

Machine Learning

PyTorch Installations

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Virtual Environment

- A virtual environment is an isolated workspace in which you can install Python packages without affecting your global system setup.
 - Different projects may require different dependencies with different versions
 - If you installed everything on the global system, you will suffer!
- Examples
 - Python's Built-in **venv**
 - **virtualenv** is a third-party package that provides more features than venv.
 - **conda** environments not only manage Python packages + other languages.
 - Developed by Anaconda Inc
 - Cross-platform, but more commonly used in Linux and macOS.
 - Comes pre-installed with the **Anaconda and Miniconda** distributions
 - Follow installations [steps](#) for your OS

Conda Example

- `conda create --name pyt`
 - This will create a conda environment: find at: <>/anaconda3/envs
- **Activating** the Virtual Environment
 - `conda activate pyt`
- **Deactivating** the Virtual Environment
 - <https://chat.openai.com/c/f26d07af-ce77-498f-99cc-09ffdee131b8conda%20deactivate>

Conda with PyCharm

- IDEs are integrated with conda
 - File (menu) ⇒ settings ⇒ Project ⇒ Interpreter
 - Find the path of python executable in the acandonda
- Let's demo

Settings

Q

▶ Appearance & Behavior

Keymap

▶ Editor

Plugins

▶ Version Control

▼ Project: most-pythons-helper-g...

Project Interpreter

Project Structure

▶ Build, Execution, Deployment

▶ Languages & Frameworks

▶ Tools

Project: most-pythons-helper-g... > Project Interpreter

For current project

Project Interpreter: Python 3.7 (pyt) ~/system-installs1/anaconda3/envs/pyt/bin/python

Package	Version	Latest version	
_libgcc_mutex	0.1		+
_openmp_mutex	4.5		-
absl-py	1.2.0		▲
addict	2.4.0		○
antlr4-python3-runtime	4.8		👁
anyio	3.5.0		
appdirs	1.4.4		
argon2-cffi	21.3.0		
argon2-cffi-bindings	21.2.0		
astunparse	1.6.3		
async_generator	1.10		
attrs	21.2.0		
babel	2.9.1		
backcall	0.2.0		
backports	1.0		
backports.functools_lru_cache	1.6.4		
black	19.10b0		
blas	1.0		
bleach	4.1.0		
bottleneck	1.3.2		
brotlipy	0.7.0		
bzip2	1.0.8		
ca-certificates	2023.7.22		
cachetools	5.2.0		
catalogue	2.0.6		
certifi	2023.7.22		

