CS470 Lab

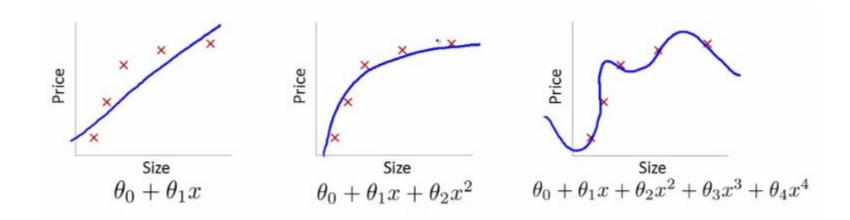
Tutorials for Colab and Pytorch

Announcement

- Team formation deadline is due this Friday!
- The first assignment will be release in the next week

Lower loss = better model?

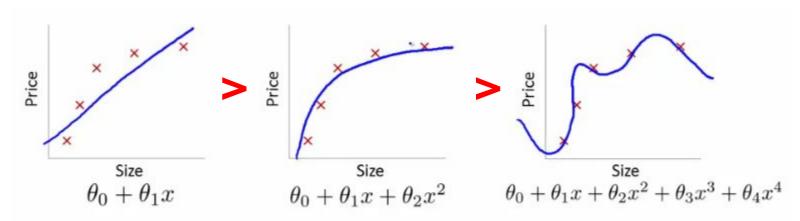
- So far, it seems like the neural network training is all about minimizing training error
- But does the lower training error always mean a better model?



Lower loss = better model?

- So far, it seems like the neural network training is all about minimizing training error
- But does the lower training error always mean a better model?

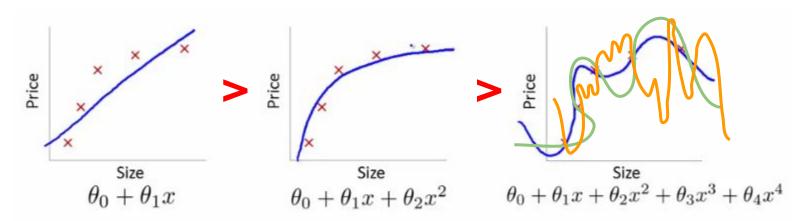
Training loss (error)



Lower loss = better model?

- So far, it seems like the neural network training is all about minimizing training error
- But does the lower training error always mean a better model?

Training loss (error)



There are also arbitrary many solutions that achieves the similar loss: which one is better?

Lower loss ≠ better model

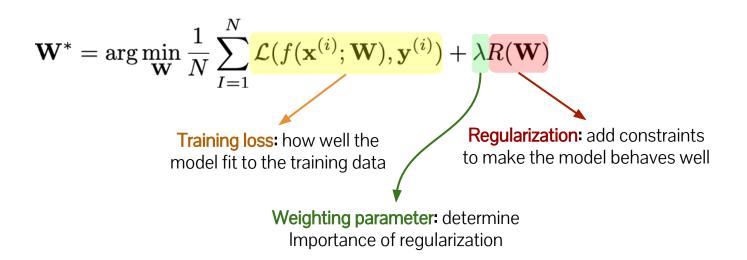
- Overfitting (memorization):
 - The model simply "memorizes" the training examples
 - Achieves very low training error, but very high test error (not generalized to unseen examples)
 - This problem is prevalent especially when **# of parameters** >> **# of training data** (can fit arbitrary complex functions to the data)

Regularizing neural network

- Option 1: weight decay
- Option 2: dropout
- Option 3: early stopping

Weight decay

Penalize complex solutions using additional constraints



Weight decay

Penalize complex solutions using additional constraints

$$\mathbf{W}^* = \arg\min_{\mathbf{W}} \frac{1}{N} \sum_{I=1}^{N} \mathcal{L}(f(\mathbf{x}^{(i)}; \mathbf{W}), \mathbf{y}^{(i)}) + \lambda \mathbf{R}(\mathbf{W})$$

Examples of regularization

- **L2** regularization **R(W)=||W||**₂: Prefer the weights roughly spreaded over all neurons
 - (i.e. make use of all neurons equally important)
- L1 regularization R(W)=||W||₁: Prefer sparse weights
 - (i.e. less complicated functions)

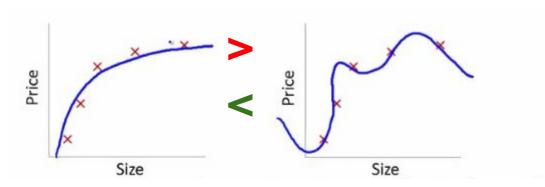
Weight decay

Penalize complex solutions using additional constraints

$$\mathbf{W}^* = \arg\min_{\mathbf{W}} \frac{1}{N} \sum_{I=1}^{N} \mathcal{L}(f(\mathbf{x}^{(i)}; \mathbf{W}), \mathbf{y}^{(i)}) + \lambda \mathbf{R}(\mathbf{W})$$

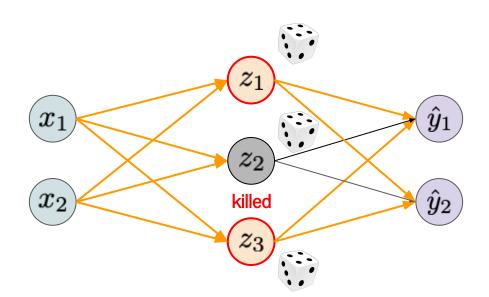
Training loss (error)

