

CS60021: Scalable Data Mining

Sourangshu Bhattacharya

CPU VS GPU

Slides taken from:

Fei-Fei Li & Justin Johnson & Serena Yeung, Stanford University

Spot the CPU!

(central processing unit)



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Spot the GPUs!

(graphics processing unit)



This image is in the public domain



CPU vs GPU

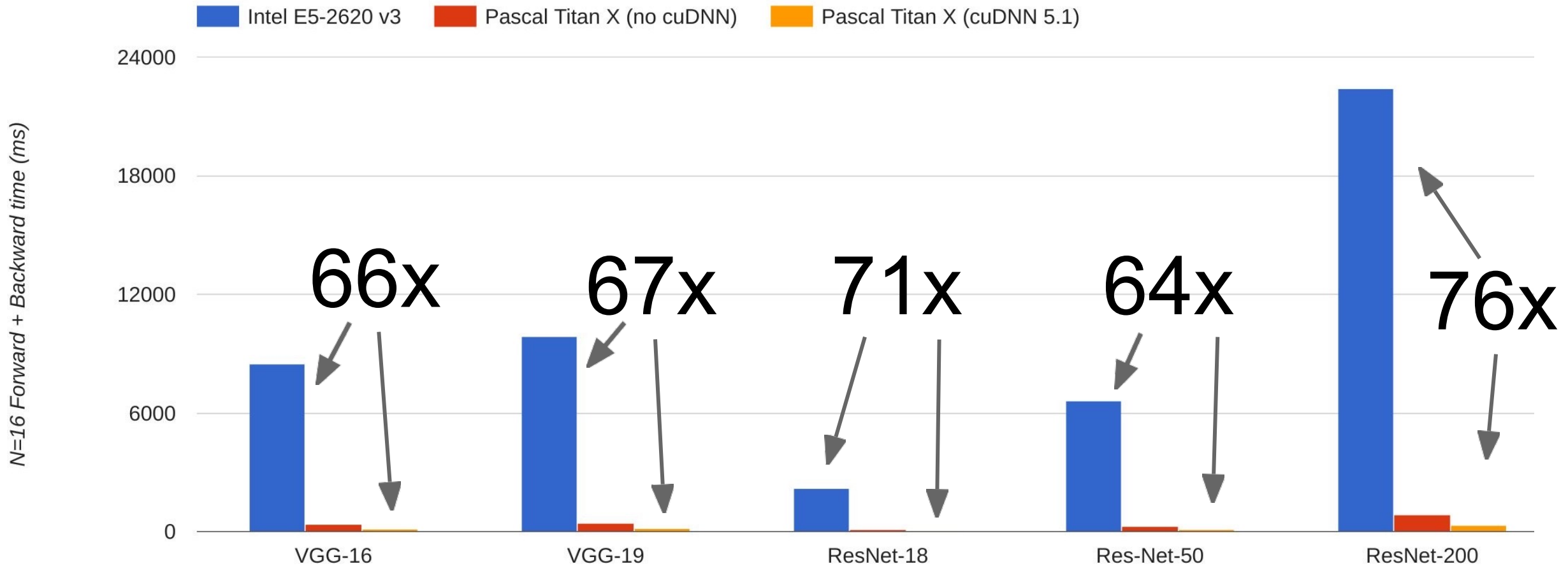
	# Cores	Clock Speed	Memory	Price
CPU (Intel Core i7-7700k)	4 (8 threads with hyperthreading)	4.4 GHz	Shared with system	\$339
CPU (Intel Core i7-6950X)	10 (20 threads with hyperthreading)	3.5 GHz	Shared with system	\$1723
GPU (NVIDIA Titan Xp)	3840	1.6 GHz	12 GB GDDR5X	\$1200
GPU (NVIDIA GTX 1070)	1920	1.68 GHz	8 GB GDDR5	\$399

CPU: Fewer cores, but each core is much faster and much more capable; great at sequential tasks

GPU: More cores, but each core is much slower and “dumber”; great for parallel tasks

