Create Your Model: PyTorch

CSE 849 Deep Learning Spring 2025

Zijun Cui

A zoo of frameworks!

PaddlePaddle Chainer (Baidu) Caffe2 Caffe (Facebook) (UC Berkeley) **MXNet CNTK** (Amazon) (Microsoft) Developed by U Washington, CMU, MIT, Hong Kong U, etc but main framework of choice at Torch **PyTorch** (Facebook) (NYU / Facebook) We'll focus on this JAX (Google) Theano **TensorFlow** (U Montreal) (Google)

The point of deep learning frameworks

- 1. Allow rapid prototyping of new ideas
- 2. Automatically compute gradients for you
- 3. Run it all efficiently on GPU (or TPU)

PyTorch

PyTorch: Versions

- For this class we are using PyTorch version 1.10
- (Released October 2021)
- Be careful if you are looking at older PyTorch code
 - the API changed a lot before 1.0 (0.3 to 0.4 had big changes!)

PyTorch: Fundamental Concepts

Tensor: Like a numpy array, but can run on GPU

Autograd: Package for building computational graphs out of Tensors, and automatically computing gradients

Module: A neural network layer; may store state or learnable weights

Running example: Train a two-layer ReLU network on random data with L2 loss

```
import torch
device = torch.device('cpu')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D_out, device=device)
w1 = torch.randn(D_in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning_rate * grad_w1
    w2 -= learning rate * grad w2
```

Create random tensors for data and weights

```
X: [64, 1000]
Y: [64, 10]
W1: [1000, 100]
W2: [100, 10]
```

```
import torch
device = torch.device('cpu')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
    w2 -= learning rate * grad w2
```

X: [64, 1000] Y: [64, 10] W1: [1000, 100] W2: [100, 10]

Forward pass: compute predictions and loss

```
h = XW1 : [64, 100]
h_relu = ReLU(h) : [64, 100]
Y_pred = h_reluW2 : [64, 10]
```

```
import torch
device = torch.device('cpu')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y_pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
    w2 -= learning rate * grad w2
```

Backward pass: manually compute gradients

```
import torch
device = torch.device('cpu')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D in, H, device=device)
w2 = torch.randn(H, D_out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
    w2 -= learning rate * grad w2
```

Gradient descent step on weights

```
import torch
device = torch.device('cpu')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
    w2 -= learning rate * grad w2
```

To run on GPU, just use a different device!

```
import torch
device = torch.device('cuda:0')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D_in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad w2 = h relu.t().mm(grad y pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    grad h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
```

w2 -= learning_rate * grad_w2

Creating Tensors with requires_grad=True enables autograd

Operations on Tensors with requires_grad=True cause PyTorch to build a computational graph