Training loss + λregularization



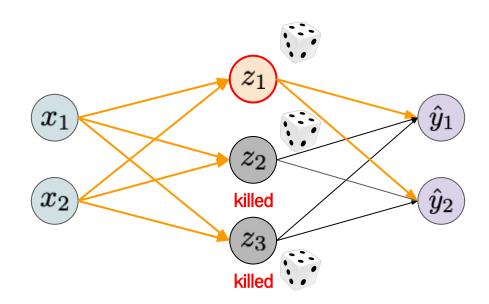
Dropout

Randomly turn off activations with some probability p



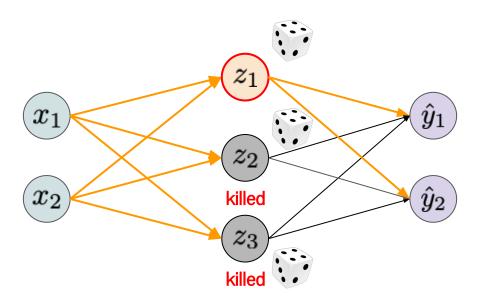
Dropout

Randomly turn off activations with some probability p

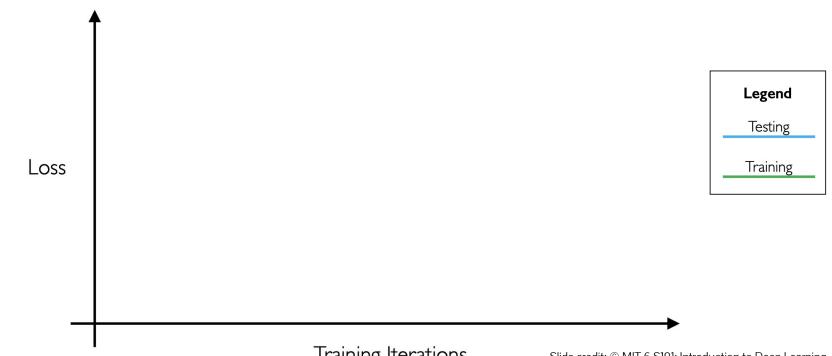


Dropout

- Randomly turn off activations with some probability p
 - Intuition: add stochasticity to the network to prevent memorization
 (every forward propagation leads to different outputs even for the same input)



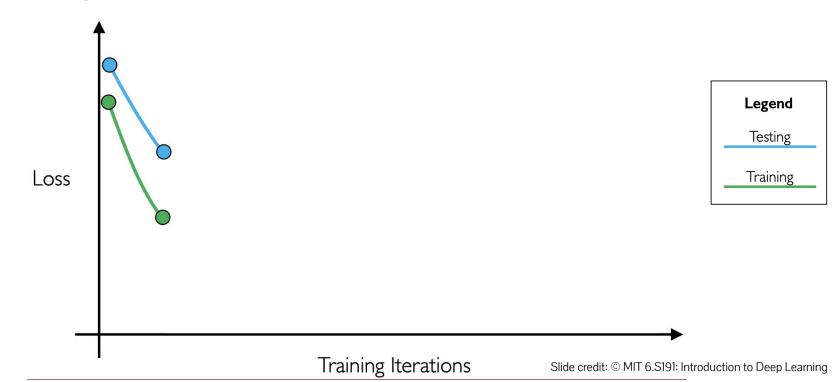
Stop training once the validation loss starts to increase



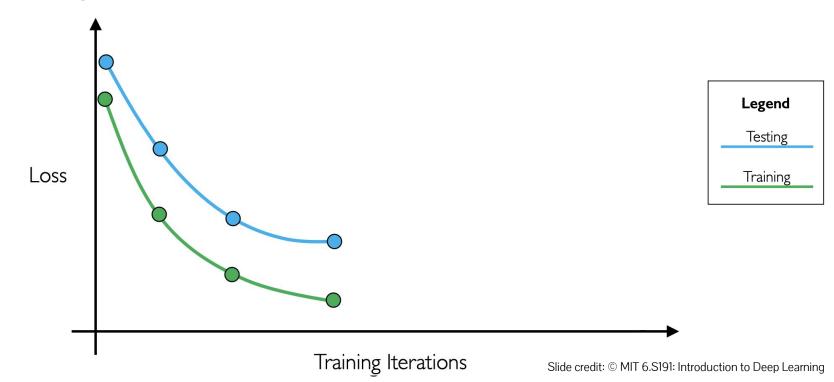
Training Iterations

Slide credit: © MIT 6.S191: Introduction to Deep Learning

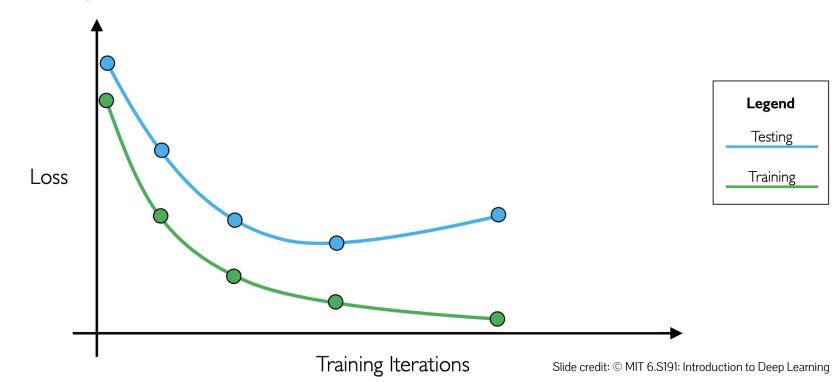
• Stop training once the validation loss starts to increase



