CIS 6930 Topics in Computing for Data Science Week 1b: Deep Learning Basics (2)

9/9/2021 Yoshihiko (Yoshi) Suhara

2pm-3:20pm & 3:30pm-4:50pm (5-6pm office hour)

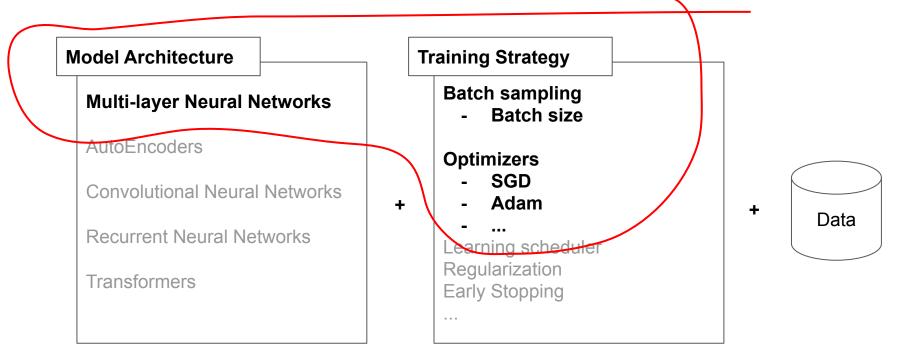
Deep Learning Basics (2)

- Part 1: Deep Learning as Building Blocks
 - Model architectures
 - Optimizers
 - Activation functions
- Part 2: PyTorch Basics
- Part 3: (Hands-on session) The first PyTorch code

Part I: Deep Learning as Building Blocks

Basic Deep-Learning Building Blocks

- (A) Model Architecture + (B) Training Strategy + (c) Data
- i.e., What to Optimize and How to Optimize



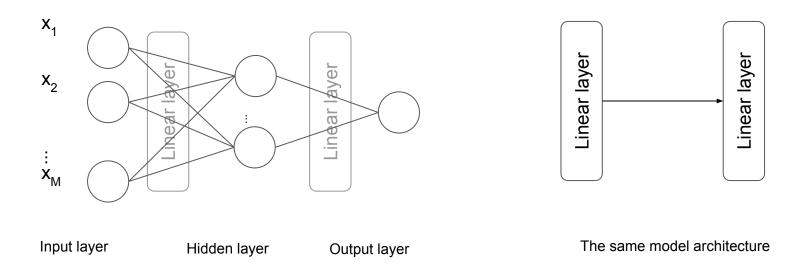
Deep-Learning Building Blocks: Starter Kit

- Layers
 - Linear Layer
- Activation functions
 - Logistic sigmoid, tanh
 - ReLU, Leaky ReLU
- Optimizers
 - SGD w/wo Momentum)
 - Adam

Layers

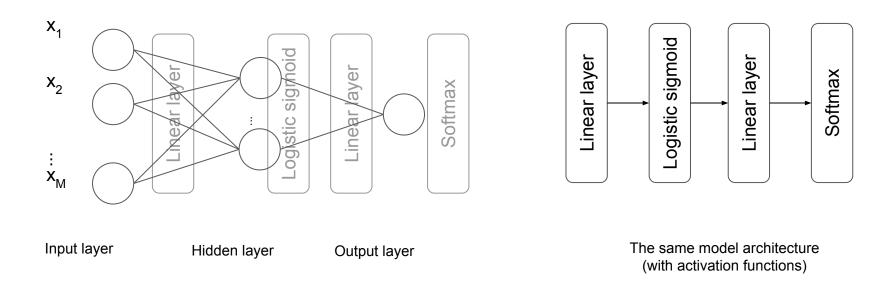
Fully-connected Layer (aka Linear Layer)

input dimension size & output dimension size (i.e., the shape of W)



Fully-connected Layer (aka Linear Layer)

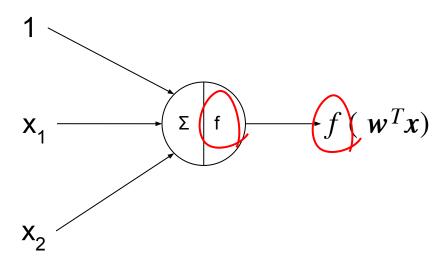
input dimension size & output dimension size (i.e., the shape of W)



Activation functions

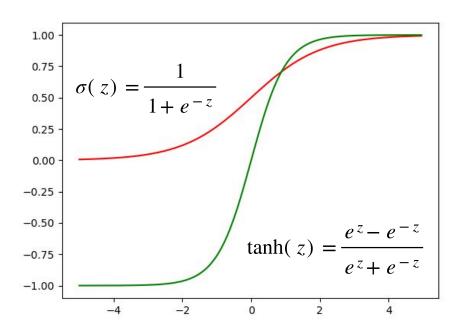
Why do we care about activation functions?

