PyTorch Crash Course: 0 to MNIST in 1 Hour

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You can download the code to follow along at:
https://github.com/markchil/pytorch-lecture

Intro

About me:

- Graduated 2016 with PhD from Course 22
- Currently a research scientist working on a variety of machine learning applications

Goals for today:

- Cover the core classes/philosophy of PyTorch
- Give you enough vocab to confidently google stuff/read the docs

Prerequisites:

- Basic familiarity with Python

You can download the code to follow along at:
https://github.com/markchil/pytorch-lecture

PyTorch Crash Course: 0 to MNIST in 1 Hour

1. Background: Machine Learning, Neural Networks, and PyTorch

2. PyTorch Fundamentals: The `Tensor` Class

3. Higher Abstractions: The `torch.nn` Module

4. Data Handling: The `Dataset` and `DataLoader` Classes

5. Putting It All Together to Solve MNIST: The "`hello, world`" of Machine Learning

6. Summary and Resources

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What Is PyTorch?

PyTorch is an open source Python **machine learning** package geared towards building **neural networks**, which provides the following key features:[1]

- Automatic differentiation
- GPU acceleration
- Many standard neural network building blocks
    - And nice abstractions which make building novel/non-standard ones easy
- Rich ecosystem of pre-trained models and open source building blocks

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[1]We'll unpack some of this jargon on the following slides

What Can You Do With PyTorch:
Machine Learning Crash Course

- **Machine learning** refers to algorithms which improve automatically through experience/data
- There are various types of machine learning (supervised, unsupervised, reinforcement, etc.)
- This crash course focuses on **supervised learning**:
  - The data takes the form of (input, output) pairs
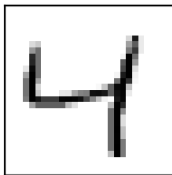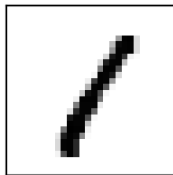 - Example: given a picture of a handwritten digit, identify which number was written
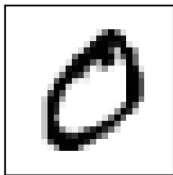
$y = 5$ $y = 0$ $y = 4$ $y = 1$

PyTorch's Flavor of Machine Learning:
Neural Network Crash Course

- PyTorch is geared to a specific family of machine learning approaches: **(deep) neural networks**
- Neural networks are a broad family of models which started out as biologically-inspired data transformations based on networks of "artificial neurons"
  - Modern practice has diverged from these biologically-inspired roots, but some of the terminology remains

Basic Neural Network Architecture: Multi-Layer Perceptron (MLP)

Most neural network approaches can be seen as an alternating sequence of linear transformations and (elementwise) non-linear functions:

$$x_i = \sigma(W_i x_{i-1} + b_i)$$

- $\sigma : \mathbb{R} \to \mathbb{R}$ is a nonlinear **activation function** which is applied separately to each element of its (vector) input
- $W_i \in \mathbb{R}^{n_{out} \times n_{in}}$ and $b_i \in \mathbb{R}^{n_{out}}$ are **learnable parameters**

# Nuts and Bolts of Neural Network Training: Gradient Descent

- In order to **train** a neural network with L layers, we need to find values for the parameters $\theta = \{W_i, b_i | 1 \le i \le L\}$
- We quantify how good specific parameter values are using a **loss function** $\mathcal{L} : \Theta \to \mathbb{R}$ which indicates how well the network matches its training data for the given parameters
  - Goal is then to find $\hat{\theta} = \arg\min_\theta \mathcal{L}(\theta)$
  - Can seek a (local) minimum using **gradient descent**: update parameters according to

$$\theta_{i+1} = \theta_i - \alpha \nabla \mathcal{L}(\theta_i)$$

Gradient Descent on Rosenbrock Function
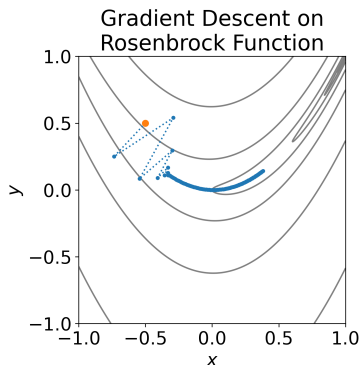
Why Not Just Write It in NumPy?
Backpropagation and Automatic Differentiation

