Tutorials for Colab and PyTorch

Jinwoo Kim

jinwoo-kim@kaist.ac.kr

Table of Contents [link to the materials]

- Google Colaboratory
 - a. Create a google account
 - b. What is Colaboratory?
 - c. How to use GPU in Colab
 - d. How to connect a Colab notebook with your google drive
 - e. Access to your google drive in Colab
- Pytorch Tutorial
 - a. Tensor and its basic operations
 - 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

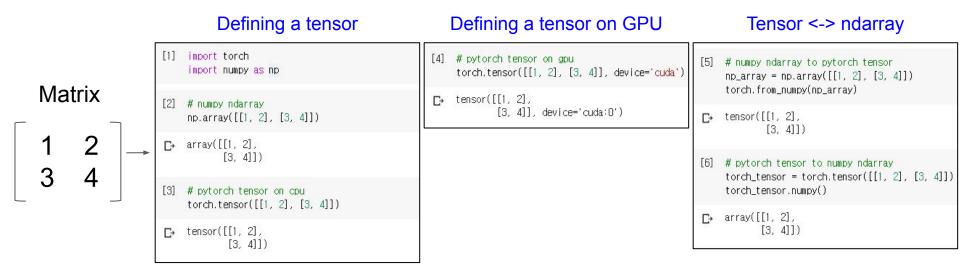
Importing PyTorch

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>

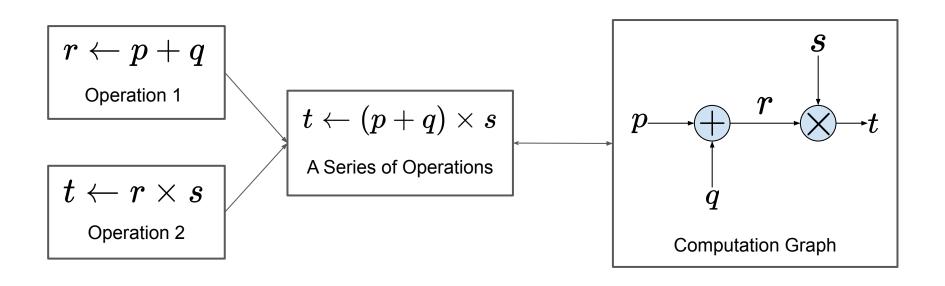


Basic arithmetic operations with tensors

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

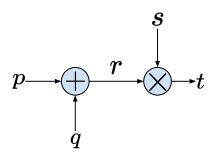
Computation graph

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

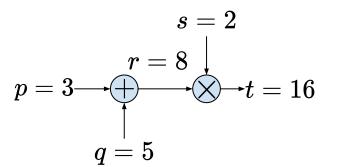


Computation graph and Forward function

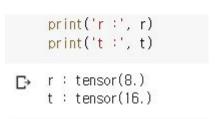
Consider below computation graph as our forward function



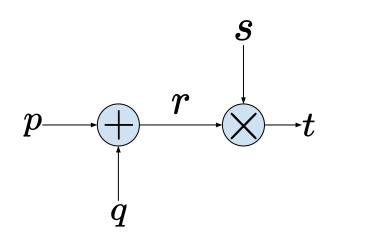
• If we assume p=3, q=5, and s=2, then we get r=8 and t=16.



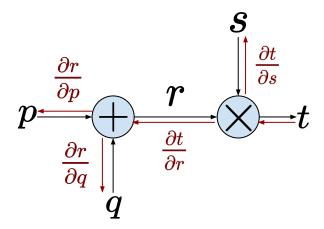
```
[14] p = torch.tensor(3.)
    q = torch.tensor(5.)
    s = torch.tensor(2.)
    r = p + q
    t = r * s
```