- For non-linearity (and better forward/backward propagation)
- It is supposed to be differentiable



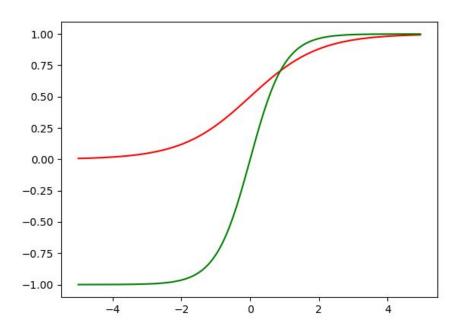
Logistic sigmoid / tanh

- Traditional choice ([0, 1] or [-1, 1])
- What's the benefit of tanh?



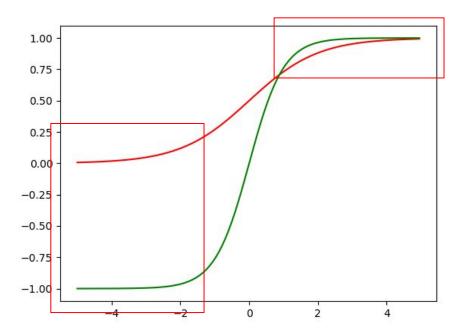
What's the issue with Logistic sigmoid / tanh?

Hint: Look at the output for small/large values of z



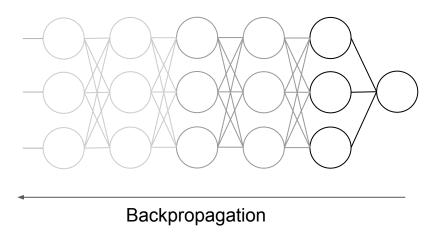
What's the issue with Logistic sigmoid / tanh?

- Hint: Look at small values of z
- Gradients can become very small at large/small input → Vanishing gradient problem



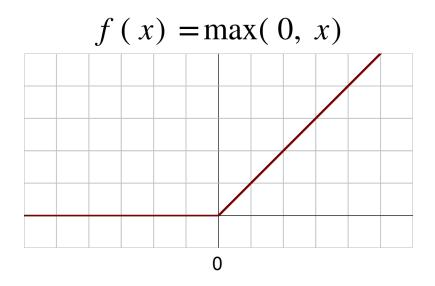
Vanishing Gradient Problem

- Errors are not propagated in the backpropagation step due to too small gradient values → Shallow layers are not appropriately updated
 - o cf. Exploding Gradient Problem (due to too large gradient values)



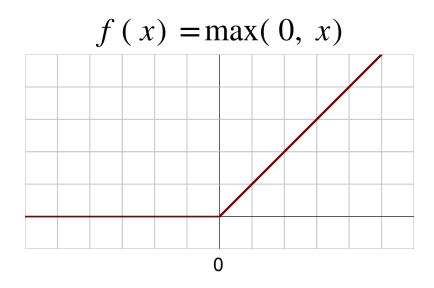
Rectified Linear Unit (ReLU)

• For better gradient propagation



Rectified Linear Unit (ReLU)

For better gradient propagation



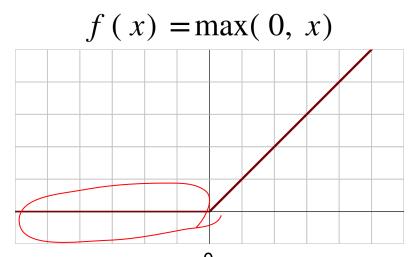
The function is not differentiable at x = 0 but we don't care about it (?!)

$$f'(x) = \begin{cases} 0 & x \le 0 \\ 1 & x > 0 \end{cases}$$

cf. subdifferentiable

Rectified Linear Unit (ReLU)

For better gradient propagation



The gradient stays 0 (for x < 0)

The function is not differentiable at x = 0 but we don't care about it (?!)

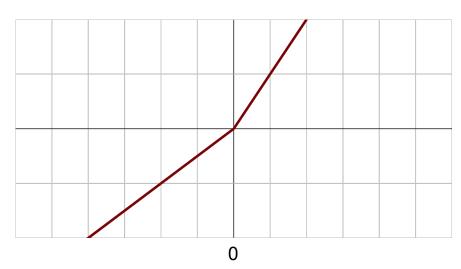
$$f'(x) = \begin{cases} 0 & x \le 0 \\ 1 & x > 0 \end{cases}$$

cf. subdifferentiable

Leaky ReLU

A ReLU variant

$$f(x) = \max(0.01x, x)$$



$$f'(x) = \begin{cases} 0.01 & x \le 0 \\ 1 & x > 0 \end{cases}$$

A list of activation functions (from Wikipedia)

