Introduction to PyTorch

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Tutorial session, STAT8056 2023 Spring

Slides and notebook available at: https://github.com/yifei-liu-stat/stat8056-intro-pytorch

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Outline

- Set up working environment
  - Coding platform
  - Practice: create conda environment for your project
- Introduction to PyTorch framework
- Deep learning with PyTorch
- Additional resources

Coding platform

On your local machine

Use Anaconda to manage packages:

- Go to anaconda.com
- Download Anaconda
- Open Anaconda Navigator (GUI)
  - Create an isolated environment for each of your projects.
  - Manage dependencies/versions of packages within the environment.
- Alternatively, one can use Anaconda in command-line style.

Notebook-style coding:

- In Anaconda Navigator, install Jupyter Notebook (if not already)
- Launch Jupyter Notebook.

Script-style coding:

- Choose an IDE to start with.
- Take VS Code for example:
  - Download VS Code.
  - Follow this tutorial to learn how to use Python in Visual Studio Code.

Coding platform

On a remote host/server

Google Colab (for this tutorial)

- Notebook-style cloud computing.
  - https://colab.research.google.com/
  - Free version runs up to 12 hrs.
- Free GPU resource:
  - Runtime | Change runtime type | Hardware accelerator | GPU
- Many libraries (numpy, torch, scikit-learn …) are pre-installed.
- Co-edit/code with collaborators.
- In sync. with your Google Drive.

Resources from MSI:

- Need to be in a research group to use the cluster. MSI access.
- Support Jupyter notebook now:
  - Connect to UMN VPN (off-campus only)
  - Visit notebooks.msi.umn.edu
  - Choose and start a server.
- Free MSI tutorial (with recordings)

Other cloud services:

- Deep-learning-in-cloud
  - A list of cloud vendors either with free or paid services (with some free credits)

UMN computing resources

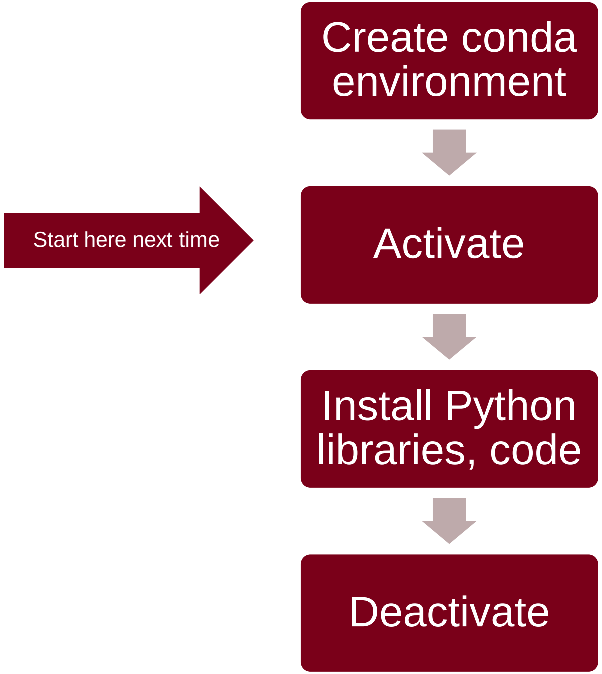
MSI: https://www.msi.umn.edu/

Introduction to Minnesota Supercomputing Institute (MSI)	This tutorial is geared to new MSI users and will provide a highlevel introduction to the facilities and computational resources at MSI.	02/01/2022
Introduction to Linux	This tutorial will provide an introduction to the Linux operating system, with particular attention paid to working from the command line	02/03/2022
Programming with Python	Introduction to fundamentals of programming using the python language.	02/08/2022
Job Submission and Scheduling at MSI	This tutorial will introduce users to MSI supercomputers, and provide an overview of how to submit calculations to the job schedulers	02/10/2022
Interactive Computing at MSI	This two part tutorial will introduce you to the concept of interactive high performance computing, and provide attendees hands-on experience running interactive parallel jobs on the Mesabi HPC	02/15/2022
Data Storage Systems and Data Analysis Workflows for Research	In this tutorial you will learn about the data storage systems available for academic research at the University of Minnesota	02/17/2022
Compiling and Debugging at MSI	This tutorial will help users learn the basics of compiling and debugging their code on MSI systems	02/24/2022
Python for Scientific Computing	This session includes efficient data processing with NumPy and Scipy, data visualization, and techniques for using python to drive parallel supercomputing tasks.	03/01/2022
RNA-Seq Analysis	This tutorial covers the basics of differential expression analysis and touches on other RNA-seq topics such as transcriptome assembly.	03/03/2022
Parallel Computing On Agate	This tutorial will help users learn the basics of parallel computation methods, including strategies for collecting calculations together for parallel execution.	03/31/2022

LATIS: https://latisresearch.umn.edu/

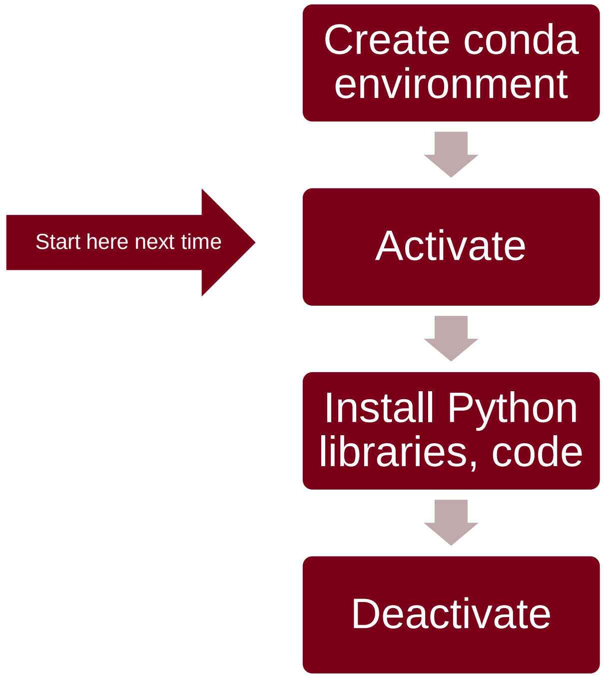
Feb. 18th | 10:00am-noon	Creating Publication Worthy Visualizations without Code	Registration
Feb. 25th | 10:00am-noon	Introduction to Computational Text Analysis	Registration
Mar. 4th | 10:00am-noon	Reproducible research practices in Excel (yes, Excel)	Registration
Mar. 9th | 10:00am-noon	Data Management in transition: Strategies for when you graduate	Registration
Mar. 18th | 10:00am-noon **[RESCHEDULED]**	Advanced Nvivo	Registration
Mar. 25th | 10:00am-noon	Introduction to parallel computing	Registration
April 1st | 10:00am-noon	Introduction to SQL and Research Databases	Registration

Create a conda environment for your Python project



- An alternative way to Virtualenv
- Manage dependencies (**different versions** of Python and some libraries) **within an isolated project**
  - An example: Python library [foolbox]()
- Key commands:
  - conda create -n <envname> python=3.8.3
  - conda activate <envname>
  - conda install <package>=<version>
  - conda deactivate
- Check [Conda Cheat Sheet]()

A hands-on exercise



- Make sure Anaconda is installed (either on your local machine or a remote host)
  - Windows: open Anaconda Prompt
  - MacOS/Linux: open terminal
  - Type `conda --version` to check availability
- Create an environment for course project
  - `conda create -n 8056proj python=3.9.13`
  - `conda activate 8056proj`
  - `conda install numpy`
  - `conda install jupyter notebook`
  - Do some coding:
    - Launch Jupyter Notebook: `jupyter notebook`
    - Launch Python terminal: `python`
  - `conda deactivate`

Installation of PyTorch

- Choose configurations and install PyTorch from http://pytorch.org/

PyTorch Build	Stable (1.11.0)	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`			

```
conda install pytorch torchvision torchaudio cudatoolkit=11.3 -c pytorch
```

Previous versions of PyTorch >

Run this within your conda environment

- If you use Google Colab, PyTorch is pre-installed with suitable configurations.

Outline

- Set up working environment
- Introduction to PyTorch framework
  - Tensor, gradient and computation graph
  - Tensor manipulation on GPU
  - Use PyTorch as a general ML framework
- Deep learning with PyTorch
- Additional resources

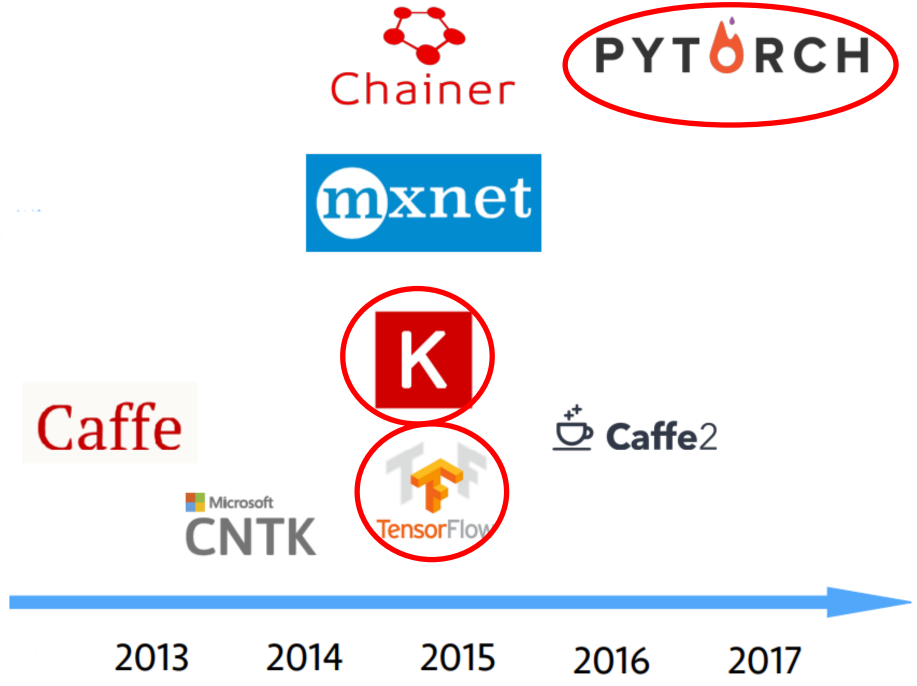
Overview of PyTorch

A fancy version of NumPy but can:

- Trace gradient via autograd
- Accelerate via GPU
- Accommodate a bunch of machine learning functionalities including but not limited to neural network

More importantly,

- Easy interface compared to others
- Easy to understand and debug
- Check this [Google Trends](#)



Credit: "Gluon: new MXNet interface to accelerate research"

Tensor

What is a tensor?

