



Machine Learning

Chapter 8.1: PyTorch

Fall 2022

Instructor: Xiaodong Gu



About PYTORCH



PyTorch is a python package that provides two high-level features:

- Tensor computation (like numpy) with strong GPU acceleration
- Neural Networks built on a tape-based autograd system

Why PYTORCH



- More **Pythonic** (imperative)
 - flexible
 - intuitive and cleaner code
 - easy to debug
- More **Neural Networks**
 - write code as the network works
 - forward/backward

PYTORCH vs Tensorflow



	PyTorch	Tensorflow
Model Definition	Dynamic computational graph	Static graph definition
Debugging	easy for debugging since computation graph is defined at runtime	you won't be able to debug any python code with it
Deployment	use Flask or another alternative to code up a REST API on top of the model.	<i>TensorFlow Serving</i> may be a better option if performance is a concern.
Data Parallelism	use <code>torch.nn.DataParallel</code> to wrap any module for parallelism over batch.	fine tune every operation to be run on specific device
A framework or a library	provides useful abstractions in certain domain and a convenient way to use them	all operations are pretty low-level

Install PYTORCH



<https://pytorch.org>

Get Started.

Select your preferences, then run the PyTorch install command.

Please ensure that you are on the latest pip and numpy packages.
Anaconda is our recommended package manager

OS	Linux	OSX	
Package Manager	conda	pip	Source
Python	2.7	3.5	3.6
CUDA	7.5	8.0	None

Run this command:

```
pip3 install http://download.pytorch.org/whl/torch-0.2.0.post3-cp36-cp36m-macosx_10_7_x86_64.whl
pip3 install torchvision
# OSX Binaries dont support CUDA, install from source if CUDA is needed
```

Hello PyTorch



```
09:40 $ python
Python 3.6.2 (v3.6.2:5fd33b5926, Jul 16 2017, 20:11:06
[GCC 4.2.1 (Apple Inc. build 5666) (dot 3)] on darwin
Type "help", "copyright", "credits" or "license" for more
information.
>>> import torch
>>> print(torch.__version__)
1.2.0_3
>>> # Happy!!
```

PYTORCH Rhythm



1 Design your model using class



2 Construct loss and optimizer (select from PyTorch API)

3 Training cycle (forward, backward, update)

How to define data?



Tensors - the basic data structure in Torch.

```
import torch
x = torch.tensor([0.1, 0.2, 0.3], dtype=torch.float)
W = torch.tensor([[0.1, 0.2, 0.3],
                  [0.4, 0.1, 0.7],
                  [0.8, 0.1, 0.2],
                  ])
r = torch.zeros([1,3], dtype=torch.long)
```

Tensors can also be defined from numpy array.

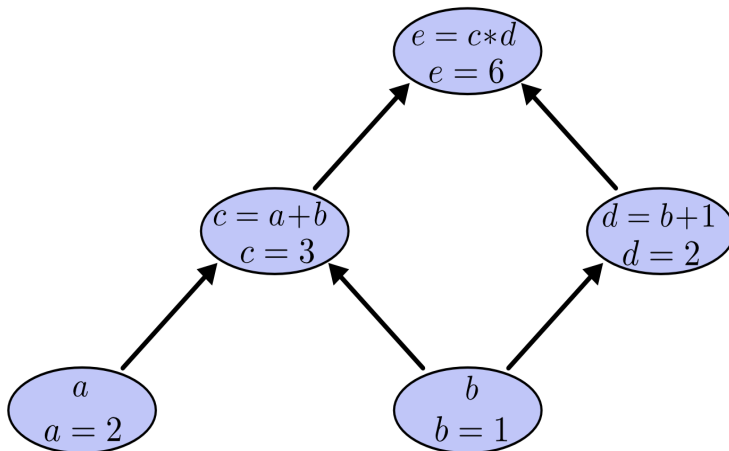
```
import numpy as np
import torch
x_np = np.array([0.1,0.2,0.3])
x_torch = torch.from_numpy(x_np)
```


Computational Graphs



- PyTorch's **tensor** object implicitly creates a **computation graph** in the background.

$$e = (a+b) \times (b+1)$$



```
a = torch.tensor(2.0,  
requires_grad=True)  
# we set requires_grad=True to let  
PyTorch know to keep the graph  
b = torch.tensor(1.0,  
requires_grad=True)  
c = a + b  
d = b + 1  
e = c * d  
print(c)  
print(d)  
print(e)
```

```
c tensor(3., grad_fn=<AddBackward0>)  
d tensor(2., grad_fn=<AddBackward0>)  
e tensor(6., grad_fn=<MulBackward0>)
```

PyTorch as an auto grad framework



- Now that we have seen that PyTorch keeps the graph around for us, let's use it to compute some **gradients** for us.
- Given $f(x)=(x-2)^2$, we want to compute $\frac{d}{dx}f(x)$ and then compute $f'(1)$.