- Gradient descent requires computing the **gradient** $\nabla\mathcal{L}(\theta_i)$
- The **backpropagation** algorithm provides an efficient way of doing this, *but needing to write explicit expressions for the gradient of your neural network would be exceedingly tedious and error-prone*
- The heart of PyTorch is the ability to perform **automatic differentiation**: you simply define the loss function computation, and PyTorch automatically computes the gradients for you

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PyTorch Fundamentals: What Is a Tensor?

A tensor **H** of valence $\left\{ \begin{matrix} \mathfrak{f} \\ \mathfrak{v} \end{matrix} \right\}$ at a point $\mathfrak{p}$ is a multilinear, real-valued function of $\mathfrak{f}$ 1-forms, and $\mathfrak{v}$ vectors, such that the value of **H** at $\mathfrak{p}$ only depends on the values of the 1-forms and vectors at $\mathfrak{p}$.[2]

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[2] *Visual Differential Geometry and Forms,* T. Needham (2021)

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lol, nope!

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[2] *Visual Differential Geometry and Forms,* T. Needham (2021)

PyTorch Fundamentals:
What Does PyTorch Think a Tensor Is?

- In machine learning, it is common to abuse the word "tensor" to refer to any *N*-dimensional array of data
- PyTorch's `Tensor` class is very similar to the `ndarray` class in NumPy, but with some extra machinery attached to:
  1. Keep track of gradients
  2. Easily move between CPU and GPU

Tensor Basics

A given `Tensor x` consists of several key elements:

- A chunk of memory
- A datatype which indicates what type of value is stored in the memory (`x.dtype`)
- A shape which indicates how the elements are arranged in an *N*-dimensional grid (`x.shape`)

Basics of Tensor Indexing

- You can index into a `Tensor` just like a Python list, with the added twist that there can be as many indices as there are dimensions:

```
1 import torch
2 x = torch.rand(3, 4, 5)  # Make a random
     Tensor
3 print(x.shape)  # torch.Size([3, 4, 5])
4 print(x[1, 0, 2])  # tensor(0.3494)
5 print(x[:, 0, 0])
6 # tensor([0.9643, 0.2863, 0.1553])
```

- There are lots of powerful things you can do by using bool and int `Tensors` to index into other `Tensors`: the examples here just barely scratch the surface

Conventional `Tensor` Shapes

There are a few conventions in use for specific meanings of various dimensions for various types of data:

- Generic data (like for an MLP): shape is (samples, features)
- Image data (like for a CNN): shape is (samples, channels, height, width)
- Sequence data (like for an RNN):
  - Defaults to (steps, samples, features) for RNN/LSTM/GRU
  - But, I prefer to use the optional (samples, steps, features) form so that the samples dimension is first

Tensor Superpowers: Autograd Example

```
1 x = torch.tensor(1.0, requires_grad=True)
2 y = torch.tensor(1.0, requires_grad=True)
3 z = x ** 2 + x + y
4 z.backward()   # Compute the gradients
5 print(x.grad)  # tensor(3.)
6 print(y.grad)  # tensor(1.)
```

- Symbolically, you would have to find $dz/dx = 2x + 1$, $dz/dy = 1$: but PyTorch does it automatically for you
- The call to z.backward() stores dz/dx into x.grad and dz/dy into y.grad

More Details on Autograd

- Use the `requires_grad` keyword to construct a `Tensor` which will have gradients computed for it
- Use the `z.backward()` method to compute gradients of `z` with respect to all `Tensors` which were involved in its computation
  - Gradients of `z` with respect to `x` are stored in `x.grad`
  - Gradients are *accumulated* with subsequent calls to `backward()`: often need to manually zero out gradients
- Tracking the computation graph can be expensive: when you do not need gradients, use the `no_grad` context manager:

```
1 with torch.no_grad():
2     y = x ** 2
```