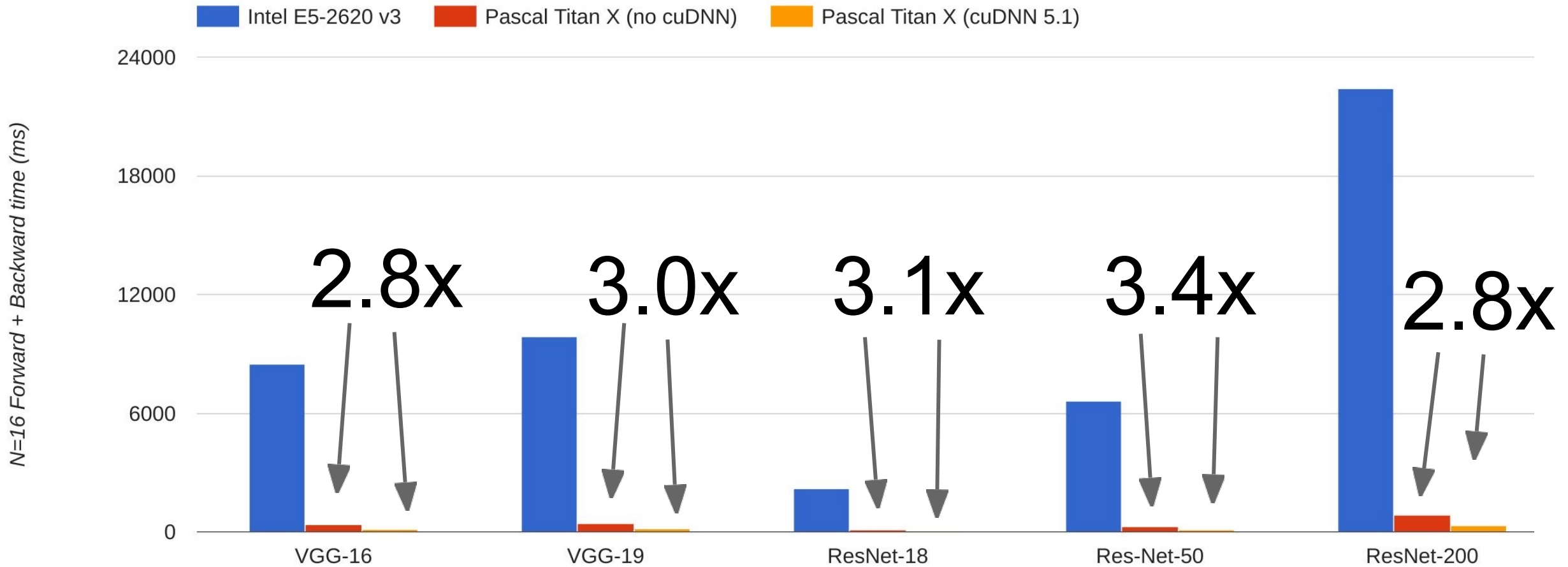
CPU vs GPU in practice

(CPU performance not well-optimized, a little unfair)