Name ¢	Plot	Function, $f(x)$	Derivative of $f, f'(x)$	Range •	Order of continuity •
Identity	_/_	x	1	$(-\infty,\infty)$	C^{∞}
Binary step		$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$\begin{cases} 0 & \text{if } x \neq 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$\{0,1\}$	C^{-1}
Logistic, sigmoid, or soft step		$\sigma(x) = \frac{1}{1+e^{-x}} {}^{\llbracket 1 \rrbracket}$	f(x)(1-f(x))	(0,1)	C^{∞}
Hyperbolic tangent (tanh)		$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$	$1-f(x)^2$	(-1,1)	C^{∞}
Rectified linear unit (ReLU) ^[9]		$\begin{cases} 0 & \text{if } x \le 0 \\ x & \text{if } x > 0 \\ & = \max\{0, x\} = x1_{x > 0} \end{cases}$	$\begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ \text{undefined} & \text{if } x = 0 \end{cases}$	$[0,\infty)$	C^0
Gaussian Error Linear Unit (GELU) ^[4]	1/	$rac{1}{2}x\left(1+\mathrm{erf}\left(rac{x}{\sqrt{2}} ight) ight) \ =x\Phi(x)$	$\Phi(x) + x\phi(x)$	$(-0.17\ldots,\infty)$	C^{∞}
Softplus ^[10]		$\ln(1+e^x)$	$\frac{1}{1+e^{-x}}$	$(0,\infty)$	C^{∞}
Exponential linear unit (ELU) ^[11]		$\begin{cases} \alpha \left(e^{x}-1\right) & \text{if } x\leq 0\\ x & \text{if } x>0 \end{cases}$ with parameter α	$\begin{cases} \alpha e^x & \text{if } x < 0 \\ 1 & \text{if } x > 0 \\ 1 & \text{if } x = 0 \text{ and } \alpha = 1 \end{cases}$	$(-lpha,\infty)$	$\left\{ \begin{aligned} &C^1 & \text{if } \alpha = 1 \\ &C^0 & \text{otherwise} \end{aligned} \right.$
Scaled exponential linear unit (SELU) ^[12]		$\lambda \begin{cases} \alpha(e^x-1) & \text{if } x<0 \\ x & \text{if } x\geq 0 \end{cases}$ with parameters $\lambda=1.0507$ and $\alpha=1.67326$	$\lambdaegin{cases} lpha e^x & ext{if } x < 0 \ 1 & ext{if } x \geq 0 \end{cases}$	$(-\lambda \alpha, \infty)$	C^0
Leaky rectified linear unit (Leaky ReLU) ^[13]		$\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$	$\begin{cases} 0.01 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}$	$(-\infty,\infty)$	C^0
Parameteric rectified linear unit (PReLU) ^[14]		$\begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameter α	$\left\{egin{array}{ll} lpha & ext{if } x < 0 \ 1 & ext{if } x \geq 0 \end{array} ight.$	$(-\infty,\infty)^{[2]}$	C^0
Sigmoid linear unit (SiLU, ^[4] Sigmoid shrinkage, ^[15] SiL, ^[16] or Swish-1 ^[17])		$\frac{x}{1+e^{-x}}$	$\frac{1 + e^{-x} + xe^{-x}}{(1 + e^{-x})^2}$	$[-0.278\ldots,\infty)$	C^{∞}
Mish [18]		$x anh(\ln(1+e^x))$	$\frac{\left(e^x(4e^{2x}+e^{3x}+4(1+x)+e^x(6+4x))\right)}{(2+2e^x+e^{2x})^2}$	$[-0.308\ldots,\infty)$	C^{∞}
Gaussian		e^{-x^2}	$-2xe^{-x^2}$	(0,1]	C^{∞}
Growing Cosine Unit (GCU)[7]		$x\cos(x)$	$\cos(x) - x\sin(x)$	$(-\infty,\infty)$	C^{∞}

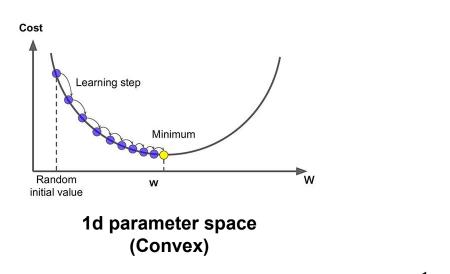
Summary: Activation functions

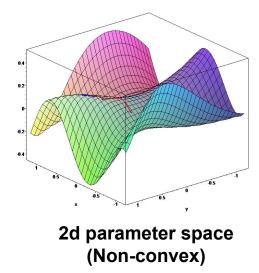
- Traditionally, Logistic sigmoid or tanh were used, which may cause the vanishing gradient problem
- The de-facto standard choice: ReLU (or ReLU variants)

Optimizers

Stochastic Gradient Descent

Optimization method based on gradient that is calculated by (randomly chosen) samples

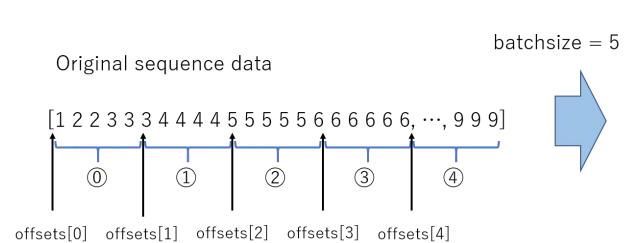




$$\mathbf{w}^t \leftarrow \mathbf{w}^{t-1} - \boldsymbol{\eta} \nabla \mathbf{w}$$

