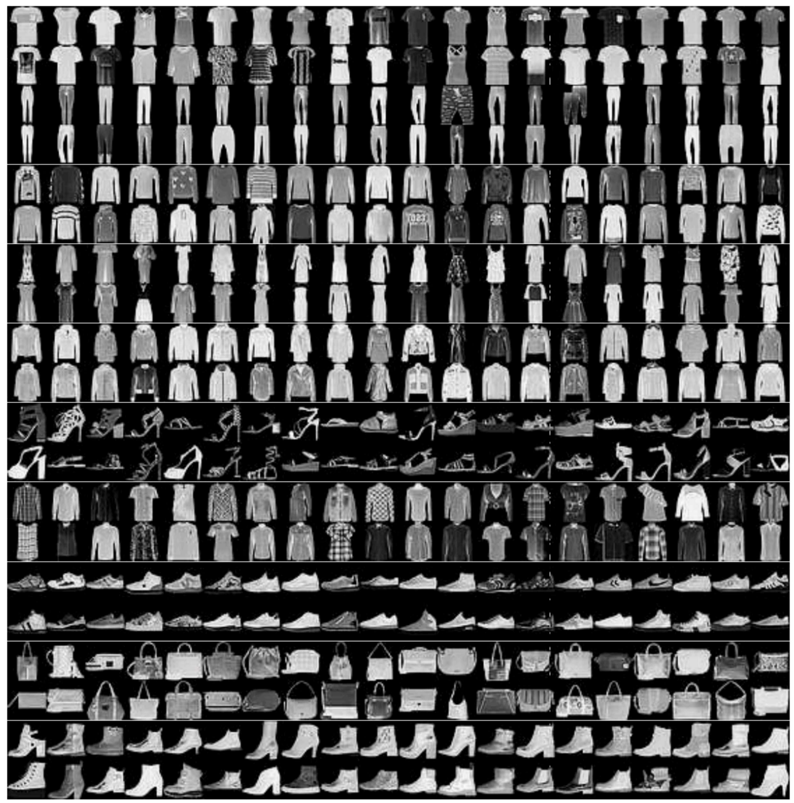
PyTorch

CS 231N PyTorch Tutorial

Drew Kaul
April 22

Fashion-MNIST

Label	Description	Examples
0	T-Shirt/Top	
1	Trouser	
2	Pullover	
3	Dress	
4	Coat	
5	Sandals	
6	Shirt	
7	Sneaker	
8	Bag	
9	Ankle boots	

Xiao et al. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. arXiv preprint arXiv:1708.07747.

Tensors

Initializing a Tensor

Directly from data

Tensors can be created directly from data. The data type is automatically inferred.

```
data = [[1, 2],[3, 4]]
x_data = torch.tensor(data)
```

From a NumPy array

Tensors can be created from NumPy arrays (and vice versa - see Bridge with NumPy).

```
np_array = np.array(data)
x_np = torch.from_numpy(np_array)
```

Initializing a Tensor

From another tensor:

The new tensor retains the properties (shape, datatype) of the argument tensor, unless explicitly overridden.

```
x_ones = torch.ones_like(x_data) # retains the properties of x_data
print(f"Ones Tensor: \n {x_ones} \n")

x_rand = torch.rand_like(x_data, dtype=torch.float) # overrides the datatype of x_data
print(f"Random Tensor: \n {x_rand} \n")
```

Out:

```
Ones Tensor:
 tensor([[1, 1],
        [1, 1]])

Random Tensor:
 tensor([[0.9152, 0.2666],
        [0.0863, 0.9133]])
```

Attributes of a Tensor

Tensor attributes describe their shape, datatype, and the device on which they are stored.

```
tensor = torch.rand(3,4)

print(f"Shape of tensor: {tensor.shape}")
print(f"Datatype of tensor: {tensor.dtype}")
print(f"Device tensor is stored on: {tensor.device}")
```

Out:

```
Shape of tensor: torch.Size([3, 4])
Datatype of tensor: torch.float32
Device tensor is stored on: cpu
```

Operations on Tensors

By default, tensors are created on the CPU. We need to explicitly move tensors to the GPU using `.to` method (after checking for GPU availability). Keep in mind that copying large tensors across devices can be expensive in terms of time and memory!

```
# We move our tensor to the GPU if available
if torch.cuda.is_available():
  tensor = tensor.to('cuda')
```