- A multidimensional array
- Some examples:
  - 0D-tensor: scalar
  - 1D-tensor: vector
  - 2D-tensor: matrix; non-RGB image
  - 3D-tensor: RGB image (3 channels)
  - 4D-tensor: one RGB video clip
  - 5D-tensor: a collection of RGB video clips
  - 6D-tensor: ???
- Tensor in PyTorch:
  - Just like arrays in Numpy
  - `t.numpy()` and `torch.from_numpy(a)`

np.array versus torch.tensor

- Similar object creations:
  - All-ones, all-zeros, identity matrix, random…
  - Check [PyTorch tensor creations]
- Similar math operations:
  - Indexing, slicing, reshape, transpose, tensor product, element-wise operation…
  - Check [PyTorch tensor math operations]

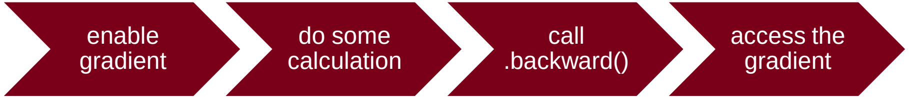
```python
import numpy as np
myarray = np.ones(3)
print(myarray)
print(myarray + 1.5)
```

```
[1. 1. 1.]
[2.5 2.5 2.5]
```

```python
import torch
mytensor = torch.ones(3)
print(mytensor)
print(mytensor + 1.5)
```

```
tensor([1., 1., 1.])
tensor([2.5000, 2.5000, 2.5000])
```

Tensor (cont.)



- Enable gradient tracing:
  - Upon any tensor creation, set `requires_grad = True`
  - For any existent tensor `t`, call `t.requires_grad_(True)`
- Calculate gradient:
  - Do some calculation from `t` and get `f`
  - Call `f.backward()` for calculation
  - Call `t.grad` to access the gradient
- Disable gradient tracing:
  - (Permanently) `t = t.detach()`
  - (Temporarily) `with torch.no_grad():`

```python
# create tensors, and enable gradient tracing
c = torch.tensor(1.)
t = torch.tensor(3., requires_grad = True)
print("Tensor c:", c)
print("Tensor t:", t)

# do some calculation
s = t**2
f = 3 * s + c

# calculate the gradient of f w.r.t. t
f.backward()

# access the gradient
print("Gradient df/dt:", t.grad)
```

```
Tensor c: tensor(1.)
Tensor t: tensor(3., requires_grad=True)
Gradient df/dt: tensor(18.)
```

Dynamic computation graph

enable gradient → do some calculation → call .backward() → access the gradient

t

c

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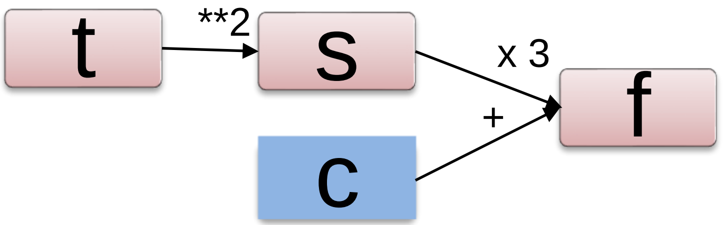


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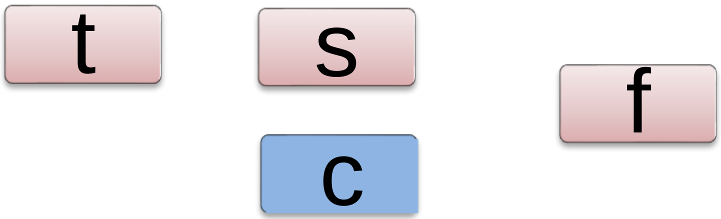
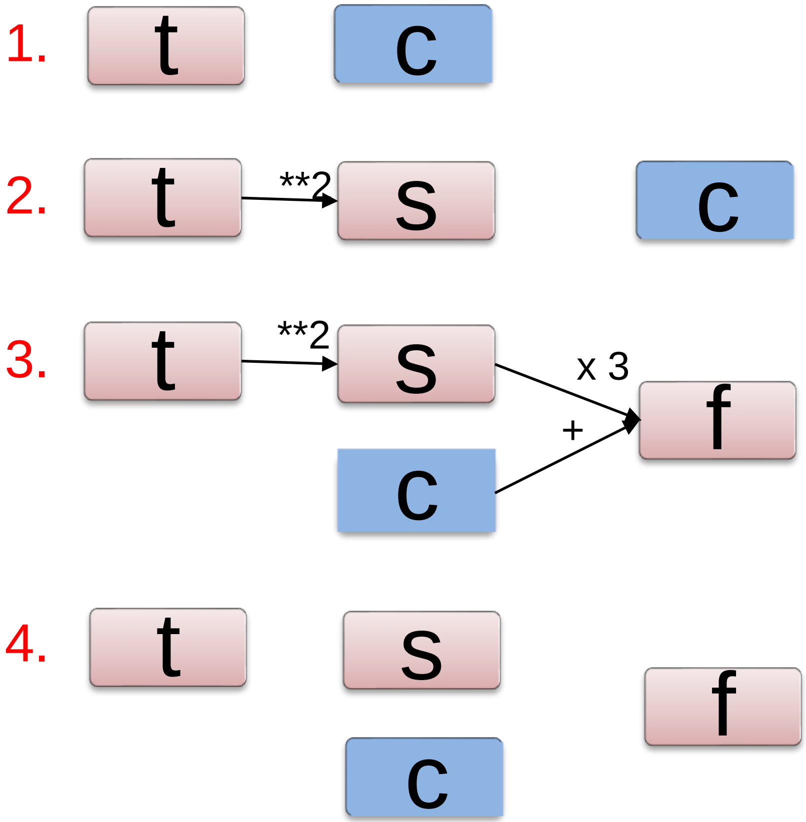
Gradient df/dt: tensor(18.)
```

The graph structure is destroyed
Once you call `.backward()`



Dynamic computation graph

enable gradient → do some calculation → call .backward() → access the gradient

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Gradient df/dt: tensor(18.)
```

Why should we understand PyTorch computation graph?

- Essentially, PyTorch is using chain rule to calculate the gradient
- A computation graph defines how the chain rule applies to your calculation
- Common MISTAKES:
  - Call `.backward()` when there is no graph
  - Retrieve gradient of non-leaf nodes
  - Gradient accumulation. To solve this problem, call `t.grad.zero_()` before building the second graph

Illustration of gradient accumulation

```python
# first back propagation
t = torch.tensor(3., requires_grad = True)
s = t**2
s.backward()
print("Gradient ds/dt:", t.grad)

# second back propagation
f = 5 * t + 1
f.backward()
print("Gradient df/dt (without emptying t.grad):", t.grad)
```

should be 5

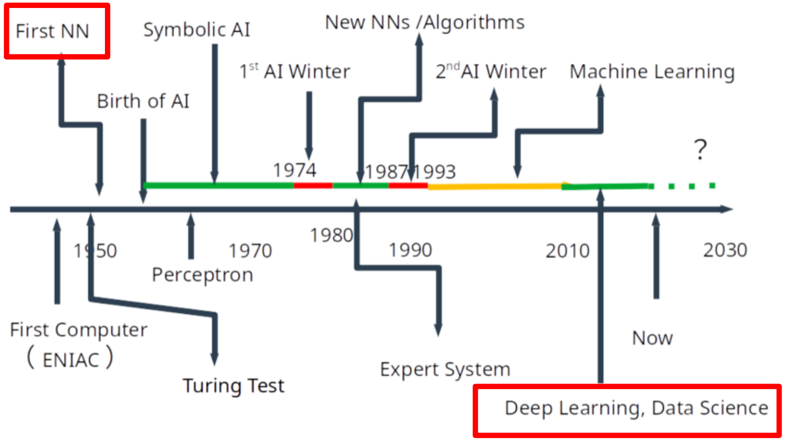
```
Gradient ds/dt: tensor(6.)
Gradient df/dt (without emptying t.grad): tensor(11.)
```

```python
t.grad.zero_() # zero out the gradient
f = 5 * t + 1
f.backward()
print("Gradient df/dt (after emptying t.grad):", t.grad)
```

```
Gradient df/dt (after emptying t.grad): tensor(5.)
```

Calculation on GPU

- Neural network dates back to 1950s, but became popular only recently (last decade) due to huge improvements in computation



Credit: CSCI 5980/8980: Think Deep Learning offered by Ju Sun, UMN

- GPU allows faster large-scale matrix multiplication (or tensor product)
- Use GPU on PyTorch:
  - `torch.cuda.is_available() # GPU?`
  - `t = t.cuda() # move to GPU`
  - `t = t.cpu() # move to CPU`
  - `t.device # cpu or cuda: index`
  - The transfer time can be long
  - Make sure all tensor manipulations are performed on the same device
- Advanced: [train on multiple GPUs]()

Time comparison: matrix multiplication on CPU and GPU

- We want to perform matrix multiplication C = AB where both A and B are 3000 x 3000 matrices

- Enable GPU on [Google Colab](#)(free!)
  1. Runtime
  2. Change runtime type
  3. Hardware Accelerator: GPU
  4. Runtime -> Restart Runtime

- Much faster on GPU for large problem!

```python
np.random.seed(8056)

d = 3000

# C = A B with numpy on CPU
A = np.random.rand(d, d)
B = np.random.rand(d, d)
begin = time.time()
C = A.dot(B)
print(f"CPU time (numpy): {time.time() - begin} s")

# C = A B with torch on CPU
A_t_cpu = torch.tensor(A)
B_t_cpu = torch.tensor(B)
begin = time.time()
C = torch.mm(A_t_cpu, B_t_cpu)
print(f"CPU time (torch): {time.time() - begin} s")

# C = A B with torch on GPU
# make sure GPU is available
A_t_gpu = torch.tensor(A).cuda()
B_t_gpu = torch.tensor(B).cuda()
begin = time.time()
C = torch.mm(A_t_gpu, B_t_gpu)
print(f"GPU time (torch): {time.time() - begin} s")
```

```
CPU time (numpy): 1.0066237449645996 s
CPU time (torch): 0.8800492286682129 s
GPU time (torch): 0.0038247108459472656 s
```