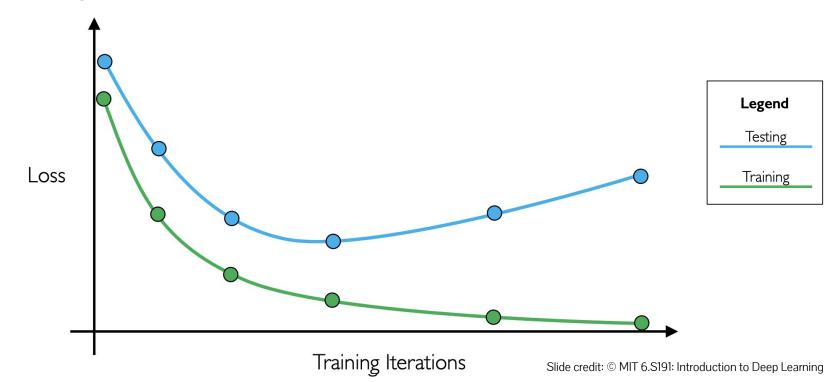
• Stop training once the validation loss starts to increase



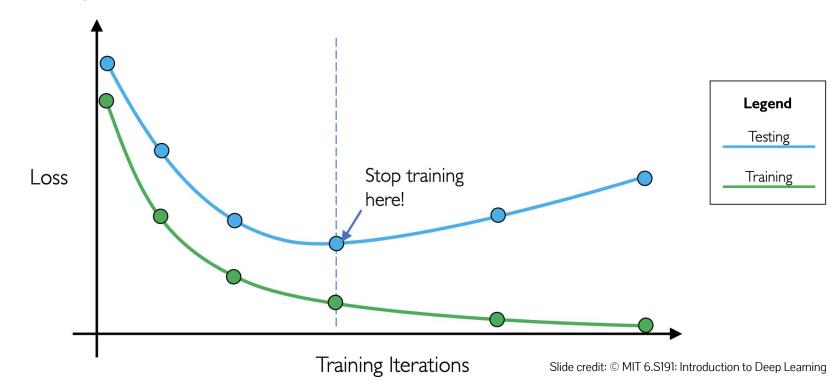
Stop training once the validation loss starts to increase



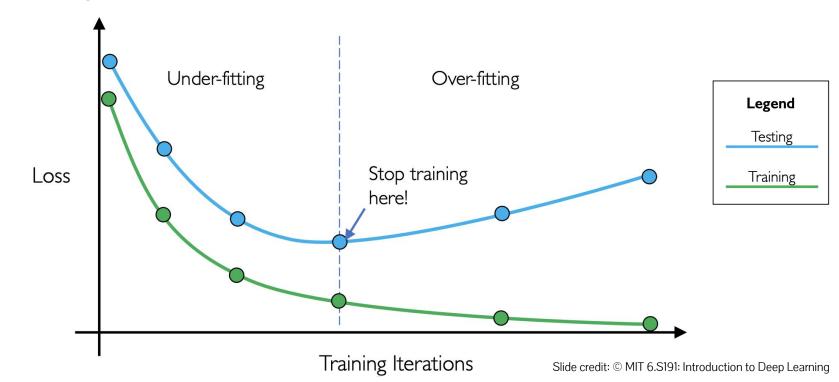
• Stop training once the validation loss starts to increase



• Stop training once the validation loss starts to increase



Stop training once the validation loss starts to increase



Summary:

- Overfitting: low training error, high testing error
 - Add regularizations to prevent memorization
 - Popular regularizations: weight decay, dropout, early stopping
- Underfitting: high training/testing error
 - Increase the model capacity/learning rate or train longer
- Improving generalization is an active research area
 - We will also discuss some other approaches in later parts of this course

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 - e. Access to your google drive in Colab
- Pytorch Tutorial
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 - b. Autograd and automatic differentiation
 - c. Building neural networks and optimizers
 - d. Data pipeline
 - e. Train and Test a simple MLP-based MNIST classifier

PyTorch Tutorial

Basics components and operations

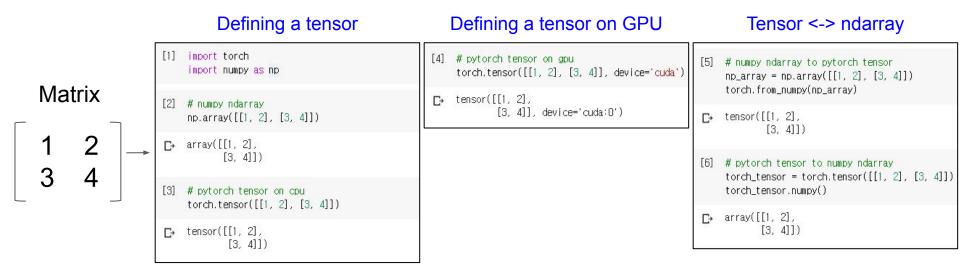
Importing PyTorch

Colab supports PyTorch by default

```
[1] 1 import torch 2 3 torch.__version__
```

Tensors: basic computing unit of Pytorch

- Basically, tensors are for representing scalars, vectors, and matrices
- Similar to NumPy's ndarrays, but <u>supports GPU acceleration</u>

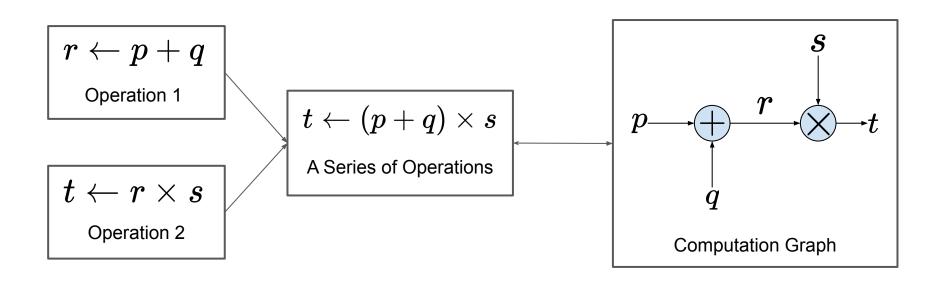


Basic arithmetic operations with tensors

a = torch.tensor([[1., 2.], [3., 4.]])