Optimization method = Gradient (direction) + Learning rate (Step size)

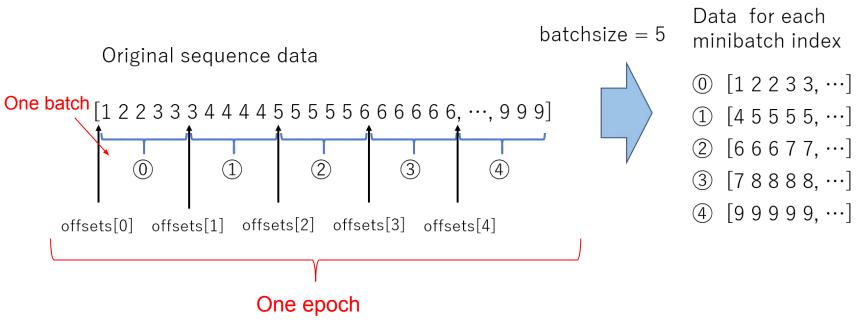
Mini-batch Sampling



Data for each minibatch index

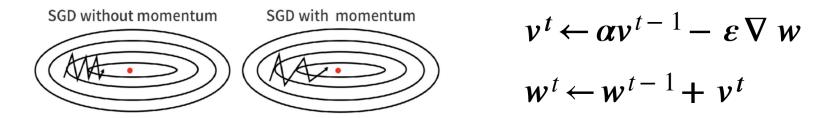
- ① [1 2 2 3 3, ···]
- ① [45555, ...]
- ② [66677,···]
- ③ [7 8 8 8 8, …]
- 4 [99999, ···]

Mini-batch Sampling



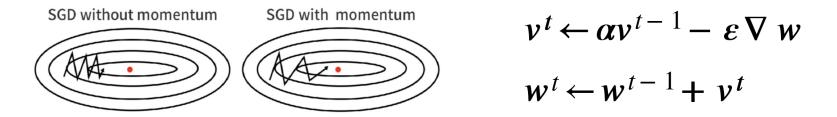
SGD + Momentum

- Adding the notion of velocity (v) to SGD
 - Intuition: "Momentum" should help the optimization step less sensitive to the current sample (especially when the batch size is small)



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Algorithms with Adaptive Learning Rates

- AdaGrad
- RMSProp
- ...
- Adam

Adam (Adaptive moments) (Kingma and Ba 2014)

- SGD + first-order moment
- + Second-order moment

+ Bias correction

$$\begin{aligned} m^t &\leftarrow \beta_1 m^{t-1} + \left(1 - \beta_1\right) \nabla w^t \\ v_t &\leftarrow \beta_2 v^{t-1} + \left(1 - \beta_2\right) (\nabla w^t)^2 \end{aligned}$$

$$\widehat{m}^t \leftarrow \frac{m^t}{1 - \left(\beta_1\right)^t}$$

$$\widehat{v}^t \leftarrow \frac{v^t}{1 - \left(\beta_2\right)^t}$$

$$w^{t+1} \leftarrow w^t - \frac{\eta}{\sqrt{\widehat{v}^t + \varepsilon}} \widehat{m}^t$$

$$\beta_1 = 0.9, \ \beta_2 = 0.999, \ \varepsilon = 10^{-8}$$

Suggested hyper-parameters

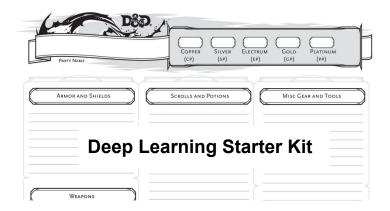
Summary: Optimizers

- Grand Design: SGD + mini-batch sampling
- Learning rate tuning is key → Algorithms with adaptive learning rates
- The de-facto standard choice: Adam

Further reading: An overview of gradient descent optimization algorithms
[2007.01547] Descending through a Crowded Valley - Benchmarking Deep Learning Optimizers

Inventory

- Layers
 - Linear Layer
- Activation functions
 - Logistic sigmoid, tanh
 - o ReLU, Leaky ReLU
- Optimizers
 - SGD w/wo Momentum
 - Adam



Part II: PyTorch Basics

PyTorch Basics

- Quick overview of PyTorch
- PyTorch sample code for training a machine learning model
 - (1) Dataset class
 - (2) Model class
 - (3) Training iteration

The aim of this part is **NOT** reproducing (excellent) tutorials **BUT** to help you get a feel for PyTorch

... and share some sample code

O PyTorch

Why PyTorch?