Forward & Backward functions

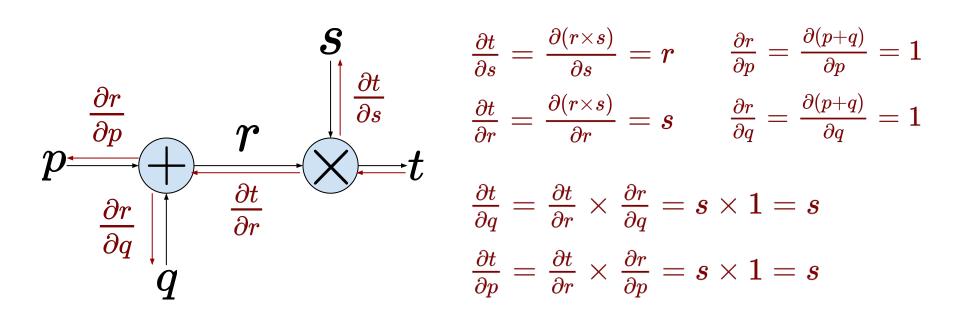






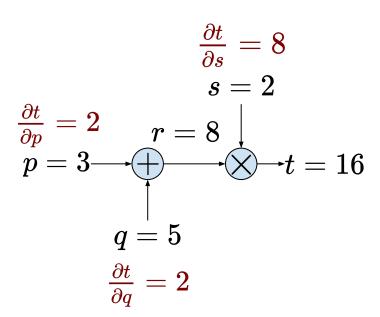
Backward Function

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
```

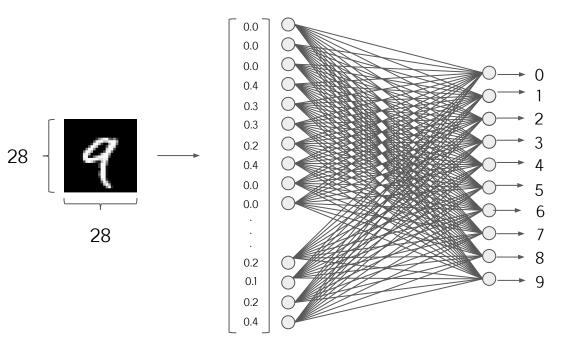
```
16 # Backward Propagation
17 t.backward()
18
19 print('dt/dp:', p.grad.item())
20 print('dt/dq:', q.grad.item())
21 print('dt/ds:', s.grad.item())
dt/dq: 2.0
dt/ds: 8.0
```

PyTorch Tutorial

Building a neural network

Let's build a one-layer baby network

One-layer classifier for MNIST digit classification



X: 784-dim

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

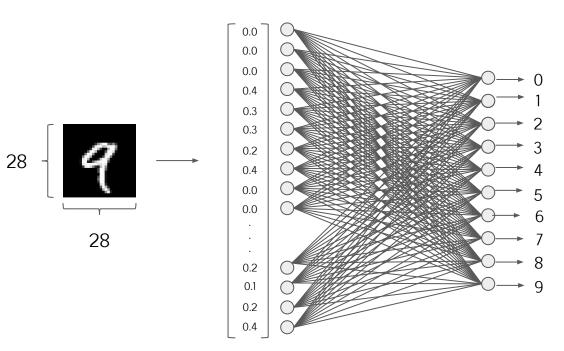
Size of W? [784, 10]

Size of b? [1, 10]

y: 10-dim

Let's build a one-layer baby network

One-layer classifier for MNIST digit classification



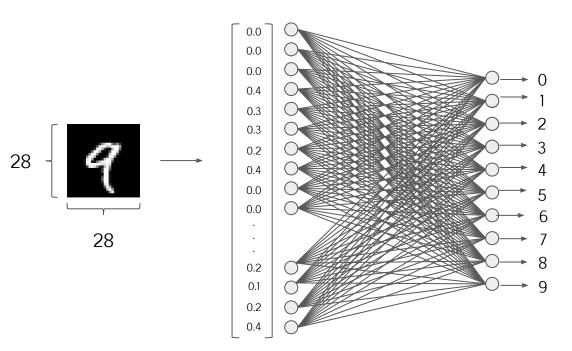
X: 784-dim

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

y: 10-dim

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

Code credit: Jeremy Howard

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?

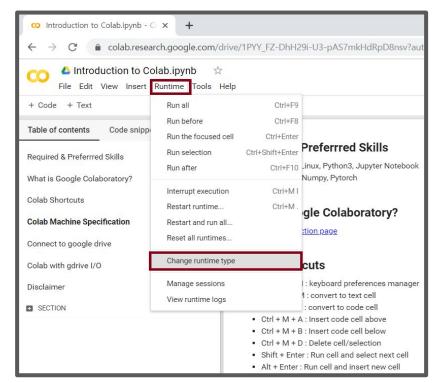
- Colaboratory is a free Jupyter notebook environment that requires no setup and runs entirely in the cloud.
- With Colaboratory you can write and execute code, save and share your analyses, and access powerful computing resources, all for free from your browser.
