PyTorch Basics

CS HUFS

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

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

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

```python
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.]]).view(-1)  # infer
dimension size
torch.tensor([[5., 3.]]).view(2)
tensor([ 5.,  3.,])


torch.tensor([[5., 3.]]).size()
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")          # a CUDA device object
    x = torch.ones(2, device=device)       # directly create a tensor on GPU
    y = torch.ones(2).to(device)           # or just use strings `.to("cuda")`
    z = x + y
    print(z)                               # z is on GPU
    print(z.to("cpu", torch.double))       # to(‘cpu’) moves array to CPU

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

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

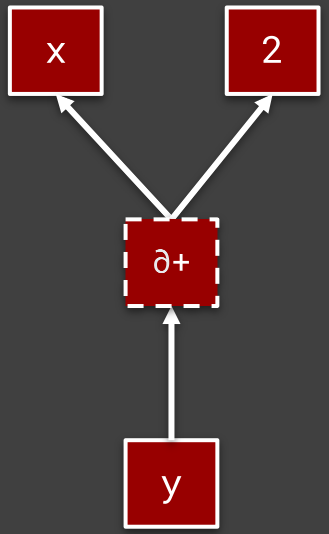
```
import torch.nn.functional as F

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>)
```

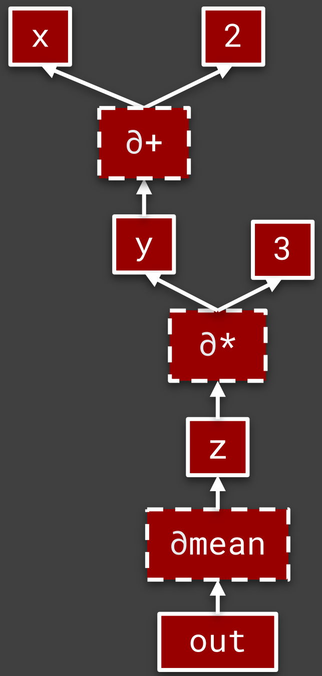


Building Blocks

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

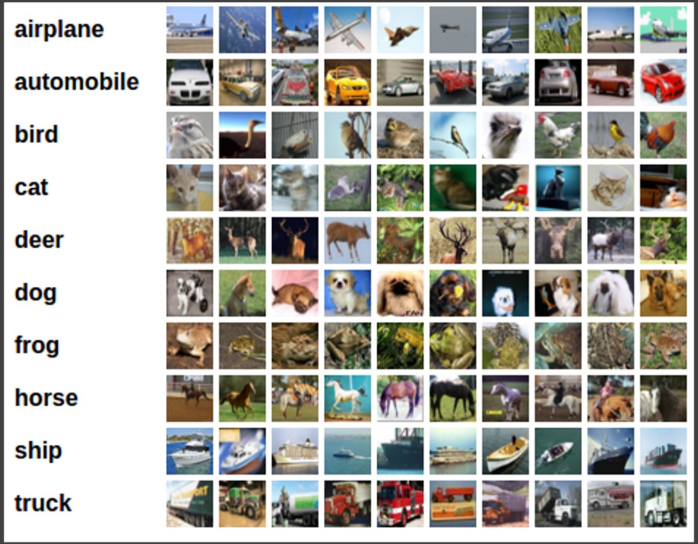
Operations / Module

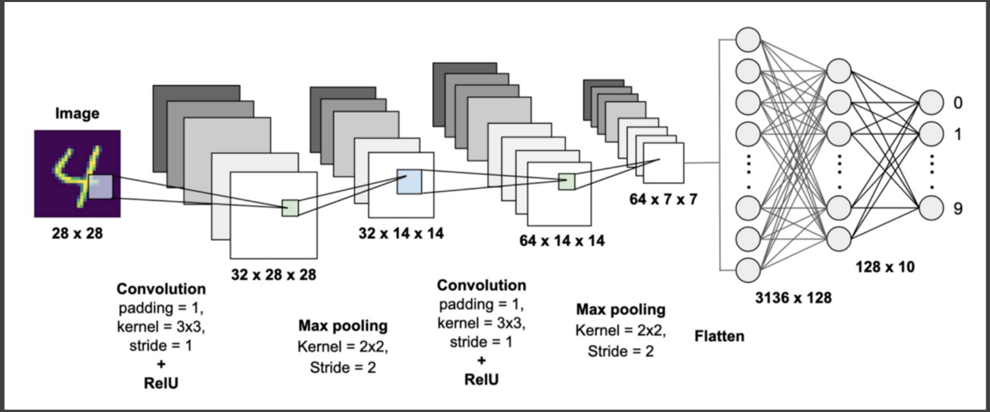
```
import torch.nn as nn

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()
```

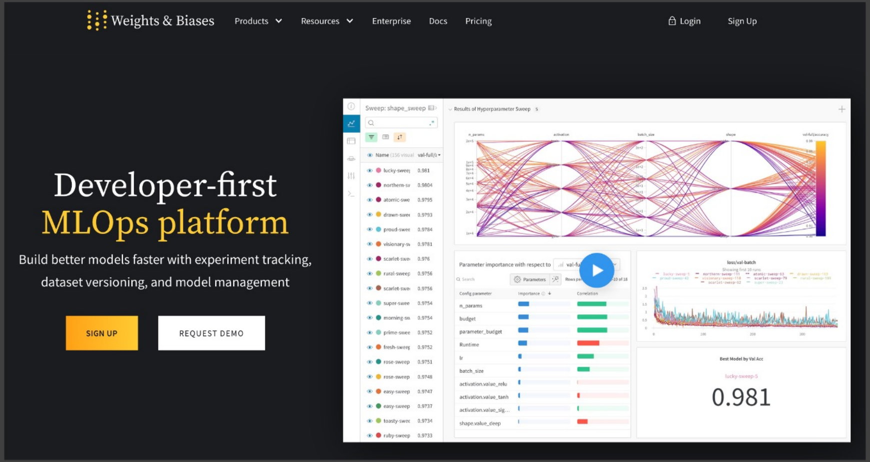
Examples

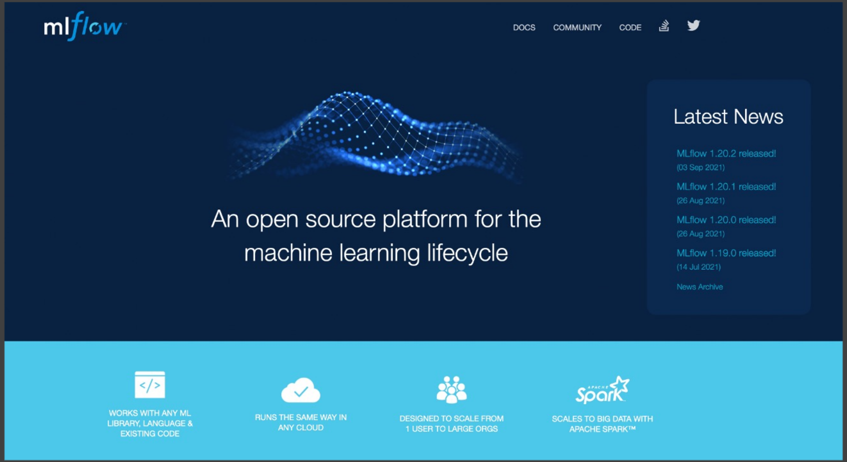
MNIST / Recap

```
... 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

Tools / Keep Track of experiments, artifacts





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