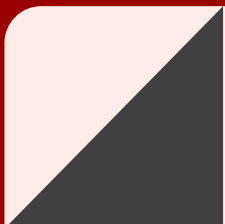


Introduction to PyTorch

CS236 Section, Autumn 2024
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What is Pytorch?

A machine learning framework that accelerates the path from research prototyping to production deployment

Machine learning framework

Deep learning primitives such as data loading, NN layer types, activations, loss functions, and optimizers

Hardware acceleration on NVIDIA GPUs

Libraries for vision, NLP, and audio applications

Research prototyping

Models are Python code, Automatic differentiation, and eager mode

Production deployment

TorchScript, TorchServe, quantization

Overview

Motivations

Python

NumPy

Building Blocks

Tensors

Operations

Modules

Examples

MNIST

Beyond PyTorch

Tools

High Level Libraries

Domain Specific Libraries

Motivations

Python vs. NumPy

```
X = [1] * 10000
Y = [0.5] * 10000
Z = [None] * 10000
for i in range(10000):
    Z[i] = X[i] * Y[i]
```

```
# 2.772092819213867 ms
# Interpreter Overhead
# 64 bit
```

```
X = np.full((10000,), 1)
Y = np.full((10000,), 0.5)
Z = X * Y
```

```
# 0.08273124694824219 ms
# Low Level Implementation
# Vectorization
```

Motivations

NumPy vs. PyTorch

```
X = np.full((10000,), 1)
Y = np.full((10000,), 0.5)
Z = X * Y
```

```
# 0.08273124694824219 ms
# Low Level Implementation
# Vectorization
```

```
X = torch.full((10000,), 1).cuda()
Y = torch.full((10000,), 0.5).cuda()
Z = X * Y
```

```
# 0.3185272216796875 ms
# GPU Acceleration
```

```
Z.sum().backward()
dX = X.grad
```

```
# Automatic Differentiation
```

Building Blocks

TENSORS

Building Blocks

Tensors / Initialization

```
torch.tensor([5., 3.])  
tensor([ 5.,  3.,]) # defaults to  
torch.float32
```

```
torch.from_numpy(np.array([5., 3.]))  
tensor([ 5.,  3.,], dtype=torch.float64) #  
because numpy defaults to 64bit
```

```
torch.tensor([5., 3.]).numpy()  
array([5., 3.], dtype=float32)
```

Building Blocks

Tensors / Initialization

```
torch.ones(5, 3)
tensor([[1., 1., 1.],
        [1., 1., 1.],
        [1., 1., 1.],
        [1., 1., 1.],
        [1., 1., 1.]], dtype=torch.float64)
```


Building Blocks

Tensors / Initialization

```
torch.randn(5, 3)
```

```
tensor([[ 0.2349, -0.0427, -0.5053],  
        [ 0.6455,  0.1199,  0.4239],  
        [ 0.1279,  0.1105,  1.4637],  
        [ 0.4259, -0.0763, -0.9671],  
        [ 0.6856,  0.5047,  0.4250]])
```

Building Blocks

Tensors / Initialization

```
torch.ones_like(tensor)
Input: tensor([[ 0.2349, -0.0427, -0.5053],
               [ 0.6455,  0.1199,
0.4239]])
Output: tensor([[1., 1., 1.],
               [1., 1., 1.],
dtype=torch.float64)
```

Building Blocks

Tensors / Initialization

```
torch.empty(5, 3)
tensor([[ 0.0000e+00,  2.5244e-29,  0.0000e+00],
        [ 2.5244e-29,  1.4569e-19,  2.7517e+12],
        [ 7.5338e+28,  3.0313e+32,  6.3828e+28],
        [ 1.4603e-19,  1.0899e+27,  6.8943e+34],
        [ 1.1835e+22,  7.0976e+22,  1.8515e+28]])
```

```
# The values are not initialized
```

Building Blocks

Tensors / Indexing & Reshaping

```
torch.tensor([[5., 3.]])[0, :]  
tensor([ 5.,  3.,])
```

```
torch.tensor([[5., 3.]])  
dimension size  
torch.tensor([[5., 3.]])  
tensor([ 5.,  3.,])
```

```
torch.tensor([[5., 3.]])  
torch.Size([1, 2])
```

Building Blocks

Tensors / Broadcasting

```
X = torch.ones((3, 3, 3))
Y = torch.ones((1, 1, 3))
Z = X * Y
Z.size()
```

```
torch.Size([3, 3, 3])
```

