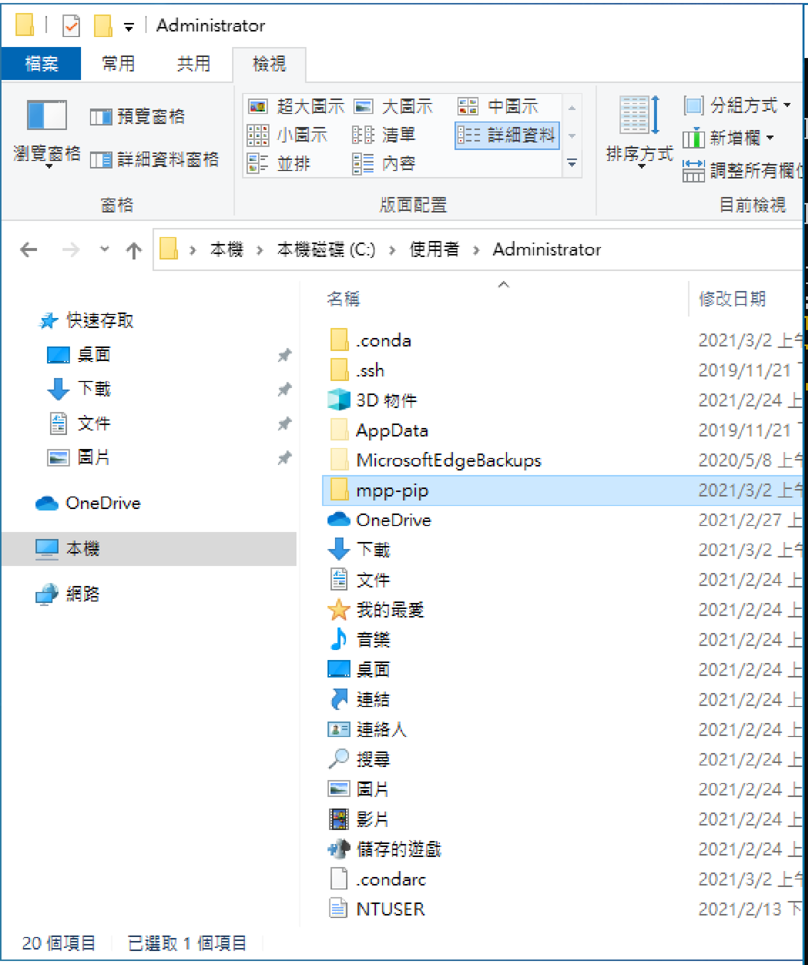
C:\Users\Administrator>C:\Users\Administrator\AppData\Local\Programs\Python\Python38\python.exe -V
Python 3.8.8

C:\Users\Administrator>C:\Users\Administrator\AppData\Local\Programs\Python\Python38\Scripts\pip3 list
Package    Version
---------- -------
pip        20.2.3
setuptools 49.2.1
WARNING: You are using pip version 20.2.3; however, version 21.0.1 is available.
You should consider upgrading via the 'c:\users\administrator\appdata\local\programs\python\python38\python.exe -m pip i
nstall --upgrade pip' command.

C:\Users\Administrator>C:\Users\Administrator\AppData\Local\Programs\Python\Python38\Scripts\pip3 install virtualenv
Collecting virtualenv
  Using cached virtualenv-20.4.2-py2.py3-none-any.whl (7.2 MB)
Collecting distlib<1,>=0.3.1
  Using cached distlib-0.3.1-py2.py3-none-any.whl (335 kB)
Collecting filelock<4,>=3.0.0
  Using cached filelock-3.0.12-py3-none-any.whl (7.6 kB)
Collecting appdirs<2,>=1.4.3
  Using cached appdirs-1.4.4-py2.py3-none-any.whl (9.6 kB)
Collecting six<2,>=1.9.0
  Using cached six-1.15.0-py2.py3-none-any.whl (10 kB)
Installing collected packages: distlib, filelock, appdirs, six, virtualenv
  WARNING: The script virtualenv.exe is installed in 'c:\users\administrator\appdata\local\programs\python\python38\Scri
pts' which is not on PATH.
  Consider adding this directory to PATH or, if you prefer to suppress this warning, use --no-warn-script-location.
Successfully installed appdirs-1.4.4 distlib-0.3.1 filelock-3.0.12 six-1.15.0 virtualenv-20.4.2
WARNING: You are using pip version 20.2.3; however, version 21.0.1 is available.
You should consider upgrading via the 'c:\users\administrator\appdata\local\programs\python\python38\python.exe -m pip i
nstall --upgrade pip' command.

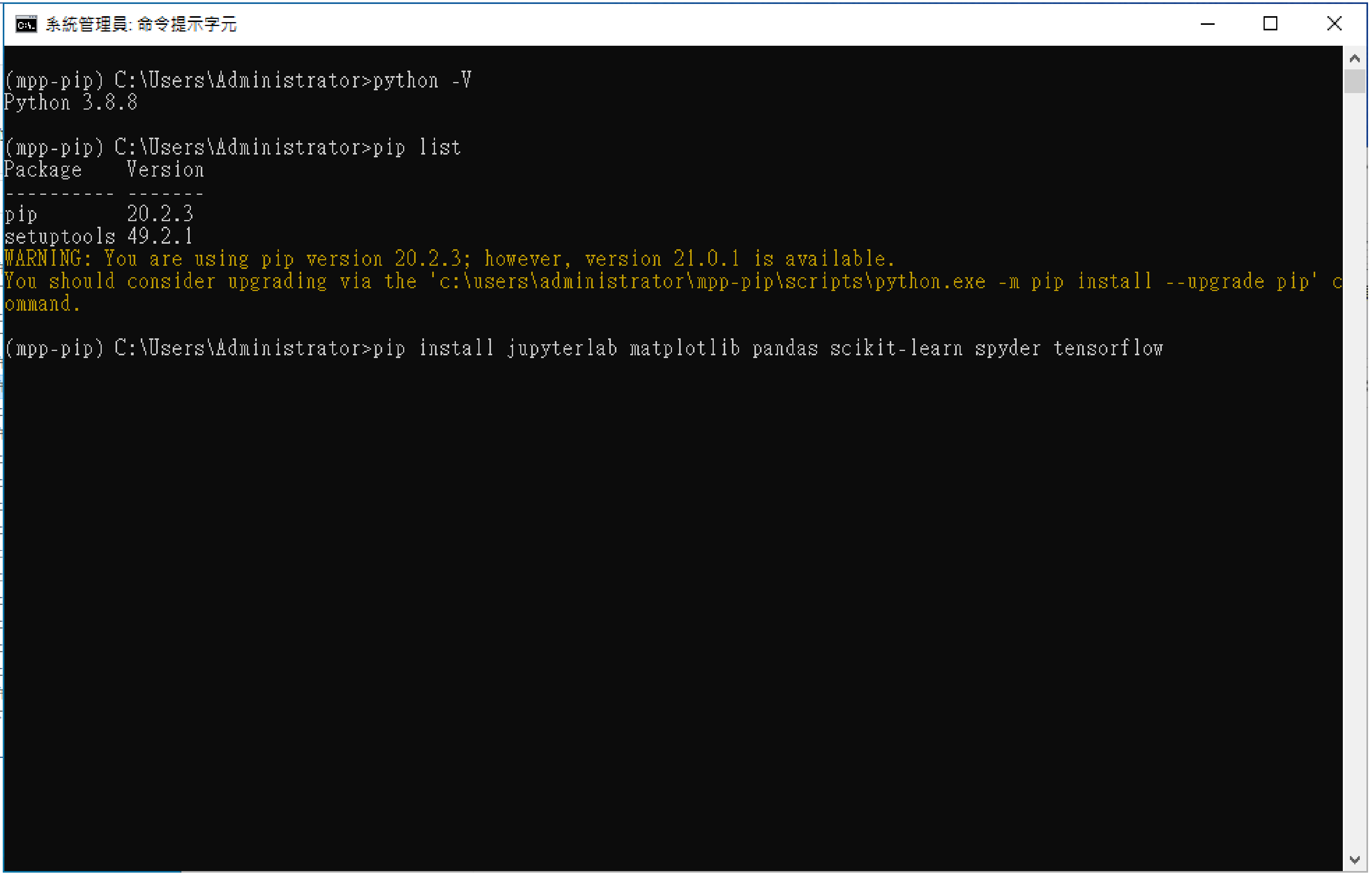
C:\Users\Administrator>
```

有看到Successfully installed…就是成功了



名稱	修改日期
.conda	2021/3/2 上午
.ssh	2019/11/21
3D 物件	2021/2/24 上
AppData	2019/11/21
MicrosoftEdgeBackups	2020/5/8 上午
mpp-pip	2021/3/2 上午
OneDrive	2021/2/27 上
下載	2021/3/2 上午
文件	2021/2/24 上
我的最愛	2021/2/24 上
音樂	2021/2/24 上
桌面	2021/2/24 上
連結	2021/2/24 上
連絡人	2021/2/24 上
搜尋	2021/2/24 上
圖片	2021/2/24 上
影片	2021/2/24 上
儲存的遊戲	2021/2/24 上
.condarc	2021/3/2 上午
NTUSER	2021/2/13 下

20 個項目　已選取 1 個項目



系統管理員: 命令提示字元