- De-facto standard library for CV/NLP research
- Why not TensorFlow?
 - No significant difference b/w PyTorch and TensorFlow anymore
 - Tensorflow has TensorFlow eager (for define-by-run)
 - PyTorch has TorchScript (for define-and-run)
- More research code assets written with PyTorch than Tensorflow

What is PyTorch?

- PyTorch != scikit-learn
 - PyTorch is NOT a machine learning/DL library

- PyTorch =~ NumPy
 - PyTorch is a fundamental library (designed for neural networks)

NumPy

- Everything is ndarray
- ndarray has data type

```
>>> import numpy as np
>>> a = np.array([1, 2, 3])
>>> a
array([1, 2, 3])
>>> a.tolist()
[1, 2, 3]
>>> a.dtype
dtype('int64')
```

PyTorch

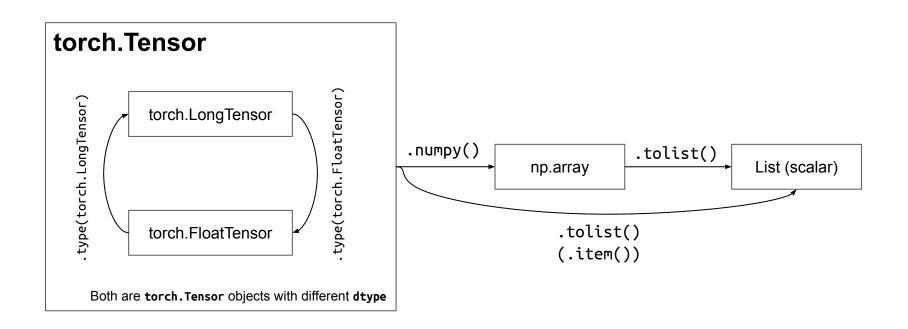
- Everything is torch.Tensor
- Tensor has data type

```
>>> import torch
>>> t = torch.Tensor([1, 2, 3])
>>> t
tensor([1., 2., 3.])

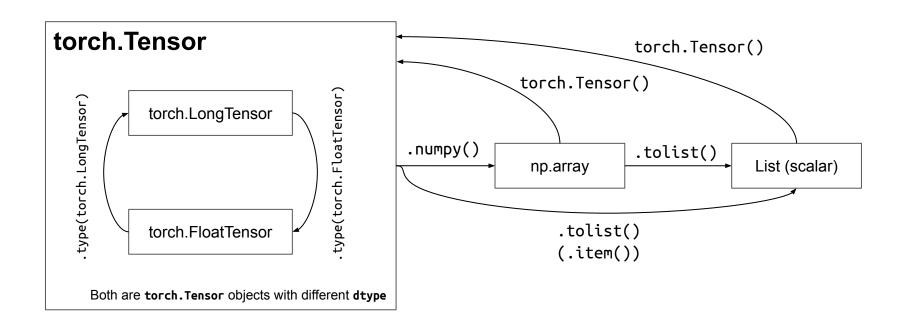
>>> t.tolist()
[1.0, 2.0, 3.0]

>>> t.dtype
torch.float32
```

PyTorch ⇔ NumPy ⇔ built-in objects



PyTorch ⇔ NumPy ⇔ built-in objects



Data type	dtype	CPU tensor	GPU tensor
32-bit floating point	torch.float32 or torch.float	torch.FloatTensor	torch.cuda.FloatTensor
64-bit floating point	torch.float64 or torch.double	torch.DoubleTensor	torch.cuda.DoubleTensor
16-bit floating point	torch.float16 or torch.half	torch.HalfTensor	torch.cuda.HalfTensor
8-bit integer (unsigned)	torch.uint8	torch.ByteTensor	torch.cuda.ByteTensor
8-bit integer (signed)	torch.int8	torch.CharTensor	torch.cuda.CharTensor
16-bit integer (signed)	torch.int16 or torch.short	torch.ShortTensor	torch.cuda.ShortTensor
32-bit integer (signed)	torch.int32 or torch.int	torch.IntTensor	torch.cuda.IntTensor
64-bit integer (signed)	torch.int64 or torch.long	torch.LongTensor	torch.cuda.LongTensor
Boolean	torch.bool	torch.BoolTensor	torch.cuda.BoolTensor

CPU ⇔ GPU

- Company Compan
- Use .to() method to transfer object to/from GPU
- PyTorch methods are device-agnostic
 - Note: Objects that are used for calculation need to be in the same "world"

```
>>> import torch
>>> device = torch.device('cuda')
>>> t = torch.Tensor([1, 2, 3])
>>> t
tensor([1., 2., 3.])
>>> t = t.to(device) # Not destructive method
>>> t * 3
tensor([3., 6., 9.], device='cuda:0')
>>> t.detach().cpu() * 2
tensor([2., 4., 6.])
```

Tips: GPU/CPU compatible code

Template

```
import torch
import torch.nn as nn
import torch.nn.functional as F

device = torch.device("cuda" if torch.cuda.is_available() else "cpu")
```