Operations on Tensors

Standard numpy-like indexing and slicing:

```
tensor = torch.ones(4, 4)
print('First row: ',tensor[0])
print('First column: ', tensor[:, 0])
print('Last column:', tensor[..., -1])
tensor[:,1] = 0
print(tensor)
```

Out:

```
First row:  tensor([1., 1., 1., 1.])
First column:  tensor([1., 1., 1., 1.])
Last column: tensor([1., 1., 1., 1.])
tensor([[1., 0., 1., 1.],
        [1., 0., 1., 1.],
        [1., 0., 1., 1.],
        [1., 0., 1., 1.]])
```

Operations on Tensors

Arithmetic operations

```
# This computes the matrix multiplication between two tensors. y1, y2, y3 will have the same value
y1 = tensor @ tensor.T
y2 = tensor.matmul(tensor.T)

y3 = torch.rand_like(tensor)
torch.matmul(tensor, tensor.T, out=y3)


# This computes the element-wise product. z1, z2, z3 will have the same value
z1 = tensor * tensor
z2 = tensor.mul(tensor)

z3 = torch.rand_like(tensor)
torch.mul(tensor, tensor, out=z3)
```

Datasets & DataLoaders

Loading a Dataset

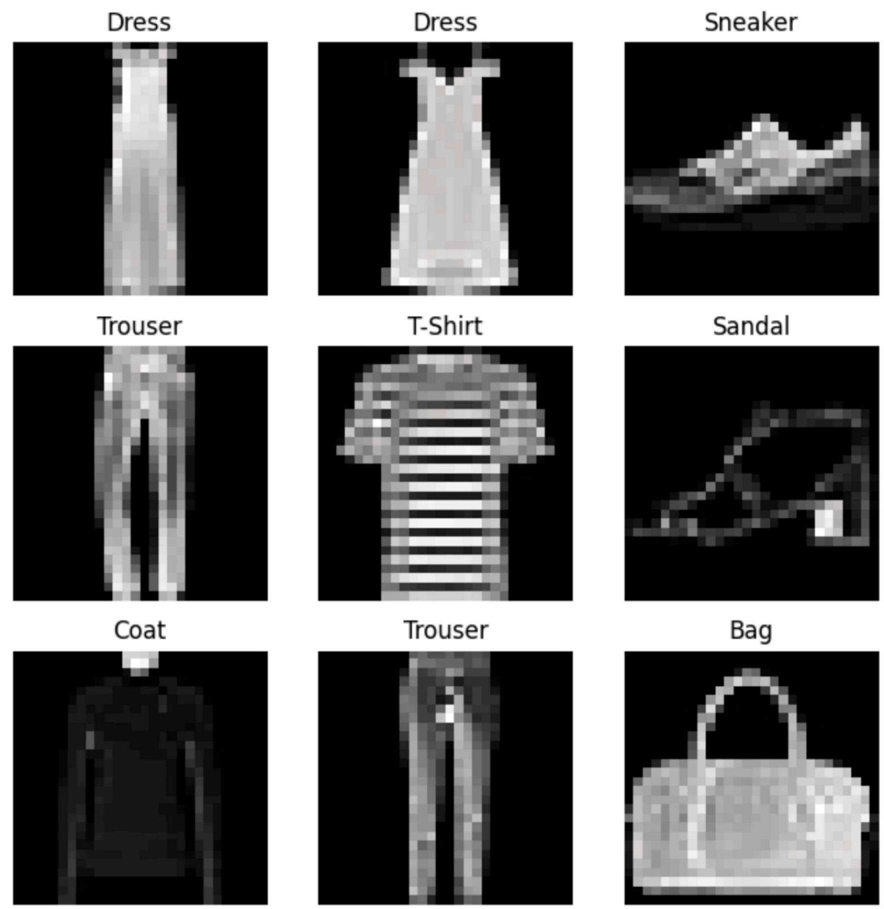
```python
import torch
from torch.utils.data import Dataset
from torchvision import datasets
from torchvision.transforms import ToTensor, Lambda
import matplotlib.pyplot as plt


training_data = datasets.FashionMNIST(
    root="data",
    train=True,
    download=True,
    transform=ToTensor()
)

test_data = datasets.FashionMNIST(
    root="data",
    train=False,
    download=True,
    transform=ToTensor()
)
```

