

Deep Learning

Software installation & Code implementation

Lu Lu

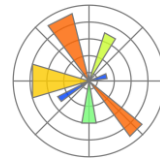
Department of Chemical and Biomolecular Engineering
Penn Institute for Computational Science
University of Pennsylvania

Tianyuan Mathematical Center in Southeast China
Dec 8, 2021

Softwares

- Python 


- Python libraries: NumPy, SciPy, Matplotlib, etc.



- Deep learning frameworks: TensorFlow, PyTorch, etc.



Python

- Anaconda  **ANACONDA**
- <https://www.anaconda.com>
- Linux
- Windows Subsystem for Linux

PyTorch

- <https://pytorch.org>

CPU

PyTorch Build	Stable (1.10)		Preview (Nightly)		LTS (1.8.2)
Your OS	Linux		Mac		Windows
Package	Conda	Pip		LibTorch	Source
Language	Python			C++ / Java	
Compute Platform	CUDA 10.2	CUDA 11.3	ROCm 4.2 (beta)		CPU
Run this Command:	conda install pytorch torchvision torchaudio cpuonly -c pytorch				

GPU

PyTorch Build	Stable (1.10)		Preview (Nightly)		LTS (1.8.2)	
Your OS	Linux		Mac		Windows	
Package	Conda	Pip		LibTorch		Source
Language	Python			C++ / Java		
Compute Platform	CUDA 10.2	CUDA 11.3		ROCm 4.2 (beta)		CPU
Run this Command:	conda install pytorch torchvision torchaudio cudatoolkit=11.3 -c pytorch					

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
cuda toolkit	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

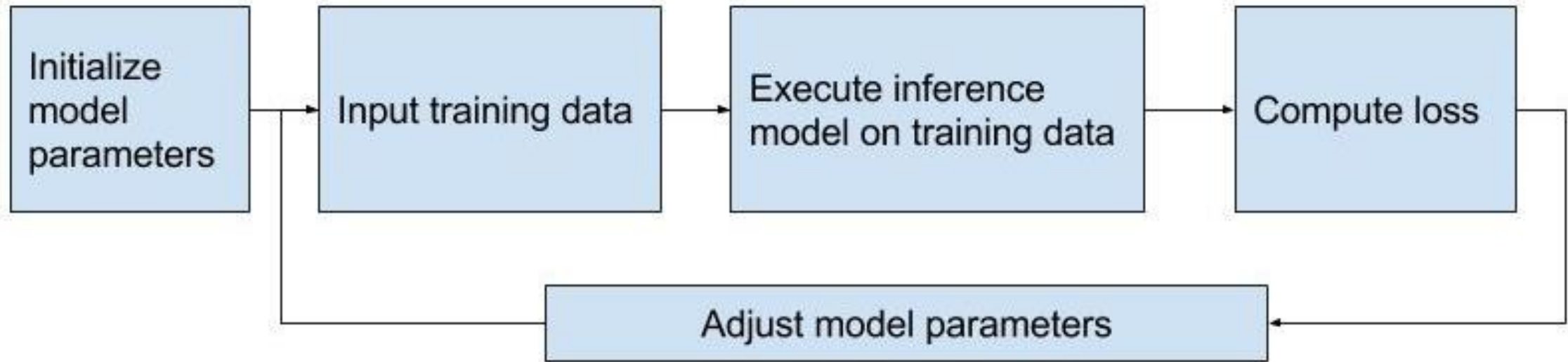
DeepXDE

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

GPU

- Monitoring 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