Switching GPU IDs using the environment variable CUDA_VISIBLE_DEVICES

```
$ CUDA_VISIBLE_DEVICES=0 python train.py # Force to use GPU0 (if exists)
$ CUDA_VISIBLE_DEVICES="" python train.py # Force to use CPU
```

Basic Operations

Arithmetic operations

```
0 +, -
```

Matrix operations

```
o .dot()
o .matmul()
```

Concatenation

```
o torch.cat()
```

Cheatsheet

Math operations

Numpy	PyTorch	Notes
x+y	<pre>x+y y.add_(x) torch.add(x,y)</pre>	addition
<pre>np.dot(x,y) np.matmul(x,y)</pre>	<pre>torch.mm(x,y) x.mm(y)</pre>	matrix multiplication
x*y	x*y	element-wise multiplication
np.max(x)	torch.max(x)	
np.argmax(x)	torch.argmax(x)	
x**2	x**2	Element-wise powers

Array creation

Numpy	PyTorch	Notes
np.empty((2, 2))	<pre>torch.empty(5, 3)</pre>	empty array
np.random.rand(3,2)	torch.rand(5, 3)	random
np.zeros((5,3))	torch.zeros(5, 3)	zeros
np.array([5.3, 3])	<pre>torch.tensor([5.3, 3])</pre>	from list
np.random.randn(*a.shape)	<pre>torch.randn_like(a)</pre>	
np.arange(16)	torch.range(0,15)	array starting from 0 ending at 15 (inclusive)

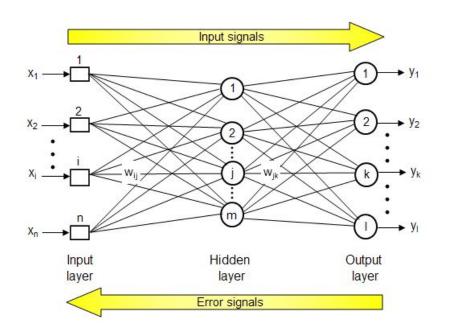
Array manipulations

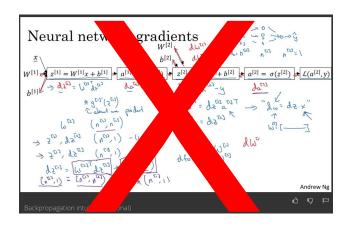
Numpy	PyTorch	Notes
<pre>x.T np.transpose(x)</pre>	<pre>torch.transpose(x, 0, 1) torch.transpose(x, 1, 0)</pre>	transpose
a = a.reshape(-1, 2)	a = a.view(-1,2)	reshape array to have two columns and however as many rows
<pre>np.concatenate([a, b])</pre>	torch.cat([a,b])	concatenate list of arrays/tensors

Training Flow with PyTorch

Forward and Backward propagation

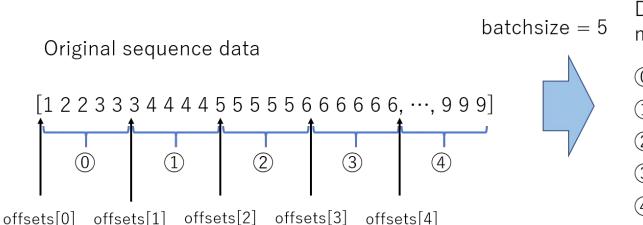
Backward propagation = Gradient calculation





Only need to define **forward propagation** function PyTorch **AutoGrad** takes care of backward propagation :)

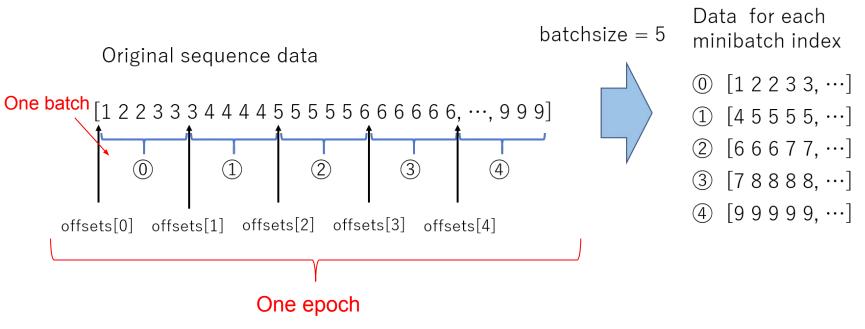
Mini-batch Sampling



Data for each minibatch index

- ① [1 2 2 3 3, ···]
- \bigcirc [45555, ...]
- ② [66677,···]
- ③ [78888, …]
- (4) [9 9 9 9 9, ···]

Mini-batch Sampling



Pseudo Code for Training

Training script has double loops: One for epochs and the other for batches

```
Input: parameters, data, NumEpoch, BatchSize

For i = 1 to NumEpoch
   batches ← CreateMiniBatch(data, BatchSize)
   For j = 1 to len(Batches)
     batch ← batches[j]
     update_parameters(parameters, batch)
```