```
(mpp-pip) C:\Users\Administrator>python -V
Python 3.8.8

(mpp-pip) C:\Users\Administrator>pip list
Package    Version
---------- -------
pip        20.2.3
setuptools 49.2.1
WARNING: You are using pip version 20.2.3; however, version 21.0.1 is available.
You should consider upgrading via the 'c:\users\administrator\mpp-pip\scripts\python.exe -m pip install --upgrade pip' c
ommand.

(mpp-pip) C:\Users\Administrator>pip install jupyterlab matplotlib pandas scikit-learn spyder tensorflow
```

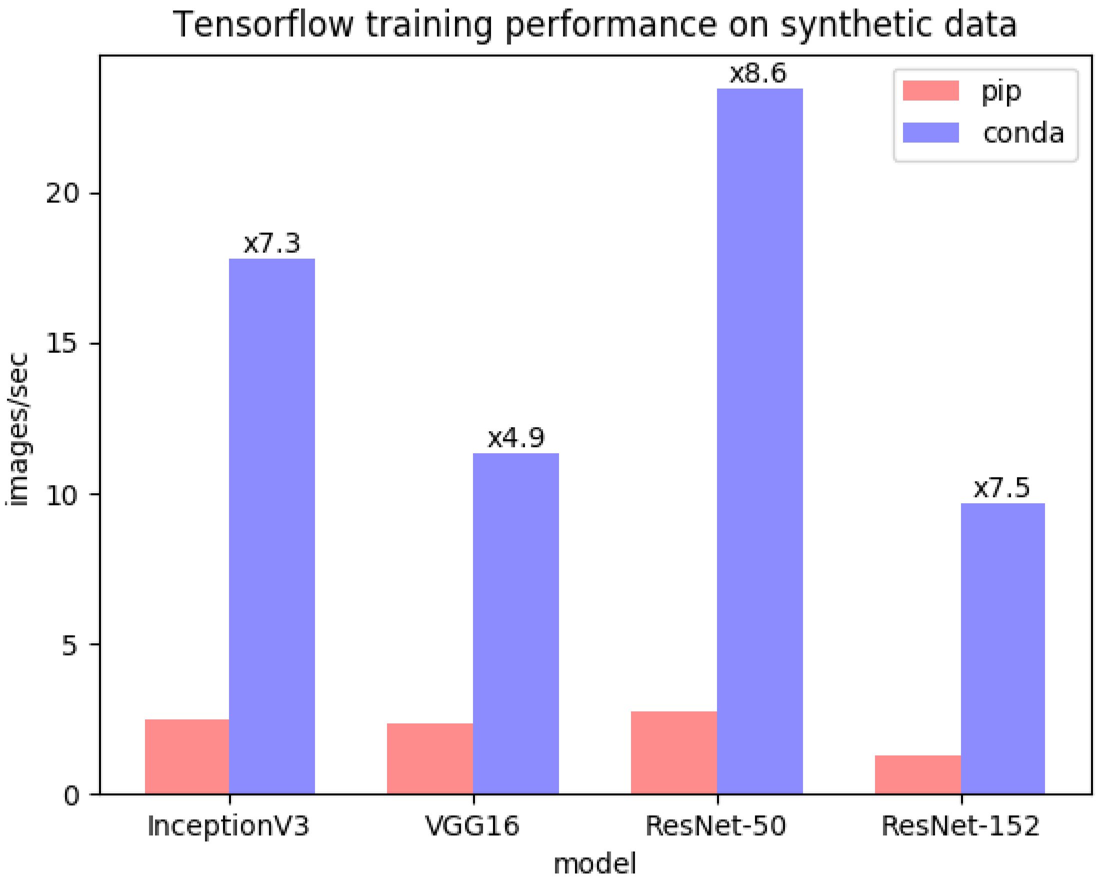
Two reasons why you should install Tensorflow using conda instead of pip

1. Much Faster CPU Performance

   The conda packages leverage the Intel Math Kernel Library for Deep Neural Networks. Not only does the MKL library speed up Tensorflow, it also speeds up other libraries like NumPy, SciPy, and Scikit-Learn.

2. Simpler install for the GPU version

   The conda install will automatically install the CUDA and CuDNN libraries needed for GPU support. The pip install will require you to do that manually.



加分題(期末總分1分):
重現右圖的任一case比較，要有環境recipe，可順利執行的程式碼和最多兩面的A4書面報告。
提示:
注意軟體以及程式碼的版本匹配。
期限:待宣布(通常跟著期末作業繳交期限)

https://www.kdnuggets.com/2018/10/stop-installing-tensorflow-using-pip-performance-sake.html

Build your own Development Environment

Use pip on CoLab

Google Colab (Colaboratory)是Google提供的雲端Jupyter Notebook開發環境。

最大賣點是提供了**免費**的GPU(型號看當時閒置資源而動態分配，有Tesla P100 GPU)和TPU。

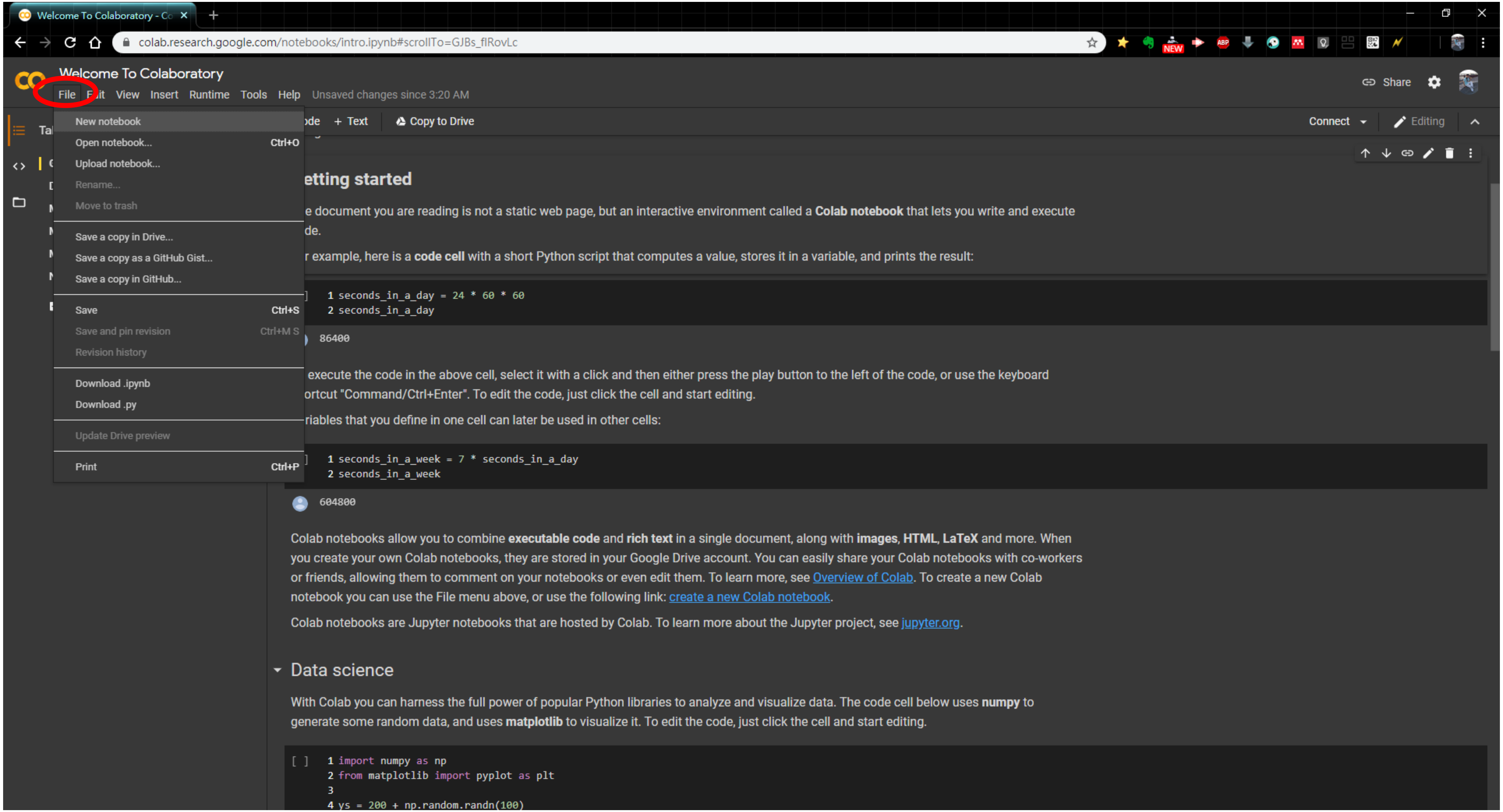
每次開啟有12小時的連續使用時間限制，12小時過後虛擬機需要重新開啟才能繼續運行，也就是說不能在Colab上運行一個需要跑超過12小時的程式。

使用條件

1.要有 google的帳號

2.會操作 Jupyter Notebook。

3.要會用pip自己安裝環境。



etting started

e document you are reading is not a static web page, but an interactive environment called a **Colab notebook** that lets you write and execute de.

r example, here is a **code cell** with a short Python script that computes a value, stores it in a variable, and prints the result:

```
seconds_in_a_day = 24 * 60 * 60
seconds_in_a_day
```

```
86400
```

execute the code in the above cell, select it with a click and then either press the play button to the left of the code, or use the keyboard ortcut "Command/Ctrl+Enter". To edit the code, just click the cell and start editing.

riables that you define in one cell can later be used in other cells:

```
seconds_in_a_week = 7 * seconds_in_a_day
seconds_in_a_week
```

```
604800
```

Colab notebooks allow you to combine **executable code** and **rich text** in a single document, along with **images**, **HTML**, **LaTeX** and more. When you create your own Colab notebooks, they are stored in your Google Drive account. You can easily share your Colab notebooks with co-workers or friends, allowing them to comment on your notebooks or even edit them. To learn more, see Overview of Colab. To create a new Colab notebook you can use the File menu above, or use the following link: create a new Colab notebook.

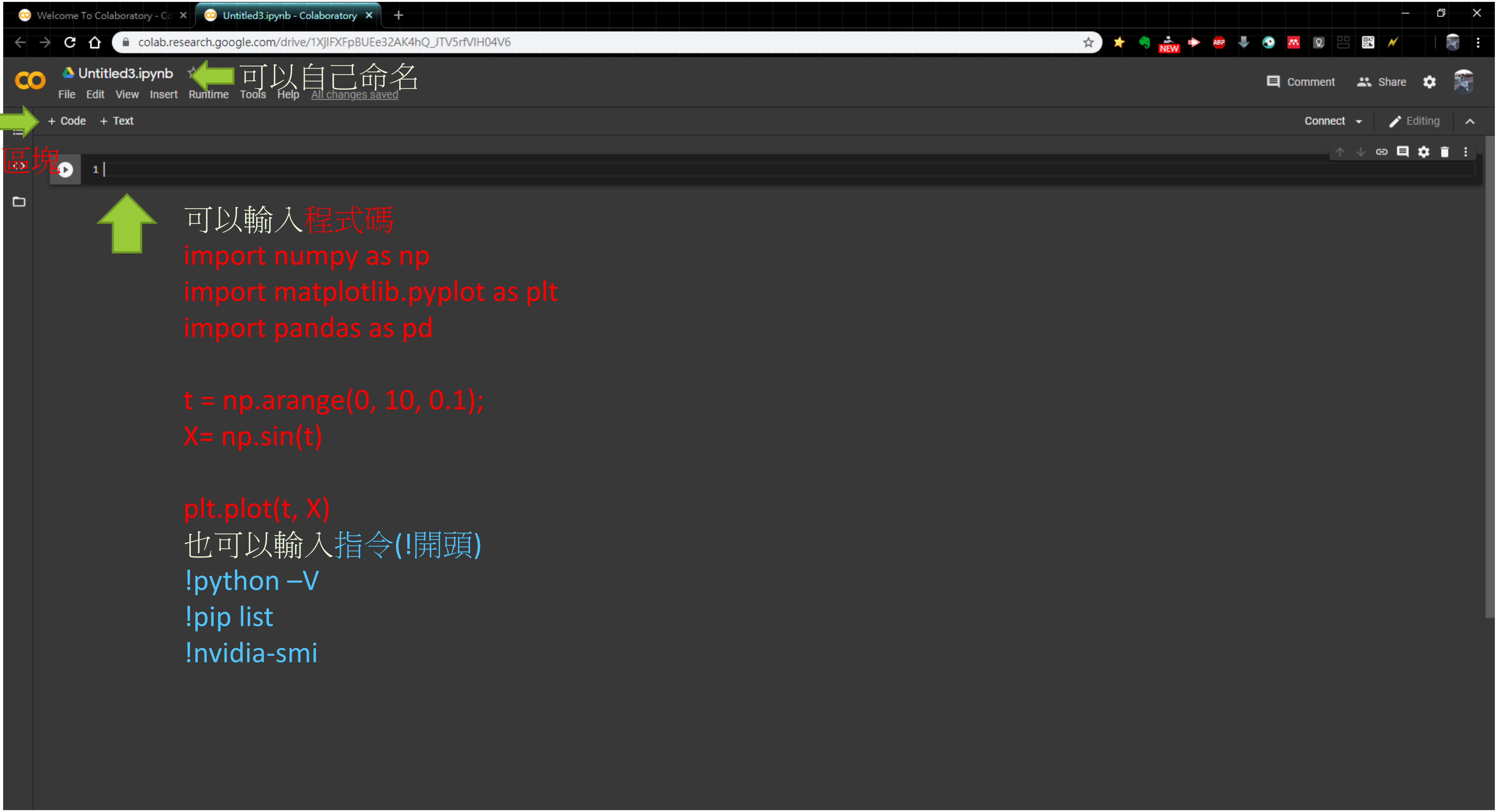
Colab notebooks are Jupyter notebooks that are hosted by Colab. To learn more about the Jupyter project, see jupyter.org.

Data science

With Colab you can harness the full power of popular Python libraries to analyze and visualize data. The code cell below uses **numpy** to generate some random data, and uses **matplotlib** to visualize it. To edit the code, just click the cell and start editing.