GPU not always better

- Calculation on GPU should be optimized smartly since
  - GPU has limited memory compared to CPU
  - Transfer/overhead time from CPU to GPU can be large

```python
d = 3000
begin = time.time()
A = torch.rand((d, d)).cuda()
B = torch.rand((d, d)).cuda()
print(f"Time from CPU to GPU: {time.time() - begin} s")
begin = time.time()
C = torch.mm(A, B)
print(f"GPU time (torch): {time.time() - begin} s")
```

```
Time from CPU to GPU: 0.15282464027404785 s
GPU time (torch): 0.0008263587951660156 s
```

```
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 440.100      Driver Version: 440.100      CUDA Version: 10.2     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|===============================+======================+======================|
|   0  TITAN RTX           Off  | 00000000:1A:00.0 Off |                  N/A |
| 41%   56C    P2   129W / 280W |  13556MiB / 24220MiB |     61%      Default |
+-------------------------------+----------------------+----------------------+
|   1  TITAN RTX           Off  | 00000000:1B:00.0 Off |                  N/A |
| 41%   55C    P2   127W / 280W |  18798MiB / 24220MiB |     60%      Default |
+-------------------------------+----------------------+----------------------+
|   2  TITAN RTX           Off  | 00000000:3D:00.0 Off |                  N/A |
| 41%   48C    P2   121W / 280W |  13616MiB / 24220MiB |     62%      Default |
+-------------------------------+----------------------+----------------------+
|   3  TITAN RTX           Off  | 00000000:3E:00.0 Off |                  N/A |
| 41%   56C    P2   121W / 280W |  20962MiB / 24220MiB |     61%      Default |
+-------------------------------+----------------------+----------------------+
|   4  TITAN RTX           Off  | 00000000:88:00.0 Off |                  N/A |
| 41%   53C    P2   162W / 280W |  13590MiB / 24220MiB |     92%      Default |
+-------------------------------+----------------------+----------------------+
|   5  TITAN RTX           Off  | 00000000:89:00.0 Off |                  N/A |
| 41%   59C    P2   155W / 280W |  18832MiB / 24220MiB |     61%      Default |
+-------------------------------+----------------------+----------------------+
|   6  TITAN RTX           Off  | 00000000:B1:00.0 Off |                  N/A |
| 41%   55C    P2   169W / 280W |  13650MiB / 24220MiB |     90%      Default |
+-------------------------------+----------------------+----------------------+
|   7  TITAN RTX           Off  | 00000000:B2:00.0 Off |                  N/A |
| 41%   56C    P2   109W / 280W |  20996MiB / 24220MiB |     91%      Default |
+-------------------------------+----------------------+----------------------+
```

ML in PyTorch

- PyTorch provides a framework for general ML modeling including but not limited to deep learning
- What is a common ML pipeline?
  - Prepare your dataset
  - Choose a training model
  - Choose a loss/objective function
  - Optimization (calculation; gradient)
  - Evaluation and inference
- The go-to optimization: SGD
  - Instead of using gradient calculated from all training samples, we only use the gradient from a randomly chosen sample
- Practical one: (Mini-) Batch SGD
  - Use gradient from a batch of samples
  - **Batch size**: # samples in one batch
  - **Epoch**: a full pass of all training samples
  - Special cases:
    - Batch size = 1: vanilla SGD
    - Batch size = n: GD

Linear regression with SGD – The naive way

- The true model: y = 2 * x + 1
- Some other setups:
  - n = 2000, x ~ Uniform(0, 1)
  - Number of epochs: 10
  - Batch size: 200 (10 batches per epoch)
  - Learning rate: 0.05
  - Initialize both intercept and slope with Uniform(0, 1)

```python
n = 2000
x = torch.rand(n)

# create dataset with true model
a0 = 2
b0 = 1
y = a0 * x + b0

# set up optimization parameter of SGD
a = torch.rand(1, requires_grad = True)
b = torch.rand(1, requires_grad = True)
nepochs = 10
batch_size = 200
lr = 0.5
```

Linear regression with SGD – The naive way

```
for epoch in range(nepochs):
  for batch in range(round(n / batch_size)):
    start = batch * batch_size
    end = start + batch_size
    # perform update on a batch
    x_batch = x[start:end]
    y_batch = y[start:end]

    # build computation graph
    y_hat = a * x_batch + b
    myloss = torch.mean((y_batch - y_hat)**2)

    # gradient calculation
    myloss.backward()

    # SGD update
    with torch.no_grad():
      a -= lr * a.grad
      b -= lr * b.grad

    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()

  print(f"Epoch: {epoch + 1} / {nepochs}")
  print(f"MSE: {myloss: .2e}; a: {a.item():.4f}; b: {b.item():.4f}")
```

Outer iteration of SGD (epoch)

Output:

```
Epoch: 1 / 10
MSE:  3.69e-02; a: 1.4460; b: 1.2822
Epoch: 2 / 10
MSE:  9.24e-03; a: 1.7226; b: 1.1413
Epoch: 3 / 10
MSE:  2.32e-03; a: 1.8611; b: 1.0707
Epoch: 4 / 10
MSE:  5.81e-04; a: 1.9305; b: 1.0354
Epoch: 5 / 10
MSE:  1.46e-04; a: 1.9652; b: 1.0177
Epoch: 6 / 10
MSE:  3.65e-05; a: 1.9826; b: 1.0089
Epoch: 7 / 10
MSE:  9.15e-06; a: 1.9913; b: 1.0044
Epoch: 8 / 10
MSE:  2.29e-06; a: 1.9956; b: 1.0022
Epoch: 9 / 10
MSE:  5.75e-07; a: 1.9978; b: 1.0011
Epoch: 10 / 10
MSE:  1.44e-07; a: 1.9989; b: 1.0006
```

Linear regression with SGD – The naive way

```
for epoch in range(nepochs):
  for batch in range(round(n / batch_size)):
    start = batch * batch_size
    end = start + batch_size
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    x_batch = x[start:end]
    y_batch = y[start:end]

    # build computation graph
    y_hat = a * x_batch + b
    myloss = torch.mean((y_batch - y_hat)**2)

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      a -= lr * a.grad
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    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()

  print(f"Epoch: {epoch + 1} / {nepochs}")
  print(f"MSE: {myloss: .2e}; a: {a.item():.4f}; b: {b.item():.4f}")
```

Inner iteration of SGD (batch)

Output:

```
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MSE:  3.69e-02; a: 1.4460; b: 1.2822
Epoch: 2 / 10
MSE:  9.24e-03; a: 1.7226; b: 1.1413
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    with torch.no_grad():
      a -= lr * a.grad
      b -= lr * b.grad

    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()

  print(f"Epoch: {epoch + 1} / {nepochs}")
  print(f"MSE: {myloss: .2e}; a: {a.item():.4f}; b: {b.item():.4f}")
```

1. Use a batch of data to build a computation graph

Output:

```
Epoch: 1 / 10
MSE:  3.69e-02; a: 1.4460; b: 1.2822
Epoch: 2 / 10
MSE:  9.24e-03; a: 1.7226; b: 1.1413
Epoch: 3 / 10
MSE:  2.32e-03; a: 1.8611; b: 1.0707
Epoch: 4 / 10
MSE:  5.81e-04; a: 1.9305; b: 1.0354
Epoch: 5 / 10
MSE:  1.46e-04; a: 1.9652; b: 1.0177
Epoch: 6 / 10
MSE:  3.65e-05; a: 1.9826; b: 1.0089
Epoch: 7 / 10
MSE:  9.15e-06; a: 1.9913; b: 1.0044
Epoch: 8 / 10
MSE:  2.29e-06; a: 1.9956; b: 1.0022
Epoch: 9 / 10
MSE:  5.75e-07; a: 1.9978; b: 1.0011
Epoch: 10 / 10
MSE:  1.44e-07; a: 1.9989; b: 1.0006
```

Linear regression with SGD – The naive way

```python
for epoch in range(nepochs):
  for batch in range(round(n / batch_size)):
    start = batch * batch_size
    end = start + batch_size
    # perform update on a batch
    x_batch = x[start:end]
    y_batch = y[start:end]

    # build computation graph
    y_hat = a * x_batch + b
    myloss = torch.mean((y_batch - y_hat)**2)

    # gradient calculation
    myloss.backward()

    # SGD update
    with torch.no_grad():
      a -= lr * a.grad
      b -= lr * b.grad

    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()

  print(f"Epoch: {epoch + 1} / {nepochs}")
  print(f"MSE: {myloss: .2e}; a: {a.item():.4f}; b: {b.item():.4f}")
```

2. Calculate gradient based on the computation graph

Output:

```
Epoch: 1 / 10
MSE:  3.69e-02; a: 1.4460; b: 1.2822
Epoch: 2 / 10
MSE:  9.24e-03; a: 1.7226; b: 1.1413
Epoch: 3 / 10
MSE:  2.32e-03; a: 1.8611; b: 1.0707
Epoch: 4 / 10
MSE:  5.81e-04; a: 1.9305; b: 1.0354
Epoch: 5 / 10
MSE:  1.46e-04; a: 1.9652; b: 1.0177
Epoch: 6 / 10
MSE:  3.65e-05; a: 1.9826; b: 1.0089
Epoch: 7 / 10
MSE:  9.15e-06; a: 1.9913; b: 1.0044
Epoch: 8 / 10
MSE:  2.29e-06; a: 1.9956; b: 1.0022
Epoch: 9 / 10
MSE:  5.75e-07; a: 1.9978; b: 1.0011
Epoch: 10 / 10
MSE:  1.44e-07; a: 1.9989; b: 1.0006
```