Writing Training Script with PyTorch

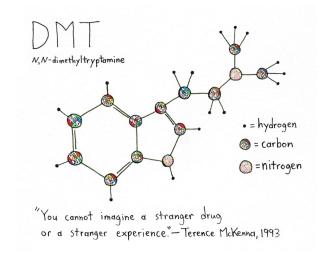
Training Script: 3 Essential Blocks (D-M-T)

- Data Preparation
- Model Preparation
- Training Iteration

Training Script: 3 Essential Blocks (D-M-T)

- Data Preparation
- Model Preparation
- Training Iteration

Not this DMT



Training Script (1): Data Preparation

- Step 1. Create a Dataset object
- Step 2. Create a DataLoader object

Training Script (1): Data Preparation

- Step 1. Create a Dataset object
- Step 2. Create a DataLoader object

Training Script (2): Model Preparation

- Step 1. Create a model object
- Step 2. Create an optimizer object. Set the parameters of the model
- Step 3. Create a loss function

```
model = MyModel()
optimizer = optim.SGD(model.parameters(), lr=0.01, momentum=0.)
criterion = nn.CrossEntropyLoss()
```

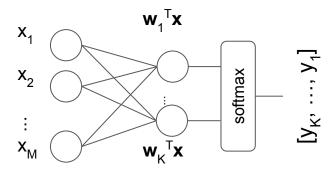
Training Script (3): Training iteration

```
for epoch in range (10):
    training loss = 0.0
   valid loss = 0.0
   model.train()
    for batch_idx, batch in enumerate(dataloader):
                                                # Initialize gradient information
        optimizer.zero grad()
       X, v = batch
                                                # Get feature/label from batch
        pred = model(X)
                                                # Get output from the model
        loss = criterion(pred, y)
                                                # Evaluate loss values
        loss.backward()
                                                # Backpropagate
        optimizer.step()
                                                # Update parameters
        training loss += loss.data.item() * batch size
    training loss /= len(train iterator)
```

Model Preparation: Design a Custom Model

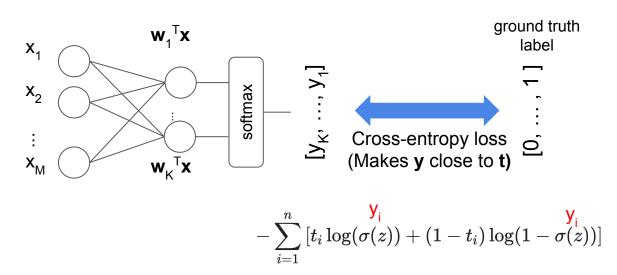
Logistic Regression as an NN model

- A single-layer NN
- (If multi-class) the final layer is a softmax function that converts output values into probabilities

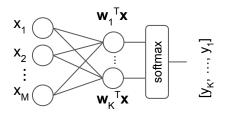


Logistic Regression as an NN model

- A single-layer NN
- (If multi-class) the final layer is a softmax function that converts output values into probabilities
- Use cross-entropy loss for training

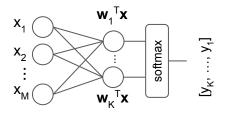


Logistic Regression



```
class LogisticRegression(nn.Module):
   def init (self,
                 num_input: int, # M
                 num output: int): # K
        super(LogisticRegression, self). init ()
        self.linear = nn.Linear(num input, num output)
    def forward(self, X):
       out = self.linear(X)
        return F.softmax(out)
```

Logistic Regression



```
class LogisticRegression(nn.Module):
   def init (self,
                num_input: int, # M
                num output: int): # K
       super(LogisticRegression, self). init ()
       self.linear = nn.Linear(num input, num output)
   def forward(self, X):
       out = self.linear(X)
       return out F.softmax(out)
```

Ref. CrossEntropyLoss

CrossEntropyLoss

CLASS torch.nn.CrossEntropyLoss(weight=None, size_average=None, ignore_index=-100, reduce=None, reduction='mean') [SOURCE]

This criterion combines nn.LogSoftmax() and nn.NLLLoss() in one single class.

It is useful when training a classification problem with C classes. If provided, the optional argument weight should be a 1D *Tensor* assigning weight to each of the classes. This is particularly useful when you have an unbalanced training set.

The *input* is expected to contain raw, unnormalized scores for each class.

Recap

D-M-T: Data Preparation

- dataset = TensorDataset(X, y)
- dataloader = DataLoader(dataset)

D-M-T: Model Preparation

model = MyModel()optimizer = Optimizer(model.parameters())criterion = LossFunction()

D-M-T: Training Iteration

• # Training model.train() • for each batch optimizer.zero grad() pred = model(X) loss = criterion(pred, batch.label) o loss.backward() optimizer.step()

Summary

Takeaway: D-M-T

- PyTorch is yet another NumPy
- Remember Dataset, Model, Training iteration
- TensorDataset wraps the conventional formats of X, y

Hands-on Time!

https://colab.research.google.com/github/suhara/cis6930-fall2021/blob/main/notebooks/cis6930_week1_deep_learning_basics.ipynb

Any Questions?