```
import numpy as np
from matplotlib import pyplot as plt

ys = 200 + np.random.randn(100)
```


Welcome To Colaboratory - Co
Untitled3.ipynb - Colaboratory
colab.research.google.com/drive/1XjIFXFpBUEe32AK4hQ_JTV5rfVIH04V6
Untitled3.ipynb
File Edit View Insert Runtime Tools Help All changes saved
Comment
Share
+ Code + Text
Connect
Editing

可以自己命名

新增區塊

可以輸入程式碼

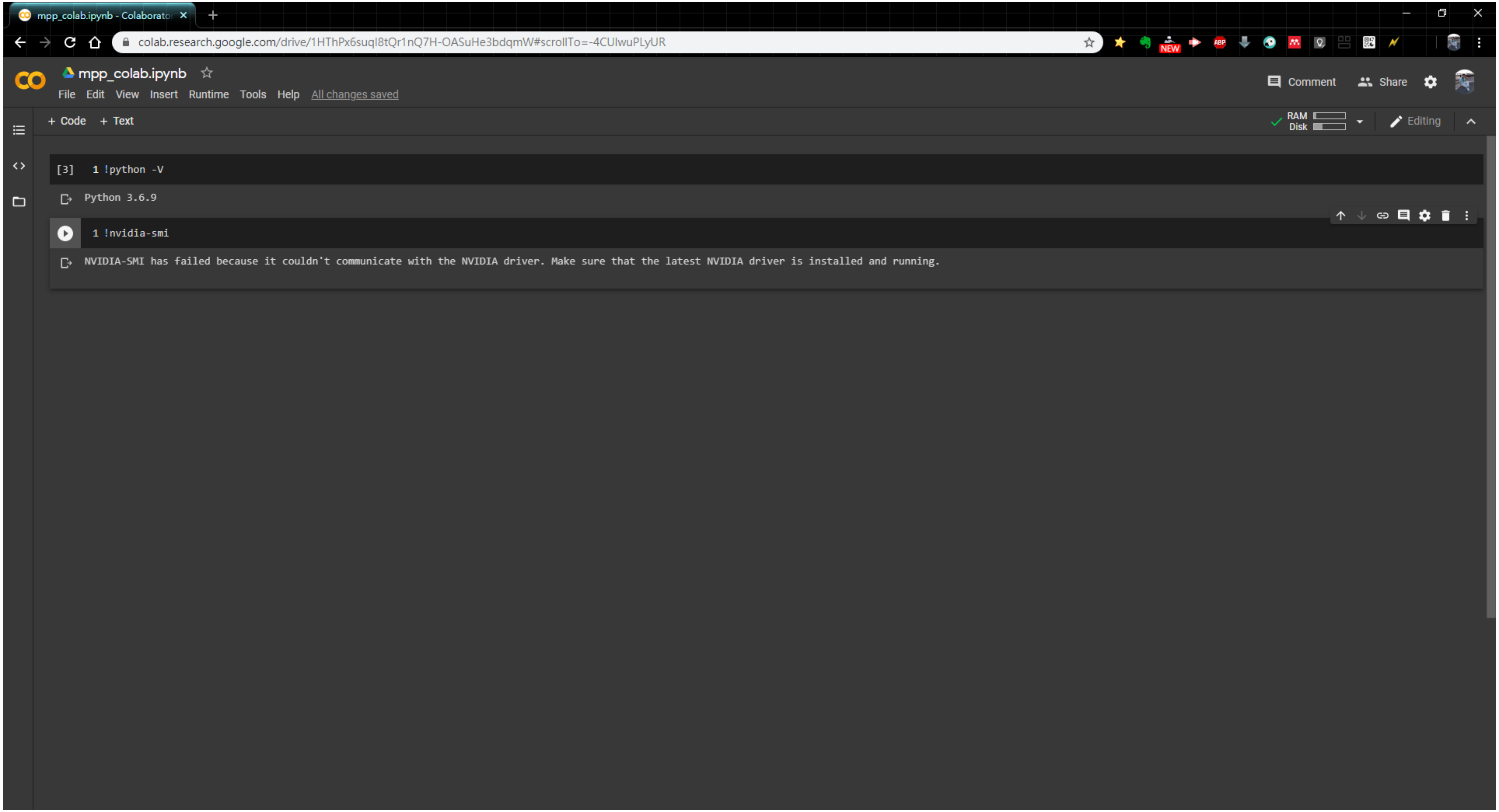
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

t = np.arange(0, 10, 0.1);
X= np.sin(t)

plt.plot(t, X)
```

也可以輸入指令(!開頭)

```
!python –V
!pip list
!nvidia-smi
```

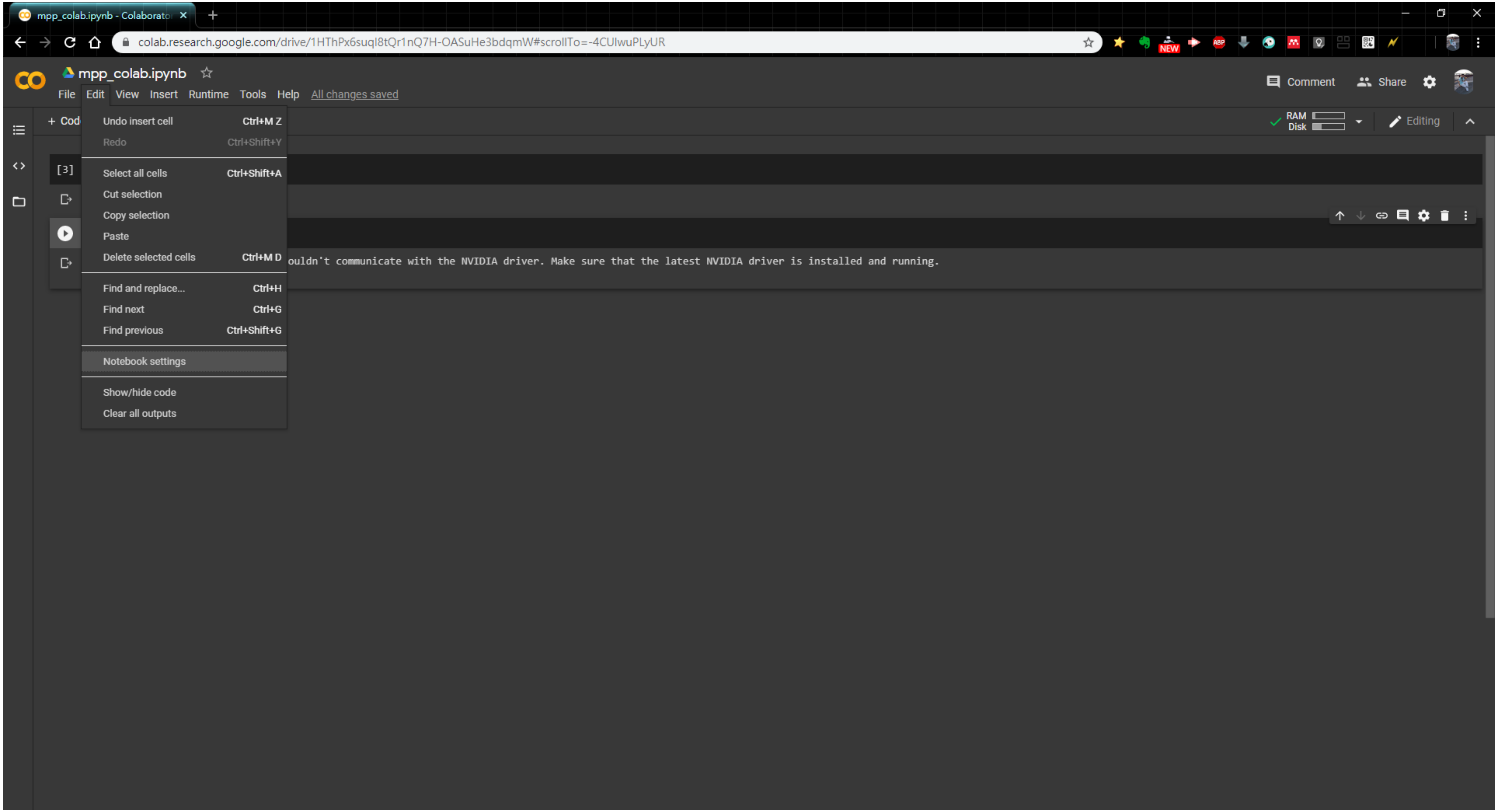

mpp_colab.ipynb - Colaborato
colab.research.google.com/drive/1HThPx6suql8tQr1nQ7H-OASuHe3bdqmW#scrollTo=-4CUlwuPLyUR
mpp_colab.ipynb
File Edit View Insert Runtime Tools Help All changes saved
Comment
Share
+ Code + Text
RAM
Disk
Editing

```
[3] !python -V
```

```
Python 3.6.9
```

```
!nvidia-smi
```

```
NVIDIA-SMI has failed because it couldn't communicate with the NVIDIA driver. Make sure that the latest NVIDIA driver is installed and running.
```