Iterating and Visualizing the Dataset

We can index `Datasets` manually like a list: `training_data[index]`. We use `matplotlib` to visualize some samples in our training data.

```python
labels_map = {
    0: "T-Shirt",
    1: "Trouser",
    2: "Pullover",
    3: "Dress",
    4: "Coat",
    5: "Sandal",
    6: "Shirt",
    7: "Sneaker",
    8: "Bag",
    9: "Ankle Boot",
}
figure = plt.figure(figsize=(8, 8))
cols, rows = 3, 3
for i in range(1, cols * rows + 1):
    sample_idx = torch.randint(len(training_data), size=(1,)).item()
    img, label = training_data[sample_idx]
    figure.add_subplot(rows, cols, i)
    plt.title(labels_map[label])
    plt.axis("off")
    plt.imshow(img.squeeze(), cmap="gray")
plt.show()
```

Iterating and Visualizing the Dataset



Creating a Custom Dataset for your files

```python
import os
import pandas as pd
from torchvision.io import read_image

class CustomImageDataset(Dataset):
    def __init__(self, annotations_file, img_dir, transform=None, target_transform=None):
        self.img_labels = pd.read_csv(annotations_file)
        self.img_dir = img_dir
        self.transform = transform
        self.target_transform = target_transform

    def __len__(self):
        return len(self.img_labels)

    def __getitem__(self, idx):
        img_path = os.path.join(self.img_dir, self.img_labels.iloc[idx, 0])
        image = read_image(img_path)
        label = self.img_labels.iloc[idx, 1]
        if self.transform:
            image = self.transform(image)
        if self.target_transform:
            label = self.target_transform(label)
        sample = {"image": image, "label": label}
        return sample
```

Creating a Custom Dataset for your files

```python
import os
import pandas as pd
from torchvision.io import read_image

class CustomImageDataset(Dataset):
    def __init__(self, annotations_file, img_dir, transform=None, target_transform=None):
        self.img_labels = pd.read_csv(annotations_file)
        self.img_dir = img_dir
        self.transform = transform
        self.target_transform = target_transform

    def __len__(self):
        return len(self.img_labels)

    def __getitem__(self, idx):
        img_path = os.path.join(self.img_dir, self.img_labels.iloc[idx, 0])
        image = read_image(img_path)
        label = self.img_labels.iloc[idx, 1]
        if self.transform:
            image = self.transform(image)
        if self.target_transform:
            label = self.target_transform(label)
        sample = {"image": image, "label": label}
        return sample
```

Creating a Custom Dataset for your files

```python
import os
import pandas as pd
from torchvision.io import read_image

class CustomImageDataset(Dataset):
    def __init__(self, annotations_file, img_dir, transform=None, target_transform=None):
        self.img_labels = pd.read_csv(annotations_file)
        self.img_dir = img_dir
        self.transform = transform
        self.target_transform = target_transform

    def __len__(self):
        return len(self.img_labels)

    def __getitem__(self, idx):
        img_path = os.path.join(self.img_dir, self.img_labels.iloc[idx, 0])
        image = read_image(img_path)
        label = self.img_labels.iloc[idx, 1]
        if self.transform:
            image = self.transform(image)
        if self.target_transform:
            label = self.target_transform(label)
        sample = {"image": image, "label": label}
        return sample
```

Creating a Custom Dataset for your files

```python
import os
import pandas as pd
from torchvision.io import read_image

class CustomImageDataset(Dataset):
    def __init__(self, annotations_file, img_dir, transform=None, target_transform=None):
        self.img_labels = pd.read_csv(annotations_file)
        self.img_dir = img_dir
        self.transform = transform
        self.target_transform = target_transform

    def __len__(self):
        return len(self.img_labels)

    def __getitem__(self, idx):
        img_path = os.path.join(self.img_dir, self.img_labels.iloc[idx, 0])
        image = read_image(img_path)
        label = self.img_labels.iloc[idx, 1]
        if self.transform:
            image = self.transform(image)
        if self.target_transform:
            label = self.target_transform(label)
        sample = {"image": image, "label": label}
        return sample
```

Preparing your data for training with DataLoaders

The `Dataset` retrieves our dataset's features and labels one sample at a time. While training a model, we typically want to pass samples in "minibatches", reshuffle the data at every epoch to reduce model overfitting, and use Python's `multiprocessing` to speed up data retrieval.

`DataLoader` is an iterable that abstracts this complexity for us in an easy API.