#

<https://pytorch.org/docs/stable/notes/broadcasting.html>

Building Blocks

Tensors / Devices

```
if torch.cuda.is_available():
    device = torch.device("cuda")
    x = torch.ones(2, device=device)
    y = torch.ones(2).to(device)
    z = x + y
    print(z)
    print(z.to("cpu", torch.double))

# `x.cuda()` and `x.cpu()` also works
```

a CUDA device object
directly create a tensor on GPU
or just use strings `.to("cuda")`
z is on GPU
to('cpu') moves array to CPU`

Building Blocks

Operations / Primitives

```
torch.tensor([5., 3.]) + torch.tensor([3., 5.])  
tensor([ 8.,  8.,])
```

```
z = torch.add(x, y)  
torch.add(x, y, out=z)  
y = y.add_(x) # inplace y += x
```

```
torch.tanh(y)  
torch.stack([x, y])
```

```
# https://pytorch.org/docs/stable/torch.html
```

Building Blocks

Operations / Functional

```
import torch.nn.functional as F

X = torch.randn((64, 3, 256, 256))
W = torch.randn((8, 3, 3, 3))

out = F.conv2d(X, W, stride=1, padding=1)

# Like SciPy
# https://pytorch.org/docs/stable/nn.functional.html
```

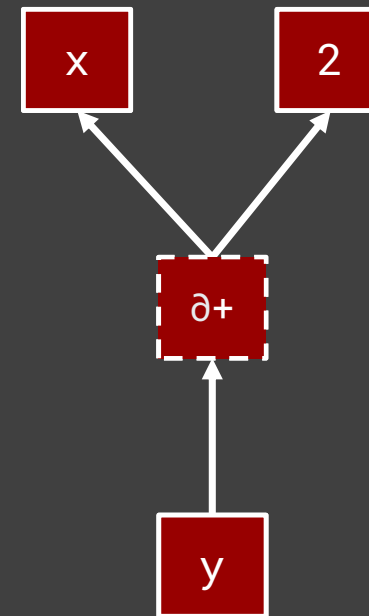

Building Blocks

Operations / Automatic Differentiation

Computation as a graph built at runtime

```
x = torch.ones(2, 2, requires_grad=True)
tensor([[1., 1.],
        [1., 1.]], requires_grad=True)

y = x + 2
tensor([[3., 3.],
        [3., 3.]], grad_fn=<AddBackward0>)
```



Building Blocks

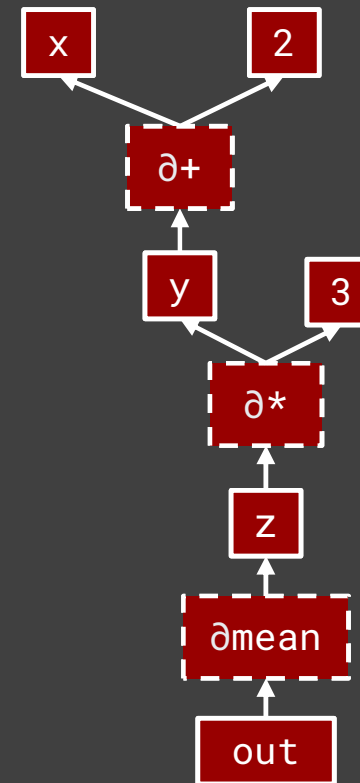
Operations / Automatic Differentiation

```
z = y * 3
out = z.mean()

tensor(9., grad_fn=<MeanBackward1>)

out.backward() # Must be scalar
print(x.grad) # Only leaf nodes have grad
```

Gradient w.r.t. the input Tensors is computed step-by-step from loss to the top in reverse



Building Blocks

Operations / Automatic Differentiation

```
x.requires_grad # True
(x ** 2).requires_grad # True

# Keeping track of activations is expensive

with torch.no_grad():
    (x ** 2).requires_grad # False

(x.detach() ** 2).requires_grad # False
```

Building Blocks

Operations / nn

```
import torch.nn as nn

X = torch.ones((64, 3, 256, 256))

conv = nn.Conv2D(in_channels=3,
                  out_channels=8,
                  kernel_size=3,
                  stride=1,
                  padding=1)

out = conv(img)
```

```
import torch.nn.functional as F

X = torch.randn((64, 3, 256, 256))
W = torch.randn((8, 3, 3, 3))

out = F.conv2d(X, W,
               stride=1, padding=1)

# Inherits from nn.Module
# Implemented using functional
# Stores internal states
```