mpp_colab.ipynb - Colaborato
colab.research.google.com/drive/1HThPx6suqI8tQr1nQ7H-OASuHe3bdqmW#scrollTo=-4CUIwuPLyUR
mpp_colab.ipynb
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Redo Ctrl+Shift+Y
Select all cells Ctrl+Shift+A
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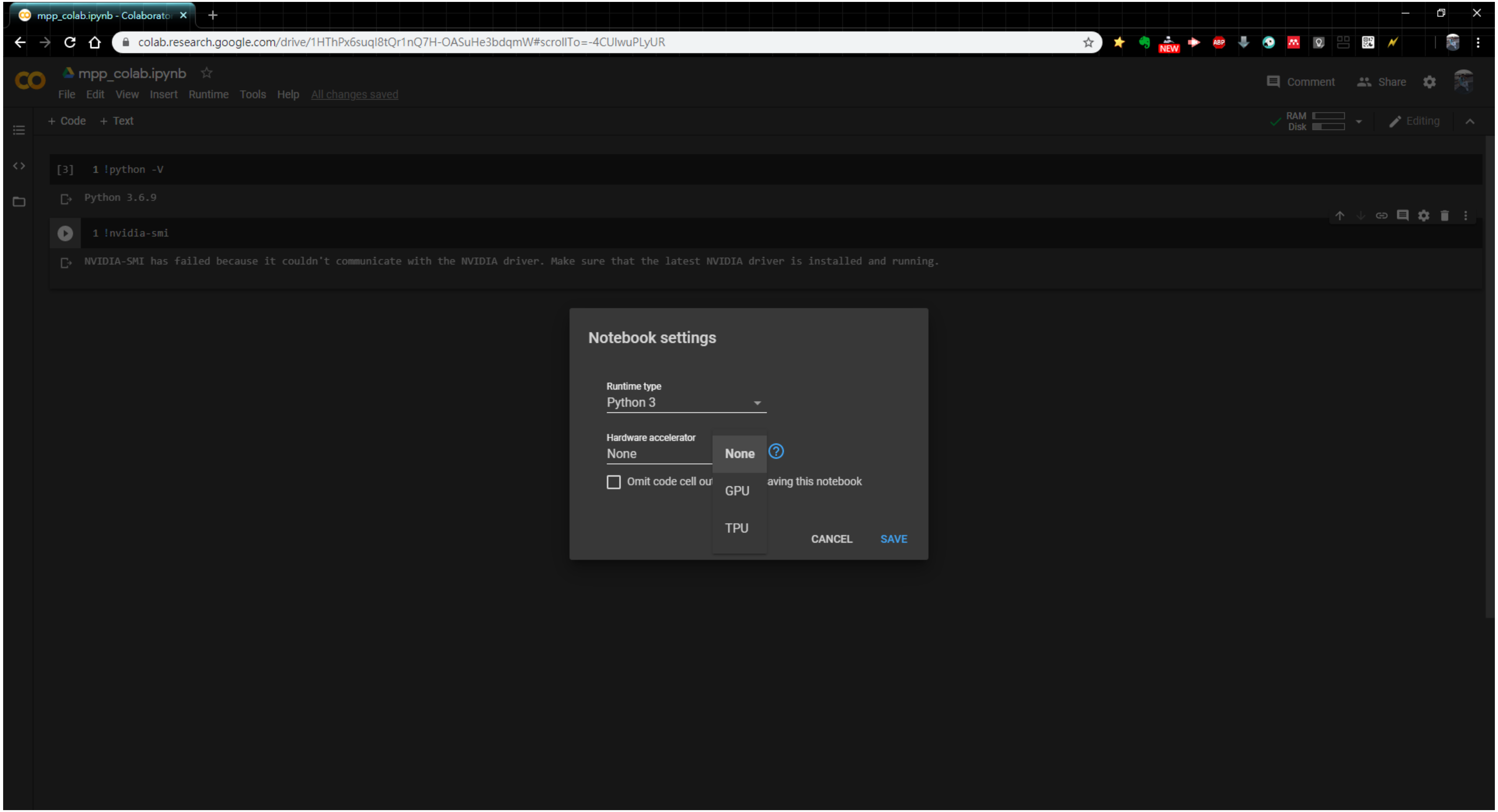
Copy selection
Paste
Delete selected cells Ctrl+M D
Find and replace... Ctrl+H
Find next Ctrl+G
Find previous Ctrl+Shift+G
Notebook settings
Show/hide code
Clear all outputs

```
ouldn't communicate with the NVIDIA driver. Make sure that the latest NVIDIA driver is installed and running.
```



```
!python -V
```

```
Python 3.6.9
```

```
!nvidia-smi
```

```
NVIDIA-SMI has failed because it couldn't communicate with the NVIDIA driver. Make sure that the latest NVIDIA driver is installed and running.
```