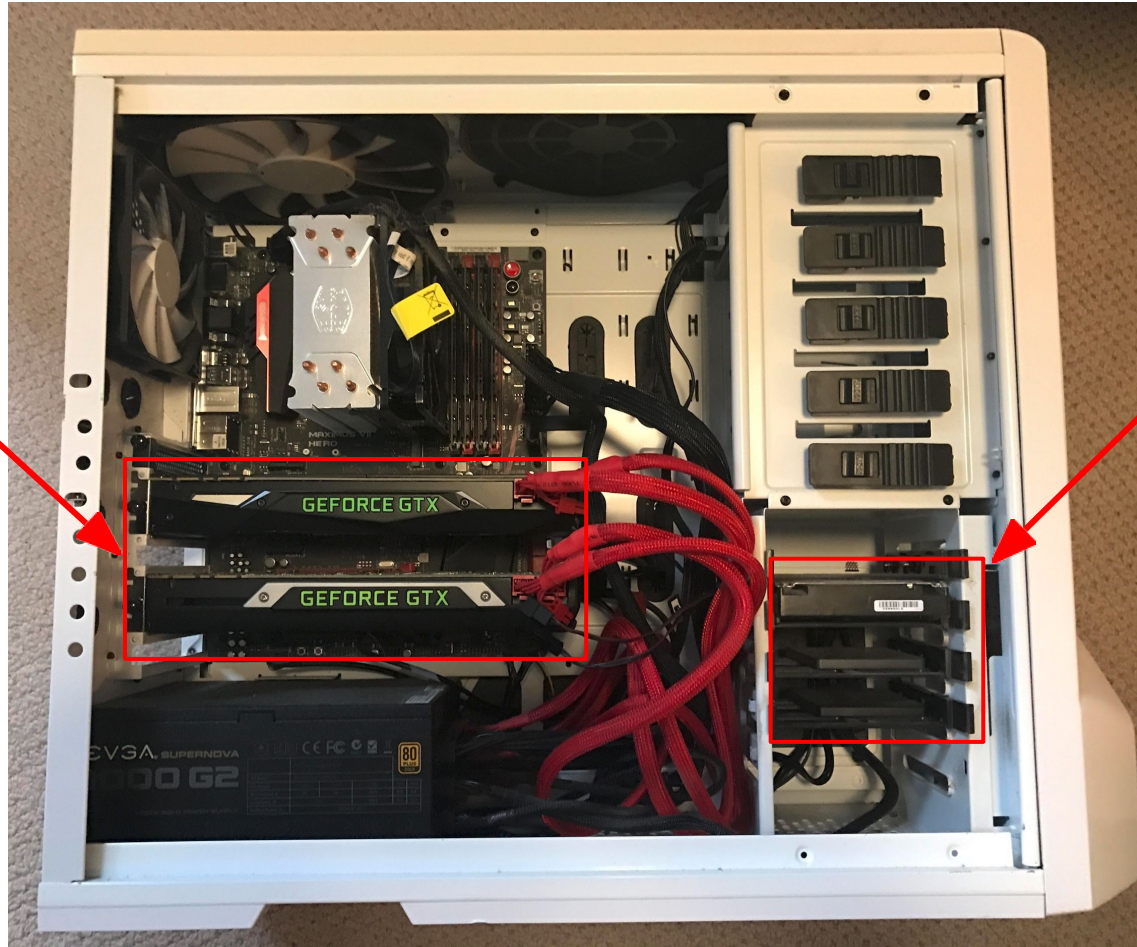
CPU vs GPU in practice

cuDNN much faster than
“unoptimized” CUDA



CPU / GPU Communication

Model
is here



Data is here

If you aren't careful, training can bottleneck on reading data and transferring to GPU!

Solutions:

- Read all data into RAM
- Use SSD instead of HDD
- Use multiple CPU threads to prefetch data

DEEP LEARNING FRAMEWORKS

Slides taken from:

Fei-Fei Li & Justin Johnson & Serena Yeung, Stanford University

Major DL Frameworks Today

Caffe
(UC Berkeley)



Caffe2
(Facebook)

Torch
(NYU / Facebook)



PyTorch
(Facebook)

Theano
(U Montreal)



TensorFlow
(Google)

Mostly these

Paddle
(Baidu)

CNTK
(Microsoft)

MXNet
(Amazon)

Developed by U Washington, CMU, MIT, Hong Kong U, etc but main framework of choice at AWS

And others...

The point of deep learning frameworks

- (1) Easily build big computational graphs
- (2) Easily compute gradients in computational graphs
- (3) Run it all efficiently on GPU (wrap cuDNN, cuBLAS, etc)

