



ECE 661  
COMP ENG ML & DEEP NEURAL NETS  
**TUTORIAL: NUMPY/PYTORCH**

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# **COLAB ENVIRONMENT**

# Overview

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- Google Colaboratory is an online interactive python IDE that provides free GPU resources
  - Already has most scientific packages (e.g., NumPy, PyTorch) installed
- You can think of it as a Jupyter Notebook running in your Google Drive
- Workflow:
  - Download .ipynb file from Sakai
  - Upload it to a folder in your Google Drive
  - From within Google Drive, open the file with Colab

# Local install

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- Alternatively, you could install PyTorch on your local machine (macOS or Linux)
  - <https://pytorch.org/get-started/locally/>
  - If you do not have a GPU w/ CUDA, your training will be very slow
  - We recommend students use Colab to leverage GPUs when training

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# NUMPY TUTORIAL

# What is Numpy?

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- NumPy is a fundamental Python package for scientific computing on CPU
- Provides us a user-friendly interface to perform fast matrix computations via vectorized backend code
- The core is the ndarray object, which is an n-dimensional array

# NumPy tutorial

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- Array
- Indexing
- Math operations
- Broadcasting
- Frequently used functions

# NumPy tutorial

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- NumPy Array

A NumPy array is a grid of values which have the same type. A NumPy array is indexed by a tuple of non-negative integers.

```
import numpy as np                # Import the numpy library
# a is a python list.
a = [2,3,4,5]
# b is a numpy array, which has the same values and shapes as a.
b = np.array([2,3,4,5])
# c is also a numpy array, which has the same values and shapes as a.
c = np.array(a)
# d is a 2x4 numpy array with all zeros.
d = np.zeros((2,4))
# e is a numpy array with all zeros with the same shape as a.
e = np.zeros_like(a)
```

The **rank** of the array is the number of dimensions.



# NumPy tutorial

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- Shape of NumPy array

The **shape** of an array is a tuple of integers giving the size of the array along each dimension.

```
import numpy as np                # Import the numpy library
# a is a numpy array.
a = np.array([[2,3],[4,5]])
# Get the shape of a.
print(a.shape)
Output: (2,2)
# Reshape a to 1x4 array.
a=np.reshape(a, (1,4))
print(a)
Output: array([[2, 3, 4, 5]])
```

# NumPy tutorial

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- Indexing of NumPy array

Unlike python list, NumPy arrays can be sliced **multidimensionally**.

```
import numpy as np                # Import the NumPy library
# a is a python list.
a = [[2,3],[4,5]]
# b is a NumPy array, which has the same values and shapes as a.
b = np.array([[2,3],[4,5]])
# Slicing a list multi-dimensionally will lead to error
a[:1, :1]
# Error: list indices must be integers or slices, not tuple
# However, NumPy array can be sliced multi-dimensionally.
b[:1, :1]
# Output: array([[2]])
```

# NumPy tutorial

---

- Boolean indexing of NumPy array

**Boolean array indexing** allows us to select arbitrary elements of an array with maximal efficiency.

```
import numpy as np
a = np.array([[1,2], [3, 4], [5, 6]])
# Find the elements of a that are greater than 2 and
bool_idx = (a > 2)
# return the corresponding boolean mask.
print(bool_idx)
Output: array([[False False] [ True True] [ True True]])
print(a[bool_idx])
Output: array([3 4 5 6])
# We can do all of the above in a single concise statement:
print(a[a > 2])
Output: [3 4 5 6]
```

# NumPy tutorial

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- Math operations of NumPy arrays

Most math operations operate **element-wise** on NumPy arrays.

```
import numpy as np
# Initialize two arrays
x = np.array([[1,2],[3,4]], dtype=np.float64)
y = np.array([[5,6],[7,8]], dtype=np.float64)
# Element-wise sum. '+' is overloaded.
print(x + y)
print(np.add(x, y))
Output: [[ 6.0  8.0] [10.0 12.0]]
# Element-wise product; both produce the array
print(x * y)
print(np.multiply(x, y))
Output: [[ 5.0 12.0] [21.0 32.0]]
# Element-wise square root; produces the array
print(np.sqrt(x))
Output: [[ 1.  1.41421356] [ 1.73205081  2.  ]]
```