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

We will not want gradients (of loss) with respect to data

Do want gradients with respect to weights

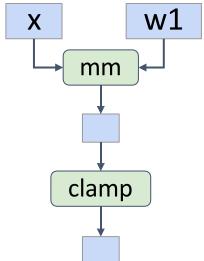
```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

Forward pass looks exactly the same as before, but we don't need to track intermediate values - PyTorch keeps track of them for us in the graph

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

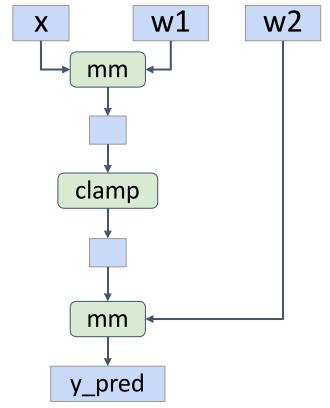
Computes gradients with respect to all inputs that have requires_grad=True!

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D out, requires grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

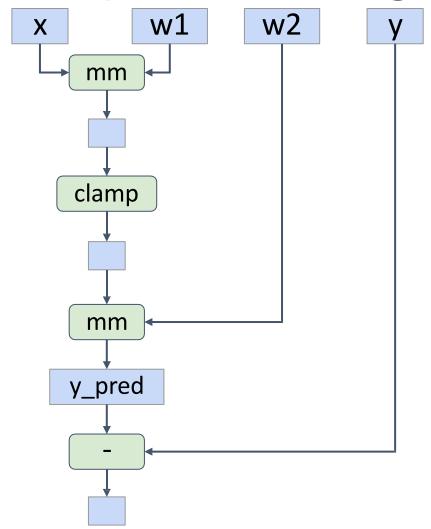


Every operation on a tensor with requires_grad=True will add to the computational graph, and the resulting tensors will also have requires_grad=True

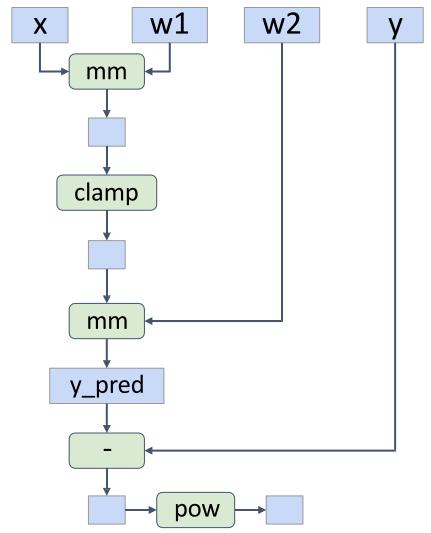
```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero_()
        w2.grad.zero ()
```



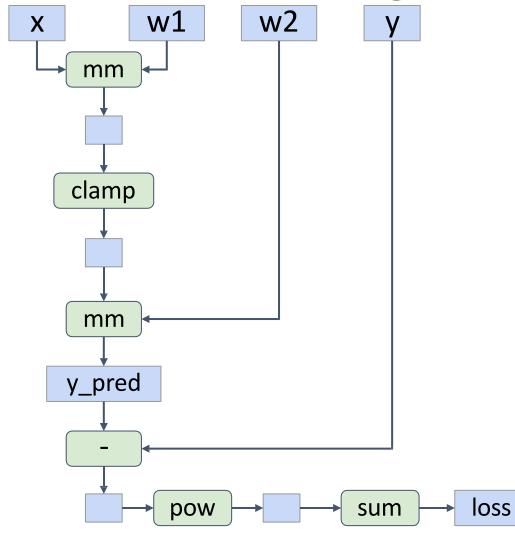
```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```



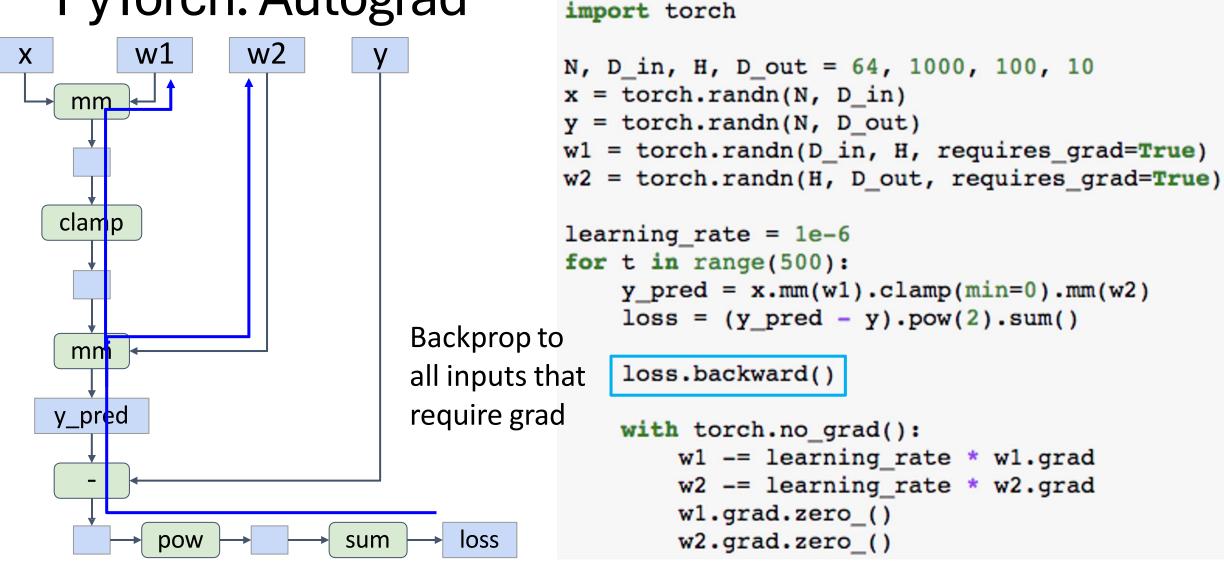
```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```