Computational Graphs

Numpy

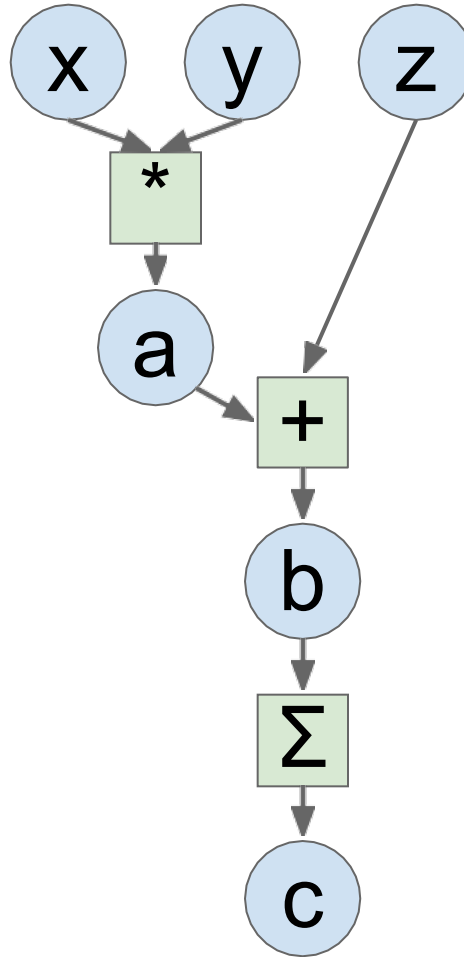
```
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)

a = x * y
b = a + z
c = np.sum(b)

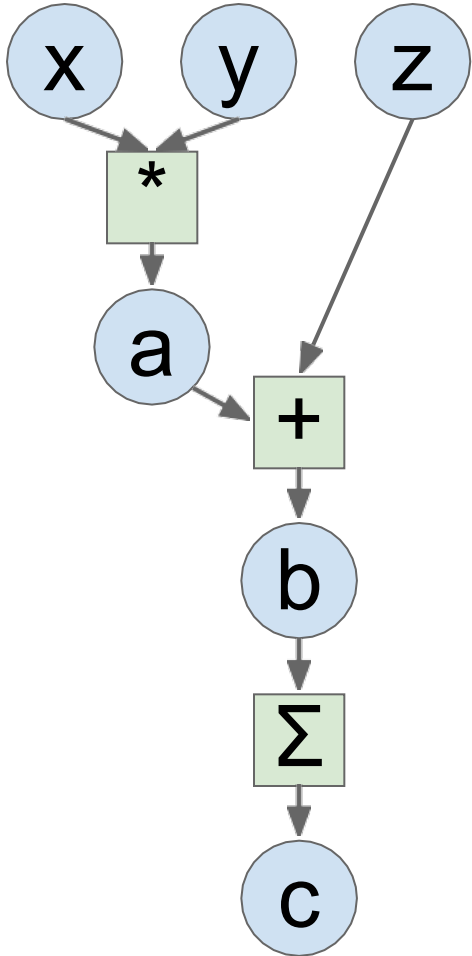
grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```



Problems:

- Can't run on GPU
- Have to compute our own gradients

Computational Graphs



PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

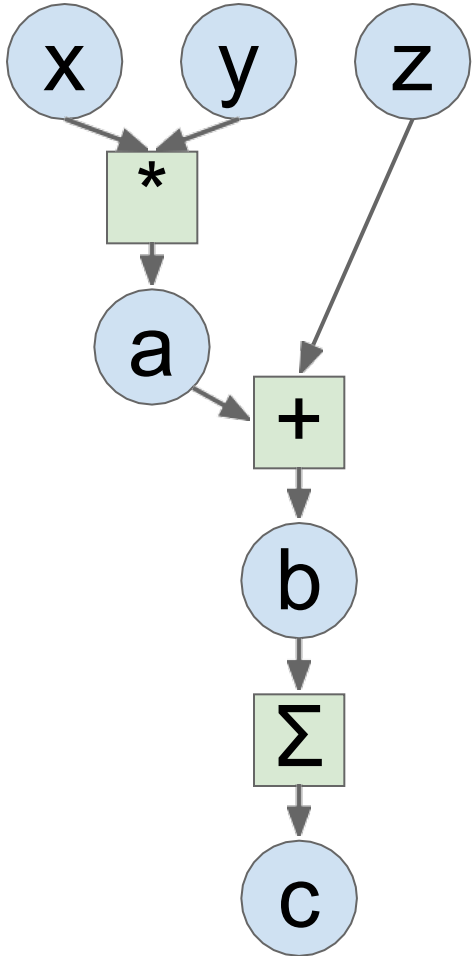
x = Variable(torch.randn(N, D),
              requires_grad=True)
y = Variable(torch.randn(N, D),
              requires_grad=True)
z = Variable(torch.randn(N, D),
              requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

Computational Graphs



Define **Variables** to start building a computational graph

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4
```