Building Blocks

Operations / Module

```
import torch.nn as nn

X = torch.ones((64, 3, 256, 256))

conv = nn.Conv2D(in_channels=3,
                  out_channels=8,
                  kernel_size=3,
                  stride=1,
                  padding=1)
```

```
# Move the module to GPUs
conv.cuda()

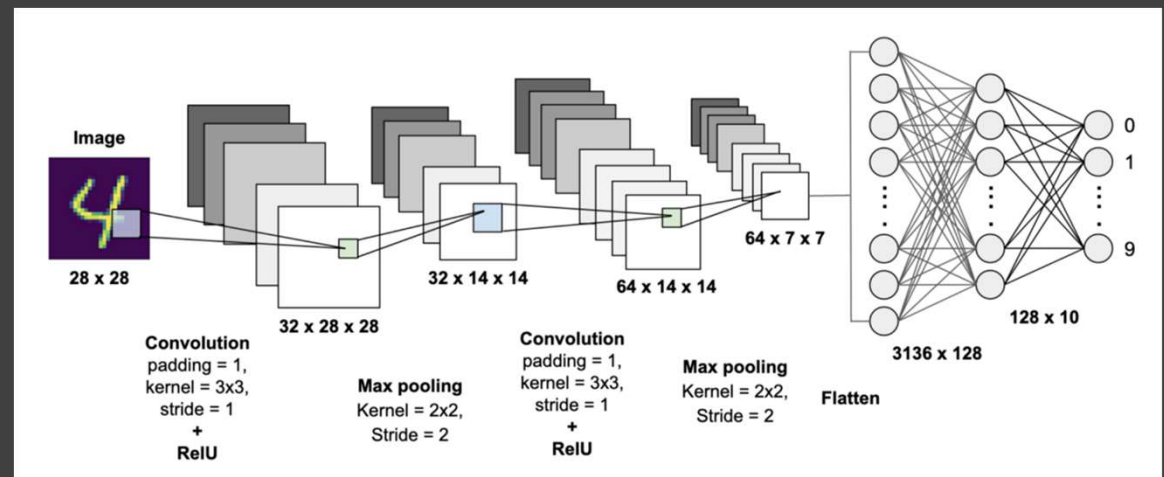
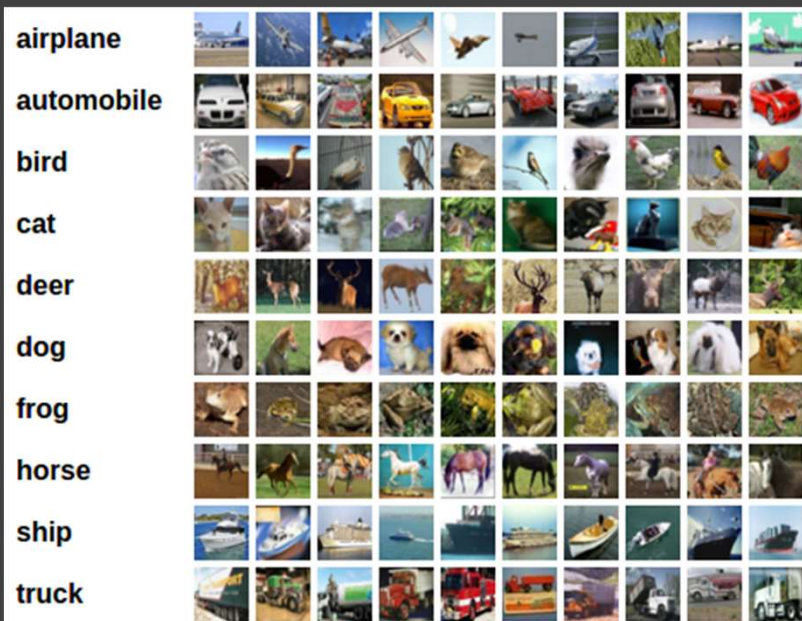
# Saves states
conv.state_dict()

# Saves trainable states
conv.parameters()

# Recursively visit child modules
conv.apply(weight_init)
```

Examples

MNIST



Example

MNIST

Preprocessing

Dataloader

Network

Optimizer

Training

Examples

MNIST / Preprocessing

```
import torchvision.transforms as transforms

transform = transforms.Compose(
    [transforms.ToTensor(),
     transforms.Normalize((0.5, 0.5, 0.5), (0.5, 0.5, 0.5))])

# Convert to Torch Tensor and perform normalization
# https://pytorch.org/vision/stable/transforms.html
# e.x Color Jitter, Five Crops
```


Examples

MNIST / Dataloader

```
Import torch
import torchvision

trainset = torchvision.datasets.CIFAR10(
    root='./data', train=True,
    download=True, transform=transform)

# Dataloaders are python iterators
trainloader = torch.utils.data.DataLoader(
    trainset, batch_size=8,
    shuffle=True, num_workers=2)
```

Examples

MNIST / Network

```
import torch.nn as nn

class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(3, 6, 5)
        self.pool = nn.MaxPool2d(2, 2)
        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)
```