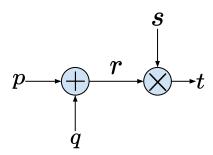
Computation graph

- A series of operations constructs a computation graph
- Any operation between tensors defines a node in the computation graph

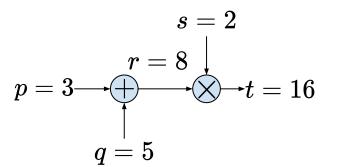


Computation graph and Forward function

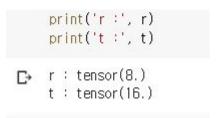
Consider below computation graph as our forward function



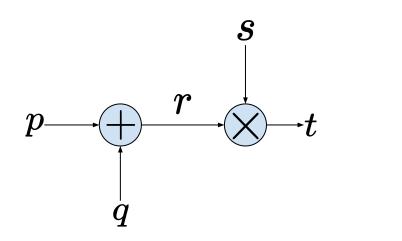
• If we assume p=3, q=5, and s=2, then we get r=8 and t=16.



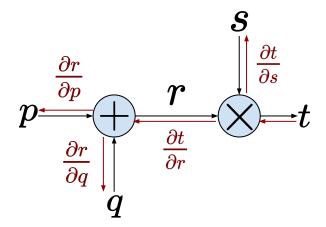
```
[14] p = torch.tensor(3.)
    q = torch.tensor(5.)
    s = torch.tensor(2.)
    r = p + q
    t = r * s
```



Forward & Backward functions

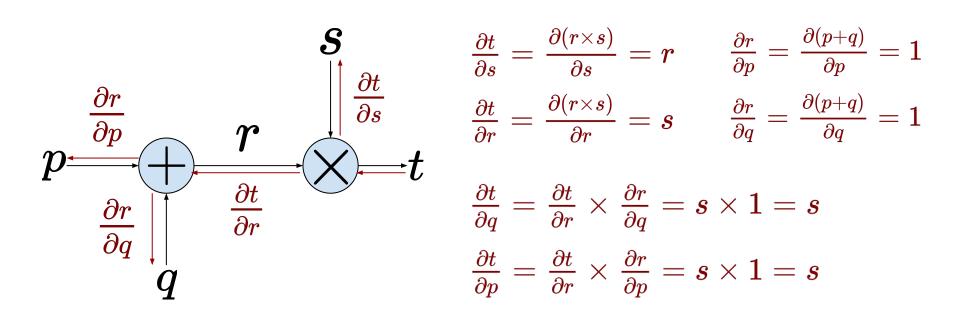






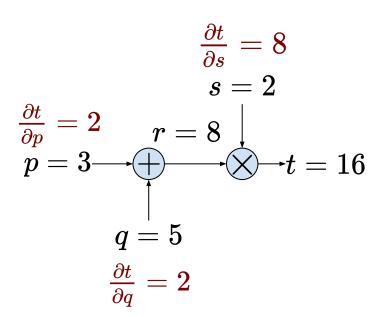
Backward Function

Backward function and Chain rule



Backward function: an example

• If we assume p=3, q=5, s=2, r=8, and t=16, then dt/ds=8, dt/dp=2 and dt/dq=2



Automatic differentiation (AutoGrad)

- Wait, then do we have to calculate all the derivatives on our own?
- What if the variables are vectors and matrices, but not scalars?
- No worries! AutoGrad Package in PyTorch will do that for us.

```
import torch
3 # Forward Propagation
4 p = torch.tensor([3.], requires_grad=True)
5 q = torch.tensor([5.], requires_grad=True)
6 s = torch.tensor([2.], requires_grad=True)
 7 r = p + a
8t = r * s
10 print('p :', p.item())
                                 p: 3.0
11 print('a :'. a.item())
12 print('s:', s.item())
                                 a: 5.0
                                 s: 2.0
13 print('r :', r.item())
                                 r: 8.0
t: 16.0
```

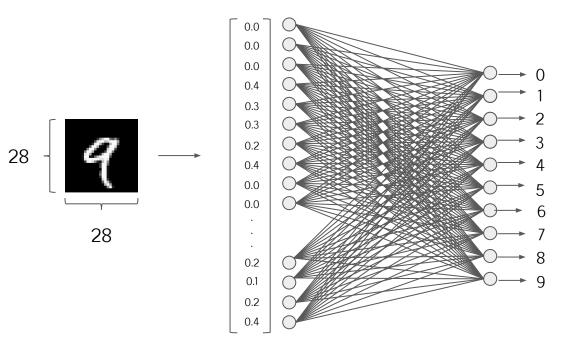
```
16 # Backward Propagation
17 t.backward()
18
19 print('dt/dp :', p.grad.item())
20 print('dt/dq :', q.grad.item())
21 print('dt/ds :', s.grad.item())
dt/dq : 2.0
dt/ds : 8.0
```