```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```



```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```



Χ

w1

w2

У

After backward finishes, gradients are accumulated into w1.grad and w2.grad and the graph is destroyed

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D out, requires grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

Χ

w1

w2

У

After backward finishes, gradients are **accumulated** into w1.grad and w2.grad and the graph is destroyed

Make gradient step on weights

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no_grad():
        w1 -= learning rate * w1.grad
        w2 -= learning rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

X

w1

w2

У

After backward finishes, gradients are **accumulated** into w1.grad and w2.grad and the graph is destroyed

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero ()
        w2.grad.zero_()
```

Set gradients to zero

-forgetting this is a common bug!

Χ

w1

w2

У

After backward finishes, gradients are **accumulated** into w1.grad and w2.grad and the graph is destroyed

Tell PyTorch not to build a graph for these operations

```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
    with torch.no grad():
        w1 -= learning rate * w1.grad
        w2 -= learning_rate * w2.grad
        wl.grad.zero ()
        w2.grad.zero ()
```

PyTorch: New functions

Can define new operations using Python functions

```
def sigmoid(x):
   return 1.0 / (1.0 + (-x).exp())
```

When our function runs, it will add to the graph Gradients computed with autograd

```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2 = torch.randn(H, D out, requires grad=True)
learning rate = 1e-6
for t in range(500):
  y pred = sigmoid(x.mm(w1)).mm(w2)
  loss = (y pred - y).pow(2).sum()
  loss.backward()
  if t % 50 == 0:
    print(t, loss.item())
  with torch.no grad():
    w1 -= learning rate * w1.grad
    w2 -= learning_rate * w2.grad
    w1.grad.zero ()
    w2.grad.zero ()
```

PyTorch: New functions

```
def sigmoid(x):
   return 1.0 / (1.0 + (-x).exp())
```

$$\frac{\partial}{\partial x} \left[\sigma(x) \right] = (1 - \sigma(x)) \sigma(x)$$

In practice this is pretty rare – in most cases Python functions are good enough

Define new autograd operators by subclassing Function, define forward and backward

```
class Sigmoid(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x):
    y = 1.0 / (1.0 + (-x).exp())
    ctx.save for backward(y)
    return y
  @staticmethod
  def backward(ctx, grad y):
    y, = ctx.saved_tensors
    grad x = grad y * y * (1.0 - y)
    return grad x
def sigmoid(x):
  return Sigmoid.apply(x)
```

Now when our function runs, it adds one node to the graph!



Higher-level wrapper for working with neural nets

Use this! It will make your life easier

```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D_out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)
    loss.backward()
    with torch.no_grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

Object-oriented API: Define model object as sequence of layers objects, each of which holds weight tensors

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D_out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    with torch.no grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

Forward pass: Feed data to model and compute loss

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse_loss(y pred, y)
    loss.backward()
    with torch.no grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

Forward pass: Feed data to model and compute loss

torch.nn.functional has useful helpers like loss functions

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    with torch.no grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

Backward pass: compute gradient with respect to all model weights (they have requires_grad=True)

Q: where did we specify requires_grad = True?

by default, all parameters of layers in torch.nn modules have requires_grad=True automatically set

```
for param in model.parameters():
    print(param.requires_grad)
    # print True for all trainable parameters
```

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)
    loss.backward()
    with torch.no grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D out))
learning rate = 1e-2
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    with torch.no grad():
        for param in model.parameters():
            param -= learning rate * param.grad
    model.zero grad()
```

Make gradient step on each model parameter (with gradients disabled)

PyTorch: optim

Use an **optimizer** for different update rules

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D_in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D_out))
learning rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                              lr=learning rate)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

PyTorch: optim

```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
          torch.nn.Linear(D_in, H),
          torch.nn.ReLU(),
          torch.nn.Linear(H, D_out))
learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                             lr=learning rate)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero_grad()
```