Linear regression with SGD – The naive way

```
for epoch in range(nepochs):
  for batch in range(round(n / batch_size)):
    start = batch * batch_size
    end = start + batch_size
    # perform update on a batch
    x_batch = x[start:end]
    y_batch = y[start:end]

    # build computation graph
    y_hat = a * x_batch + b
    myloss = torch.mean((y_batch - y_hat)**2)

    # gradient calculation
    myloss.backward()

    # SGD update
    with torch.no_grad():
      a -= lr * a.grad
      b -= lr * b.grad

    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()

  print(f"Epoch: {epoch + 1} / {nepochs}")
  print(f"MSE: {myloss: .2e}; a: {a.item():.4f}; b: {b.item():.4f}")
```

3. Update parameters and zero out gradients

Output:

```
Epoch: 1 / 10
MSE:  3.69e-02; a: 1.4460; b: 1.2822
Epoch: 2 / 10
MSE:  9.24e-03; a: 1.7226; b: 1.1413
Epoch: 3 / 10
MSE:  2.32e-03; a: 1.8611; b: 1.0707
Epoch: 4 / 10
MSE:  5.81e-04; a: 1.9305; b: 1.0354
Epoch: 5 / 10
MSE:  1.46e-04; a: 1.9652; b: 1.0177
Epoch: 6 / 10
MSE:  3.65e-05; a: 1.9826; b: 1.0089
Epoch: 7 / 10
MSE:  9.15e-06; a: 1.9913; b: 1.0044
Epoch: 8 / 10
MSE:  2.29e-06; a: 1.9956; b: 1.0022
Epoch: 9 / 10
MSE:  5.75e-07; a: 1.9978; b: 1.0011
Epoch: 10 / 10
MSE:  1.44e-07; a: 1.9989; b: 1.0006
```

Linear regression with SGD – The PyTorch way

Built-in functionalities

- Dataset preparation:
  - torch.utils.data
  - Check Datasets & DataLoaders
- Define training model:
  - Check torch.nn for all kinds of components to build your own model
- Optimization algorithms:
  - Check torch.optim for various opt methods

```
from torch import nn, optim
from torch.utils.data import Dataset, DataLoader
```

```
class SimpleLinear(Dataset):
    def __init__(self, n, a, b):
        self.n = n
        self.x = torch.rand(n, 1)
        self.y = a * self.x + b

    def __len__(self):
        return self.n

    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

# create a training model
# (cont.) also initializes a and b
mymodel = nn.Sequential(nn.Linear(1, 1))

# prepare dataset and dataloaders
mydata = SimpleLinear(n = 2000, a = 2, b = 1)
mydataloader = DataLoader(mydata, batch_size = 200)

# set up optimization with SGD
criterion = nn.MSELoss()
optimizer = optim.SGD(mymodel.parameters(), lr = 0.5)
```

Linear regression with SGD – The PyTorch way

Prepare our datasets

- `Dataset` (a Python class)
  - `__init__`: initialize the dataset
  - `__len__`: sample size of the dataset
  - `__getitem__`: fetch a sample with idx
  - As the input of `DataLoader` function
- `DataLoader` (a Python function)
  - Divide the dataset into batches
  - Check this for more advanced usages
  - Have some tricks to reduce overhead time when transferring data to GPU

```
class SimpleLinear(Dataset):
    def __init__(self, n, a, b):
      self.n = n
      self.x = torch.rand(n, 1)
      self.y = a * self.x + b

    def __len__(self):
        return self.n

    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

# create a training model
# (cont.) also initializes a and b
mymodel = nn.Sequential(nn.Linear(1, 1))

# prepare dataset and dataloaders
mydata = SimpleLinear(n = 2000, a = 2, b = 1)
mydataloader = DataLoader(mydata, batch_size = 200)

# set up optimization with SGD
criterion = nn.MSELoss()
optimizer = optim.SGD(mymodel.parameters(), lr = 0.5)
```

Linear regression with SGD – The PyTorch way

Create the training model:

- `nn.Sequential`
  – Build a model with sequential operations
  – `nn.Linear(m, n)`
    - A linear operator of shape n x m
    - A bias vector of shape n x 1 (default)
  – All parameters are initialized automatically upon creation
  – Check torch.nn for other operations

```python
class SimpleLinear(Dataset):
    def __init__(self, n, a, b):
      self.n = n
      self.x = torch.rand(n, 1)
      self.y = a * self.x + b

    def __len__(self):
        return self.n

    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

# create a training model
# (cont.) also initializes a and b
mymodel = nn.Sequential(nn.Linear(1, 1))

# prepare dataset and dataloaders
mydata = SimpleLinear(n = 2000, a = 2, b = 1)
mydataloader = DataLoader(mydata, batch_size = 200)

# set up optimization with SGD
criterion = nn.MSELoss()
optimizer = optim.SGD(mymodel.parameters(), lr = 0.5)
```

Linear regression with SGD – The PyTorch way

Set up optimization:
- The loss function
- The optimization method
- Optimization parameters

```
class SimpleLinear(Dataset):
    def __init__(self, n, a, b):
      self.n = n
      self.x = torch.rand(n, 1)
      self.y = a * self.x + b

    def __len__(self):
        return self.n

    def __getitem__(self, idx):
        return self.x[idx], self.y[idx]

# create a training model
# (cont.) also initializes a and b
mymodel = nn.Sequential(nn.Linear(1, 1))

# prepare dataset and dataloaders
mydata = SimpleLinear(n = 2000, a = 2, b = 1)
mydataloader = DataLoader(mydata, batch_size = 200)

# set up optimization with SGD
criterion = nn.MSELoss()
optimizer = optim.SGD(mymodel.parameters(), lr = 0.5)
```

Linear regression with SGD – The PyTorch way

```python
nepochs = 10
for epoch in range(nepochs):
  for x_batch, y_batch in mydataloader:
    # build computation graph
    yhat = mymodel(x_batch)
    myloss = criterion(y_batch, yhat)

    # optimization
    optimizer.zero_grad() # zero out gradient
    myloss.backward() # back propagation
    optimizer.step() # updata parameters
```

Build computation graph

Output:

```
Epoch: 1 / 10
MSE:  3.52e-02; a: 1.3904; b: 1.3368
Epoch: 2 / 10
MSE:  9.21e-03; a: 1.6882; b: 1.1722
Epoch: 3 / 10
MSE:  2.41e-03; a: 1.8406; b: 1.0881
Epoch: 4 / 10
MSE:  6.30e-04; a: 1.9185; b: 1.0450
Epoch: 5 / 10
MSE:  1.65e-04; a: 1.9583; b: 1.0230
Epoch: 6 / 10
MSE:  4.31e-05; a: 1.9787; b: 1.0118
Epoch: 7 / 10
MSE:  1.13e-05; a: 1.9891; b: 1.0060
Epoch: 8 / 10
MSE:  2.95e-06; a: 1.9944; b: 1.0031
Epoch: 9 / 10
MSE:  7.71e-07; a: 1.9971; b: 1.0016
Epoch: 10 / 10
MSE:  2.02e-07; a: 1.9985; b: 1.0008
```

Linear regression with SGD – The PyTorch way

```python
nepochs = 10
for epoch in range(nepochs):
  for x_batch, y_batch in mydataloader:
    # build computation graph
    yhat = mymodel(x_batch)
    myloss = criterion(y_batch, yhat)

    # optimization
    optimizer.zero_grad() # zero out gradient
    myloss.backward() # back propagation
    optimizer.step() # updata parameters
```

The whole optimization part

Output:

```
Epoch: 1 / 10
MSE:  3.52e-02; a: 1.3904; b: 1.3368
Epoch: 2 / 10
MSE:  9.21e-03; a: 1.6882; b: 1.1722
Epoch: 3 / 10
MSE:  2.41e-03; a: 1.8406; b: 1.0881
Epoch: 4 / 10
MSE:  6.30e-04; a: 1.9185; b: 1.0450
Epoch: 5 / 10
MSE:  1.65e-04; a: 1.9583; b: 1.0230
Epoch: 6 / 10
MSE:  4.31e-05; a: 1.9787; b: 1.0118
Epoch: 7 / 10
MSE:  1.13e-05; a: 1.9891; b: 1.0060
Epoch: 8 / 10
MSE:  2.95e-06; a: 1.9944; b: 1.0031
Epoch: 9 / 10
MSE:  7.71e-07; a: 1.9971; b: 1.0016
Epoch: 10 / 10
MSE:  2.02e-07; a: 1.9985; b: 1.0008
```

Linear regression with SGD – Comparison of two ways

The PyTorch way

```
nepochs = 10
for epoch in range(nepochs):
  for x_batch, y_batch in mydataloader:
    # build computation graph
    yhat = mymodel(x_batch)
    myloss = criterion(y_batch, yhat)

    # optimization
    optimizer.zero_grad() # zero out gradient
    myloss.backward() # back propagation
    optimizer.step() # updata parameters
```

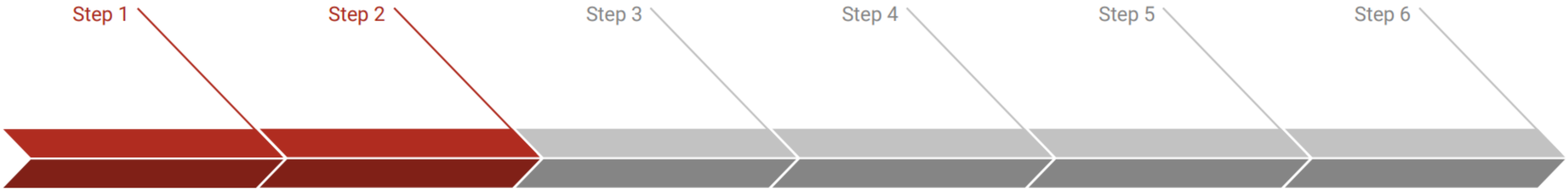
Agnostic to datasets, models, losses and optimization methods!