Tensor Superpowers: Using a GPU

- Can easily move `Tensors` between GPU and CPU:
    - Can create `Tensor` on GPU using the `device` keyword:
      `x = torch.tensor(1.0, device=torch.device('cuda'))`
    - Can copy existing `Tensor` to GPU using the `to()` method:
      `x = x.to(torch.device('cuda'))`
    - Can copy existing `Tensor` to CPU using the `cpu()` method:
      `x = x.cpu()`
- Best practice: don't hard-code the `device` keyword. Instead, make your code fail back to CPU if GPU is unavailable:

```
1 if torch.cuda.is_available():
2     device = torch.device('cuda')
3 else:
4     device = torch.device('cpu')
5
6 x = torch.tensor(1.0, device=device)
```

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Neural Network Building Blocks: The `torch.nn` Module

The `torch.nn` module has a wide array of standard neural network building blocks, including:

- Linear transformations
- Various activation functions
- Convolutional layers
- Recurrent layers

Defining an MLP Using `torch.nn`

```python
import torch.nn as nn

net = nn.Sequential(
    nn.Linear(16, 128),  # 16 in, 128 out
    nn.ReLU(),  # "ReLU" activation function
    nn.Linear(128, 4)   # 128 in, 4 out
)

x = torch.rand(1, 16)
out = net(x)
print(out.shape)  # torch.Size([1, 4])
```

The Module Class

- All of the building blocks in `torch.nn` inherit from the `torch.nn.Module` class
- A given `Module` has:
  - Parameters: `Tensors` which the optimizer should update during training
  - Buffers: `Tensors` which should be included when saving/restoring the `Module`, but which should *not* be updated by the optimizer
  - Submodules: other `Modules` which are contained within the `Module`
  - A `forward()` method which defines the actual operation performed by the `Module`
    - Important: never call `forward()` directly: `Module` provides `__call__()` which wraps `forward()` with extra steps!

Some Additional Key `Module` Methods

- `to(device)`: Move to the given device
  - A `Module` and the `Tensors` it operates on must be on the same device
- `train()`: Put into training mode
- `eval()`: Put into eval mode
- `parameters()`: Get an iterator over the trainable parameters

Implementing a Custom `Module` Class

```python
class ScaledLinear(nn.Module):
    def __init__(self, in_features, out_features,
        scale):
        super().__init__()

        self.weight = nn.Parameter(torch.empty(
            out_features, in_features))
        self.bias = nn.Parameter(torch.empty(
            out_features))
        self.register_buffer('scale', torch.
            as_tensor(scale))

    def forward(self, x):
        return self.scale * torch.nn.functional.
            linear(
            x, self.weight, self.bias
        )
```

Using the Custom `Module`

```python
1 layer = ScaledLinear(16, 4, 2.0)
2 x = torch.rand(1, 16)
3 out = layer(x)
4 print(out.shape)  # torch.Size([1, 4])
5 print(layer.state_dict().keys())
6 # odict_keys(['weight', 'bias', 'scale'])
```

Saving/Loading `Modules`

- The `state_dict()` method returns a dict which has the values of all of the parameters and buffers associated with a given `Module`
- This can be saved to disk, and restored using the `load_state_dict()` method

```
1 layer = ScaledLinear(16, 4, 2.0)
2 state_dict = layer.state_dict()
3 torch.save(state_dict, 'model.pt')
4
5 state_dict = torch.load('model.pt')
6 layer.load_state_dict(state_dict)
7 # <All keys matched successfully>
```

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Two-Stage Data Handling: `Dataset` and `DataLoader`

PyTorch breaks down data handling into two steps:

1. A `Dataset` provides a wrapper to access single (input, output) pairs at a time
2. A `DataLoader` combines multiple samples from a `Dataset` into batches

Both of these classes are defined in `torch.utils.data`

Dataset: Single-Sample Access

To get your data into PyTorch's format, you simply need to subclass `Dataset` and implement two methods:

- `__len__()`: returns the number of samples in the `Dataset`
  - It is usually safe to change the length over time: a `Dataset` can grow/shrink
- `__getitem__(idx)`: returns the sample at a given index
  - Can do arbitrary processing here: e.g., load image from disk, crop, scale, convert to `Tensor`, etc.
  - Can return fairly arbitrary output, as long as the result at each index has the same form
  - Do not always need to return the same value for a given index: a `Dataset` can perform random data augmentations or even data generation