PyTorch Tutorial

Building a neural network

Let's build a one-layer baby network

One-layer classifier for MNIST digit classification



X: 784-dim

$$\mathbf{y} = \mathbf{x} \mathbf{W} + \mathbf{b}$$

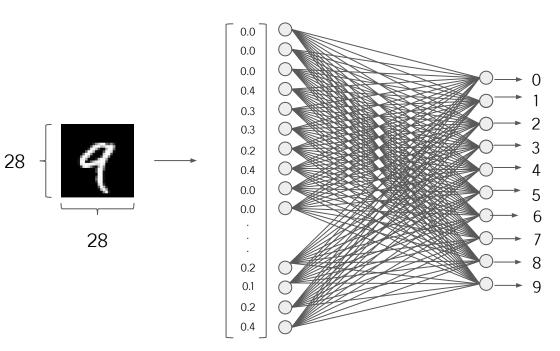
Size of W? [784, 10]

Size of b? [1, 10]

y: 10-dim

Let's build a one-layer baby network

One-layer classifier for MNIST digit classification



X: 784-dim

```
import math

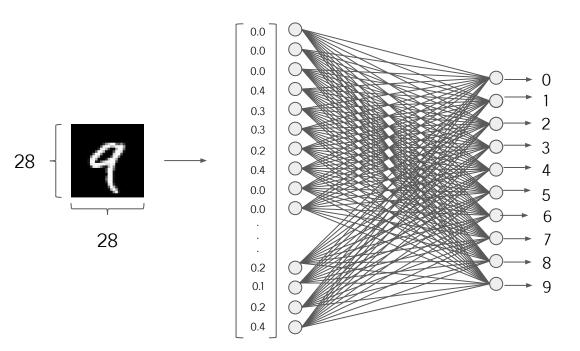
weights = torch.randn(784, 10) / math.sqrt(784)
weights.requires_grad_()
bias = torch.zeros(10, requires_grad=True)
```

y: 10-dim

Code credit: Jeremy Howard

Let's build a one-layer baby network

One-layer classifier for MNIST digit classification



X: 784-dim

y = xW + b

```
import math

weights = torch.randn(784, 10) / math.sqrt(784)
weights.requires_grad_()
bias = torch.zeros(10, requires_grad=True)
```

```
def log_softmax(x):
    return x - x.exp().sum(-1).log().unsqueeze(-1)

def model(xb):
    return log_softmax(xb @ weights + bias)
```

y: 10-dim

Baby network: forward propagation

```
bs = 64 # batch size

xb = x_train[0:bs] # a mini-batch from x
preds = model(xb) # predictions
preds[0], preds.shape
print(preds[0], preds.shape)
```

output:

```
tensor([-1.9759, -2.1991, -1.9989, -2.4762, -2.6573, -2.2036, -2.7582, -2.5692, -2.2971, -2.2089], grad_fn=<SelectBackward>) torch.Size([64, 10])
```

Baby network: loss function

Binary cross-entropy loss

```
def nll(input, target):
    return -input[range(target.shape[0]), target].mean()

loss_func = nll
```

Baby network: a training loop

```
from IPython.core.debugger import set_trace
lr = 0.5 # learning rate
epochs = 2 # how many epochs to train for
for epoch in range(epochs):
    for i in range((n - 1) // bs + 1):
                 set trace()
        start i = i * bs
        end_i = start_i + bs
       xb = x_train[start_i:end_i]
       yb = y_train[start_i:end_i]
       pred = model(xb)
       loss = loss_func(pred, yb)
```

loss.backward()

Sampling the minibatch (of the size bs)

Forward & loss computation

Gradient update step

with torch.no_grad():
 weights -= weights.grad * lr
 bias -= bias.grad * lr
 weights.grad.zero_()
 bias.grad.zero_()

Code credit: Jeremy Howard

What should we have for this single-layer network?

- Network parameters
 - Tensors for weight and bias
- Forward and backward mechanisms
 - y=xW + b in this case
- Gradient of parameters
 - All parameters in the network should hold the gradient of the loss w.r.t itself
- Loss function
 - A binary cross entropy loss in this case
- Optimizations
 - Weight initialization, a naive gradient update mechanism (SGD)

How about more complicated networks?

A single linear network



of layers: 1

A matrix multiplication and addition

Inception (GoogleNet)



of layers: a lot

Parallel convolution with different filter sizes, nonlinear functions, batch norm, average and max poolings, multi-head loss, ...

Solution: modularize the computations

Modularize a layer using a class, which comes with handy utility functions
 (e.g. managing parameters/gradients, forward/backward, switching b/w training/evaluation modes, etc)

```
from torch import nn

class Mnist_Logistic (nn.Module):
    def __init__(self):
        super().__init__()
        self.weights = nn.Parameter(torch.randn(784, 10) / math.sqrt(784))
        self.bias = nn.Parameter(torch.zeros(10))

def forward(self, xb):
    return xb @ self.weights + self.bias
```

It inherits other utility functions defined in torch.nn.Module

Solution: modularize the computations

Modularize a layer using a class, which comes with handy utility functions
 (e.g. managing parameters/gradients, forward/backward, switching b/w training/evaluation modes, etc)

```
class Linear(Module):
   constants = ['in features', 'out features']
   def __init__(self, in_features, out_features, bias=True):
       super(Linear, self).__init__()
       self.in features = in features
       self.out_features = out_features
       self.weight = Parameter(torch.Tensor(out_features, in_features))
       if bias:
           self.bias = Parameter(torch.Tensor(out features))
       else:
           self.register parameter('bias', None)
       self.reset parameters()
   def reset parameters(self):
       init.kaiming_uniform_(self.weight, a=math.sqrt(5))
       if self.bias is not None:
           fan_in, _ = init._calculate_fan_in_and_fan_out(self.weight)
           bound = 1 / math.sqrt(fan in)
           init.uniform_(self.bias, -bound, bound)
   def forward(self, input):
       return F.linear(input, self.weight, self.bias)
```

Example:

Actual definition of fully-connected layer in PyTorch

Solution: modularize the computations

- Modularize a layer using a class, which comes with handy utility functions
 (e.g. managing parameters/gradients, forward/backward, switching b/w training/evaluation modes, etc)
- We can build a complicated neural network by simply composing these layers

Google Colaboratory

Before we start ...