After computing gradients, use optimizer to update and zero gradients

A PyTorch **Module** is a neural net layer; it inputs and outputs Tensors

Modules can contain weights or other modules

Very common to define your own models or layers as custom Modules

```
import torch
class TwoLayerNet(torch.nn.Module):
    def init (self, D in, H, D out):
        super(TwoLayerNet, self). init ()
        self.linear1 = torch.nn.Linear(D in, H)
        self.linear2 = torch.nn.Linear(H, D out)
    def forward(self, x):
        h relu = self.linear1(x).clamp(min=0)
        y pred = self.linear2(h relu)
        return y pred
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

Define our whole model as a single Module

```
import torch
class TwoLayerNet(torch.nn.Module):
    def init (self, D in, H, D out):
        super(TwoLayerNet, self). init ()
        self.linear1 = torch.nn.Linear(D in, H)
        self.linear2 = torch.nn.Linear(H, D out)
    def forward(self, x):
        h relu = self.linear1(x).clamp(min=0)
        y pred = self.linear2(h relu)
        return y pred
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

Initializer sets up two children

Modules can contain modules

In this case, self.linear 1 and self.linear 2 are submodules of the TwoLayerNet module.

```
import torch
class TwoLayerNet(torch.nn.Module):
    def init (self, D in, H, D out):
        super(TwoLayerNet, self). init ()
        self.linear1 = torch.nn.Linear(D in, H)
        self.linear2 = torch.nn.Linear(H, D out)
    def forward(self, x):
        h relu = self.linear1(x).clamp(min=0)
        y pred = self.linear2(h relu)
        return y pred
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

Define forward pass using child modules and tensor operations

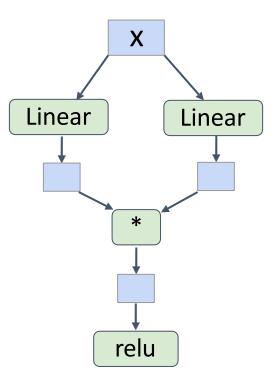
No need to define backward - autograd will handle it

```
import torch
class TwoLayerNet(torch.nn.Module):
    def init (self, D in, H, D out):
        super(TwoLayerNet, self). init ()
        self.linear1 = torch.nn.Linear(D in, H)
        self.linear2 = torch.nn.Linear(H, D out)
    def forward(self, x):
        h relu = self.linear1(x).clamp(min=0)
        y pred = self.linear2(h relu)
        return y pred
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
   y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

Very common to mix and match custom Module subclasses and Sequential containers

```
import torch
class ParallelBlock(torch.nn.Module):
    def init (self, D in, D out):
        super(ParallelBlock, self). init ()
        self.linear1 = torch.nn.Linear(D in, D out)
        self.linear2 = torch.nn.Linear(D in, D out)
    def forward(self, x):
        h1 = self.linear1(x)
        h2 = self.linear2(x)
        return (h1 * h2).clamp(min=0)
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
            ParallelBlock(D_in, H),
            ParallelBlock(H, H),
            torch.nn.Linear(H, D out))
optimizer = torch.optim.Adam(model.parameters(), lr=1e-4)
for t in range(500):
    y pred = model(x)
   loss = torch.nn.functional.mse loss(y pred, y)
   loss.backward()
   optimizer.step()
    optimizer.zero grad()
```

Define network component as a Module subclass



import torch

```
class ParallelBlock(torch.nn.Module):
    def __init__(self, D_in, D_out):
        super(ParallelBlock, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, D_out)
        self.linear2 = torch.nn.Linear(D_in, D_out)

def forward(self, x):
    h1 = self.linear1(x)
    h2 = self.linear2(x)
    return (h1 * h2).clamp(min=0)
```

Stack multiple instances of the component in a sequential

Very easy to quickly build complex network architectures!