OK

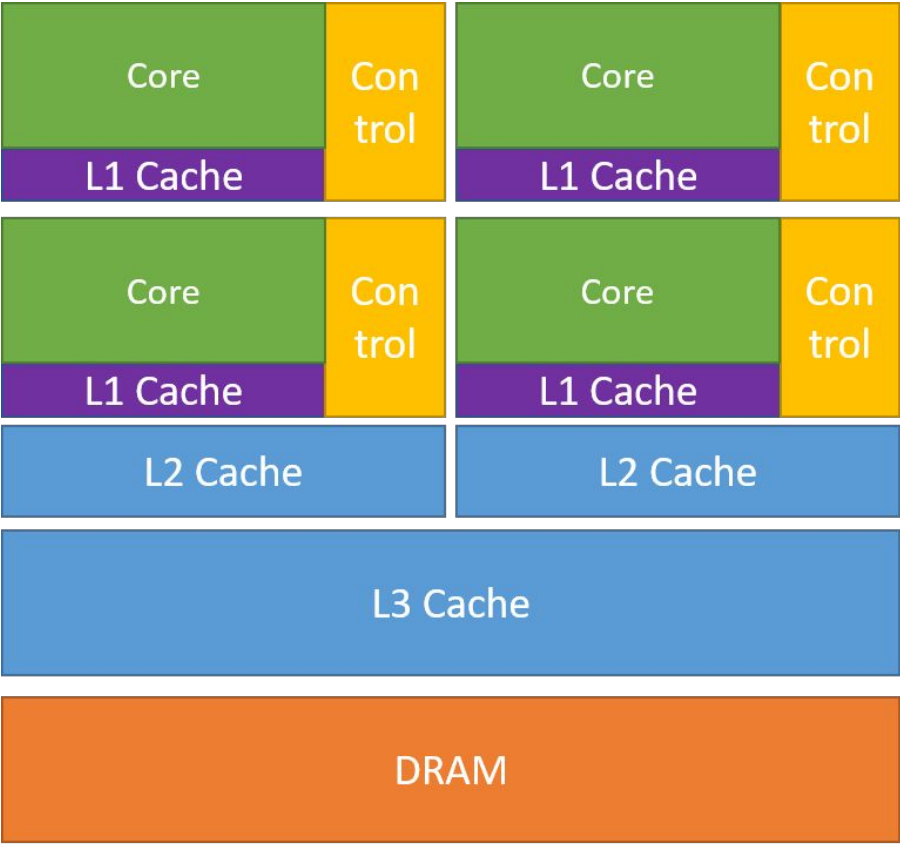
Cancel

Apply

Help

CPU vs GPU

- CPUs (Central Processing Unit) are jacks-of-all-trades, optimized for **single-threaded** performance and general-purpose / **sequential** tasks.
- GPUs (Graphics Processing Units) are specialized for highly **parallel** tasks like graphics **rendering** and matrix **operations**
 - Simpler memory hierarchy, optimized for high-throughput data access.
 - Specialized programming models (e.g., **CUDA**, OpenCL) required for computation.
 - Designed such that **more transistors** are devoted to data processing rather than data **caching** and **flow** control



CPU



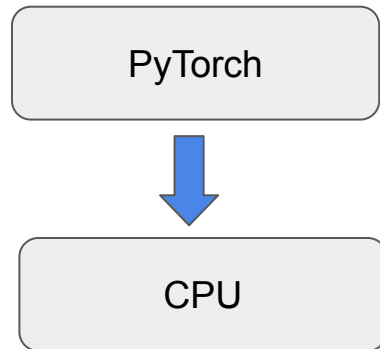
GPU

Check GPU (terminal)

- First, Check for NVIDIA GPU
- Use lspci
 - lspci is a command that prints detailed information about all PCI buses and devices
- As we want only to check nvidia, use grep command
 - Very useful one
 - short for “global regular expression print”, is a command used in searching and matching text files contained in the regular expressions.
- **lspci | grep -i nvidia**
 - Match with pattern (nvidia). -i means ignore case (lower/uppercase)
 - 01:00.0 VGA compatible controller: NVIDIA Corporation GP106M [**GeForce GTX 1060 Mobile**] (rev a1)
 - 01:00.1 Audio device: NVIDIA Corporation **GP106** High Definition Audio Controller (rev a1)

PyTorch Installations

- In practice, we always install frameworks to work with GPUs
 - However, this comes with several challenges
- An easier initial start is just to install to work with **CPUs**
 - You can even develop in this mode and launch later code on some GPU cloud