# NumPy tutorial

---

- Broadcasting on NumPy array

**Broadcasting** is a powerful mechanism that allows NumPy to work with arrays of different shapes when performing arithmetic operations.

```
import numpy as np
# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = x + v                                # v is expanded to
[[1,0,1],[1,0,1],[1,0,1],[1,0,1]]
# Add v to each row of x using broadcasting
print(y)
Output: [[ 2  2  4] [ 5  5  7] [ 8  8 10] [11 11 13]]
```

Note: We recommend you use broadcasting carry on matrix operations. Avoid using loops as it is quite inefficient.

# NumPy tutorial

---

- Always remember to import NumPy:

```
import numpy as np
```

## Frequently used functions:

Function	Description
<code>np.concatenate</code>	Concatenate two arrays
<code>np.random.random</code>	Generate random arrays
<code>np.random.permutation</code>	Generate random sequence
<code>np.sum/np.mean/np.std</code>	Get sum/mean/variance of an array
<code>np.argsort</code>	Get the indices that would sort an array
<code>np.random.choice</code>	Randomly choose elements from an array
<code>np.min/np.max</code>	Get the max/min value of an array

**Refer to NumPy documentation for more details:**

<https://numpy.org/doc/1.19/>

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# PYTORCH TUTORIAL

# PyTorch tutorial

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- PyTorch basics
- Setting up training pipelines
- Case study: Dynamic Net
- Advanced PyTorch functions



# What is **PYTORCH**?

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- A GPU-version of the NumPy library. The NumPy way of processing arrays can be reused.
- A deep learning framework that provides maximum flexibility and speed on training deep neural networks on various tasks.
- Deep learning models are represented as computation graphs in PyTorch.

# Imports

---

- Essential imports for PyTorch utilities.

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

**torch.nn.functional:** Contains all functions such as non-linear activation functions.

**torch.nn:** Contains all neural network modules.

**torchvision:** PyTorch computer vision utilities.

- Other utilities

**torch.optim:** Contains all PyTorch-supported optimizers.

**torch.utils.data:** Data loader.

**torch.backends:** PyTorch backend.

# Tensors

---

- PyTorch uses **Tensors** to hold weights and activations during neural network computation.
- **Tensors** are similar to NumPy's ndarrays.
- **Tensors** can also be processed and executed on a GPU to accelerate computing.

# Generating PyTorch Tensors

---

- A toy example

```
from __future__ import print_function
import torch
# Create a 5x3 matrix, uninitialized:
x = torch.empty(5, 3)
# Create a random initialized 5x3 matrix:
x = torch.rand(5, 3)
# Create a matrix filled of zeros with dtype long:
x = torch.zeros(5, 3, dtype=torch.long)
# Output for visualization
print(x)
```

Out:

```
Tensor([[0,0,0],
        [0,0,0], [0,0,0],
        [0,0,0], [0,0,0]])
```

Tensors are placed on **CPU** by default. Use **`x = x.cuda()`** to place tensor `x` on GPUs.

# PyTorch vs. NumPy Tensors

---

## How to convert PyTorch and NumPy tensors from one to another?

- Convert NumPy Tensor to PyTorch Tensor

```
a = np.ones(5)  
b = torch.from_numpy(a)
```

- Convert PyTorch Tensor to NumPy Tensor

```
a = torch.ones(5)  
b = a.numpy()
```

- If the designated torch tensor is on **GPU**, you may use:

```
a = torch.ones(5)  
b = a.cpu().numpy()
```

# Best practices on using NumPy and PyTorch

---

- Always refer to the document when you have confusion about using library functions.
- Avoid using loops. Instead, try vectorized representations to make your code compact and efficient.
- You may ‘Google’ the questions (e.g., error message) you encountered when using NumPy/PyTorch.
  - However, please **DO NOT** copy the code without reference, as we hope you learn from this process.