The naive way

```
for epoch in range(nepochs):
  for batch in range(round(n / batch_size)):
    start = batch * batch_size
    end = start + batch_size
    # perform update on a batch
    x_batch = x[start:end]
    y_batch = y[start:end]

    # build computation graph
    y_hat = a * x_batch + b
    myloss = torch.mean((y_batch - y_hat)**2)

    # gradient calculation
    myloss.backward()

    # SGD update
    with torch.no_grad():
      a -= lr * a.grad
      b -= lr * b.grad

    # avoid gradient accumulation
    a.grad.zero_()
    b.grad.zero_()
```

ML workflow in PyTorch

Credit: HPRC Short Course by Jian Tao, TAMU



Definition

Iteration

Forward Propagation

Loss Calculation

Backward Propagation

Updating

- Define training model using `torch.nn`;
- Define Dataset using `Dataset` class;
- Define loss function;
- Define optimizer with `torch.optim`

Iterate through dataset using `DataLoader` function; (to perform batch-optimization)

```
# forward pass
yhat = mymodel(inputs)
myloss = criterion(labels, yhat)
```

```
# zero out the gradient
optimizer.zero_grad()
# backward propagation
myloss.backward()
# update the model
optimizer.step()
```

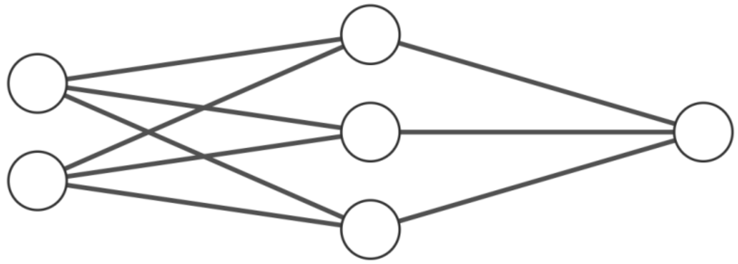
Outline

- Set up working environment
- Introduction to PyTorch framework
- Deep learning with PyTorch
  - Regression using ReLU neural net
  - Image classification with CNN
- Additional resources

From linear model to shallow ReLU network

Usage: nn.Linear(in_features, n_out_features)

Shallow ReLU neural net



$$\text{ReLUnn2: } \boldsymbol{x} \in \mathbb{R}^2 \mapsto \boldsymbol{w}_2^\intercal(\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{b}_1)_+ + b_2 \in \mathbb{R}$$

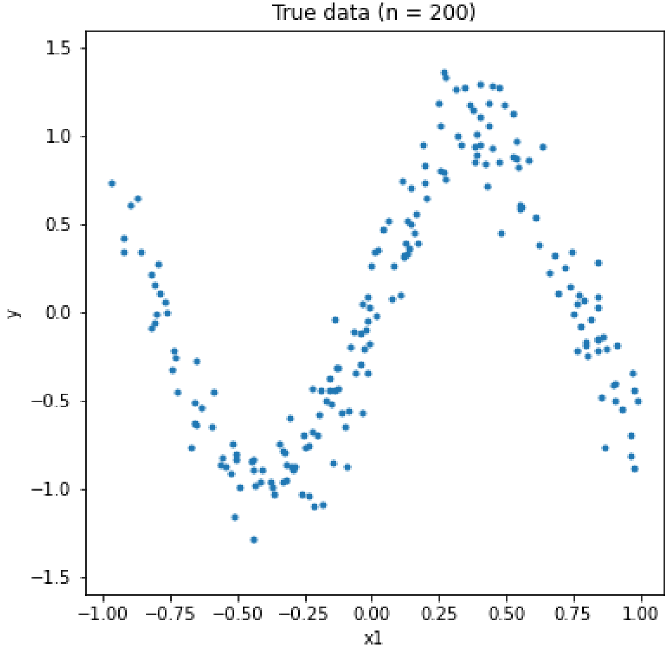
$$\boldsymbol{W}_1 \in \mathbb{R}^{3\times 2}, \boldsymbol{b}_1 \in \mathbb{R}^3, \boldsymbol{w}_2 \in \mathbb{R}^3, b_2 \in \mathbb{R}$$

```python
# shallow relu net
ReLUnn2 = nn.Sequential(
    nn.Linear(2, 3),
    nn.ReLU(),
    nn.Linear(3, 1)
)
for param in ReLUnn2.parameters():
    print(type(param.data), param.shape)
```

```
<class 'torch.Tensor'> torch.Size([3, 2])
<class 'torch.Tensor'> torch.Size([3])
<class 'torch.Tensor'> torch.Size([1, 3])
<class 'torch.Tensor'> torch.Size([1])
```

Fit a ReLU neural network to Sine function

What dose the data look like?



$$y = 4\sin(x_1) + \mathcal{N}(0,1) \text{ where } \boldsymbol{x} \sim \mathrm{Unif}([-1,1]^5)$$

What is our training model?

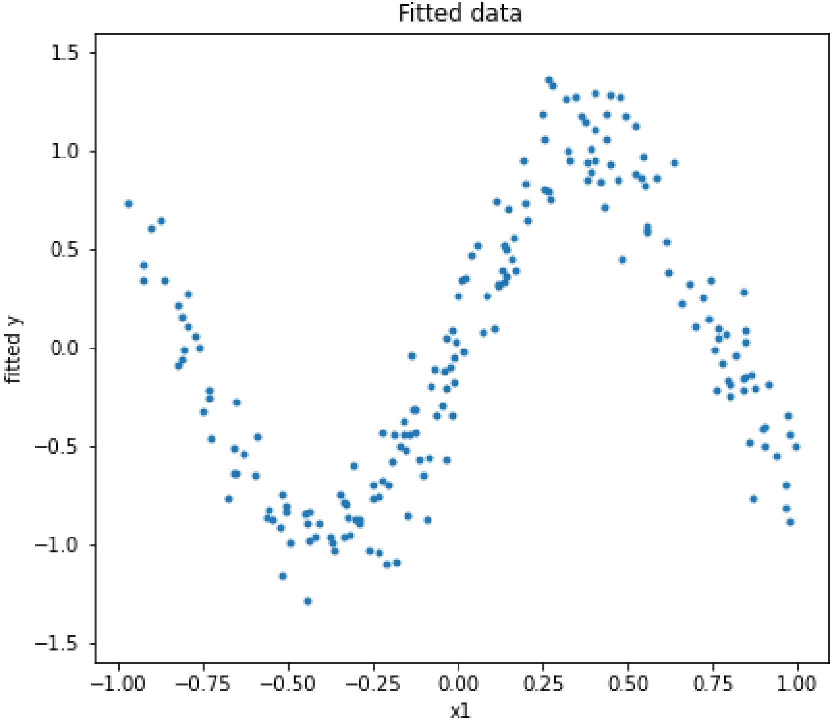
```python
# initialize a training model
train_model = nn.Sequential(
    nn.Linear(5, 256),
    nn.ReLU(),
    nn.Linear(256, 128),
    nn.ReLU(),
    nn.Linear(128, 1)
)
train_model
```

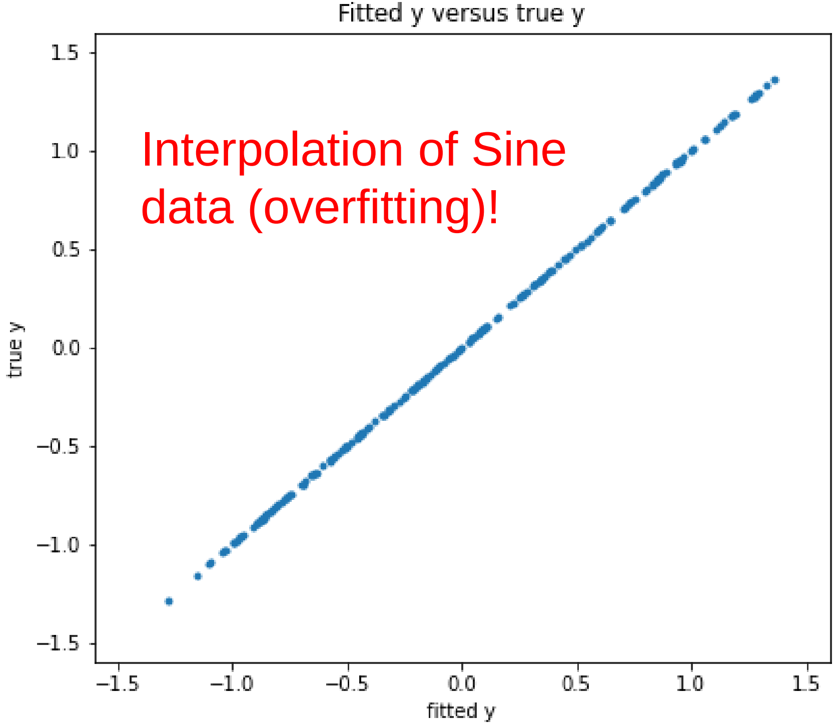
```
Sequential(
  (0): Linear(in_features=5, out_features=256, bias=True)
  (1): ReLU()
  (2): Linear(in_features=256, out_features=128, bias=True)
  (3): ReLU()
  (4): Linear(in_features=128, out_features=1, bias=True)
)
```

- A two-layer ReLU neural network with 256 hidden units in the first layer, and 128 hidden units in the second layer