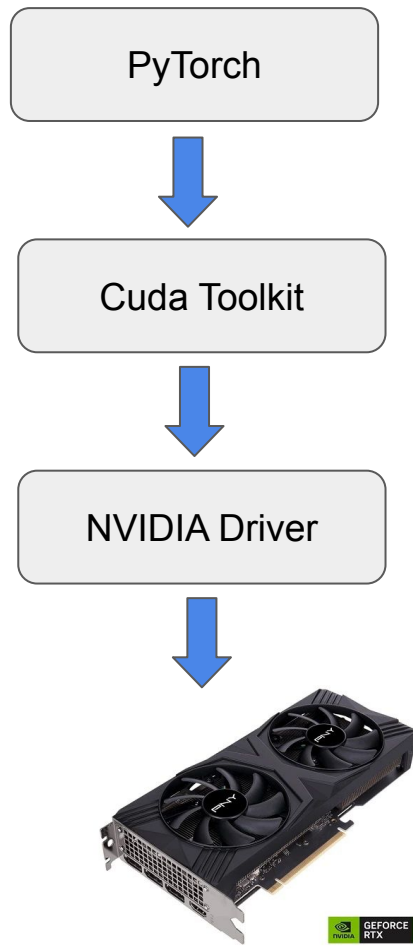
Pytorch CPU

- Go to: <https://pytorch.org/get-started/locally/>
 - Make different selections, including conda and cpu
 - E.g. inside your conda run: **conda install** pytorch torchvision torchaudio cpuonly -c pytorch

PyTorch Build	Stable (2.1.0)		Preview (Nightly)	
Your OS	Linux	Mac		Windows
Package	Conda	Pip	LibTorch	Source
Language	Python		C++ / Java	
Compute Platform	CUDA 11.8	CUDA 12.1	ROCm 5.6	CPU
Run this Command:	conda install pytorch torchvision torchaudio cpuonly -c pytorch			

PyTorch Installations on GPU (Ubuntu)

- 3 steps in order
- 1) NVIDIA Driver
 - Installed on the OPERATING SYSTEM
- 2) Cuda toolkit
 - Installed on
 - Either install on OS locally and your framework use it
 - With your framework directly (in step 3) so no step 2
 - Must match a **minimum version** of the **driver**.
- 3) PyTorch
 - Installed on your conda / pip



- This page is updated with CUDA Toolkit and [Corresponding](#) Driver Versions

CUDA Toolkit	Linux x86_64 Driver Version	Windows x86_64 Driver Version
CUDA 12.3	>=545.23.06 ubuntu 20+	>=545.84
CUDA 12.0	>=525.60.13 ubuntu 18+	>=527.41
CUDA 11.7	>=515.48.07 ubuntu 18+	>=516.31
CUDA 11.6	>=510.47.03 ubuntu 18+	>=511.65
CUDA 11.4	>=470.82.01 ubuntu 18+	>=472.50
CUDA 11.3	>= 465.19.01 ubuntu 18+	>=465.89
CUDA 10.1	>= 418.39 ubuntu 18+	>= 418.96
CUDA 9.0	>= 384.81 ubuntu 16+	>= 385.54
CUDA 8.0	>= 367.48	>= 369.30

[February 02, 2023](#): Deprecation of CUDA 11.6 and Python 3.7 Support

NVIDIA driver

- A software package that enables the operating system to communicate with NVIDIA GPUs. It includes
 - **CUDA Driver**: The interface between CUDA applications and the GPU
 - **Graphics Driver** for rendering 2D and 3D graphics.
 - **Display Driver**: Includes Control Panel GUI for configuring GPU settings / rendering
 - **nvidia-smi** [tool](#): command-line utility to manage NVIDIA GPUs. [Details](#)
 - `nvidia-smi`
 - `watch nvidia-smi` (keep refreshing - very useful)
 - `nvidia-smi -a` (comprehensive details)
 - SDKs like **cuDNN**

nvidia-smi

```
moustafa@moustafa-Aspire-VN7-793G:~/system-installs1/pycharm-community-2018.2/bin$ nvidia-smi
Mon Oct 30 18:32:12 2023
```

NVIDIA-SMI 470.182.03					Driver Version: 470.182.03		CUDA Version: 11.4	
GPU	Name	Persistence-M	Bus-Id	Disp.A	Volatile	Uncorr. ECC		
Fan	Temp	Perf	Pwr:Usage/Cap	Memory-Usage	GPU-Util	Compute M.		
						MIG M.		
0	NVIDIA GeForce ...	Off	00000000:01:00.0	Off		N/A		
N/A	60C	P0	26W / N/A	740MiB / 6078MiB	32%	Default		
						N/A		