Today's Star

```
Linear
```

```
import torch
class ParallelBlock(torch.nn.Module):
    def init (self, D in, D out):
        super(ParallelBlock, self). init ()
        self.linear1 = torch.nn.Linear(D in, D out)
        self.linear2 = torch.nn.Linear(D in, D out)
    def forward(self, x):
        h1 = self.linear1(x)
        h2 = self.linear2(x)
        return (h1 * h2).clamp(min=0)
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
model = torch.nn.Sequential(
            ParallelBlock(D_in, H),
            ParallelBlock(H, H),
            torch.nn.Linear(H, D out))
optimizer = torch.optim.Adam(model.parameters(), lr=1e-4)
for t in range(500):
    y pred = model(x)
    loss = torch.nn.functional.mse loss(y pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero grad()
```

PyTorch: DataLoaders

A **DataLoader** wraps a **Dataset** and provides minibatching, shuffling, multithreading, for you

When you need to load custom data, just write your own Dataset class

Iterate over loader to form minibatches

```
import torch
from torch.utils.data import TensorDataset, DataLoader
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
loader = DataLoader(TensorDataset(x, y), batch_size=8)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-2)
for epoch in range(20):
    for x batch, y batch in loader:
        y pred = model(x batch)
        loss = torch.nn.functional.mse_loss(y_pred, y_batch)
        loss.backward()
        optimizer.step()
        optimizer.zero grad()
```

Pytorch

- Tensors; Autograd; with new function
- nn; optim; define modules
- dataloaders

```
import torch
device = torch.device('cuda:0')
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in, device=device)
y = torch.randn(N, D out, device=device)
w1 = torch.randn(D_in, H, device=device)
w2 = torch.randn(H, D out, device=device)
learning rate = 1e-6
for t in range(500):
    h = x.mm(w1)
    h relu = h.clamp(min=0)
    y pred = h relu.mm(w2)
    loss = (y pred - y).pow(2).sum()
    grad y pred = 2.0 * (y pred - y)
    grad_w2 = h_relu.t().mm(grad_y_pred)
    grad h relu = grad y pred.mm(w2.t())
    grad h = grad h relu.clone()
    \operatorname{grad} h[h < 0] = 0
    grad w1 = x.t().mm(grad h)
    w1 -= learning rate * grad w1
    w2 -= learning rate * grad w2
```

```
import torch
from torch.utils.data import TensorDataset, DataLoader
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
loader = DataLoader(TensorDataset(x, y), batch size=8)
model = TwoLayerNet(D in, H, D out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-2)
for epoch in range(20):
    for x batch, y batch in loader:
        y pred = model(x batch)
        loss = torch.nn.functional.mse loss(y pred, y batch)
        loss.backward()
        optimizer.step()
        optimizer.zero grad()
```

PyTorch: Pretrained Models

Super easy to use pretrained models with torchvision https://github.com/pytorch/vision

```
import torch
import torchvision

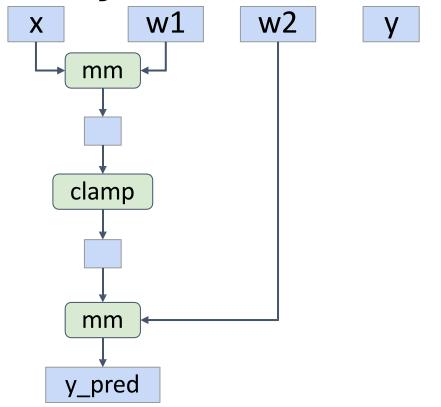
alexnet = torchvision.models.alexnet(pretrained=True)
vgg16 = torchvision.models.vgg16(pretrained=True)
resnet101 = torchvision.models.resnet101(pretrained=True)
```

```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

x w1 w2 y

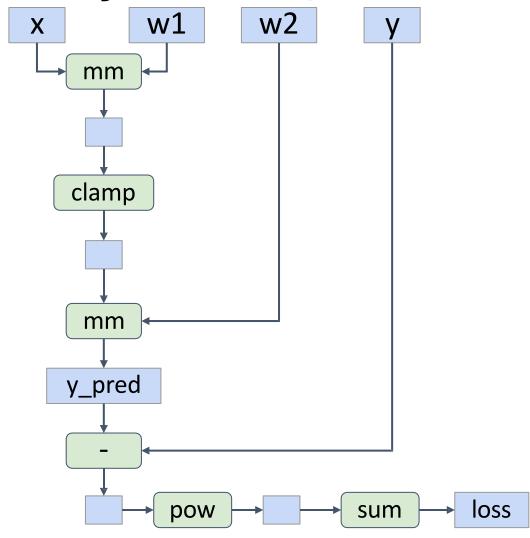
```
import torch
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Create Tensor objects