We make a `backward()` call on the leaf variable (`y`) in the computation, computing all the gradients of `y` at once.

```
def f(x):  
    return (x-2)**2  
def fp(x):  
    return 2*(x-2)  
x = torch.tensor([1.0], requires_grad=True)  
y = f(x)  
y.backward()  
print('Analytical f\'(x):', fp(x))  
print('PyTorch\'s f\'(x):', x.grad)
```

```
Analytical f'(x): tensor([-2.], grad_fn=<MulBackward0>)  
PyTorch's f'(x): tensor([-2.])
```

PyTorch as an auto grad framework



- It can also find **gradients** of functions.

Let $w=[w_1, w_2]^T$

Consider $g(w)=2w_1w_2+w_2\cos(w_1)$

Q: Compute $\nabla_w g(w)$ and verify $\nabla_w g([\pi, 1])=[2, \pi-1]^T$

```
def g(w):  
    return 2*w[0]*w[1]+w[1]*torch.cos(w[0])  
def grad_g(w):  
    return torch.tensor([2*w[1]-w[1]*torch.sin(w[0]), 2*w[0]+  
torch.cos(w[0])])  
w = torch.tensor([np.pi, 1], requires_grad=True)  
z = g(w)  
z.backward()  
print('Analytical grad g(w)', grad_g(w))  
print('PyTorch\'s grad g(w)', w.grad)
```

Analytical grad $g(w)$ tensor([2.0000, 5.2832])

PyTorch's grad $g(w)$ tensor([2.0000, 5.2832])

Define a Machine Learning Model



- A machine Learning model can be defined by inheriting the `torch.nn.Module`.
- You should customize the `forward()` function which defines the computational graph for the model.

```
class Model(torch.nn.Module):
    def __init__(self):
        """
        In the constructor we instantiate two nn.Linear module
        """
        super(Model, self).__init__()
        self.linear = torch.nn.Linear(1, 1) # One in and one out

    def forward(self, x):
        """
        In the forward function we accept a Variable of input data and we must return
        a Variable of output data. We can use Modules defined in the constructor as
        well as arbitrary operators on Variables.
        """
        y_pred = self.linear(x)
        return y_pred

# our model
model = Model()
```

Define a Machine Learning Model



Building the model may require submodules provided by PyTorch such as:

- Basic Modules(e.g., Linear,)
- Functions (e.g., activations,)
- Containers (e.g., sequential, concat,)
- Other Developed Models



Define Loss functions

- PyTorch implements many common loss functions including the **MSELoss** and the **CrossEntropyLoss**.

```
mse_loss_fn = nn.MSELoss()  
input = torch.tensor([[0., 0, 0]])  
target = torch.tensor([[1., 0, -1]])  
loss = mse_loss_fn(input, target)  
print(loss)
```

```
tensor(0.6667)
```

Choose an Optimizer



- PyTorch implements a number of gradient-based optimization methods in `torch.optim`, including Gradient Descent. At the minimum, it takes in the `model parameters` and a `learning rate`.
- Optimizers do not compute the gradients for you, so you must call `backward()` yourself.
- You also must call the `optim.zero_grad()` function before calling `backward()` since by default PyTorch does an inplace add to the `.grad` member variable rather than overwriting it.

Optimizers



```
# create a simple model
model = nn.Linear(1, 1)
# create a simple dataset
X_simple = torch.tensor([[1.]])
y_simple = torch.tensor([[2.]])
# create our optimizer
optim = torch.optim.SGD(model.parameters(), lr=1e-2)
loss_fn = nn.MSELoss()
y_hat = model(X_simple)
print('model params before:', model.weight)
loss = loss_fn(y_hat, y_simple)
optim.zero_grad()
loss.backward()
optim.step()
print('model params after:', model.weight)
```


Dataset



`torch.utils.data.Dataset` is an abstract class representing a dataset. Your custom dataset should inherit `Dataset` and override the following methods:

- `__len__` so that `len(dataset)` returns the size of the dataset.
- `__getitem__` to support the indexing such that `dataset[i]` can be used to get i -th sample

```
class MyDataset(Dataset):
    def __init__(self, csv_file):
        self.sentences = pd.read_csv(csv_file)
    def __len__(self):
        return len(self.sentences)
    def __getitem__(self, idx):
        sample = self.sentences[idx]
        sample = sample.lower()
        return sample
```



Data Loader

To efficiently load data into model (instead of a simple for loop), the `torch.utils.data.DataLoader` is an iterator which provides:

- **batching** the data
- **shuffling** the data
- **load** the data in parallel using multiprocessing workers.

```
dataloader = DataLoader(my_dataset, batch_size=4,
                        shuffle=True, num_workers=4)
for i_batch, sample_batched in enumerate(dataloader):
    print(i_batch, sample_batched['image'].size())
    .....
```

Training: forward, loss, backward, step



```
# Construct our loss function and an Optimizer. The call to model.parameters()
# in the SGD constructor will contain the learnable parameters of the two
# nn.Linear modules which are members of the model.
criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=0.01)

# Training loop
for epoch in range(500):
    # Forward pass: Compute predicted y by passing x to the model
    y_pred = model(x_data)

    # Compute and print loss
    loss = criterion(y_pred, y_data)
    print(epoch, loss.data[0])

    # Zero gradients, perform a backward pass, and update the weights.
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

    for x_val, y_val in zip(x_data, y_data):
        ...
        w.data = w.data - 0.01 * w.grad.data
```