Processes:						
GPU	GI ID	CI ID	PID	Type	Process name	GPU Memory Usage
0	N/A	N/A	3062	G	/usr/lib/xorg/Xorg	347MiB
0	N/A	N/A	3226	G	/usr/bin/gnome-shell	209MiB
0	N/A	N/A	31838	G	...061346670394462259,262144	108MiB
0	N/A	N/A	32449	G	...veSuggestionsOnlyOnDemand	71MiB

Installing NVIDIA Driver: GUI

- From the GUI, go to your Ubuntu Software and Update
 - Click Additional Drivers
 - Select one and install
 - Restart after installation
- The higher the driver version, the higher cuda toolkit and PyTorch version
 - However, many of these listed version may fail to be installed
 - Due to your OS / Hardware / Driver code itself

Ubuntu Software

Other Software

Updates

Authentication

Additional Drivers

Developer Options

Ubuntu Pro

**NVIDIA Corporation: GP106M [GeForce GTX 1060 Mobile]**

This device is using the recommended driver.

- ☒ Using NVIDIA driver metapackage from nvidia-driver-470 (proprietary, tested)
- ☐ Using NVIDIA driver metapackage from nvidia-driver-530 (proprietary)
- ☐ Using NVIDIA driver metapackage from nvidia-driver-510 (proprietary)
- ☐ Using NVIDIA driver metapackage from nvidia-driver-390 (proprietary)
- ☐ Using NVIDIA Server Driver metapackage from nvidia-driver-470-server (proprietary)
- ☐ Using NVIDIA driver metapackage from nvidia-driver-525 (proprietary)
- ☐ Using NVIDIA Server Driver metapackage from nvidia-driver-515-server (proprietary)
- ☐ Using NVIDIA Server Driver metapackage from nvidia-driver-450-server (proprietary)
- ☐ Using NVIDIA Server Driver metapackage from nvidia-driver-418-server (proprietary)
- ☐ Using NVIDIA driver metapackage from nvidia-driver-515 (proprietary)
- ☐ Using NVIDIA Server Driver metapackage from nvidia-driver-525-server (proprietary)
- ☐ Using X.Org X server – Nouveau display driver from xserver-xorg-video-nouveau (open source)

1 proprietary driver in use.

Revert

Apply Changes

A proprietary driver has private code that Ubuntu developers can't review or improve. Security and other updates are dependent on the driver vendor.

Close

Installing NVIDIA Driver: Terminal

- To check drivers for your card
 - `sudo ubuntu-drivers list`
 - driver : nvidia-driver-470-server - distro non-free
 - driver : nvidia-driver-515-server - distro non-free
 - driver : nvidia-driver-470 - distro non-free **recommended**
 - driver : nvidia-driver-525-server - distro non-free
- `sudo apt update`
- `sudo apt install nvidia-<driver number>`
 - `sudo apt install nvidia-470`
- Or `sudo ubuntu-drivers install`
 - will install the driver that is considered the **best match** for your hardware
- Restart after installation

Installing NVIDIA Driver: Troubleshooting

- Installing the driver can easily go wrong after restarting
 - Login page doesn't appear
 - Login loop problem: login returns you to login
- Don't rush to OS reinstallation: Google the error and get help for commands to run
- To run commands, you may Switch to Console Mode
 - Press **Ctrl + Alt + F1** to switch from the graphical interface to a console terminal.
 - You can also use F2, F3, etc., to switch to different terminals.
 - **Login** (numpad may not work)
 - **Stop the Display Manager:** `sudo systemctl stop gdm`
 - Uninstall Old Drivers:
 - `sudo apt-get purge nvidia*` **then** `sudo apt-get autoremove` **then** `sudo apt-get autoclean`
 - You may now restart or try installing another driver from the terminal
 - **Restart** the Display Manager: `sudo systemctl start gdm`
 - **Reboot:** `sudo reboot`
- For windows: Boot into Safe Mode (e.g. F8 or Shift F8)

