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

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What Is PyTorch?

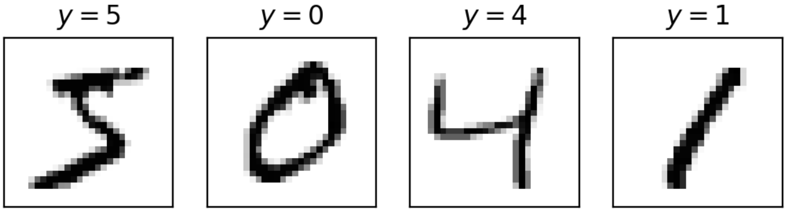
PyTorch is an open source Python **machine learning** package geared towards building **neural networks**, which provides the following key features:[1]

- 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

[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



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

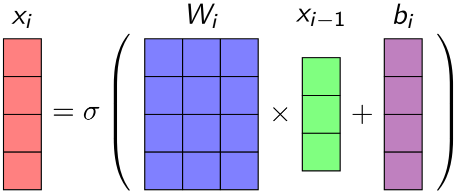
- PyTorch is geared to a specific family of machine learning approaches: **(deep) neural networks**
- Neural networks are a broad family of models which started out as biologically-inspired data transformations based on networks of "artificial neurons"
    - Modern practice has diverged from these biologically-inspired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

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

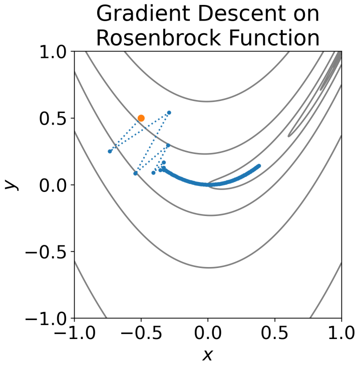
- $\sigma : \mathbb{R} \to \mathbb{R}$ is a nonlinear **activation function** which is applied separately to each element of its (vector) input
- $W_i \in \mathbb{R}^{n_{\text{out}} \times n_{\text{in}}}$ and $b_i \in \mathbb{R}^{n_{\text{out}}}$ are **learnable parameters**



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 $\theta = \{W_i, b_i | 1 \leq i \leq L\}$
- 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

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



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

PyTorch Fundamentals: What Is a Tensor?

A tensor $\mathbf{H}$ of valence $\begin{Bmatrix} \mathfrak{f} \\ \mathfrak{v} \end{Bmatrix}$ 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 $\mathbf{H}$ at $\mathfrak{p}$ only depends on the values of the 1-forms and vectors at $\mathfrak{p}$.[2]

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

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lol, nope!

[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:

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

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

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

```
with torch.no_grad():
    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:

```
if torch.cuda.is_available():
    device = torch.device('cuda')
else:
    device = torch.device('cpu')

x = torch.tensor(1.0, device=device)
```

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

```
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

```
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
layer = ScaledLinear(16, 4, 2.0)
x = torch.rand(1, 16)
out = layer(x)
print(out.shape)  # torch.Size([1, 4])
print(layer.state_dict().keys())
# 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

```
layer = ScaledLinear(16, 4, 2.0)
state_dict = layer.state_dict()
torch.save(state_dict, 'model.pt')

state_dict = torch.load('model.pt')
layer.load_state_dict(state_dict)
# <All keys matched successfully>
```

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:

```
x = torch.rand(500, 10, dtype=torch.float)
y = torch.randint(low=0, high=5, size=(500,),
    dtype=torch.long)
dataset = TensorDataset(x, y)

x_0, y_0 = dataset[0]
print(x_0.shape)  # torch.Size([10])
print(y_0)  # tensor(1)
```

DataLoader: Sampling and Batching

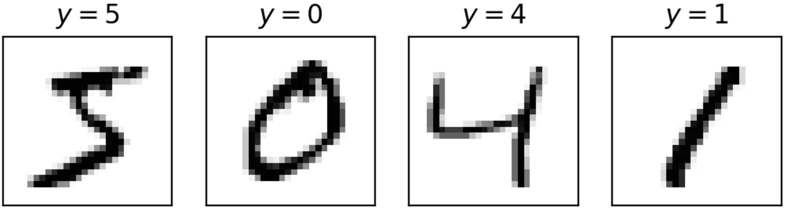
- Typically train using **mini-batch stochastic gradient descent**: update the trainable parameters using gradients computed from a random subset of the training data
- DataLoader wraps a Dataset and enables iteration over batches

```python
x = torch.rand(500, 10, dtype=torch.float)
y = torch.randint(low=0, high=5, size=(500,), dtype
    =torch.long)
dataset = TensorDataset(x, y)
loader = DataLoader(dataset, batch_size=5, shuffle=
    True)

x_0, y_0 = next(iter(loader))
print(x_0.shape)  # torch.Size([5, 10])
print(y_0.shape)  # torch.Size([5])
```

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



Solution Script (Walk Through Full Code in Editor)

```
train_loader, val_loader, test_loader = get_data(
    drop_last=True, batch_size=128
)

num_class = 10
layer_widths = [256, 128, 64]
model = MLPNet(train_loader.dataset[0][0].shape, num_class,
    layer_widths)
model.to(device)

optimizer = optim.Adam(model.parameters())

loss_fn = nn.CrossEntropyLoss(reduction='sum')

num_epoch = 10
run_training_loop(
    train_loader, val_loader, model, loss_fn, device,
        optimizer, num_epoch
)
torch.save(model.state_dict(), 'model.pt')

test_loss, test_acc = epoch(test_loader, model, loss_fn,
    device)
print('\n\t\tLoss\tAcc.')
print(f'Test:\t\t{test_loss:.3f}\t{test_acc:.3f}')
```

Example Output (Last Few Lines)

```
Epoch 7:     Loss    Acc.
Train:       0.025   0.992
Val:         0.094   0.973

Epoch 8:     Loss    Acc.
Train:       0.022   0.993
Val:         0.094   0.976

Epoch 9:     Loss    Acc.
Train:       0.020   0.994
Val:         0.086   0.979

             Loss    Acc.
Test:        0.078   0.980
```

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/