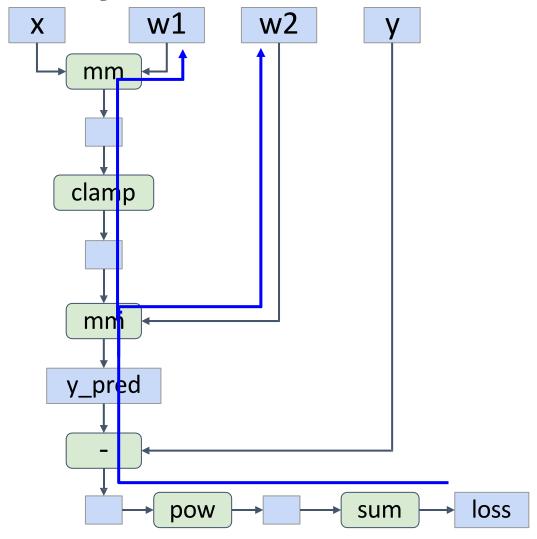
```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Build graph data structure AND perform computation



```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Build graph data structure AND perform computation



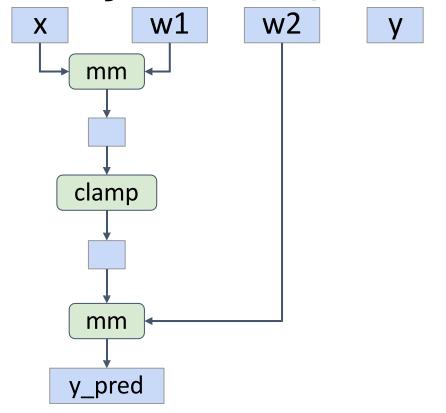
```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y_{pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Perform backprop, throw away graph

x w1 w2 y

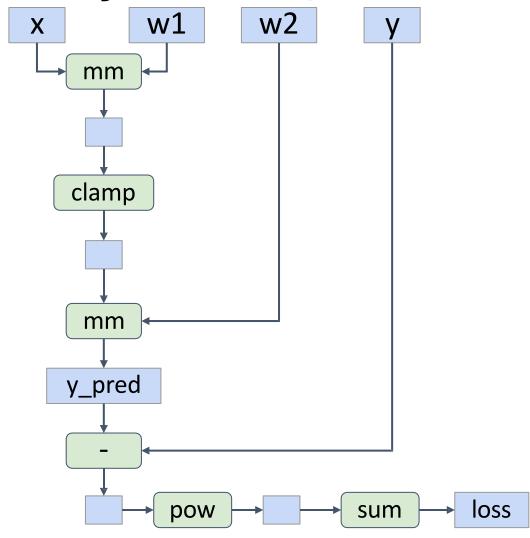
```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Perform backprop, throw away graph



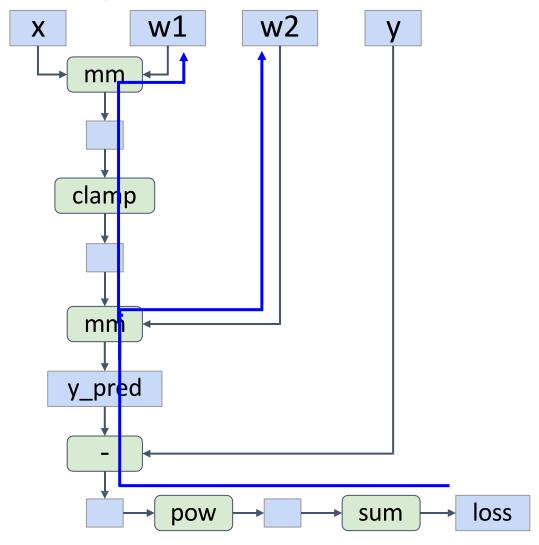
```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Build graph data structure AND perform computation



```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Build graph data structure AND perform computation



```
import torch
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)
learning_rate = 1e-6
for t in range(500):
    y \text{ pred} = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y pred - y).pow(2).sum()
    loss.backward()
```