CUDA Toolkit

- The **CUDA Toolkit** is a development environment for **building applications** (GPU-accelerated).
 - Include libraries, compiler, linker tools, debugging/ optimization, APIs, and runtime libraries.
- Below are some key components:
 - **CUDA Libraries:**
 - **cuBLAS**: for Linear Algebra / matrix operations.
 - **NCCL** (NVIDIA Collective **Communications** Library): For multi-GPU / multi-node
 - cuFFT, cuRAND, cuSPARSE, cuSOLVER, NPP, Thrust (parallel algorithms)
 - CUDA Compiler (**nvcc**) and Linker (nvlink)
 - Profiling and Debugging Tools: Nsight Compute / CUDA-GDB / CUDA-MEMCHECK
 - APIs: CUDA Runtime (high-level) and CUDA Driver (low-level) APIs
 - Utilities: Visual Profiler / Bandwidth Test Utilities
- Tip: Download .deb file and install it

CUDA Toolkit

- The official page will have the latest toolkit, but you can google a version
 - E.g. CUDA Toolkit 11.7 Update 1 Downloads
 - Make choices and select deb

Operating System	Linux	Windows								
Architecture	x86_64	ppc64le	arm64-sbsa							
Distribution	CentOS	Debian	Fedora	OpenSUSE	RHEL	Rocky	SLES	Ubuntu	WSL-Ubuntu	
Version	18.04	20.04	22.04							
Installer Type	deb (local)	deb (network)	runfile (local)							

CUDA Toolkit

- Follow the commands. Google the internet for errors

Installation Instructions:

```
$ wget https://developer.download.nvidia.com/compute/cuda/repos/ubuntu1804/x86_64/cuda-ubuntu1804.pin
$ sudo mv cuda-ubuntu1804.pin /etc/apt/preferences.d/cuda-repository-pin-600
$ wget https://developer.download.nvidia.com/compute/cuda/11.7.1/local_installers/cuda-repo-ubuntu1804-11-7-local_11.7.1-515.65.01-1_amd64.deb
$ sudo dpkg -i cuda-repo-ubuntu1804-11-7-local_11.7.1-515.65.01-1_amd64.deb
$ sudo cp /var/cuda-repo-ubuntu1804-11-7-local/cuda-*-keyring.gpg /usr/share/keyrings/
$ sudo apt-get update
$ sudo apt-get -y install cuda
```

CUDA Toolkit: Troubleshooting

- Sometimes the cuda is not seen by something
- You need to add it to your .bashrc
- Add the following lines to your .bashrc
 - export **PATH**=/usr/local/cuda-<version>/bin\${PATH:+:\${PATH}}
 - export **LD_LIBRARY_PATH**=/usr/local/cuda-<version>/lib64\${LD_LIBRARY_PATH:+:\${LD_LIBRARY_PATH}}
 - Tip: verify the paths
- Run **source ~/.bashrc** to refresh your **environment** variables.
 -

Installing PyTorch GPU

- Go to: <https://pytorch.org/get-started/locally/>
 - Now select the cuda version
 - However, this is always the latest
 - `pip3 install torch torchvision torchaudio --index-url https://download.pytorch.org/whl/cu118`
 - Then google target version
 - Many versions [here](#)
 - `conda install pytorch==2.0.0 torchvision==0.15.0 torchaudio==2.0.0 pytorch-cuda=11.7 -c pytorch -c nvidia`
 - `conda install pytorch==1.13.1 torchvision==0.14.1 torchaudio==0.13.1 pytorch-cuda=11.7 -c pytorch -c nvidia`
 - `conda install pytorch==1.12.1 torchvision==0.13.1 torchaudio==0.12.1 cudatoolkit=11.3 -c pytorch`
 - `conda install pytorch==1.9.1 torchvision==0.10.1 torchaudio==0.9.1 cudatoolkit=11.3 -c pytorch -c conda-forge`
 - `conda install pytorch==1.13.1 torchvision==0.14.1 torchaudio==0.13.1 pytorch-cuda=11.6 -c pytorch -c nvidia`
 - `conda install pytorch==1.11.0 torchvision==0.12.0 torchaudio==0.11.0 cudatoolkit=10.2 -c pytorch`