Appendix: Tips

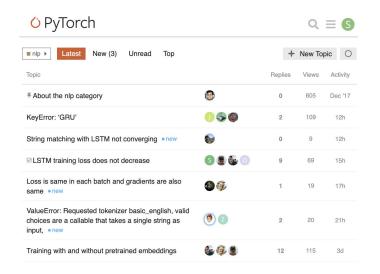
Getting Started

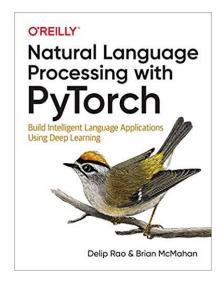






https://pytorch.org/tutorials/





Define MyDataset

Only 2 methods to implement: __len__() and __getitem__()

```
class MyDataset(Dataset):
    def __len__(self):
        """Returns # of instances."""
        pass

def __getitem__(self, idx):
        """Returns single instane."""
        pass
```

Example

train.csv

data

label

		į .
	1	0.72
<pre>class MyDataset(Dataset): def init (self):</pre>	0	0.56
self.df = pd.read_csv("train.csv")	1	0.67
<pre>deflen(self):</pre>		
return len(self.df)		

Returned value does not have to be Dict[str, torch.Tensor]
For example, it can be a hierarchical dictionary Dict[str, Dict[str, torch.Tensor]]

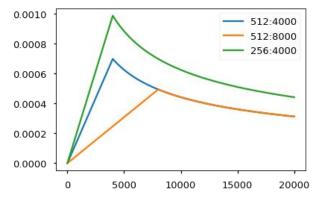
Appendix: Customized Optimizer for Transformer

Optimizer

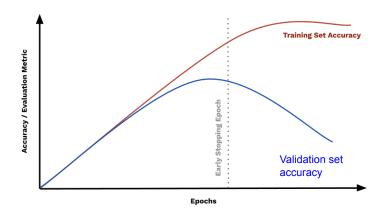
We used the Adam optimizer (cite) with \$\beta_1=0.9\$, \$\beta_2=0.98\$ and \$\epsilon=10^{-9}\$. We varied the learning rate over the course of training, according to the formula: This corresponds to increasing the learning rate linearly for the first \$\swarmup_steps\$ training steps, and decreasing it thereafter proportionally to the inverse square root of the step number. We used \$\swarmup_steps=4000\$.

Note: This part is very important. Need to train with this setup of the model.

```
class NoamOpt:
    "Optim wrapper that implements rate."
   def __init__(self, model_size, factor, warmup, optimizer):
       self.optimizer = optimizer
       self. step = 0
       self.warmup = warmup
       self.factor = factor
       self.model_size = model_size
       self. rate = 0
   def step(self):
        "Update parameters and rate"
       self. step += 1
       rate = self.rate()
       for p in self.optimizer.param_groups:
           p['lr'] = rate
       self. rate = rate
       self.optimizer.step()
   def rate(self, step = None):
        "Implement `lrate` above"
       if step is None:
           step = self._step
       return self.factor * \
           (self.model_size ** (-0.5) *
           min(step ** (-0.5), step * self.warmup ** (-1.5)))
def get std opt(model):
   return NoamOpt(model.src_embed[0].d_model, 2, 4000,
           torch.optim.Adam(model.parameters(), lr=0, betas=(0.9, 0.98), eps=1e-9))
```



Tips: Early Stopping



```
best_val_loss = None
earlystop counter = 0
for epoch_idx in range(num_epochs):
    # Training
    model.train()
    for batch_idx, batch in enumerate(train_dataloader):
    # Validation
    model.eval()
    for batch idx, batch in enumerate(valid dataloader):
    # Early stopping checkpoint
        if best val loss is None or \
           running_val_loss < best_val_loss:</pre>
        best_val_loss = running_val_loss
        earlystop counter = 0
    else:
        earlystop counter += 1
    if earlystop_counter >= patience:
        print("Early stopping.")
        break
```

Tips: Transferring data to GPU

- "data" must be in the GPU world if you use GPU
 - One solution is to wrap DataLoader and call .to(device) method for each data
 - The following code can handle

```
def generate_batches(dataset,
                     batch size,
                     shuffle=True,
                     drop_last=True,
                     device="cpu"):
    dataloader = DataLoader(dataset=dataset,
                            batch_size=batch_size,
                            shuffle=shuffle,
                            drop last=drop last)
    for data dict in dataloader:
        if device == "cpu":
            yield data_dict
        else:
            out_data_dict = {}
            for name, tensor in data dict.items():
                if type(tensor) == dict:
                    out_data_dict[name] = {}
                    for n, t in tensor.items():
                        out data dict[name][n] = data dict[name][n].to(device)
                else:
                    out_data_dict[name] = data_dict[name].to(device)
            yield out data dict
```