PyTorch forward/backward

```
w = torch.Tensor([1.0]) # Any random value
```

```
# our model forward pass
```

```
def forward(x):  
    return x * w
```

```
# Loss function
```

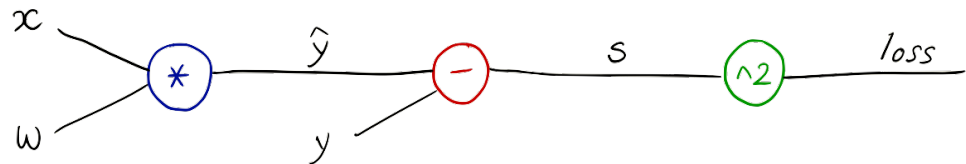
```
def loss(x, y):  
    y_pred = forward(x)  
    return (y_pred - y) * (y_pred - y)
```

```
# Training Loop
```

```
for epoch in range(10):  
    for x_val, y_val in zip(x_data, y_data):  
        l = loss(x_val, y_val)  
        l.backward()  
        print("\tgrad: ", x_val, y_val, w.grad.data[0])  
        w.data = w.data - 0.01 * w.grad.data
```

```
# Manually zero the gradients after updating weights
```

```
w.grad.data.zero_()  
print("progress:", epoch, l.data[0])
```



Hello World



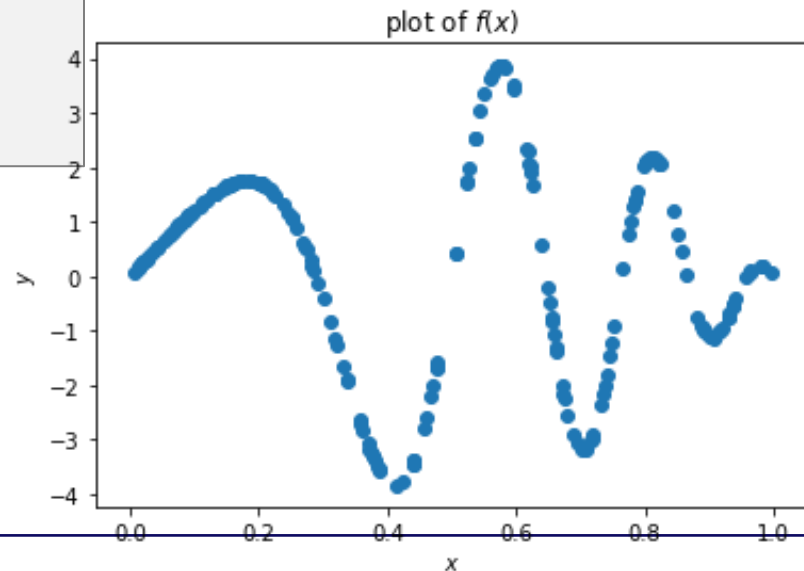
Implementing an MLP using PyTorch



MLP using PyTorch

- Create a simple dataset

```
d = 1
n = 200
X = torch.rand(n,d)
y = 4 * torch.sin(np.pi * X) *
torch.cos(6*np.pi*X**2)
plt.scatter(X.numpy(), y.numpy())
plt.title('plot of  $f(x)$ ')
plt.xlabel('$x$')
plt.ylabel('$y$')
plt.show()
```



MLP using PyTorch



- **define the model**

```
n_hidden_1 = 32
n_hidden_2 = 32
d_out = 1

neural_network = nn.Sequential(
    nn.Linear(d, n_hidden_1),
    nn.Tanh(),
    nn.Linear(n_hidden_1, n_hidden_2),
    nn.Tanh(),
    nn.Linear(n_hidden_2, d_out)
)
```



MLP using PyTorch

- Training

```
step_size = 0.05
n_epochs = 6000
loss_func = nn.MSELoss()
optim = torch.optim.SGD(
    neural_network.parameters(), lr=step_size
)
print('iter, \tloss')
for i in range(n_epochs):
    y_hat = neural_network(X)
    loss = loss_func(y_hat, y)
    optim.zero_grad()
    loss.backward()
    optim.step()
    if i % (n_epochs // 10) == 0:
        print(f'{i}, {loss.item()}')
```

iter,	loss
0,	3.96
600,	3.69
1200,	2.58
1800,	1.10
2400,	0.85
3000,	0.60
3600,	0.14
4200,	0.08
4800,	0.06
5400,	0.24

MLP using PyTorch



- Prediction and Visualization

```
X_grid =  
torch.from_numpy(np.linspace(0,1,50)).float().view(-1, d)  
y_hat = neural_network(X_grid)  
plt.scatter(X_numpy(), y_numpy(),  
plt.plot(X_grid.numpy(), y_hat.numpy(),  
'r')  
plt.title('plot of  $f(x)$  and  $\hat{f}(x)$ ')  
plt.xlabel('$x$')  
plt.ylabel('$y$')  
plt.show()
```