# PyTorch operations

---

- In PyTorch, you can simply use arithmetic operations the same as NumPy operations.

```
# For example, If you want to add two tensors:  
torch.add(x,y) and x+y are equivalent.
```

- Use `torch.view` to reshape a tensor.

```
x = torch.randn(4, 4)  
y = x.view(16)  
z = x.view(-1, 8) # the size -1 is inferred from other dimensions  
print(x.size(), y.size(), z.size())
```

```
Out:  
torch.Size([4, 4])  
torch.Size([16])  
torch.Size([2, 8])
```

This is useful when you want to feed the output of final convolution layer to fully connected layers.

# Autograd

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- PyTorch provides automated differentiation for all operations on Tensors. Thus, you don't need to rewrite the backpropagation parts.

**Example:** Differentiating  $\mathbf{Z} = \frac{3}{4} ||(\mathbf{X} + \mathbf{2}) \odot (\mathbf{X} + \mathbf{2})||_1, \mathbf{X} = \mathbf{1}$

```
x = torch.ones(2, 2, requires_grad=True)
y = x + 2
z = y * y * 3
out = z.mean()
print(z, out)
# Use autograd to compute gradient
out.backward()
print(x.grad)
```

Out:

```
tensor([[27., 27.], [27., 27.]],
      grad_fn=<MulBackward0>) tensor(27.,
      grad_fn=<MeanBackward0>)
```

Out:

```
tensor([[4.5000, 4.5000], [4.5000, 4.5000]])
```

If you see something like <MulBackward0>, your tensor has a backward gradient computed by the Autograd engine.



# Setting up training pipeline

---

- Step 0: Write the DNN model
- Step 1: Setup transformation (Preprocessing)
- Step 2: Setup Data Loader (I/O)
- Step 3: Setup Dataset (I/O)
- Step 4: Setup Loss Function
- Step 5: Setup Optimizer

# How to write your own DNN model?

- Custom PyTorch Block: Template

**Please follow this template.** Otherwise, your PyTorch code cannot run normally.

```
import torch.nn as nn
class Block(nn.Module):
    def __init__(self):
        super(Block, self).__init__()
        ...

    def forward(self, x):
        ...
```

Each block must inherit parent class **nn.Module** to be recognized as a component of DNN in PyTorch. You must super the parent class.

Variables are defined and initialized in the **\_\_init\_\_** method.

Each block must have a method called **forward**. Computational graph is constructed in the forward method.

The above block can be instantiated by:

```
net = Block()
```

# How to write your own DNN model?

---

- **Example:** Building a LeNet-5 for MNIST

```
import torch.nn as nn
class LeNet(nn.Module):
    def init (self):
        super(LeNet, self).__init__()
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.conv2 = nn.Conv2d(6, 16, 5)
        self.fc1    = nn.Linear(16*5*5, 120)
        self.fc2    = nn.Linear(120, 84)
        self.fc3    = nn.Linear(84, 10)

    def forward(self, x):
        out = F.relu(self.conv1(x))
        out = F.max_pool2d(out, 2)
        out = F.relu(self.conv2(out))
        out = F.max_pool2d(out, 2)
        out = out.view(out.size(0), -1)
        out = F.relu(self.fc1(out))
        out = F.relu(self.fc2(out))
        out = self.fc3(out)
        return out
```

**Super your class to initialize from parent class in `__init__` function.** Layer definitions are defined in the `__init__` method. Weights for convolutional/linear layers are initialized.

**Computation graph** of a neural network is constructed. That means connections between layers and the flow of tensors are defined here.

# How to write your own DNN model?

---

- Modularize your DNN

```
import torch.nn as nn
class Block(nn.Module):
    def __init__(self):
        super(Block, self).__init__()
        ...

    def forward(self, x):
        ...
        return output

class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.layer = Block()
        ...

    def forward(self, x):
        output = self.layer()
        ...
        return output
```

Larger blocks can be constructed by reusing smaller blocks.

Modularization relieves the trouble of debugging and makes the code more readable.

**Important: remember to use super to initialize each of your custom module from parent class.**

# Setting up pipeline I: Transformation

---

Data transformation is a preprocessing step for your target dataset.

```
import torchvision.transforms as transforms
```

Use functions from **torchvision.transforms** to do data preprocessing as well as data augmentation.