Fit a ReLU neural network to Sine function

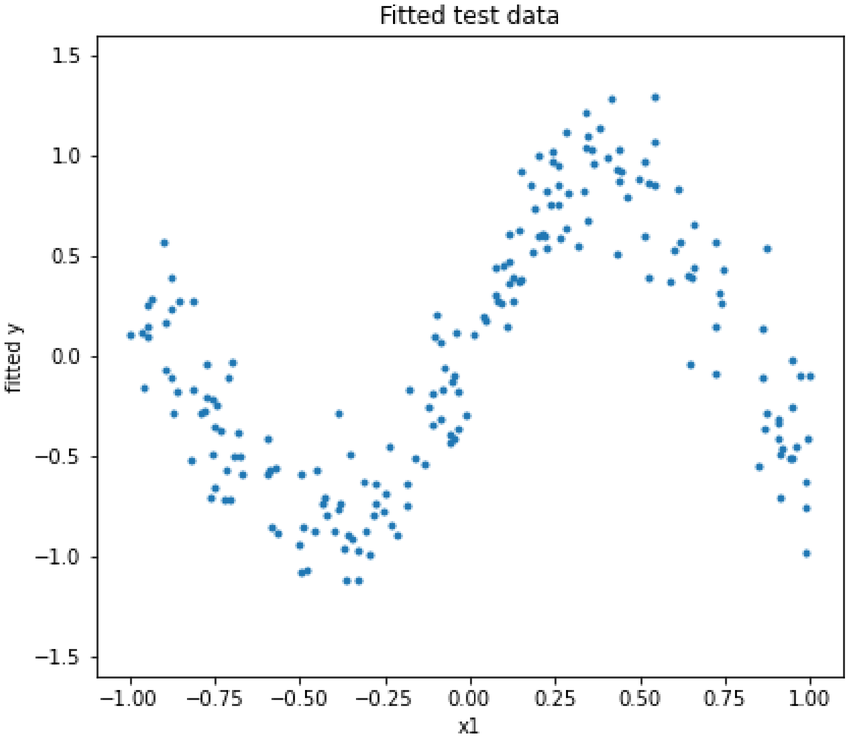
Trained model on **TRAINING** data

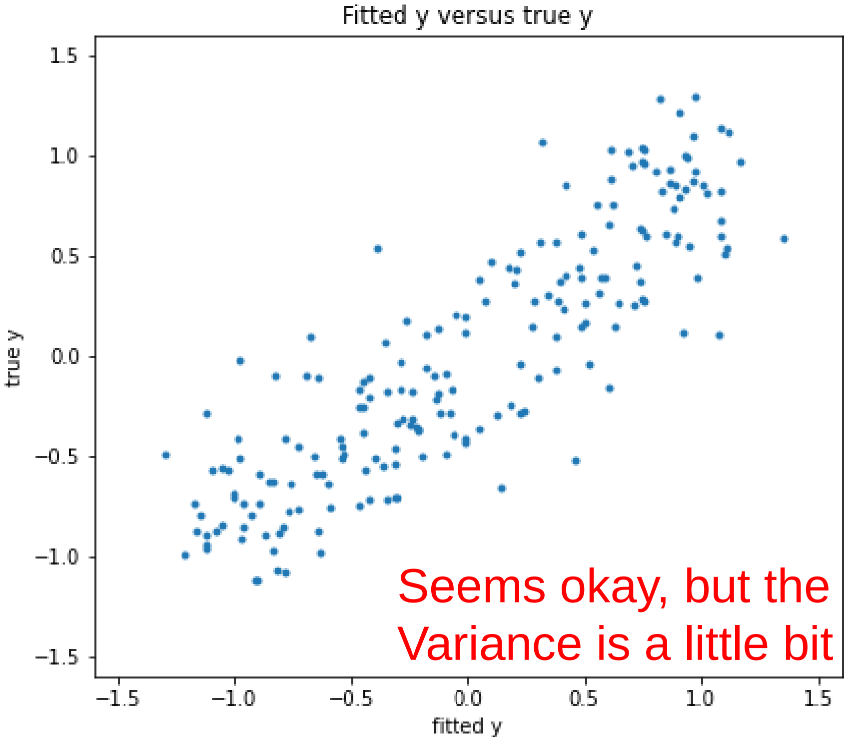




Fit a ReLU neural network to Sine function

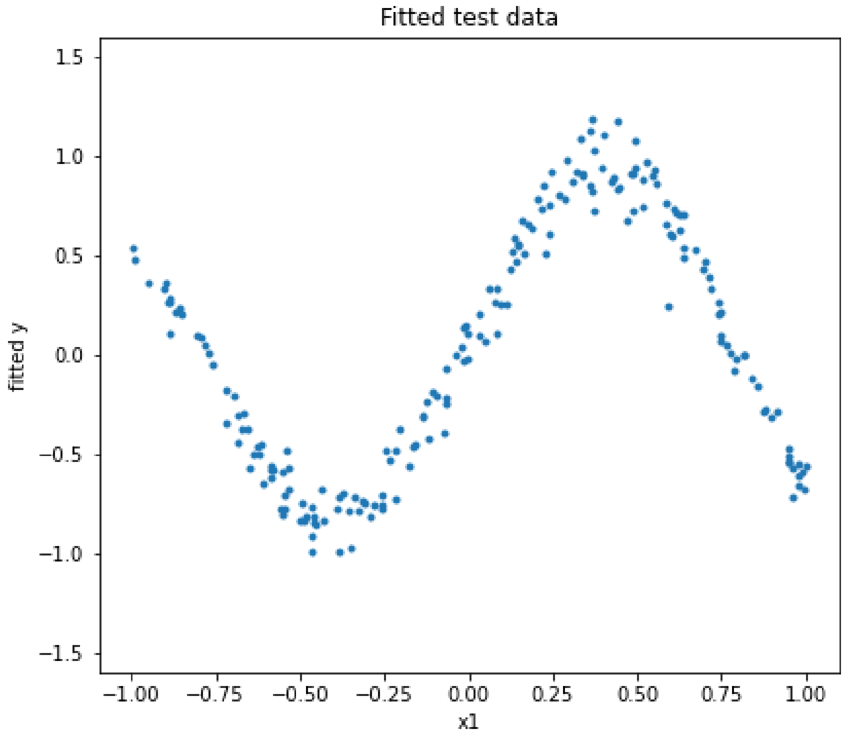
Trained model on **TESTING** data



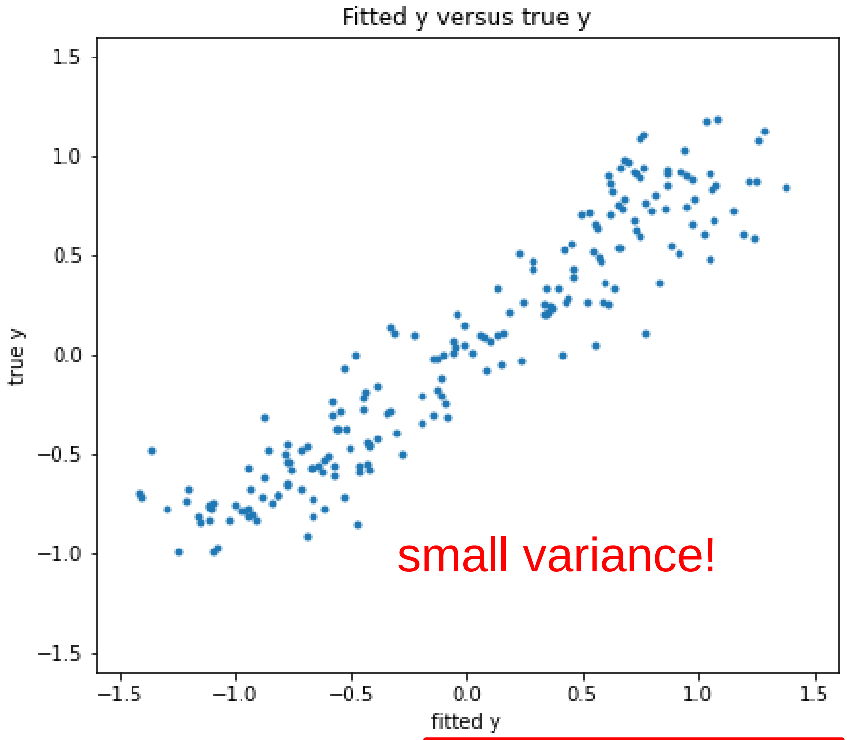


Seems okay, but the Variance is a little bit large

Fit a ReLU neural network to Sine function



Trained model on TESTING data and with REGULARIZATION



Code:

```
optimizer = optim.Adam(train_model.parameters(), lr = 0.001, weight_decay = 0.01)
```

Regularization of neural net
- To achieve better generalization

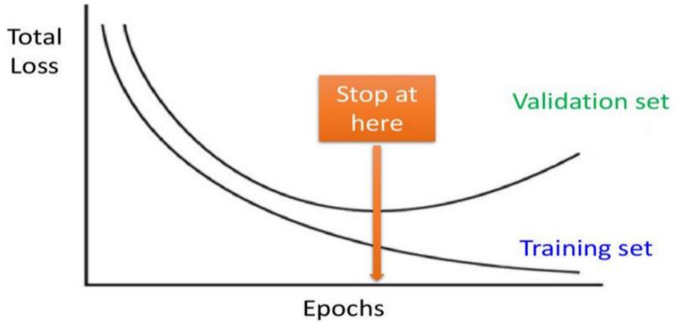
- Explicit regularization:

$$\min_{\boldsymbol{W}} \ \frac{1}{m}\sum_{i=1}^{m} \ell\left(\boldsymbol{y}_i, \mathrm{DNN}_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) + \lambda\Omega\left(\boldsymbol{W}\right)$$

  - Norms of weight matrices
  - Norms of gradients / Jacobians
  - …

- Miscellaneous: A neural net structure can also induce regularization. E.g. The convolutional neural net (CNN)

- Implicit regularization:
  - The regularization that is not built in the objective function (the loss)
  - Regularization induced by an optimization algorithm: SGD tends to find a solution with small norm (regularized solution)
  - Early stopping; batch normalization; dropout

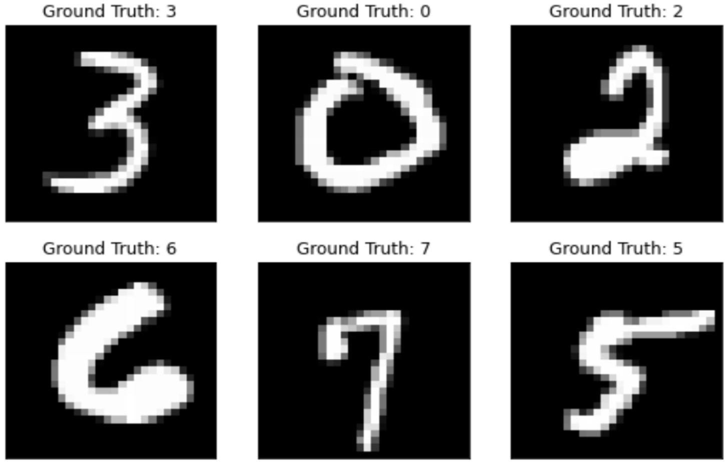


Credit: CSCI 5980/8980: Think Deep Learning offered by Ju Sun, UMN

Image classification using CNN

Dataset: MNIST

- One of the benchmark datasets of deep learning for image classification
- Classifying digits as 0, 1, …, 9