Check PyTorch GPU

- You can do so in the console
- `import torch`
- `print(torch.version.cuda)`
- `print(torch.cuda.is_available())`
- `print(torch.cuda.device_count())`
- If nvidia-smi shows a GPU but device_count = 0, then some **mismatch** in installations


```
(test) moustafa@moustafa-Aspire-VN7-793G:~/system-installs1/pycharm-community-2018.2/bin$ conda list | grep pytorch
ffmpeg                4.3                hf484d3e_0      pytorch
pytorch                1.12.0             py3.9_cuda11.3_cudnn8.3.2_0  pytorch
pytorch-mutex         1.0                cuda            pytorch
torchaudio            0.12.0             py39_cu113      pytorch
torchvision           0.13.0             py39_cu113      pytorch
(test) moustafa@moustafa-Aspire-VN7-793G:~/system-installs1/pycharm-community-2018.2/bin$ python
Python 3.9.18 | packaged by conda-forge | (main, Aug 30 2023, 03:49:32)
[GCC 12.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> print(torch.version.cuda)
11.3
>>> print(torch.cuda.is_available())
True
>>> print(torch.cuda.device_count())
1
>>> exit()
(test) moustafa@moustafa-Aspire-VN7-793G:~/system-installs1/pycharm-community-2018.2/bin$
```

Prepackaged Toolkit

- It seems latest PyTorch binaries come **pre-packaged** with their own copies of **CUDA libraries** such as cuBLAS, cuDNN, and NCCL.
 - This setup is designed to make it easier to get started with PyTorch without having to manually manage CUDA dependencies
- This suggests we don't need to do step 2 explicitly (toolkit installation).
- So try step 1 and step 3. If still facing problems, add step 2

Upgrades

- Sometimes, you would like to make an upgrade to a different PyTorch version
- Don't just start installations
- First, identify the corresponding toolkit and then the driver
- If your target driver is higher than the installed one, you will need to install a new driver (which may come with troubles)
 - First remove existing nvidia driver
- If you succeeded, then install the new toolkit
 - Better in a new conda env to not lose the old one

nvcc

- The NVIDIA CUDA Compiler (nvcc) is a command-line tool that serves as a wrapper around the **NVIDIA C/C++ compiler** (nvcc).
 - It compiles CUDA source files to generate object code or executables that can run on NVIDIA GPUs.
 - nvcc enables developers to include CUDA C/C++ code in the form of source code or device functions within host code, which is typically written in C/C++.
- Most of the time, you don't need to worry about it
- If you want it and you don't find it installed, you may install with
 - `sudo apt install nvidia-cuda-toolkit`

Suitable GPU

- Speed and GPU RAM are critical factors
- During my PhD/Work, I found 12 **GPU Ram (VRAM)** are a must for training
 - With nowadays transformers / LLMs, one may need 24+
- Don't aim for a laptop to **train** Deep Networks
 - It will be very expensive (4k+) - hard to replace the GPU
 - You can use a cheap NVIDIA GPU to **do inference** or basic training cycle for validation
 - Then you need some cloud service that trains for you
 - Also, training on your local laptop will noisy and busy for hours/days to train
 - If you can afford it, you can build a desktop for 5k USD
 - Consider also machine RAM 16+ / SSD 1T / 4T HDD
- Educate yourself: [here](#) / [here](#)
- Tip: there are websites to evaluate if components work together

“Acquire knowledge and impart it to the people.”

“Seek knowledge from the Cradle to the Grave.”