Function Name	Description
<code>torchvision.transforms.ToTensor</code>	Converting an NumPy array to a torch tensor. Also, normalize the given array to range [0,1].
<code>torchvision.transforms.Normalize</code>	Normalize the input with given mean and standard deviation.
<code>torchvision.transforms.RandomHorizontalFlip</code>	Randomly do a horizontal flip on the input image. This is for data augmentation.
<code>torchvision.transforms.RandomCrop</code>	Randomly crop an image to target size. This function will first add a given padding to the image, then randomly crop it to get the target image.

# Setting up pipeline I: Transformation

---

- Use **transforms.Compose** to compose different transforms to formulate a pipeline.

```
import torchvision.transforms as transforms
# Data transformation for training dataset
transform_train = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.4914, 0.4822, 0.4465), (0.2023, 0.1994,
0.2010)),
])
# Data transformation for testing dataset
transform_test = transforms.Compose([
    transforms.ToTensor(),
    transforms.Normalize((0.4914, 0.4822, 0.4465), (0.2023, 0.1994,
0.2010)),
])
```

Note: data transformation for training/testing dataset should be consistent. For example, use the same normalization value for both training and validation dataset.

# Setting up pipeline II: Data loader

---

- Data loader sets the I/O pipeline and process your data efficiently.
- Data loaders can be imported from **torch.utils.data.DataLoader**.

```
CLASS torch.utils.data.DataLoader(dataset, batch_size=1, shuffle=False, sampler=None,  
    batch_sampler=None, num_workers=0, collate_fn=None, pin_memory=False, drop_last=False, [SOURCE]  
    timeout=0, worker_init_fn=None, multiprocessing_context=None, generator=None)
```

Data loader. Combines a dataset and a sampler, and provides an iterable over the given dataset.

- You should specify some training settings in the data loader, including **batch\_size**, **shuffle** etc.
- **num\_workers** is usually configured to be the number of available CPU cores on your system. Please use it sparingly.

# Setting up pipeline III: Dataset

---

- **Torchvision.datasets** prepares the dataset for you. Pass it to the data loader finishes the I/O pipeline.
- **Torchvision.datasets** covers a various of public vision datasets, including MNIST, CIFAR-10 etc.

## TORCHVISION.DATASETS

All datasets are subclasses of `torch.utils.data.Dataset` i.e, they have `__getitem__` and `__len__` methods implemented. Hence, they can all be passed to a `torch.utils.data.DataLoader` which can load multiple samples parallely using `torch.multiprocessing` workers. For example:

```
imagenet_data = torchvision.datasets.ImageNet('path/to/imagenet_root/')
data_loader = torch.utils.data.DataLoader(imagenet_data,
                                          batch_size=4,
                                          shuffle=True,
                                          num_workers=args.nThreads)
```



# Setting up pipeline III: Dataset

---

- Example: data loader for CIFAR-10 dataset

```
import torchvision

trainset = torchvision.datasets.CIFAR10(root='./data', train=True,
download=True, transform=transform_train)
trainloader = torch.utils.data.DataLoader(trainset, batch_size=128,
shuffle=True, num_workers=4)

testset = torchvision.datasets.CIFAR10(root='./data', train=False,
download=True, transform=transform_test)
testloader = torch.utils.data.DataLoader(testset, batch_size=100,
shuffle=False, num_workers=4)
```

Note: This is for general use. We will use an alternative dataset loader as a part of requirements in Lab 2.

# Setting up pipeline IV: Loss function

---

- For most of the problems here, we will use the **cross-entropy** loss function.

```
import torch.nn as nn
criterion = nn.CrossEntropyLoss()
```

- We recommend looking at the source code of PyTorch. This loss function takes two arguments as the input:

```
class CrossEntropyLoss(_WeightedLoss):
    def __init__(self, weight=None, size_average=None, ignore_index=-100,
                  reduce=None, reduction='mean'):
        super(CrossEntropyLoss, self).__init__(weight, size_average, reduce, reduction)
        self.ignore_index = ignore_index

    def forward(self, input, target):
        return F.cross_entropy(input, target, weight=self.weight,
                               ignore_index=self.ignore_index, reduction=self.reduction)
```

- Therefore, the correct way to use cross entropy loss here is:

```
loss = nn.CrossEntropyLoss(outputs, targets)
```

