Book recommended for Machine Learning:

# **Machine Learning with PyTorch and Scikit-Learn: Develop machine learning and deep learning models with Python 1st Edition, Kindle Edition**

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**COMPUTER PREPARATION**

**1. Install the Anaconda distribution**, free for Mac, Windows, and Linux, from [https://www.anaconda.com/download.](https://www.anaconda.com/download)

**2. Install Microsoft Visual Studio Code**, also free for Mac, Windows, and Linux, from [https://code.visualstudio.com.](https://code.visualstudio.com/)

**3. Create a *conda* virtual environment for machine learning (ml).** The sequence of installation steps will be shown here for a typical Mac or Linux device. Instructions on how to do the installation in a Window computers are very similar, but additional details can be found at:

<https://docs.conda.io/projects/conda/en/latest/user-guide/install/windows.html>.

**IMPORTANT**: All the installation steps must be carried out from a terminal window (Mac,Linux) or the Anaconda Prompt window (Windows). The Anaconda Prompt window will appear as one of the applications that can be launched from the Windows desktop.

After opening a terminal your prompt will appear as something like:

tcsh-% (for tcsh shell), bash-3.2$ (for bash shell), user: (dos shell)

At the prompt, type the exact sequence of commands shown below, one line at a time, and wait for the completion of each command execution before typing the next command.

conda --version (yes, 2 minus signs in front of version)

conda create -n ml\_310 python=3.10.14

conda env list (this command should show the existence of two environments: base and ml\_310. **VERY IMPORTANT:** **do not do any further installation of programs in the base environment**.

conda activate ml\_310 (this command brings you inside the ml\_310 virtual env: the prompt will change to  (ml\_310) tcsh-%.

Next, we will install all the programs. Inside a virtual env, programs can be installed either with conda install or with pip install. While you will probably find on the web a general recommendation to use conda install, in our case this installation command produces some inconsistencies between libraries used by the different programs inside the environment. For this reason, we will use instead pip install):

pip install scikit-learn

pip install pandas

pip install openpyxl

pip install matplotlib

pip install ipykernel  
  
pip install jupyter

 1. for Linux, Windows, or Mac without AMD GPU or M chip  
  
pip install torch torchvision torchaudio --index-url <https://download.pytorch.org/whl/cpu>

2. for Linux, Windows with Nvidia Cuda 11.8

pip install torch torchvision torchaudio --index-url https://download.pytorch.org/whl/cu118

3. for Linux, Windows with Nvidia Cuda 12.1

pip install torch torchvision torchaudio --index-url https://download.pytorch.org/whl/cu121

4. for Mac with AMD GPU or M chip

pip install --pre torch torchvision torchaudio --extra-index-url https://download.pytorch.org/whl/nightly/cpu

**Check the version of torch installed using 'pip list', then change the following line accordingly. For example, if torch 2.1.1 then:**  
  
pip install torch\_scatter torch\_sparse torch\_cluster torch\_spline\_conv torch\_geometric -f [https://data.pyg.org/whl/torch-2.1.1+cpu.html](https://data.pyg.org/whl/torch-2.3.0+cpu.html)

pip install lightning

pip install ogb

pip install ipympl  
  
pip install torchmetrics  
  
pip install torchsummary  
  
pip install pytorch-lightning  
  
pip install tensorboard (real time display of training progression)  
  
pip install transformers  
  
pip install h5py  
  
pip install nltk  
  
pip install gdown  
  
pip install pyprind  
  
pip install umap-learn   
  
pip install xgboost  
  
pip install seaborn

pip install rdkit-pypi

pip install ipywidgets

pip install nglview

pip install jupyterlab

pip install neo4j

pip install graphdatascience

pip install torchdrug

pip list or conda list (this will show you all the programs that were installed)

conda deactivate (this brings you out of the virtual env)

**4.  Visual Studio Code settings**

By now you must have been able to create your 'conda' environment and install all the programs (if not, we will troubleshoot any problems).

We can now proceed to continue the setup of Visual Studio Code (VS).

In the past you might have had the opportunity to use a Jupyter Notebook or the Jupyter Lab Graphic Interphase to open files of Jupyter Notebooks type (i.e., 'myprogram.ipynb). However, in order to open, edit, and execute these files it may be convenient to use VS instead of the native Jupyter Notebook application. In order to do it we need to complete the VS installation.

1. Launch VS
2. In the bar on the left side of the workspace you will see a little icon with 4 little squares one of which is detached:

Click on the icon. It will open the 'Extension' section. Here is where you will install additional extension to VS. Some extension will appear already in the section as 'Recommended Extensions'. If some of all the extensions that you will need in your work are not already recommended, you can search for them in the text window at the top which shows: 'Search extensions in the marketplace'.

You will need to install the following extensions:

* Jupyter
* Jupyter Cell Tag
* Jupyter Keymap
* Jupyter Notebook Renderers
* Jupyter Slide Show
* Pylance
* Python
* Vscode-pdf

**Do NOT install** 'Kite AutoComplete AI code' and 'Vim', even if recommended.