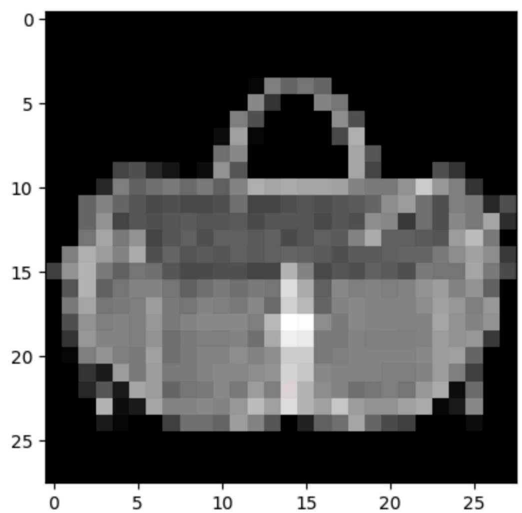
```
from torch.utils.data import DataLoader

train_dataloader = DataLoader(training_data, batch_size=64, shuffle=True)
test_dataloader = DataLoader(test_data, batch_size=64, shuffle=True)
```

Iterate through the DataLoader

We have loaded that dataset into the `Dataloader` and can iterate through the dataset as needed. Each iteration below returns a batch of `train_features` and `train_labels``(containing` ``batch_size=64` features and labels respectively). Because we specified `shuffle=True`, after we iterate over all batches the data is shuffled (for finer-grained control over the data loading order, take a look at Samplers).

```
# Display image and label.
train_features, train_labels = next(iter(train_dataloader))
print(f"Feature batch shape: {train_features.size()}")
print(f"Labels batch shape: {train_labels.size()}")
img = train_features[0].squeeze()
label = train_labels[0]
plt.imshow(img, cmap="gray")
plt.show()
print(f"Label: {label}")
```

Iterate through the DataLoader



Out:

```
Feature batch shape: torch.Size([64, 1, 28, 28])
Labels batch shape: torch.Size([64])
Label: 8
```

Neural Network

torch.nn.Module

```
import os
import torch
from torch import nn
from torch.utils.data import DataLoader
from torchvision import datasets, transforms
```

Get Device for Training

We want to be able to train our model on a hardware accelerator like the GPU, if it is available. Let's check to see if torch.cuda is available, else we continue to use the CPU.

```
device = 'cuda' if torch.cuda.is_available() else 'cpu'
print('Using {} device'.format(device))
```

Out:

```
Using cuda device
```

Define the Class

We define our neural network by subclassing `nn.Module`, and initialize the neural network layers in `__init__`. Every `nn.Module` subclass implements the operations on input data in the `forward` method.

```
class NeuralNetwork(nn.Module):
    def __init__(self):
        super(NeuralNetwork, self).__init__()
        self.flatten = nn.Flatten()
        self.linear_relu_stack = nn.Sequential(
            nn.Linear(28*28, 512),
            nn.ReLU(),
            nn.Linear(512, 512),
            nn.ReLU(),
            nn.Linear(512, 10),
            nn.ReLU()
        )

    def forward(self, x):
        x = self.flatten(x)
        logits = self.linear_relu_stack(x)
        return logits
```

Define the Class

We create an instance of `NeuralNetwork`, and move it to the `device`, and print it’s structure.

```
model = NeuralNetwork().to(device)
print(model)
```

Out:

```
NeuralNetwork(
  (flatten): Flatten(start_dim=1, end_dim=-1)
  (linear_relu_stack): Sequential(
    (0): Linear(in_features=784, out_features=512, bias=True)
    (1): ReLU()
    (2): Linear(in_features=512, out_features=512, bias=True)
    (3): ReLU()
    (4): Linear(in_features=512, out_features=10, bias=True)
    (5): ReLU()
  )
)
```

Define the Class

To use the model, we pass it the input data. This executes the model's `forward`, along with some background operations. Do not call `model.forward()` directly!

Calling the model on the input returns a 10-dimensional tensor with raw predicted values for each class. We get the prediction probabilities by passing it through an instance of the `nn.Softmax` module.

```
X = torch.rand(1, 28, 28, device=device)
logits = model(X)
pred_probab = nn.Softmax(dim=1)(logits)
y_pred = pred_probab.argmax(1)
print(f"Predicted class: {y_pred}")
```

Out:

```
Predicted class: tensor([2], device='cuda:0')
```

Optimizing Model Params

Loss Function

Common loss functions include nn.MSELoss (Mean Square Error) for regression tasks, and nn.NLLLoss (Negative Log Likelihood) for classification. nn.CrossEntropyLoss combines `nn.LogSoftmax` and `nn.NLLLoss`.