- Colaboratory is run on a Ubuntu 18.04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

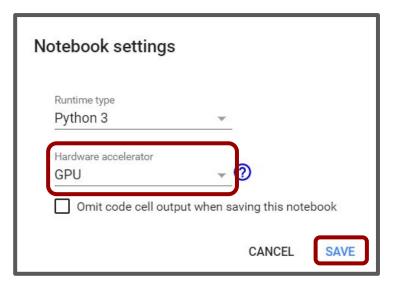
Handy shortcuts

- 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

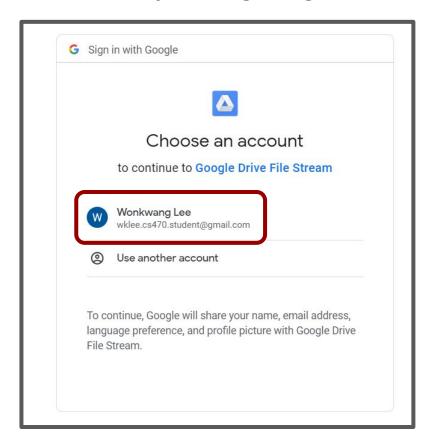
If you succeed, then you'll see "Mounted at /gdrive"

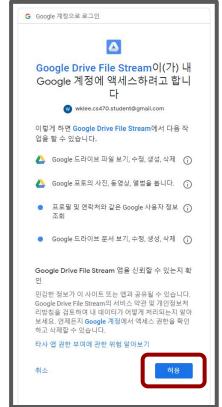
Note: This step should be repeated everytime you initialize the runtime sesison



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

Enter your authorization code:







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:





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))

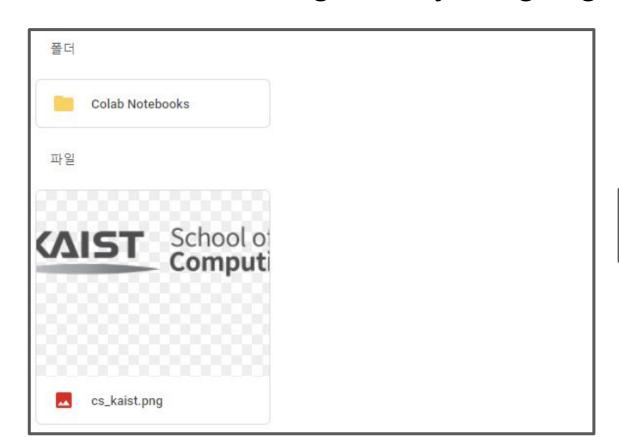
notebook_dir = os.path.join(gdrive_root, 'Colab Notebooks') print('In Colab Notebooks :', os.listdir(notebook_dir))

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
- Go to this <u>Link</u> and open
 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

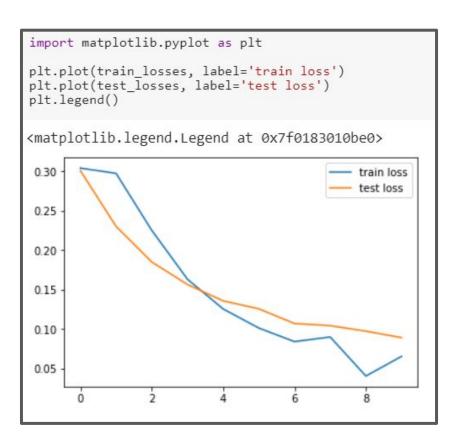
 It is always a good idea to save the checkpoints periodically, otherwise you'll lose everything you've trained if the session is expired.

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

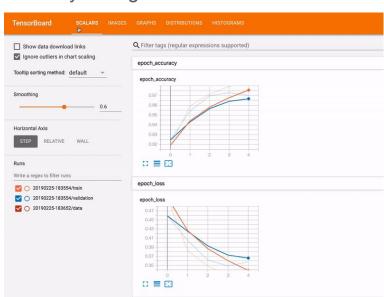


9. Visualize and analyze the results - 2