# Setting up pipeline IV: Loss function

- Now let's take a deeper look into the documentation.

```
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.

*input* has to be a *Tensor* of size either  $(minibatch, C)$  or  $(minibatch, C, d_1, d_2, \dots, d_K)$  with  $K \geq 1$  for the  $K$ -dimensional case (described later).

This criterion expects a class index in the range  $[0, C - 1]$  as the *target* for each value of a 1D *tensor* of size *minibatch*; if *ignore\_index* is specified, this criterion also accepts this class index (this index may not necessarily be in the class range).

The loss can be described as:

$$\text{loss}(x, \text{class}) = -\log \left( \frac{\exp(x[\text{class}])}{\sum_j \exp(x[j])} \right) = -x[\text{class}] + \log \left( \sum_j \exp(x[j]) \right)$$

or in the case of the `weight` argument being specified:

$$\text{loss}(x, \text{class}) = \text{weight}[\text{class}] \left( -x[\text{class}] + \log \left( \sum_j \exp(x[j]) \right) \right)$$

The losses are averaged across observations for each minibatch.

Can also be used for higher dimension inputs, such as 2D images, by providing an input of size  $(minibatch, C, d_1, d_2, \dots, d_K)$  with  $K \geq 1$ , where  $K$  is the number of dimensions, and a target of appropriate shape (see below).

DO NOT use softmax activation in the last layer. The softmax operation is fused into cross entropy loss in PyTorch.

Note:

In situation of any confusion, always look at source code or documentation of PyTorch.

<https://pytorch.org/docs/stable/index.html>

# Setting up pipeline V: Optimizer

---

- Optimizer is what we use to optimize the loss function during training. The optimizers are defined in **torch.optim** package.
- Some popular optimizers are:

Optimizer Name	Description
<code>torch.optim.Adadelta</code>	Implements Adadelta algorithm.
<code>torch.optim.Adagrad</code>	Implements Adagrad algorithm.
<code>torch.optim.Adam</code>	Implements Adam algorithm.
<code>torch.optim.ASGD</code>	Implements Averaged Stochastic Gradient Descent.
<code>torch.optim.RMSprop</code>	Implements RMSprop algorithm.
<code>torch.optim.SGD</code>	Implements stochastic gradient descent (optionally with momentum).

We will use **torch.optim.SGD** under most cases.

# Setting up pipeline V: Optimizer

---

Optimizer should be defined after the computational graph (your custom module) is finalized.

Suppose we have instantiated a neural network called `net`.

**Example:** Define an optimizer using SGD with momentum

```
import torch.optim as optim

optimizer = optim.SGD(net.parameters(), lr=0.01, momentum=0.9,
weight_decay=1e-4)
```

To achieve the best performance, it is recommended to leave all parameters in their default settings. We will talk about hyperparameter tuning in the next few lectures.

# Setting up pipeline V: Optimizer

---

- How to compute gradients and apply it to update the weights?
- **Step 1: Zero the gradients.** This ensures that the gradient computation is correct.

```
optimizer.zero_grad()
```

- Step 2: Compute gradients use back propagation

```
loss.backward()
```

- Step 3: Take the optimization step to apply gradients

```
optimizer.step()
```

Repeat this 3-step loop and you can train your neural network model gradually.

# Setting up pipeline V: Optimizer

---

- Learning rate can be scheduled in the optimizer to achieve maximum performance.

```
import torch.optim as optim
optimizer = optim.SGD(net.parameters(), lr=0.01, momentum=0.9,
weight_decay=1e-4)
for param_group in optimizer.param_groups:
    param_group['lr'] = 0.01           # Setting up a new lr.
```

- You can also use existing learning rate scheduler in `torch.optim.lr_scheduler`.