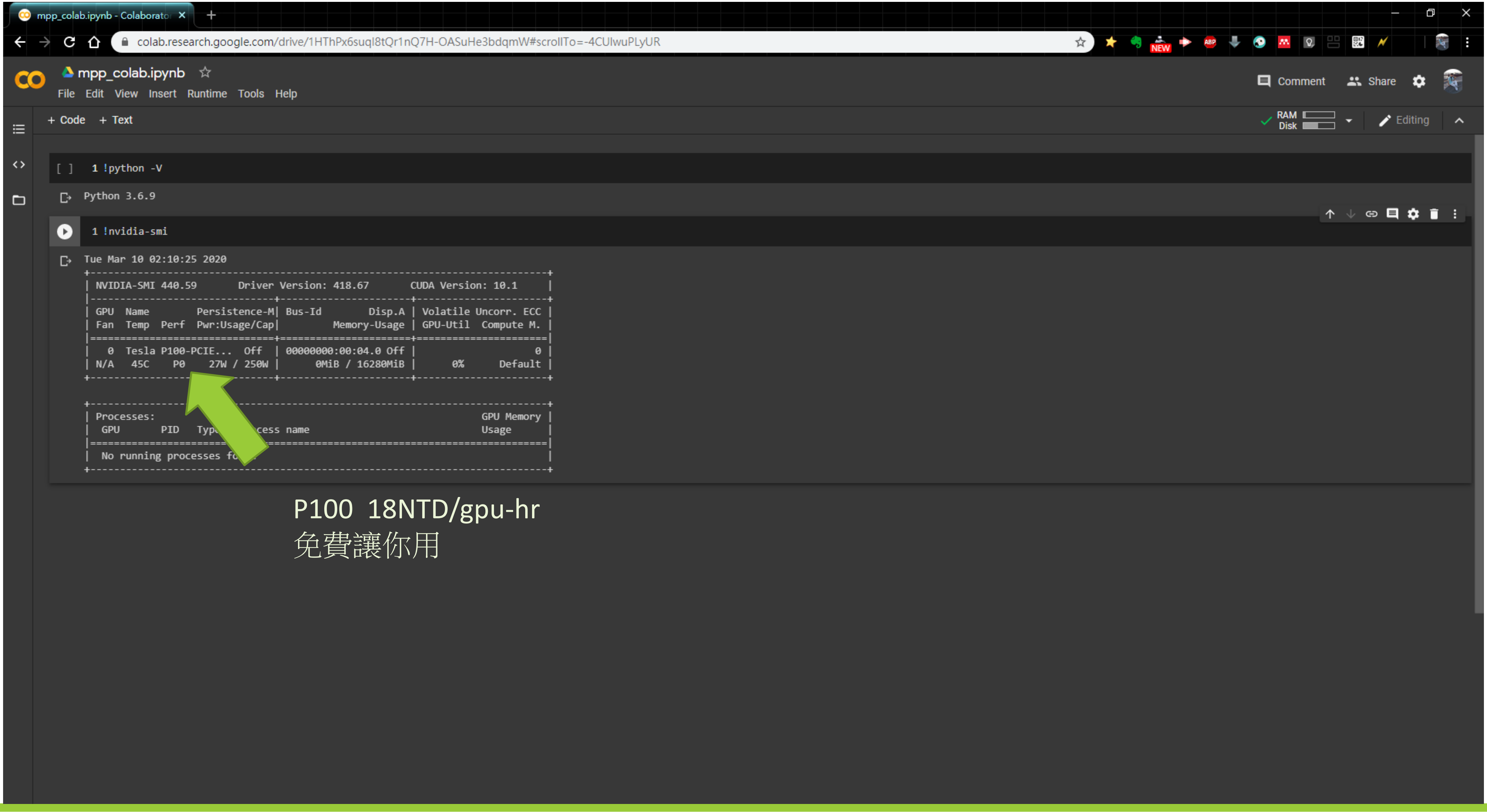
Notebook settings

Runtime type
Python 3

Hardware accelerator
None

None
GPU
TPU

□ Omit code cell out aving this notebook


mpp_colab.ipynb - Colaborator
colab.research.google.com/drive/1HThPx6suql8tQr1nQ7H-OASuHe3bdqmW#scrollTo=-4CUlwuPLyUR
mpp_colab.ipynb
File Edit View Insert Runtime Tools Help
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RAM
Disk
Editing

```
!python -V
```

```
Python 3.6.9
```

```
!nvidia-smi
```

```
Tue Mar 10 02:10:25 2020
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 440.59       Driver Version: 418.67       CUDA Version: 10.1     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  Tesla P100-PCIE...  Off  | 00000000:00:04.0 Off |                    0 |
| N/A   45C    P0    27W / 250W |      0MiB / 16280MiB |      0%      Default |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                       GPU Memory |
|  GPU       PID   Typ      cess name                             Usage      |
|=============================================================================|
|  No running processes fo                                                    |
+-----------------------------------------------------------------------------+
```

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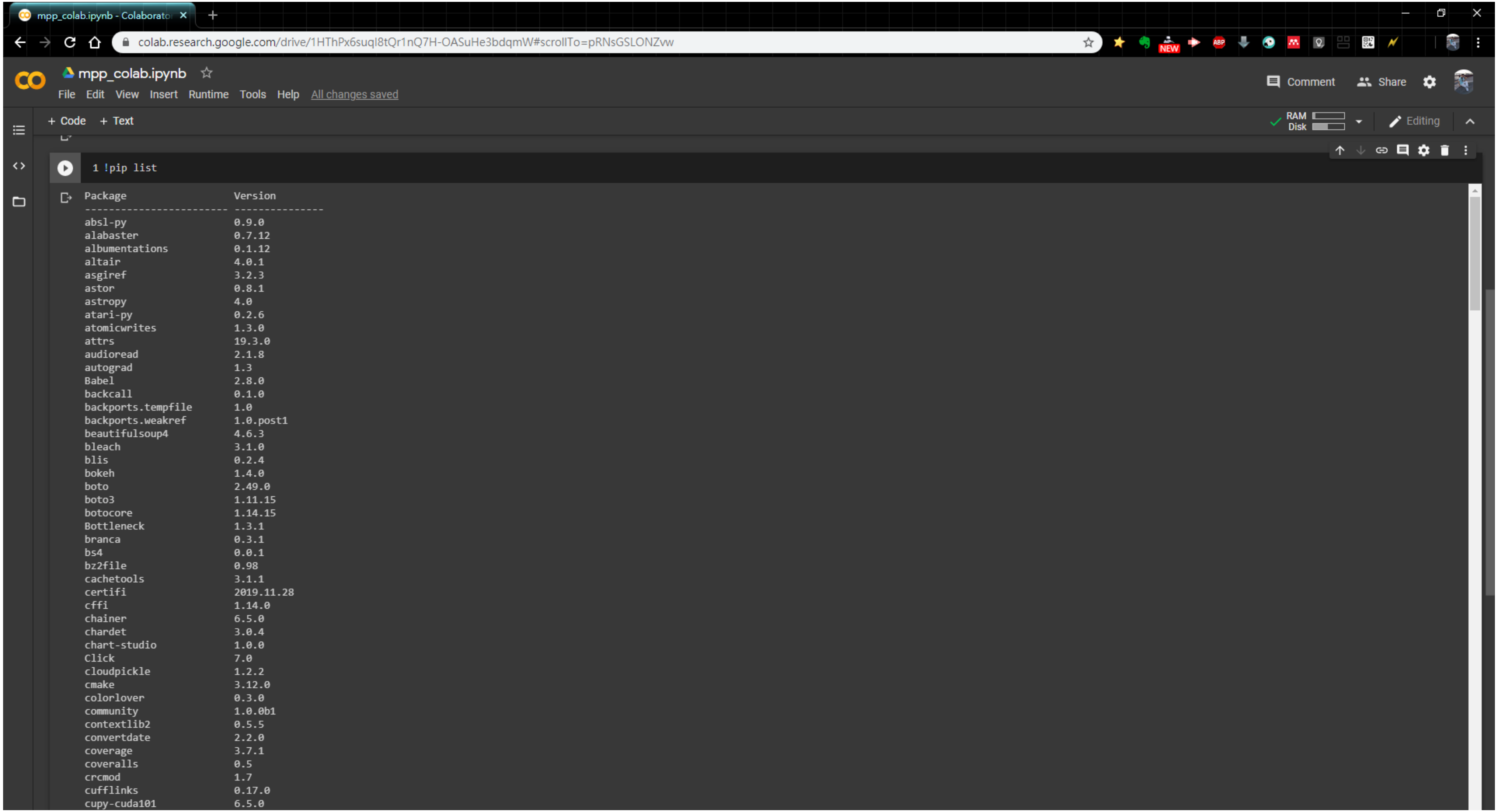
mpp_colab.ipynb - Colaborato
colab.research.google.com/drive/1HThPx6suql8tQr1nQ7H-OASuHe3bdqmW#scrollTo=pRNsGSLONZvw
mpp_colab.ipynb
File
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Runtime
Tools
Help