```
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
```

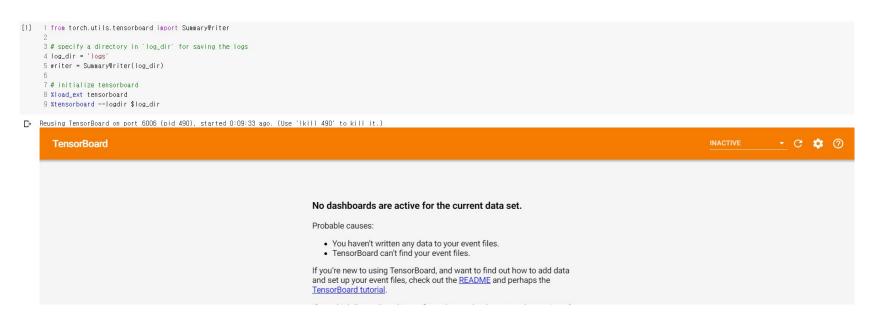
Monitoring the training: Tensorboard

- Tracking and visualizing metrics such as loss and accuracy
- Visualizing the model graph (ops and layers)
- Viewing histograms of weights, biases, or other tensors as they change over time
- Projecting embeddings to a lower dimensional space
- Displaying images, text, and audio data
- Profiling TensorFlow programs
- And much more



Monitoring the training: Tensorboard

- Colab supports tensorboard by default
- At first, it doesn't show anything since no logs are saved in the directory



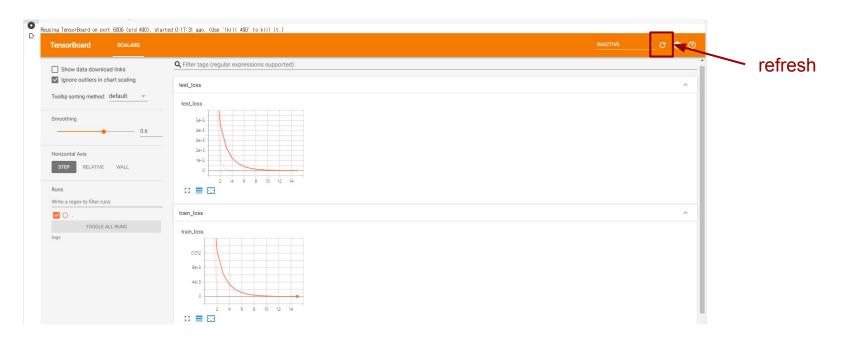
Monitoring the training: T

Just add <u>two more lines</u>
 into the loop
 to save and visualize the losses

```
1 # train & test the model
 2 \text{ max\_epoch} = 50
 3 best_test_loss = 999999
 4 for epoch in range(max_epoch):
    train_loss = 0.
    for train_iteration, (x, y) in enumerate(train_dataloader):
      # train_dataloader gives us minibatch data (x, y) at each iteration
      # forward x through the network
      y_pred = regressor(x)
      # compute loss
      loss = compute_loss(y_pred, y)
      train_loss += loss.item()/num_train_data
      # flush previously computed gradients
      optimizer.zero_grad()
      # backward the loss to compute gradients
      loss.backward()
      # update weights using the gradients
      optimizer.step()
21
    print('epoch : %02d | train loss : %.10f' % (epoch+1, train_loss))
    # log train_loss
    writer.add_scalar('train_loss', train_loss, epoch+1)
    num\_test\_sample = 0.
    test loss = 0.
    for x, y in test_dataloader:
      # test_dataloader gives us minibatch data (x, y) at each iteration
30
      # forward x through the network
      y_pred = regressor(x)
      # compute loss
      loss = compute_loss(v_pred, v)
      test_loss += loss.item()/num_test_data
    print('epoch : %02d | test loss : %.10f' % (epoch+1, test_loss))
    # log test_loss
    writer.add_scalar('test_loss', test_loss, epoch+1)
    # checkpoint the model weights if necessary (e.g. when the model achieved the best test loss.)
    torch.save(regressor.state_dict(), 'latest_weight.pt')
     if best_test_loss > test_loss:
      best_test_loss = test_loss
      torch.save(regressor.state_dict(), 'best_weight.pt')
```

Monitoring the training: Tensorboard

Go back to the tensorboard, and press refresh button



More resources

- Official PyTorch tutorials
 - Highly recommend you to go through all four tutorials in it