Perform backprop, throw away graph

Initialize two different weight matrices for second layer

Decide which one to use at each layer based on loss at previous iteration

```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D out, requires grad=True)
learning rate = 1e-6
prev loss = 5.0
for t in range(500):
  w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  loss.backward()
  prev loss = loss.item()
```

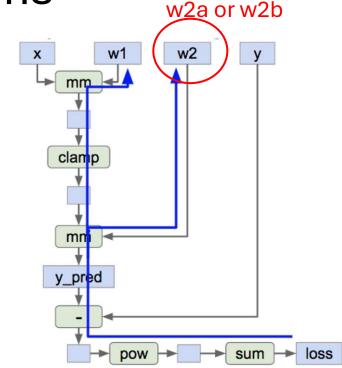
Note: this model is only a simple dynamic example, doesn't make much sense in real applications.

With Static Computation Graphs

Static graphs

Step 1: Build computational graph describing our computation (including finding paths for backprop)

Step 2: Reuse the same graph on every iteration



Solution with Dynamic Computation Graph?

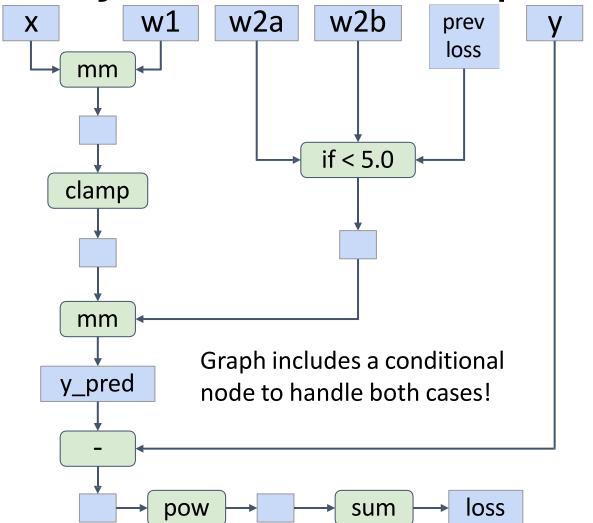
Define model as a Python function

```
import torch
def model(x, y, w1, w2a, w2b, prev loss):
  w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  return loss
N, D_{in}, H, D_{out} = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D_in, H, requires grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D out, requires grad=True)
graph = torch.jit.script(model)
prev loss = 5.0
learning rate = 1e-6
for t in range(500):
  loss = graph(x, y, w1, w2a, w2b, prev loss)
  loss.backward()
  prev loss = loss.item()
```

Just-In-Time compilation: Introspect the source code of the function, **compile** it into a graph object.

Lots of magic here!

```
import torch
def model(x, y, w1, w2a, w2b, prev loss):
  w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  return loss
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D_in, H, requires grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D out, requires grad=True)
graph = torch.jit.script(model)
prev loss = 5.0
learning rate = 1e-6
for t in range(500):
  loss = graph(x, y, w1, w2a, w2b, prev loss)
  loss.backward()
  prev loss = loss.item()
```



```
import torch
def model(x, y, w1, w2a, w2b, prev loss):
  w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  return loss
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2a = torch.randn(H, D out, requires grad=True)
w2b = torch.randn(H, D out, requires grad=True)
graph = torch.jit.script(model)
prev loss = 5.0
learning rate = 1e-6
for t in range(500):
  loss = graph(x, y, w1, w2a, w2b, prev loss)
  loss.backward()
  prev loss = loss.item()
```

Use our compiled graph object at each forward pass

```
import torch
def model(x, y, w1, w2a, w2b, prev loss):
  w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  return loss
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D_in, H, requires grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D out, requires grad=True)
graph = torch.jit.script(model)
prev loss = 5.0
learning rate = 1e-6
for t in range(500):
 loss = graph(x, y, w1, w2a, w2b, prev_loss)
  loss.backward()
  prev loss = loss.item()
```

Even easier: add **annotation** to function, Python function compiled to a graph when it is defined

Calling function uses graph

```
import torch
@torch.jit.script
def model(x, y, w1, w2a, w2b, prev loss):
  w2 = w2a if prev loss < 5.0 else w2b
 y pred = x.mm(w1).clamp(min=0).mm(w2)
 loss = (y pred - y).pow(2).sum()
  return loss
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D_out)
w1 = torch.randn(D in, H, requires grad=True)
w2a = torch.randn(H, D out, requires grad=True)
w2b = torch.randn(H, D out, requires grad=True)
prev loss = 5.0
learning rate = 1e-6
for t in range(500):
  loss = model(x, y, w1, w2a, w2b, prev loss)
  loss.backward()
  prev loss = loss.item()
```

Static vs Dynamic Graphs: Flexibility

Static computation graphs (e.g., Tensorflow 1.x) can handle if or for theoretically, but require special mechanisms instead of regular Python control flow.