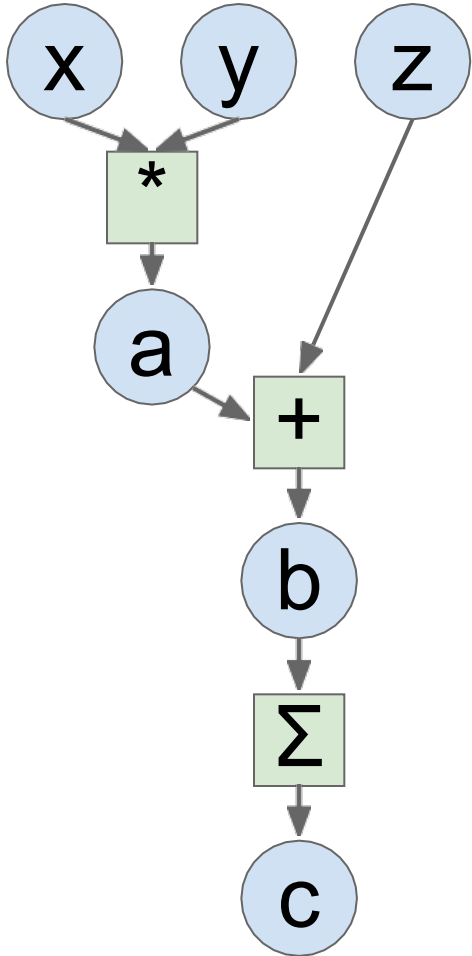
```
x = Variable(torch.randn(N, D),
              requires_grad=True)
y = Variable(torch.randn(N, D),
              requires_grad=True)
z = Variable(torch.randn(N, D),
              requires_grad=True)
```

```
a = x * y
b = a + z
c = torch.sum(b)
```

```
c.backward()
```

```
print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

Computational Graphs



Forward pass
looks just like numpy

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

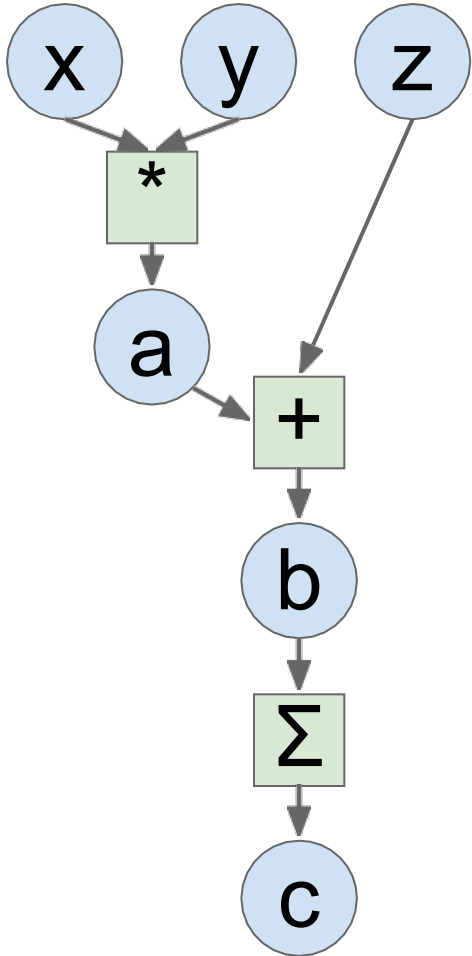
x = Variable(torch.randn(N, D),
              requires_grad=True)
y = Variable(torch.randn(N, D),
              requires_grad=True)
z = Variable(torch.randn(N, D),
              requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

Computational Graphs



Calling `c.backward()`
computes all gradients

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

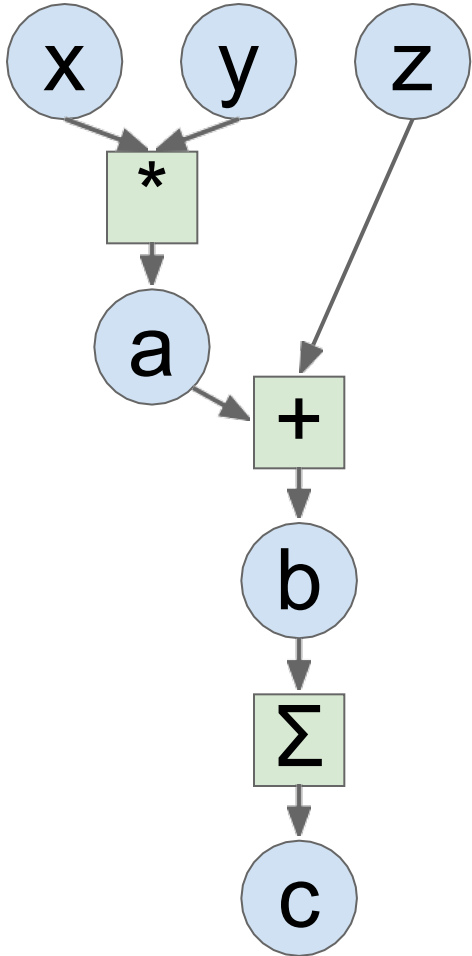
x = Variable(torch.randn(N, D),
              requires_grad=True)
y = Variable(torch.randn(N, D),
              requires_grad=True)
z = Variable(torch.randn(N, D),
              requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```


Computational Graphs



Run on GPU by casting to `.cuda()`

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

x = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)
y = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)
z = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

Numpy