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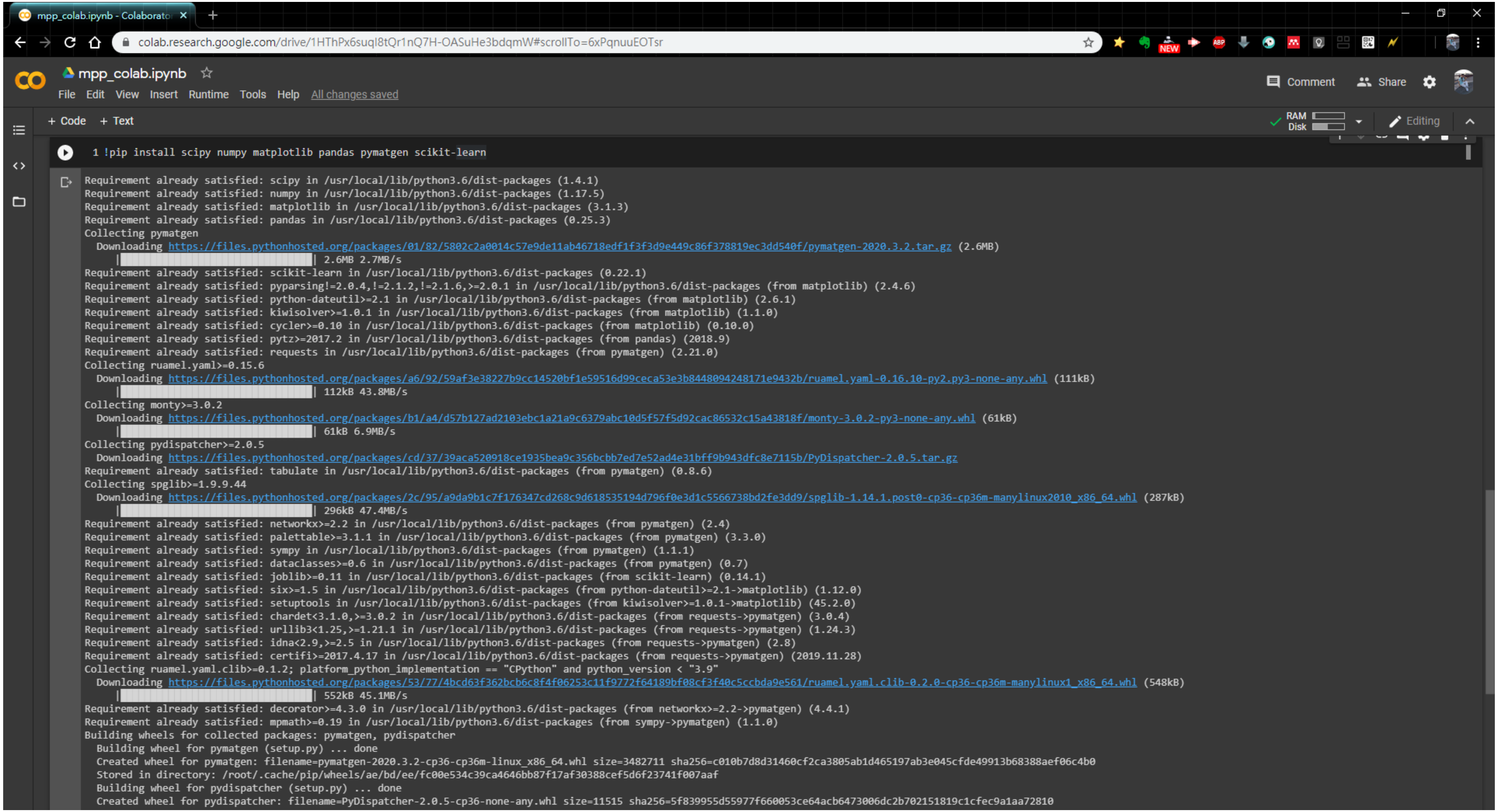
```
!pip list
```

```
Package                  Version
------------------------ ---------------
absl-py                  0.9.0
alabaster                0.7.12
albumentations           0.1.12
altair                   4.0.1
asgiref                  3.2.3
astor                    0.8.1
astropy                  4.0
atari-py                 0.2.6
atomicwrites             1.3.0
attrs                    19.3.0
audioread                2.1.8
autograd                 1.3
Babel                    2.8.0
backcall                 0.1.0
backports.tempfile       1.0
backports.weakref        1.0.post1
beautifulsoup4           4.6.3
bleach                   3.1.0
blis                     0.2.4
bokeh                    1.4.0
boto                     2.49.0
boto3                    1.11.15
botocore                 1.14.15
Bottleneck               1.3.1
branca                   0.3.1
bs4                      0.0.1
bz2file                  0.98
cachetools               3.1.1
certifi                  2019.11.28
cffi                     1.14.0
chainer                  6.5.0
chardet                  3.0.4
chart-studio             1.0.0
Click                    7.0
cloudpickle              1.2.2
cmake                    3.12.0
colorlover               0.3.0
community                1.0.0b1
contextlib2              0.5.5
convertdate              2.2.0
coverage                 3.7.1
coveralls                0.5
crcmod                   1.7
cufflinks                0.17.0
cupy-cuda101             6.5.0
```