We pass our model's output logits to `nn.CrossEntropyLoss`, which will normalize the logits and compute the prediction error.

```
# Initialize the loss function
loss_fn = nn.CrossEntropyLoss()
```

Optimizer

We initialize the optimizer by registering the model's parameters that need to be trained, and passing in the learning rate hyperparameter.

```
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)
```

Inside the training loop, optimization happens in three steps:

- Call `optimizer.zero_grad()` to reset the gradients of model parameters. Gradients by default add up; to prevent double-counting, we explicitly zero them at each iteration.
- Backpropagate the prediction loss with a call to `loss.backwards()`. PyTorch deposits the gradients of the loss w.r.t. each parameter.
- Once we have our gradients, we call `optimizer.step()` to adjust the parameters by the gradients collected in the backward pass.

Full Implementation – Train Loop

```python
def train_loop(dataloader, model, loss_fn, optimizer):
    size = len(dataloader.dataset)
    for batch, (X, y) in enumerate(dataloader):
        # Compute prediction and loss
        pred = model(X)
        loss = loss_fn(pred, y)

        # Backpropagation
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if batch % 100 == 0:
            loss, current = loss.item(), batch * len(X)
            print(f"loss: {loss:>7f}  [{current:>5d}/{size:>5d}]")
```

Full Implementation – Test Loop

```
def test_loop(dataloader, model, loss_fn):
    size = len(dataloader.dataset)
    test_loss, correct = 0, 0

    with torch.no_grad():
        for X, y in dataloader:
            pred = model(X)
            test_loss += loss_fn(pred, y).item()
            correct += (pred.argmax(1) == y).type(torch.float).sum().item()

    test_loss /= size
    correct /= size
    print(f"Test Error: \n Accuracy: {(100*correct):>0.1f}%, Avg loss: {test_loss:>8f} \n")
```

Full Implementation

```
loss_fn = nn.CrossEntropyLoss()
optimizer = torch.optim.SGD(model.parameters(), lr=learning_rate)

epochs = 10
for t in range(epochs):
    print(f"Epoch {t+1}\n-------------------------------")
    train_loop(train_dataloader, model, loss_fn, optimizer)
    test_loop(test_dataloader, model, loss_fn)
print("Done!")
```

Full Implementation

Out:

```
Epoch 1
-------------------------------
loss: 2.299511  [    0/60000]
loss: 2.301767  [ 6400/60000]
loss: 2.289777  [12800/60000]
loss: 2.291731  [19200/60000]
loss: 2.269755  [25600/60000]
loss: 2.261175  [32000/60000]
loss: 2.258553  [38400/60000]
loss: 2.240743  [44800/60000]
loss: 2.260818  [51200/60000]
loss: 2.243683  [57600/60000]
Test Error:
 Accuracy: 37.3%, Avg loss: 0.035121

Epoch 2
-------------------------------
loss: 2.229830  [    0/60000]
loss: 2.241497  [ 6400/60000]
loss: 2.221580  [12800/60000]
```

Save and Load the Model

Saving and Loading Model Weights

PyTorch models store the learned parameters in an internal state dictionary, called `state_dict`. These can be persisted via the `torch.save` method:

```
model = models.vgg16(pretrained=True)
torch.save(model.state_dict(), 'model_weights.pth')
```

To load model weights, you need to create an instance of the same model first, and then load the parameters using `load_state_dict()` method.

```
model = models.vgg16() # we do not specify pretrained=True, i.e. do not load default weights
model.load_state_dict(torch.load('model_weights.pth'))
model.eval()
```

Saving and Loading Models with Shapes

When loading model weights, we needed to instantiate the model class first, because the class defines the structure of a network. We might want to save the structure of this class together with the model, in which case we can pass `model` (and not `model.state_dict()`) to the saving function:

```
torch.save(model, 'model.pth')
```

We can then load the model like this:

```
model = torch.load('model.pth')
```

Acknowledgment

- PyTorch Official Tutorial: https://pytorch.org/tutorials/beginner/basics/intro.html

- Feel free to check out the tutorial for more details!