- 1. Create your google account if you don't have one
- 2. Go to this Link and open Introduction to Colab.ipynb
- 3. Click `File` tab -> Click `Save a copy in drive` button
 - This will save the notebook file in your google drive, which is necessary to follow the tutorial
 - Check `Colab Notebooks` directory in your google drive if the notebook is saved successfully

What is Colaboratory?

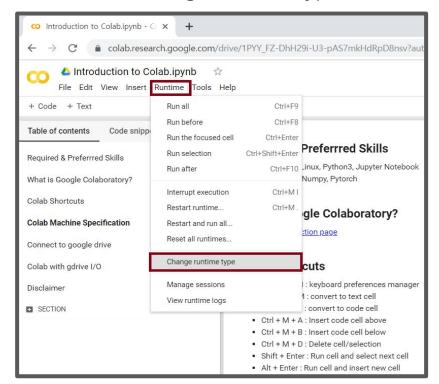
- Colaboratory is a free Jupyter notebook environment that requires no setup and runs entirely in the cloud.
- With Colaboratory you can write and execute code, save and share your analyses, and access powerful computing resources, all for free from your browser.
- Colaboratory is run on a Ubuntu 18.04 virtual machine equipped with 13GB RAM, ~310GB Storage limits, and GPUs (K80, TPU).

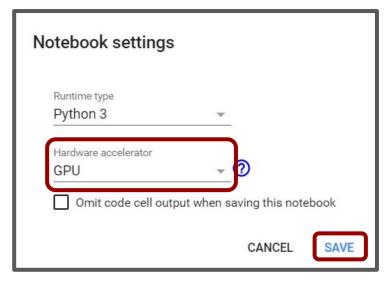
Handy shortcuts

- Ctrl + M + H : keyboard preferences manager
- Ctrl + M + M : convert to text cell
- Ctrl + M + Y : convert to code cell
- Ctrl + M + A : Insert code cell above
- Ctrl + M + B : Insert code cell below
- Ctrl + M + D : Delete cell/selection
- Shift + Enter : Run cell and select next cell
- Alt + Enter : Run cell and insert new cell
- Ctrl + M + I : Interrupt execution
- Ctrl + M + . : Restart Runtime
- Ctrl + / : comment/uncomment

How to setup GPU

Runtime -> Change runtime type -> Set Hardware accelerator to GPU -> Save





Run the script below, and follow the instruction. Namely,

- 1. Go to the given URL in a browser
- 2. Select your cs470 account and log-in
- 3. Allow access to the google account
- 4. Copy the given authorization code, and paste it into the blank below

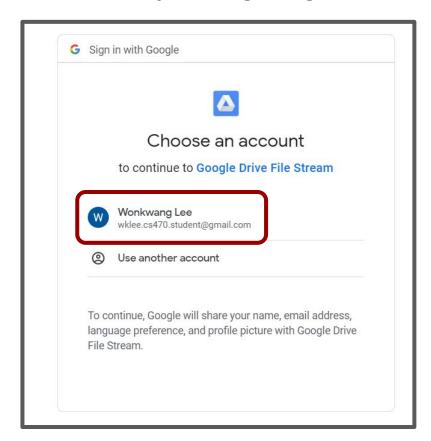
If you succeed, then you'll see "Mounted at /gdrive"

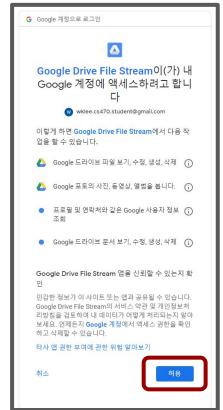
Note: This step should be repeated everytime you initialize the runtime sesison



••• Go to this URL in a browser: https://accounts.google.com/o/oauth2/auth?client_id=947318989803-6bn6qk8qdgf4n

Enter your authorization code:







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••• Go to this URL in a browser: https://accounts.google.com/o/oauth2/auth?client_id=947318989803-6bn6qk8qdgf4n-

Enter your authorization code:





Access to your google drive in Colab

```
# check what's in the mounted gdrive using Colab import os

gdrive_root = '/gdrive/My Drive' print('In gdrive :', os.listdir(gdrive_root))

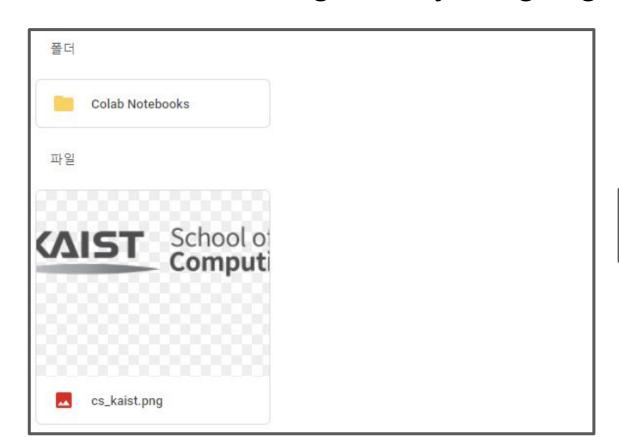
notebook_dir = os.path.join(gdrive_root, 'Colab Notebooks') print('In Colab Notebooks :', os.listdir(notebook_dir))

The gdrive : ['Colab Notebooks'] In Colab Notebooks : ['Copy of Introduction to Colab.ipynb']
```