Examples

MNIST / Network

```
import torch.nn.functional as F

class Net(nn.Module):
    def __init__(self):
        ...
    def forward(self, x):
        x = self.pool(F.relu(self.conv1(x)))
        x = torch.flatten(self.pool(F.relu(self.conv2(x))))
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        return self.fc3(x)
```

Examples

MNIST / Optimizer

```
import torch.optim as optim

# Instantiate nn.Module (Use default weights)
net = Net().to("cuda")

# Define loss function
criterion = nn.CrossEntropyLoss()

# Create optimizer: https://pytorch.org/docs/stable/optim.html
optimizer = optim.SGD(net.parameters(), lr=0.001, momentum=0.9)
```

Examples

MNIST / Training

```
net.train() # Set to training mode (there is also `net.eval()`)

for epoch in range(2):
    for inputs, labels in trainloader:
        # zero the parameter gradients
        optimizer.zero_grad()
        # forward + backward + optimize
        outputs = net(inputs.to("cuda"))
        loss = criterion(outputs, labels.to("cuda"))
        loss.backward()
        optimizer.step()
```


Examples

MNIST / Recap

```
... transforms.Compose( ... # Define preprocessing transforms
... torch.utils.data.DataLoader( ... # Create Dataloader
... def Net(nn.Module): ... # Define Network
... criterion = nn.CrossEntropyLoss() ... # Define loss function
... optim.SGD(net.parameters(), ... # Create Optimizer
... for x, y in trainloader: ... # Iterate over Dataloader
... outputs = net(inputs) # Forward Pass
... criterion(outputs, labels) ... # Compute Loss
... optimizer.zero_grad() ... # Zero out gradients
... loss.backward() ... # Back Propagate
... optimizer.step() ... # Update weights
```

Beyond PyTorch

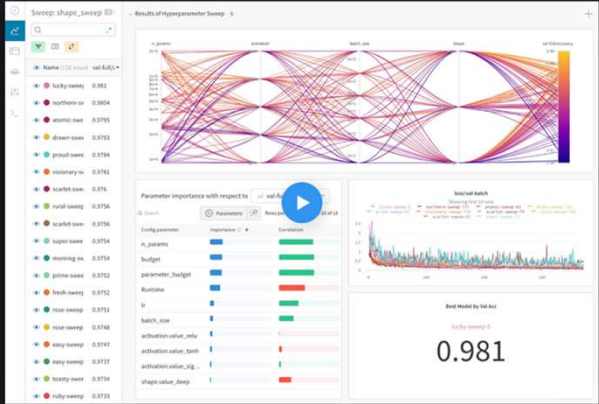
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- MLflow 1.20.0 released! (26 Aug 2021)
- MLflow 1.19.0 released! (14 Jul 2021)


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Beyond PyTorch

High Level Libraries / Distributed & Mixed Precision Training

LIGHTNING CODE

```
# Train
model = LitAutoEncoder()
trainer = pl.Trainer(tpu_cores=8)
trainer.fit(model, mnist_train, mnist_val)
```

GPU available: True, used: False
TPU available: True, using: 8 TPU cores
training on 8 TPU cores

Epoch 2:

LIGHTNING CODE

```
# model
class LitAutoEncoder(pl.LightningModule):
    def __init__(self):
        super().__init__()
        self.encoder = nn.Sequential(n.Linear(28 * 28, 64), n.ReLU(), nn.Linear(64, 3))
        self.decoder = nn.Sequential(nn.Linear(28 * 28, 64), nn.Linear(3, 64), nn.ReLU(), nn.Linear(64, 28 * 28))

    def forward(self, x):
        embedding = self.encoder(x)
        return embedding

    def configure_optimizers(self):
        optimizer = torch.optim.Adam(self.parameters, lr=1e-3)
        return optimizer


    def training_step(self, train_batch, batch_idx):
        x, y = train_batch
        x = x.view(x.size(0), -1)
        z = self.encoder(x)
        x_hat = self.decoder(z)
        loss = F.mse_loss(x_hat, x)
        self.log('train_loss', loss)
        return loss

    def validation_step(self, val_batch, batch_idx):
        x, y = val_batch
        x = x.view(x.size(0), -1)
        z = self.encoder(x)
        x_hat = self.decoder(z)
        loss = F.mse_loss(x_hat, x)
        self.log('val_loss', loss)

    def backward(self, trainer, loss, optimizer, optimizer_idx):
        loss.backward()
```


Beyond PyTorch


Domain Specific Libraries / Graph, RL, Probabilistic Programming

**PyG**NEWSDOCS

PyG is the ultimate library for Graph Neural Networks


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**Gym**

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**PYRO**

Deep Universal Probabilistic Programming