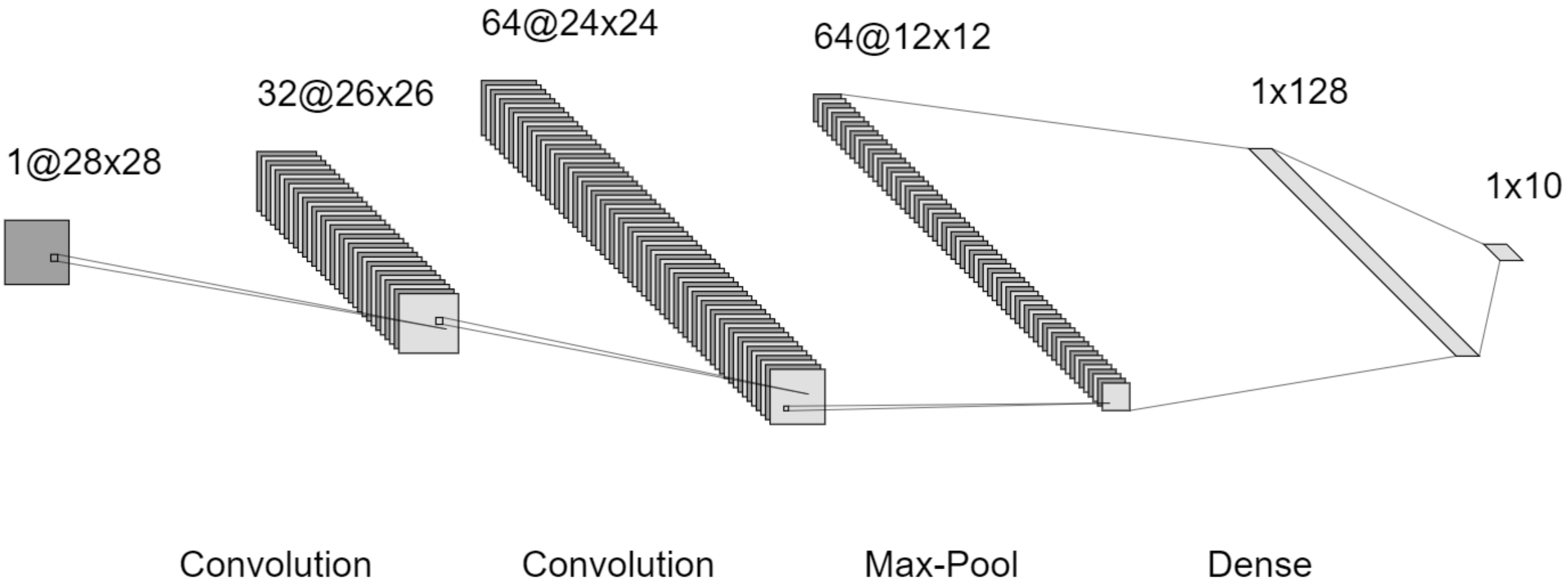


Our CNN model

```
model = nn.Sequential(
    nn.Conv2d(1, 32, 3, 1),
    nn.ReLU(),
    nn.Conv2d(32, 64, 3, 1),
    nn.ReLU(),
    nn.MaxPool2d(2),
    nn.Dropout(0.25),
    nn.Flatten(),
    nn.Linear(9216, 128),
    nn.ReLU(),
    nn.Dropout(0.5),
    nn.Linear(128, 10),
    nn.LogSoftmax(dim = 1)
)
```

Image classification using CNN

Our CNN structure with activation functions, dropout regularization in between layers.

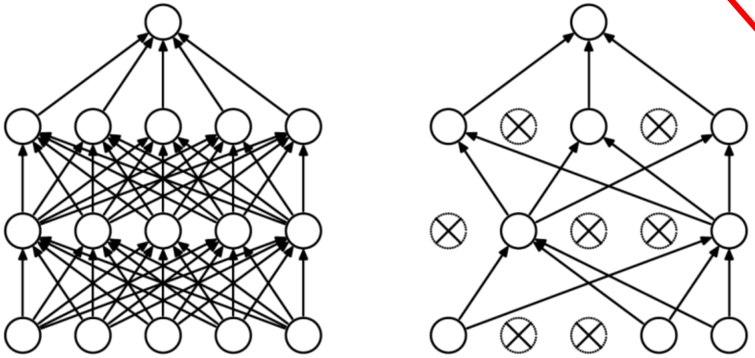


`nn.Conv2d()` `nn.MaxPool2d()` `nn.Linear()`

Image classification using CNN

Dropout for regularization:

- randomly kills inner neurons with some probability p



(a) Standard Neural Net (b) After applying dropout.

Credit: Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: a simple way to prevent neural networks from overfitting. The journal of machine learning research, 15(1), 1929-1958.

Our CNN model

```
model = nn.Sequential(
    nn.Conv2d(1, 32, 3, 1),
    nn.ReLU(),
    nn.Conv2d(32, 64, 3, 1),
    nn.ReLU(),
    nn.MaxPool2d(2),
    nn.Dropout(0.25),
    nn.Flatten(),
    nn.Linear(9216, 128),
    nn.ReLU(),
    nn.Dropout(0.5),
    nn.Linear(128, 10),
    nn.LogSoftmax(dim = 1)
)
```

Image classification using CNN

The total number of trainable parameters is 1,199,882!

```
---------------------------------------------------------------------------
        Layer (type)        Input Shape         Param #     Tr. Param #
===========================================================================
            Conv2d-1      [1, 1, 28, 28]             320             320
              ReLU-2     [1, 32, 26, 26]               0               0
            Conv2d-3     [1, 32, 26, 26]          18,496          18,496
              ReLU-4     [1, 64, 24, 24]               0               0
         MaxPool2d-5     [1, 64, 24, 24]               0               0
           Dropout-6     [1, 64, 12, 12]               0               0
           Flatten-7     [1, 64, 12, 12]               0               0
            Linear-8           [1, 9216]       1,179,776       1,179,776
              ReLU-9            [1, 128]               0               0
        Dropout-10            [1, 128]               0               0
         Linear-11            [1, 128]           1,290           1,290
     LogSoftmax-12             [1, 10]               0               0
===========================================================================
Total params: 1,199,882
Trainable params: 1,199,882
Non-trainable params: 0
---------------------------------------------------------------------------
```

Check GPU availability

CPU

```
# check device availability
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(device)
```

```
cpu
```

GPU

```
# check device availability
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
print(device)
```

```
cuda
```

Download and preprocess the MNIST training / testing dataset

Other transforms: cropping, translation, rotation, padding…

```
# define image transformation
transform=transforms.Compose([
                              transforms.ToTensor(),
                              transforms.Normalize((0.1307,), (0.3081,))
                              ])

# import MNIST dataset
dataset1 = datasets.MNIST('../data', train = True, download = True, transform = transform)
dataset2 = datasets.MNIST('../data', train = False, transform = transform)

# only use 2000 training images and 20 testing images
train_index = np.random.choice(range(60000), 2000, replace = False)
test_index = np.random.choice(range(10000), 20, replace = False)
train_data = Subset(dataset1, train_index)
test_data = Subset(dataset2, test_index)
```

Download and preprocess the MNIST training / testing dataset

Most popular benchmark datasets can be loaded via `torchvision` library

```
# define image transformation
transform=transforms.Compose([
                              transforms.ToTensor(),
                              transforms.Normalize((0.1307,), (0.3081,))
                              ])

# import MNIST dataset
dataset1 = datasets.MNIST('../data', train = True, download = True, transform = transform)
dataset2 = datasets.MNIST('../data', train = False, transform = transform)

# only use 2000 training images and 20 testing images
train_index = np.random.choice(range(60000), 2000, replace = False)
test_index = np.random.choice(range(10000), 20, replace = False)
train_data = Subset(dataset1, train_index)
test_data = Subset(dataset2, test_index)
```

and don't forget to prepare `DataLoader` for training

Define a training utils function

```python
# a utils function for training
def train(model, device, train_loader, optimizer, epoch):
    model.train() # enable dropout
    correct = 0
    for batch_idx, (data, target) in enumerate(train_loader):
        # transfer batches of data to specified device
        data, target = data.to(device), target.to(device)

        # build computation graph
        output = model(data)
        loss = F.nll_loss(output, target)

        # the optimization part
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        # count the corrected classified cases
        pred = output.argmax(dim = 1, keepdim = True)  # get the index of the max log-probability
        correct += pred.eq(target.view_as(pred)).sum().item()

    print(f"Epoch {epoch + 1}:")
    print(f"Training accuracy: {100. * correct / len(train_loader.dataset): .2f} %")
```

Similar as before, nothing new

Train our CNN

```
# the training
model = model.to(device)
optimizer = optim.Adam(model.parameters(), lr = 0.005)

nepochs = 10
for epoch in range(nepochs):
  train(model, device, train_loader, optimizer, epoch)
  test(model, device, test_loader)
```

```
Epoch 1: Training accuracy:  41.10 %; Testing accuracy: 154/200 (77%)
Epoch 2: Training accuracy:  78.35 %; Testing accuracy: 179/200 (90%)
Epoch 3: Training accuracy:  88.25 %; Testing accuracy: 186/200 (93%)
Epoch 4: Training accuracy:  92.25 %; Testing accuracy: 185/200 (92%)
Epoch 5: Training accuracy:  94.15 %; Testing accuracy: 195/200 (98%)
Epoch 6: Training accuracy:  96.05 %; Testing accuracy: 191/200 (96%)
Epoch 7: Training accuracy:  97.00 %; Testing accuracy: 192/200 (96%)
Epoch 8: Training accuracy:  96.55 %; Testing accuracy: 193/200 (96%)
Epoch 9: Training accuracy:  96.85 %; Testing accuracy: 194/200 (97%)
Epoch 10: Training accuracy:  97.60 %; Testing accuracy: 195/200 (98%)
```

Save / load the trained model

- State dictionary method: only save parameter values:

```
# save parameter values
torch.save(model.state_dict(), "model_dict.pt")

# When one wants to use saved model next time:
# 1. initialize the same CNN model
model_new = myCNN()
# 2. load parameter values
model_new.load_state_dict(torch.load("model_dict.pt"))
model_new.eval()
```