Dynamic graphs (PyTorch) let you use regular Python control flow (if condition, for loops) during the forward pass.

All you need is to call JIT

```
import torch
N, D in, H, D out = 64, 1000, 100, 10
x = torch.randn(N, D in)
y = torch.randn(N, D out)
w1 = torch.randn(D in, H, requires grad=True)
w2a = torch.randn(H, D out, requires grad=True)
w2b = torch.randn(H, D out, requires grad=True)
learning rate = 1e-6
prev loss = 5.0
for t in range(500):
 w2 = w2a if prev loss < 5.0 else w2b
  y pred = x.mm(w1).clamp(min=0).mm(w2)
  loss = (y pred - y).pow(2).sum()
  loss.backward()
  prev loss = loss.item()
```

Static vs Dynamic Graphs: Optimization

With static graphs, framework can **optimize** the graph for you before it runs.

The graph you wrote

Conv ReLU Conv ReLU Conv ReLU

Equivalent graph with **fused operations**

Conv+ReLU
Conv+ReLU
Conv+ReLU

Static vs Dynamic Graphs: Serialization

Static

• Once graph is built, can **serialize** it (save it as a standalone file) and run it without the code that built the graph!

e.g. train model in Python, deploy
 in C++

Dynamic

Graph building and execution are intertwined, so always need to keep code around

Today's Star

Q: PyTorch checkpoints are instances for serialization?

A: No.

PyTorch Checkpoints

Saving Model Weights and State:

torch.save({'model_state_dict': model.state_dict(), 'epoch': epoch,}, "checkpoint.pth")

Reloading Checkpoints:

```
model = MyModel() # You need to define the model architecture here.
checkpoint = torch.load("checkpoint.pth")
model.load_state_dict(checkpoint['model_state_dict'])
```

The checkpoints requires the model's definition to recreate the computation graph first. Otherwise, PyTorch can't interpret model state_dict entries and will throw errors

Static vs Dynamic Graphs: Debugging

Static

Lots of indirection between the code you write and the code that runs – can be hard to debug, benchmark, etc

Dynamic

The code you write is the code that runs! Easy to reason about, debug, profile, etc

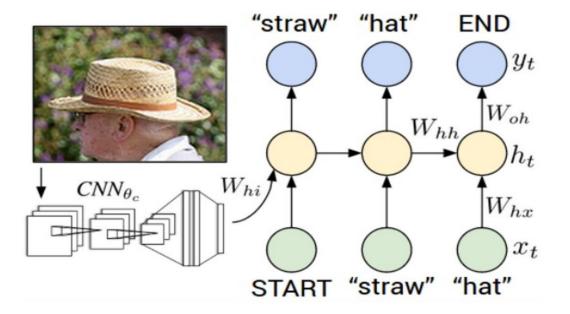
Dynamic Graph Applications?

Your idea here!

Dynamic Graph Applications

Model structure depends on the input:

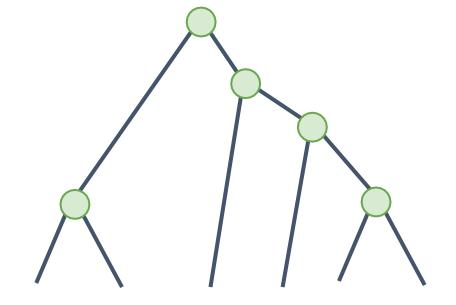
- Recurrent Networks



Dynamic Graph Applications

Model structure depends on the input:

- Recurrent Networks
- Recursive Networks



The cat ate a big rat

Dynamic Graph Applications

Model structure depends on the input:

- Recurrent Networks
- Recursive Networks
- Modular Networks