TensorDataset Example

If your data are already stored in `Tensors`, can simply wrap them with a `TensorDataset`:

```
1 x = torch.rand(500, 10, dtype=torch.float)
2 y = torch.randint(low=0, high=5, size=(500,),
    dtype=torch.long)
3 dataset = TensorDataset(x, y)
4
5 x_0, y_0 = dataset[0]
6 print(x_0.shape)  # torch.Size([10])
7 print(y_0)  # tensor(1)
```

DataLoader: Sampling and Batching

- Typically train using **mini-batch stochastic gradient descent**: update the trainable parameters using gradients computed from a random subset of the training data

- DataLoader wraps a Dataset and enables iteration over batches

```
1 x = torch.rand(500, 10, dtype=torch.float)
2 y = torch.randint(low=0, high=5, size=(500,), dtype
      =torch.long)
3 dataset = TensorDataset(x, y)
4 loader = DataLoader(dataset, batch_size=5, shuffle=
      True)
5
6 x_0, y_0 = next(iter(loader))
7 print(x_0.shape)  # torch.Size([5, 10])
8 print(y_0.shape)  # torch.Size([5])
```

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MNIST: The "`hello, world`" of Machine Learning

- One of the standard image processing benchmark datasets for many years
- Consists of 28×28 grayscale images of handwritten digits: 60 000 training images and 10 000 test images
  - Data are very clean: only one digit per image, nicely centered/scaled, etc.
- Fairly small/easy by today's standards, but good for education because you can successfully train models on the CPU
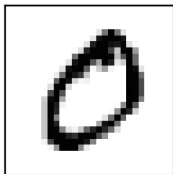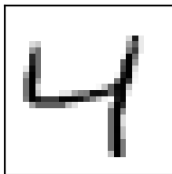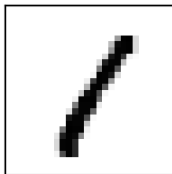

$y = 5$ $\qquad$ $y = 0$ $\qquad$ $y = 4$ $\qquad$ $y = 1$

Solution Script (Walk Through Full Code in Editor)

```
1    train_loader, val_loader, test_loader = get_data(
2        drop_last=True, batch_size=128
3    )
4
5    num_class = 10
6    layer_widths = [256, 128, 64]
7    model = MLPNet(train_loader.dataset[0][0].shape, num_class,
         layer_widths)
8    model.to(device)
9
10   optimizer = optim.Adam(model.parameters())
11
12   loss_fn = nn.CrossEntropyLoss(reduction='sum')
13
14   num_epoch = 10
15   run_training_loop(
16       train_loader, val_loader, model, loss_fn, device,
             optimizer, num_epoch
17   )
18   torch.save(model.state_dict(), 'model.pt')
19
20   test_loss, test_acc = epoch(test_loader, model, loss_fn,
         device)
21   print('\n\t\tLoss\tAcc.')
22   print(f'Test:\t\t{test_loss:.3f}\t{test_acc:.3f}')
```

Example Output (Last Few Lines)

```
1  Epoch 7:     Loss    Acc.
2  Train:       0.025   0.992
3  Val:         0.094   0.973
4
5  Epoch 8:     Loss    Acc.
6  Train:       0.022   0.993
7  Val:         0.094   0.976
8
9  Epoch 9:     Loss    Acc.
10 Train:       0.020   0.994
11 Val:         0.086   0.979
12
13              Loss    Acc.
14 Test:        0.078   0.980
```

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Summary and Additional Resources

PyTorch-specific resources:

- PyTorch documentation:
  https://pytorch.org/docs/stable/index.html
- PyTorch tutorials: https://pytorch.org/tutorials/
- PyTorch book: https://pytorch.org/assets/deep-learning/
  Deep-Learning-with-PyTorch.pdf

General machine learning/deep learning resources:

- Introduction to Statistical Learning (R-focused, but very
  popular for learning the fundamentals):
  https://www.statlearning.com/
- Probabilistic Machine Learning (book series):
  https://probml.github.io/pml-book/
- Deep Learning: https://www.deeplearningbook.org/