Download an image into your google drive

```
# download and save an image
!wget https://cs.kaist.ac.kr/common/images/header/logo top.png -0 '/gdrive/My Drive/cs kaist.png'
print('In gdrive :', os.listdir(gdrive root))
# Go to the google drive hompage(https://drive.google.com/drive/my-drive),
# log-in using your CS470 account,
# and browse your gdrive directory to check if the image is downloaded successfully
--2019-09-08 12:12:39-- https://cs.kaist.ac.kr/common/images/header/logo_top.png
Resolving cs.kaist.ac.kr (cs.kaist.ac.kr)... 192.249.19.36
Connecting to cs.kaist.ac.kr (cs.kaist.ac.kr) 192.249.19.36:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 6313 (6.2K) [image/png]
Saving to: '/gdrive/My Drive/cs kaist.png'
in 0s
2019-09-08 12:12:41 (13.3 MB/s) - '/gdrive/My Drive/cs_kaist.png' saved [6313/6313]
In gdrive : ['Colab Notebooks', 'cs_kaist.png']
```

Download an image into your google drive





Load the image from your google drive

```
# load the saved image
from PIL import Image

image_path = os.path.join(gdrive_root, 'cs_kaist.png')
img = Image.open(image_path)
img

School of
Computing
```

Disclaimer

- Runtime session will last at most 12 hours, regardless of devices (e.g. CPU, GPU, and TPU)
 - o if you left the browser opened, probably the session will last at most 12 hours
 - o if you closed the browser, probably the session will last at most 90 minutes
- Therefore, it is highly recommended that you periodically back-up your data/outputs to your gdrive and resume your training by re-loading your saved data. Otherwise, you'll lose everything you've trained as soon as the session is recycled.

PyTorch + Colab

Train and test a simple MLP-based MNIST classifier

Again,

- 1. Create your google account if you don't have one
- 2. Go to this <u>Link</u> and open5. Train and Test a simple MLP-based MNIST classifier.ipynb
- 3. Click `File` tab -> Click `Save a copy in drive` button
 - This will save the notebook file in your google drive, which is necessary to follow the tutorial
 - Check `Colab Notebooks` directory in your google drive if the notebook is saved successfully

Common steps for training a neural network in Colab

- 1. Connect to your google drive
- 2. Import modules
- 3. Configure the experiments (e.g. hyper-parameters)
- 4. Construct data pipeline
- 5. Construct a neural network builder
- 6. Initialize the network and optimizer
- 7. Load pre-trained weight if exists
- 8. Train the network
- Visualize and analyze the results

1. Connect to your google drive

 This step is required if you want to save checkpoints into your drive and load them later on

```
from google.colab import drive

drive.mount('/gdrive')
gdrive_root = '/gdrive/My Drive'

Go to this URL in a browser: https://accounts.google.com/o/oauth2/auth?c

Enter your authorization code:
.........

Mounted at /gdrive
```

2. Import modules

```
import os

import torch
import torch.optim as optim
import torch.nn as nn
import torch.nn.functional as F
from torch.utils.data import DataLoader
from torchvision import transforms
from torchvision.datasets import MNIST
```

3. Configure the experiments

```
# training & optimization hyper-parameters
max_epoch = 10
learning_rate = 0.0001
batch_size = 200
device = 'cuda'

# model hyper-parameters
input_dim = 784 # 28x28=784
hidden_dim = 512
output_dim = 10
```

4. Construct data pipeline

- torchvision.datasets.MNIST will automatically construct MNIST dataset.
- torch.utils.data.DataLoader receives MNIST dataset and does followings
 - parse data using multi-processing
 - make mini-batches of data
 - shuffle data when make a mini-batch

```
data_dir = os.path.join(gdrive_root, 'my_data')
transform = transforms.ToTensor()
train_dataset = MNIST(data_dir, train=True, download=True, transform=transform)
train_dataloader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True, drop_last=True)
test_dataset = MNIST(data_dir, train=False, download=True, transform=transform)
test_dataloader = DataLoader(test_dataset, batch_size=batch_size, shuffle=False, drop_last=False)
```

5. Construct a neural network builder

 Here we're going to train a simple MLP-based neural network with ReLU non-linear activation functions.

```
class MyClassifier(nn.Module):
  def __init__(self, input_dim=784, hidden_dim=512, output_dim=10):
    super(MyClassifier, self).__init__()
    self.layers = nn.Sequential(
      nn.Linear(input dim, hidden dim),
      nn.ReLU(),
      nn.Linear(hidden dim, hidden dim),
      nn.ReLU(),
      nn.Linear(hidden dim, hidden dim),
     nn.ReLU(),
      nn.Linear(hidden dim, output dim),
  def forward(self, x):
    batch size = x.size(0)
   x = x.view(batch_size, -1)
   outputs = self.layers(x)
    return outputs
```

6. Initialize the network and optimizer

Initialize the network and pass its parameters to the optimizer

```
my_classifier = MyClassifier(input_dim, hidden_dim, output_dim)
my_classifier = my_classifier.to(device)
optimizer = optim.Adam(my_classifier.parameters(), lr=learning_rate)
```