```
import torch.optim as optim
optimizer = optim.SGD(net.parameters(), lr=0.01, momentum=0.9,
weight_decay=1e-4)
# Apply 0.1 learning rate decay for every 30 epochs.
optimizer = optim.lr_scheduler.StepLR(optimizer, step_size=30,
gamma=0.1)
```

# Case study: Dynamic Net

---

- Putting the 5-stage pipeline all-together, you are able to train a real neural network smoothly!
- Let's have a more concrete example. We are going to create a neural network with dynamic depth. That means, we will randomly choose 0-3 hidden layers for forward propagation. Note that weights for hidden layers are shared despite of the number of hidden layers chosen in forward/backward propagation.
- This toy example mainly focuses on setting up the model and launching training. We will see more complicated examples in our labs.



# Case study: Dynamic Net

---

- Import essentials

```
import torch
import random
```

- For more complicated neural architecture design, it is recommended to import all of the following packages:

```
import torch.nn as nn
import torch.optim as optim
import torch.nn.functional as F
import torch.backends.cudnn as cudnn
import torchvision
import torchvision.transforms as transforms
```

# Case study: Dynamic Net

- Create the dynamic net module

```
class DynamicNet(torch.nn.Module):
    def __init__(self, D_in, H, D_out):
        super(DynamicNet, self).__init__()
        self.input_linear = torch.nn.Linear(D_in, H)
        self.middle_linear = torch.nn.Linear(H, H)
        self.output_linear = torch.nn.Linear(H,
D_out)

    def forward(self, x):
        h_relu = self.input_linear(x).clamp(min=0)
        for _ in range(random.randint(0, 3)):
            h_relu =
self.middle_linear(h_relu).clamp(min=0)
        y_pred = self.output_linear(h_relu)
        return y_pred
```

Important: initialize the parent class.

Initialize layer/weight configuration

Specify the connection relationship.

Randomly choose 0-3 hidden layers.

The module can be instantiated by:

```
model = DynamicNet(D_in, H, D_out)
```

# Case study: Dynamic Net

---

- Generate toy data

```
# N is batch size; D_in is input dimension;  
# H is hidden dimension; D_out is output dimension.  
N, D_in, H, D_out = 64, 1000, 100, 10  
  
# Create random Tensors to hold inputs and outputs  
x = torch.randn(N, D_in)  
y = torch.randn(N, D_out)
```

- As we are using toy data here, we may skip step 2 and step 3 in this example. You may expect to see these steps on a real dataset in Lab 2 and beyond.
- **Exercise:** Try to change some of these parameters. What will you observe?

# Case study: Dynamic Net

---

- Instantiate model, create loss function and optimization op.

```
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)

# Construct our loss function and an Optimizer. Training this strange
model with vanilla stochastic gradient descent is tough, so we use
momentum
criterion = torch.nn.MSELoss(reduction='sum')
#Use mean squared error as loss function.
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4, momentum=0.9)
```

Since the data is not normalized, we use a smaller learning rate  $1e-4$  to prevent gradient explosion. Usually, if we use a normalized data, default learning rate parameter for momentum optimizer should be set to 0.01.

# Case study: Dynamic Net

---

- Up to now, the training pipeline is all set!
- Let's try to start it by running the forward/backward pass

```
for t in range(500):  
    # Zero gradients, perform a backward pass, and update the weights.  
    optimizer.zero_grad()  
  
    # Forward pass: Compute predicted y by passing x to the model  
    y_pred = model(x)  
  
    # Compute and print loss  
    loss = criterion(y_pred, y)  
    print(t, loss.item())  
  
    # Backward pass: Compute predicted y by passing x to the model  
    loss.backward()  
    optimizer.step()
```

Note: remember to copy inputs and labels to GPU device if you are using the GPU version of PyTorch.

# Advanced PyTorch topics

---

- Train/Eval mode
- Training on GPU
- Model load/save
- Data parallel
- Learning rate scheduler

# Train/Evaluation mode

---

- Some neural network layers (e.g. dropout, batch normalization) have completely different behavior during training and evaluation. **It is important to set the correct mode for both training and evaluation.**

```
import torch
...
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
...
# Set to train mode before running the training process
model.train()
... # Training code
# Set to eval mode before running the evaluation process
model.eval()
... # Evaluation code
```

- Examples:** Dropout, BatchNorm, ...

# Training on GPU

---

- GPU gives a considerable acceleration on training speed compared to CPUs. As computation graph are placed on CPU by default, you have to manually deploy it on GPU.

## Deploy models on GPU

```
import torch
# Find if GPU device is available
device = 'cuda' if torch.cuda.is_available() else 'cpu'
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
# Copy to CUDA device. This is very important.
model.to(device)
```

**Note: this must be run on an instance with GPU configuration and CUDA compatibility.**



# Training on GPU

---

- Don't forget to copy **all** inputs to GPU devices during training!