mpp_colab.ipynb - Colaborato
colab.research.google.com/drive/1HThPx6suql8tQr1nQ7H-OASuHe3bdqmW#scrollTo=6xPqnuuEOTsr
mpp_colab.ipynb
File Edit View Insert Runtime Tools Help All changes saved
Comment
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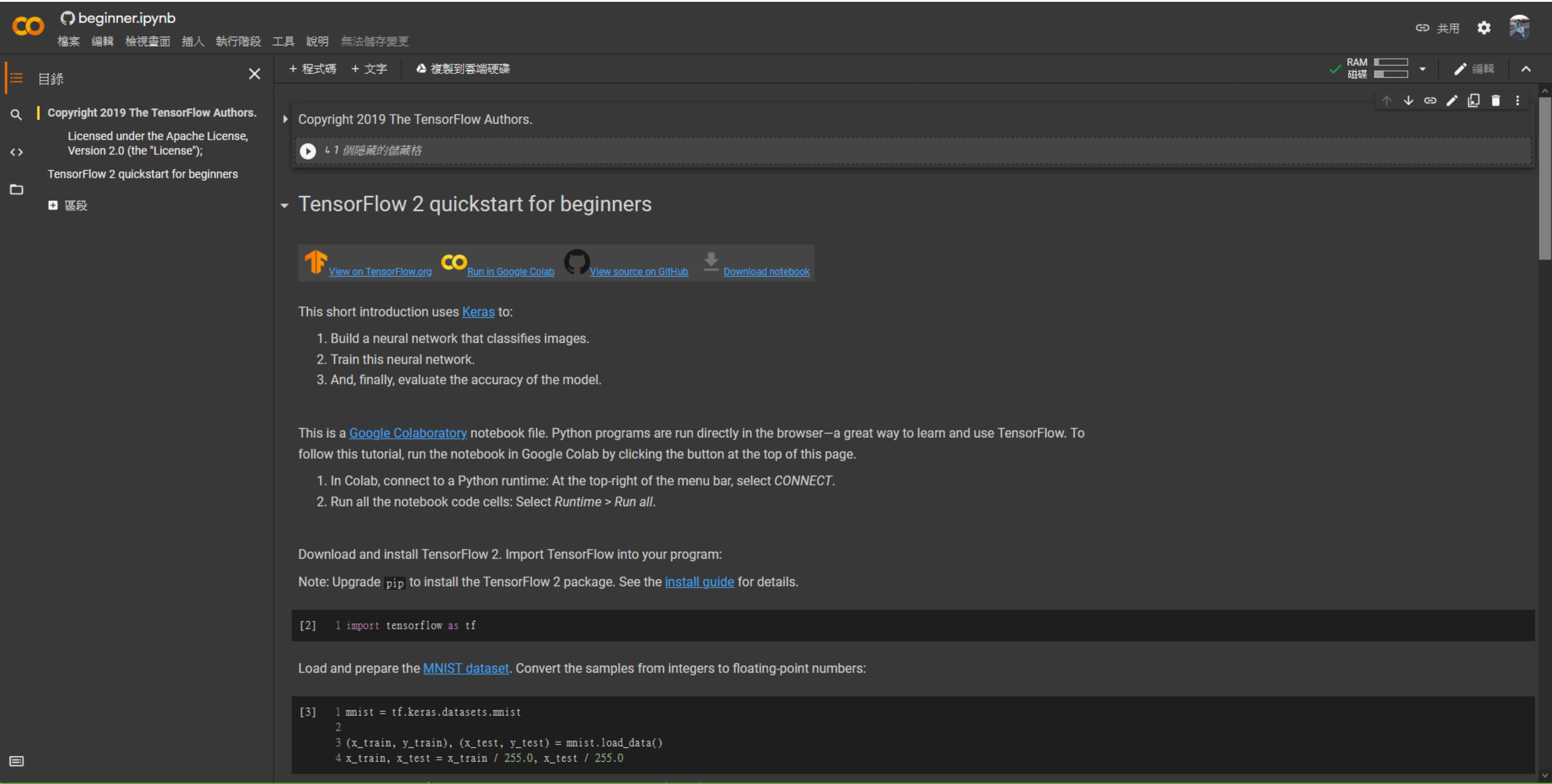
```
1 !pip install scipy numpy matplotlib pandas pymatgen scikit-learn
```

```
Requirement already satisfied: scipy in /usr/local/lib/python3.6/dist-packages (1.4.1)
Requirement already satisfied: numpy in /usr/local/lib/python3.6/dist-packages (1.17.5)
Requirement already satisfied: matplotlib in /usr/local/lib/python3.6/dist-packages (3.1.3)
Requirement already satisfied: pandas in /usr/local/lib/python3.6/dist-packages (0.25.3)
Collecting pymatgen
  Downloading https://files.pythonhosted.org/packages/01/82/5802c2a0014c57e9de11ab46718edf1f3f3d9e449c86f378819ec3dd540f/pymatgen-2020.3.2.tar.gz (2.6MB)
     |████████████████████████████████| 2.6MB 2.7MB/s
Requirement already satisfied: scikit-learn in /usr/local/lib/python3.6/dist-packages (0.22.1)
Requirement already satisfied: pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.1 in /usr/local/lib/python3.6/dist-packages (from matplotlib) (2.4.6)
Requirement already satisfied: python-dateutil>=2.1 in /usr/local/lib/python3.6/dist-packages (from matplotlib) (2.6.1)
Requirement already satisfied: kiwisolver>=1.0.1 in /usr/local/lib/python3.6/dist-packages (from matplotlib) (1.1.0)
Requirement already satisfied: cycler>=0.10 in /usr/local/lib/python3.6/dist-packages (from matplotlib) (0.10.0)
Requirement already satisfied: pytz>=2017.2 in /usr/local/lib/python3.6/dist-packages (from pandas) (2018.9)
Requirement already satisfied: requests in /usr/local/lib/python3.6/dist-packages (from pymatgen) (2.21.0)
Collecting ruamel.yaml>=0.15.6
  Downloading https://files.pythonhosted.org/packages/a6/92/59af3e38227b9cc14520bf1e59516d99ceca53e3b8448094248171e9432b/ruamel.yaml-0.16.10-py2.py3-none-any.whl (111kB)
     |████████████████████████████████| 112kB 43.8MB/s
Collecting monty>=3.0.2
  Downloading https://files.pythonhosted.org/packages/b1/a4/d57b127ad2103ebc1a21a9c6379abc10d5f57f5d92cac86532c15a43818f/monty-3.0.2-py3-none-any.whl (61kB)
     |████████████████████████████████| 61kB 6.9MB/s
Collecting pydispatcher>=2.0.5
  Downloading https://files.pythonhosted.org/packages/cd/37/39aca520918ce1935bea9c356bcbb7ed7e52ad4e31bff9b943dfc8e7115b/PyDispatcher-2.0.5.tar.gz
Requirement already satisfied: tabulate in /usr/local/lib/python3.6/dist-packages (from pymatgen) (0.8.6)
Collecting spglib>=1.9.9.44
  Downloading https://files.pythonhosted.org/packages/2c/95/a9da9b1c7f176347cd268c9d618535194d796f0e3d1c5566738bd2fe3dd9/spglib-1.14.1.post0-cp36-cp36m-manylinux2010_x86_64.whl (287kB)
     |████████████████████████████████| 296kB 47.4MB/s
Requirement already satisfied: networkx>=2.2 in /usr/local/lib/python3.6/dist-packages (from pymatgen) (2.4)
Requirement already satisfied: palettable>=3.1.1 in /usr/local/lib/python3.6/dist-packages (from pymatgen) (3.3.0)
Requirement already satisfied: sympy in /usr/local/lib/python3.6/dist-packages (from pymatgen) (1.1.1)
Requirement already satisfied: dataclasses>=0.6 in /usr/local/lib/python3.6/dist-packages (from pymatgen) (0.7)
Requirement already satisfied: joblib>=0.11 in /usr/local/lib/python3.6/dist-packages (from scikit-learn) (0.14.1)
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.6/dist-packages (from python-dateutil>=2.1->matplotlib) (1.12.0)
Requirement already satisfied: setuptools in /usr/local/lib/python3.6/dist-packages (from kiwisolver>=1.0.1->matplotlib) (45.2.0)
Requirement already satisfied: chardet<3.1.0,>=3.0.2 in /usr/local/lib/python3.6/dist-packages (from requests->pymatgen) (3.0.4)
Requirement already satisfied: urllib3<1.25,>=1.21.1 in /usr/local/lib/python3.6/dist-packages (from requests->pymatgen) (1.24.3)
Requirement already satisfied: idna<2.9,>=2.5 in /usr/local/lib/python3.6/dist-packages (from requests->pymatgen) (2.8)
Requirement already satisfied: certifi>=2017.4.17 in /usr/local/lib/python3.6/dist-packages (from requests->pymatgen) (2019.11.28)
Collecting ruamel.yaml.clib>=0.1.2; platform_python_implementation == "CPython" and python_version < "3.9"
  Downloading https://files.pythonhosted.org/packages/53/77/4bcd63f362bcb6c8f4f06253c11f9772f64189bf08cf3f40c5ccbda9e561/ruamel.yaml.clib-0.2.0-cp36-cp36m-manylinux1_x86_64.whl (548kB)
     |████████████████████████████████| 552kB 45.1MB/s
Requirement already satisfied: decorator>=4.3.0 in /usr/local/lib/python3.6/dist-packages (from networkx>=2.2->pymatgen) (4.4.1)
Requirement already satisfied: mpmath>=0.19 in /usr/local/lib/python3.6/dist-packages (from sympy->pymatgen) (1.1.0)
Building wheels for collected packages: pymatgen, pydispatcher
  Building wheel for pymatgen (setup.py) ... done
  Created wheel for pymatgen: filename=pymatgen-2020.3.2-cp36-cp36m-linux_x86_64.whl size=3482711 sha256=c010b7d8d31460cf2ca3805ab1d465197ab3e045cfde49913b68388aef06c4b0
  Stored in directory: /root/.cache/pip/wheels/ae/bd/ee/fc00e534c39ca4646bb87f17af30388cef5d6f23741f007aaf
  Building wheel for pydispatcher (setup.py) ... done
  Created wheel for pydispatcher: filename=PyDispatcher-2.0.5-cp36-none-any.whl size=11515 sha256=5f839955d55977f660053ce64acb6473006dc2b702151819c1cfec9a1aa72810
```

`!pip install scipy numpy matplotlib pandas pymatgen scikit-learn`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TensorFlow 2 quickstart for beginners

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This short introduction uses Keras to:

1. Build a neural network that classifies images.
2. Train this neural network.
3. And, finally, evaluate the accuracy of the model.

This is a Google Colaboratory notebook file. Python programs are run directly in the browser—a great way to learn and use TensorFlow. To follow this tutorial, run the notebook in Google Colab by clicking the button at the top of this page.

1. In Colab, connect to a Python runtime: At the top-right of the menu bar, select *CONNECT*.
2. Run all the notebook code cells: Select *Runtime* > *Run all*.

Download and install TensorFlow 2. Import TensorFlow into your program:

Note: Upgrade `pip` to install the TensorFlow 2 package. See the install guide for details.

```
[2]  import tensorflow as tf
```

Load and prepare the MNIST dataset. Convert the samples from integers to floating-point numbers:

```
[3]  mnist = tf.keras.datasets.mnist

     (x_train, y_train), (x_test, y_test) = mnist.load_data()
     x_train, x_test = x_train / 255.0, x_test / 255.0
```