Save / load the trained model

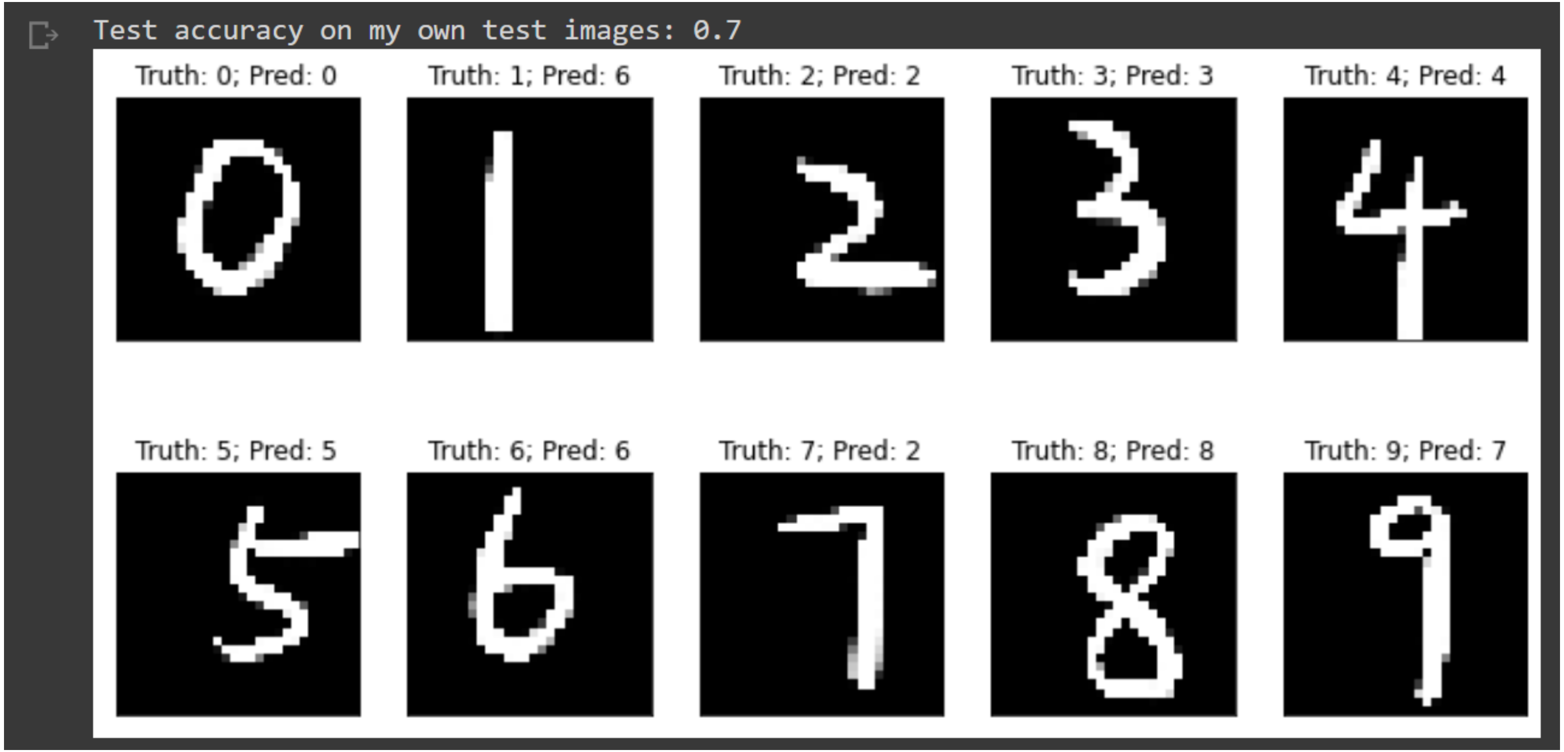
- Checkpoint method: save for resuming training later

```
# save checkpoint for resuming training
torch.save({
            'epoch': epoch,
            'model_state_dict': model.state_dict(),
            'optimizer_state_dict': optimizer.state_dict()
            }, "model_checkpoint.pt")

# When one wants to use saved model next time:
# 1. initialize class and optimizer
model_new = myCNN()
optimizer_new = optim.Adam(model_new.parameters(), lr = 0.005)
# 2. load checkpoints for both model and optimizer
checkpoint = torch.load("model_checkpoint.pt")
model_new.load_state_dict(checkpoint['model_state_dict'])
optimizer_new.load_state_dict(checkpoint['optimizer_state_dict'])
epoch = checkpoint['epoch']
# 3. do whatever you like :)
# - either - evaluate the mode and do some inference
model_new.eval()
# - or - resume training from your last checkpoint
model_new.train()
```

Check [saving and loading models] for more details

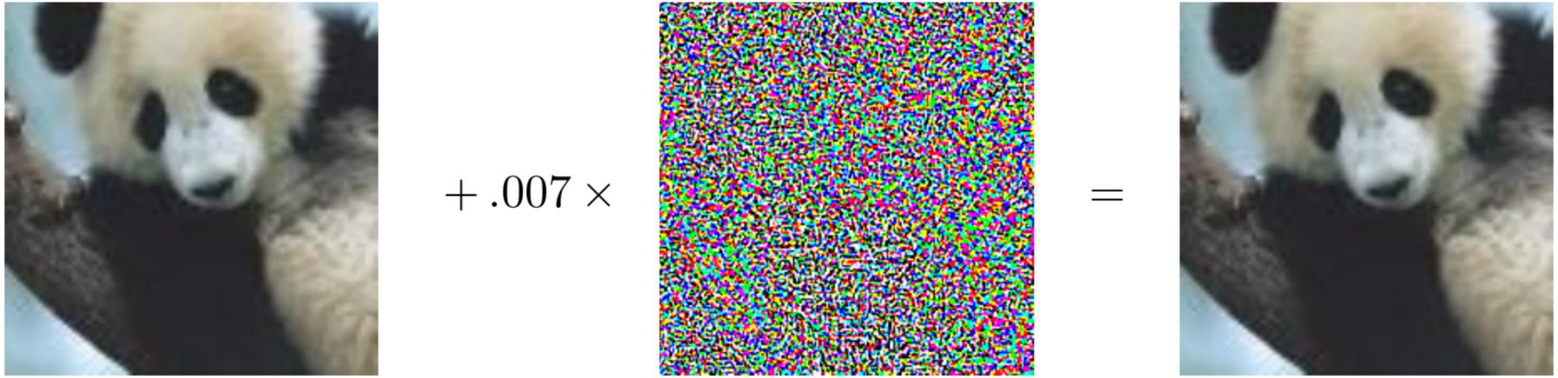
Robustness issue of CNN

Test accuracy only 0.7.
Solution: data augmentation!



Robustness issue of CNN

Solution: adversarial training!



$\boldsymbol{x}$	$\mathrm{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$	$\boldsymbol{x} + \epsilon\mathrm{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$
"panda" 57.7% confidence	"nematode" 8.2% confidence	"gibbon" 99.3 % confidence

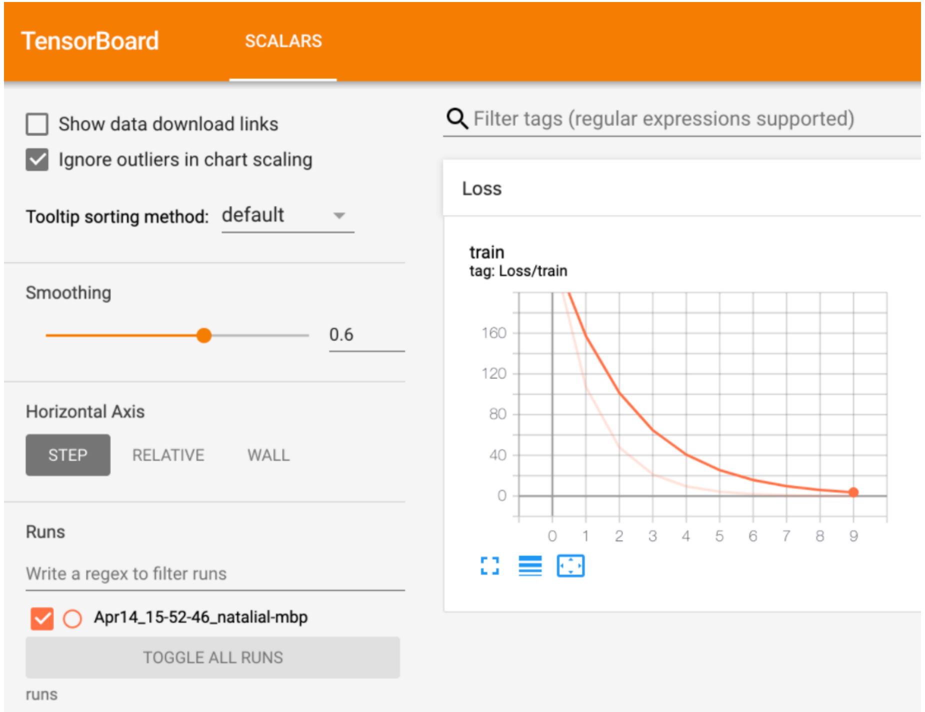
Credit: Goodfellow, I. J., Shlens, J., & Szegedy, C. (2014). Explaining and harnessing adversarial examples. arXiv preprint arXiv:1412.6572.

Outline

- Set up working environment
- Introduction to PyTorch framework
- Deep learning with PyTorch
- Other resources

Visualization with TensorBoard

- Track and visualize:
  - Metrics such as loss and accuracy
  - The model graph
  - Histograms, images and much more
- Some resources:
  - How to use TensorBoard with PyTorch
  - Visualizing models, data, and training with TensorBoard
  - PyTorch TensorBoard support



Tutorials and courses:

Books and tutorials:

- Dive into Deep Learning (livebook)
- Deep Learning by Ian Goodfellow
- Official PyTorch tutorial
- Deep learning with Python (livebook)
- UvA DL Notebooks

Courses:

- DL/ML tutorial by Hung-Yi Lee
- Deep learning course by Yann LeCun
- Deep learning with Pytorch
- Stanford STAT385 series
- Think Deep Learning by Ju Sun

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