```
for t in range(500):  
    # Copy inputs to GPU. This is very important.  
    x, y = x.to(device), y.to(device)  
    # Forward pass: Compute predicted y by passing x to the model  
    y_pred = model(x)  
  
    # Compute and print loss  
    loss = criterion(y_pred, y)  
    print(t, loss.item())  
  
    # Zero gradients, perform a backward pass, and update the weights.  
    optimizer.zero_grad()  
    loss.backward()  
    optimizer.step()
```

# Model load/save

---

- Save/Load the whole model

The model is serialized in a pickle object.

```
import torch
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
# Configure the optimizer and training
...
# Save model
torch.save(model, "dynamic_net.pth")
```

**Note:** The disadvantage of this approach is that the serialized data is bound to the specific classes and the exact directory structure used when the model is saved.

# Model load/save

---

- Load the whole model

Make sure the structure of your code is not broken before loading.

```
import torch
# Load model
model = torch.load("dynamic_net.pth")
```

**Note:** The disadvantage of this approach is that the serialized data is bound to the specific classes and the exact directory structure used when the model is loaded.

# Model load/save

---

- Save the weight parameters of a model (**Recommended**)

Only the weight parameters are saved as a state dictionary.

```
import torch
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
# Configure the optimizer and training
...
# Save weight parameters
torch.save(model.state_dict(), "dynamic_net.pt")
```

**Note:** This approach is better because weight parameters do not rely on specific classes or code structures during the saving process.

# Model load/save

---

- Load the weight parameters of a model (Recommended)

Construct the model, then load the state dictionary.

```
import torch
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
# Configure the optimizer and training
...
# Load weight parameters
model.load_state_dict(torch.load("dynamic_net.pt"))
```

Note: This approach is better because weight parameters do not rely on specific classes or code structures during the saving process.

# Data parallel

---

- Much more accelerations can be achieved using multiple GPU cards.

```
import torch
# Find if GPU device is available
device = 'cuda' if torch.cuda.is_available() else 'cpu'
# Construct our model by instantiating the class defined above
model = DynamicNet(D_in, H, D_out)
# Copy to CUDA device. This is very important.
model.to(device)
# Apply the data parallelization semantics.
model = torch.nn.DataParallel(model)
```

Note: Due to limited GPU resources we have for this class, using Data Parallel is prohibited on the JupyterLab server.

# Learning rate schedule

- Use the learning rate scheduler in **torch.optim.lr\_scheduler** package.

## Example: Schedule an exponential learning rate decay

**CLASS** `torch.optim.lr_scheduler.StepLR(optimizer, step_size, gamma=0.1, last_epoch=-1)` [\[SOURCE\]](#)

Sets the learning rate of each parameter group to the initial lr decayed by gamma every step\_size epochs. When last\_epoch=-1, sets initial lr as lr.

### Parameters

- **optimizer** (*Optimizer*) – Wrapped optimizer.
- **step\_size** (*int*) – Period of learning rate decay.
- **gamma** (*float*) – Multiplicative factor of learning rate decay. Default: 0.1.
- **last\_epoch** (*int*) – The index of last epoch. Default: -1.

### Example

```
>>> # Assuming optimizer uses lr = 0.05 for all groups
>>> # lr = 0.05      if epoch < 30
>>> # lr = 0.005     if 30 <= epoch < 60
>>> # lr = 0.0005    if 60 <= epoch < 90
>>> # ...
>>> scheduler = StepLR(optimizer, step_size=30, gamma=0.1)
>>> for epoch in range(100):
>>>     train(...)
>>>     validate(...)
>>>     scheduler.step()
```

We will see the power of learning rate schedule in the next a few lectures.

# Reference

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- **NumPy tutorial**

<http://cs231n.github.io/python-numpy-tutorial/>

- **PyTorch master documentation**

<https://pytorch.org/docs/stable/index.html>