7. Load pre-trained weight if exists

- Later when we train a neural network, we're going to save checkpoints periodically into the location 'gdrive/My Drive/checkpoints'.
- And if you have a saved checkpoint there, this block will load it and resume the training.

```
ckpt_dir = os.path.join(gdrive_root, 'checkpoints')
if not os.path.exists(ckpt_dir):
    os.makedirs(ckpt_dir)

ckpt_path = os.path.join(ckpt_dir, 'lastest.pt')
if os.path.exists(ckpt_path):
    ckpt = torch.load(ckpt_path)
    best_acc = ckpt['best_acc']
    my_classifier.load_state_dict(ckpt['my_classifier'])
    optimizer.load_state_dict(ckpt['optimizer'])
    print('checkpoint is loaded !')
    print('current best accuracy : %.2f' % best_acc)
else:
    best_acc = 0
```

8. Now train the network

- Training session consists of mainly three parts:
 - train phase
 - test phase
 - backup phase

```
it = 0
train_losses = []
test_losses = []
for epoch in range(max_epoch):
    # train phase
    # ...

# test phase
# ...

# save checkpoint whenever there is improvement in performance
# ...
```

8. Now train the network - train phase

```
it = 0
train losses = []
test losses = []
for epoch in range(max_epoch):
 # train phase
 for inputs, labels in train dataloader:
    it += 1
    # load data to the GPU.
    inputs = inputs.to(device)
   labels = labels.to(device)
    # feed data into the network and get outputs.
   logits = my classifier(inputs)
    # calculate loss
    # Note: `F.cross entropy` function receives logits, or pre-softmax outputs, rather than final probability scores.
    loss = F.cross entropy(logits, labels)
    # Note: You should flush out gradients computed at the previous step before computing gradients at the current step.
           Otherwise, gradients will accumulate.
    optimizer.zero grad()
   # backprogate loss.
   loss.backward()
   # update the weights in the network.
    optimizer.step()
    # calculate accuracy.
    acc = (logits.argmax(dim=1) == labels).float().mean()
    if it % 200 == 0:
      print('[epoch:{}, iteration:{}] train loss : {:.4f} train accuracy : {:.4f}'.format(epoch, it, loss.item(), acc.item()))
  # save losses in a list so that we can visualize them later.
  train losses.append(loss.item())
```

8. Now train the network - test phase

- test phase follows the same steps as the train phase, except that:
 - use test data instead of train data
 - do not back-propagate loss and update weights

```
# test phase
n = 0.
test_loss = 0.
test_acc = 0.
for test_inputs, test_labels in test_dataloader:
    test_inputs = test_inputs.to(device)
    test_labels = test_labels.to(device)

logits = my_classifier(test_inputs)
    test_loss += F.cross_entropy(logits, test_labels, reduction='sum')
    test_acc += (logits.argmax(dim=1) == test_labels).float().sum()
    n += inputs.size(0)

test_loss /= n
test_acc /= n
test_acc /= n
test_losses.append(test_loss.item())
print('[epoch:{}, iteration:{}] test_loss : {:.4f} test_accuracy : {:.4f}'.format(epoch, it, test_loss.item(), test_acc.item()))
```

8. Now train the network - checkpointing

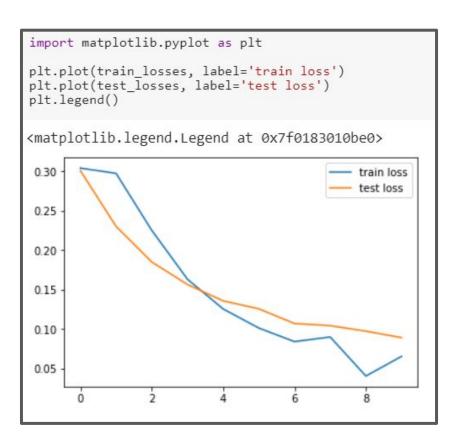
 It is always a good idea to save the checkpoints periodically, otherwise you'll lose everything you've trained if the session is expired.

8. Now train the network - results

After 10 epochs,
 you'll get near 98% accuracy on MNIST dataset

```
[epoch:5, iteration:1600] train loss: 0.1125 train accuracy: 0.9700
[epoch:5, iteration:1800] train loss: 0.1012 train accuracy: 0.9700
[epoch:5, iteration:1800] test loss: 0.1256 test accuracy: 0.9606
checkpoint is saved !
[epoch:6, iteration:2000] train loss: 0.0906 train accuracy: 0.9750
[epoch:6, iteration:2100] test loss: 0.1069 test accuracy: 0.9663
checkpoint is saved !
[epoch:7, iteration:2200] train loss: 0.0742 train accuracy: 0.9750
[epoch:7, iteration:2400] train loss: 0.0898 train accuracy: 0.9750
[epoch:7, iteration:2400] test loss: 0.1042 test accuracy: 0.9671
checkpoint is saved !
[epoch:8, iteration:2600] train loss: 0.0897 train accuracy: 0.9800
[epoch:8, iteration:2700] test loss: 0.0972 test accuracy: 0.9698
checkpoint is saved !
[epoch:9, iteration:2800] train loss: 0.0885 train accuracy: 0.9700
[epoch:9, iteration:3000] train loss: 0.0652 train accuracy: 0.9750
[epoch:9, iteration:3000] test loss: 0.0889 test accuracy: 0.9720
checkpoint is saved !
```

9. Visualize and analyze the results - 1



9. Visualize and analyze the results - 2

```
import random
from PIL import Image
num test samples = len(test dataset)
random_idx = random.randint(0, num_test_samples)
topil = transforms.transforms.ToPILImage()
test input, test label = test dataset. getitem (random idx)
test prediction = F.softmax(my classifier(test input.unsqueeze(0).to(device)), dim=1).argmax().item()
print('label : %i' % test label)
print('prediction : %i' % test prediction)
test image = topil(test input)
test image.resize((128, 128))
label: 0
prediction: 0
```