Deep Learning Software installation & Code implementation

Lu Lu

Department of Chemical and Biomolecular Engineering
Penn Institute for Computational Science
University of Pennsylvania

Tianyuan Mathematical Center in Southeast China Dec 8, 2021



Softwares



• Python libraries: NumPy, SciPy, Matplotlib, DeepXDE, etc.







• Deep learning frameworks: TensorFlow, PyTorch, etc.





Python

- Anaconda ANACONDA
- https://www.anaconda.com

- Linux
- Windows Subsystem for Linux

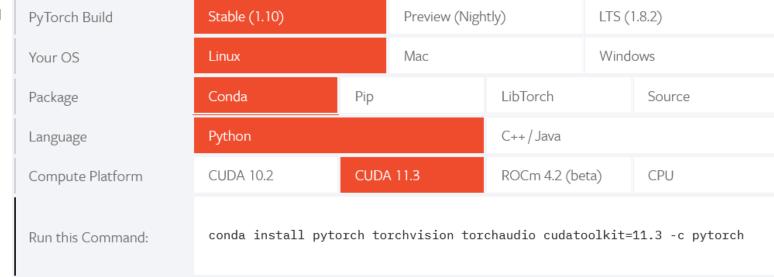
PyTorch

CPU

https://pytorch.org







TensorFlow

https://www.tensorflow.org

```
# Current stable release for CPU and GPU
$ pip install tensorflow
```

- GPU: compatible versions of NVIDIA driver, CUDA, cuDNN
 - Can be directly installed on OS
 - Install CUDA and cuDNN in Anaconda

Package	Version	Source
cudatoolkit	11.2.2	conda-forge
cudnn	8.1.0.77	conda-forge
TensorFlow	2.6.2	pip
tensorflow-probability	0.14.1	pip
tensorflow-addons	0.14.0	pip

Updated on 11/17/2021

DeepXDE

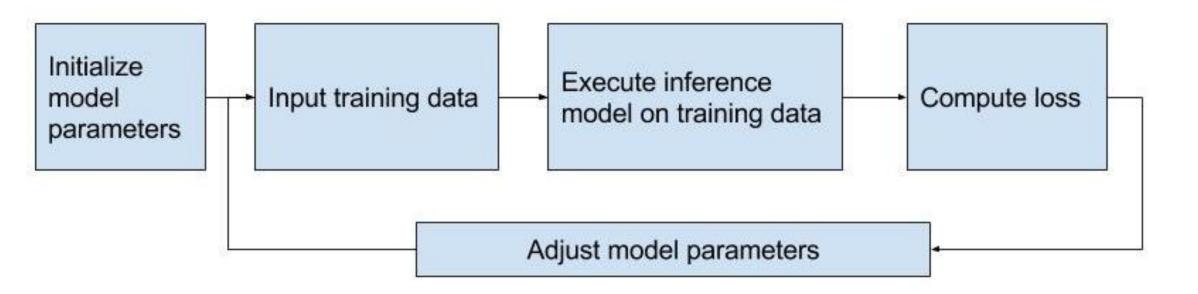
- https://github.com/lululxvi/deepxde
- https://deepxde.readthedocs.io

GPU

- Monitor GPU status
 - \$ nvidia-smi
 - \$ gpustat https://github.com/wookayin/gpustat

- Run on GPU 0
 - \$ CUDA_VISIBLE_DEVICES=0 python nn.py
- Run on CPU
 - \$ CUDA_VISIBLE_DEVICES=-1 python nn.py

Training loop



Hands-on