```
import numpy as np
np.random.seed(0)

N, D = 3, 4

x = np.random.randn(N, D)
y = np.random.randn(N, D)
z = np.random.randn(N, D)

a = x * y
b = a + z
c = np.sum(b)

grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

x = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)
y = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)
z = Variable(torch.randn(N, D).cuda(),
              requires_grad=True)

a = x * y
b = a + z
c = torch.sum(b)

c.backward()

print(x.grad.data)
print(y.grad.data)
print(z.grad.data)
```

PyTorch (more detail)

PyTorch: Three Levels of Abstraction

	TensorFlow equivalent
<ul style="list-style-type: none">• Tensor: Imperative ndarray, but runs on GPU	Numpy array
<ul style="list-style-type: none">• Variable: Node in a computational graph; stores data and gradient	Tensor, Variable, Placeholder
<ul style="list-style-type: none">• Module: A neural network layer; may store state or learnable weights	tf.layers, or TFSlim, or TFLearn, or Sonnet, or

PyTorch: Tensors

PyTorch Tensors are just like numpy arrays, but they can run on GPU.

No built-in notion of computational graph, or gradients, or deep learning.

Here we fit a two-layer net using PyTorch Tensors:

```
import torch

dtype = torch.FloatTensor

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in).type(dtype)
y = torch.randn(N, D_out).type(dtype)
w1 = torch.randn(D_in, H).type(dtype)
w2 = torch.randn(H, D_out).type(dtype)

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
```

PyTorch: Tensors

Create random tensors
for data and weights



```
import torch
```

```
dtype = torch.FloatTensor
```

```
N, D_in, H, D_out = 64, 1000, 100, 10  
x = torch.randn(N, D_in).type(dtype)  
y = torch.randn(N, D_out).type(dtype)  
w1 = torch.randn(D_in, H).type(dtype)  
w2 = torch.randn(H, D_out).type(dtype)
```

```
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
```

PyTorch: Tensors

Forward pass: compute predictions and loss

```
import torch
```

```
dtype = torch.FloatTensor
```

```
N, D_in, H, D_out = 64, 1000, 100, 10  
x = torch.randn(N, D_in).type(dtype)  
y = torch.randn(N, D_out).type(dtype)  
w1 = torch.randn(D_in, H).type(dtype)  
w2 = torch.randn(H, D_out).type(dtype)
```

```
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
```

PyTorch: Tensors

Backward pass:
manually compute
gradients



```
import torch

dtype = torch.FloatTensor

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in).type(dtype)
y = torch.randn(N, D_out).type(dtype)
w1 = torch.randn(D_in, H).type(dtype)
w2 = torch.randn(H, D_out).type(dtype)

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
```


PyTorch: Tensors

Gradient descent
step on weights

```
import torch

dtype = torch.FloatTensor

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in).type(dtype)
y = torch.randn(N, D_out).type(dtype)
w1 = torch.randn(D_in, H).type(dtype)
w2 = torch.randn(H, D_out).type(dtype)

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
```

PyTorch: Tensors

To run on GPU, just cast tensors to a cuda datatype!

```
import torch
```

```
dtype = torch.cuda.FloatTensor
```

```
N, D_in, H, D_out = 64, 1000, 100, 10
```

```
x = torch.randn(N, D_in).type(dtype)
```

```
y = torch.randn(N, D_out).type(dtype)
```

```
w1 = torch.randn(D_in, H).type(dtype)
```

```
w2 = torch.randn(H, D_out).type(dtype)
```

```
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
```

PyTorch: Autograd

A PyTorch **Variable** is a node in a computational graph

x.data is a Tensor

x.grad is a Variable of gradients
(same shape as x.data)

x.grad.data is a Tensor of gradients

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

PyTorch: Autograd

PyTorch Tensors and Variables
have the same API!

Variables remember how they were
created (for backprop)

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

PyTorch: Autograd

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

Do want gradients with
respect to weights

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

PyTorch: Autograd

Forward pass looks exactly the same as the Tensor version, but everything is a variable now

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

PyTorch: Autograd

Compute gradient of loss with respect to w1 and w2 (zero out grads first)

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

PyTorch: Autograd

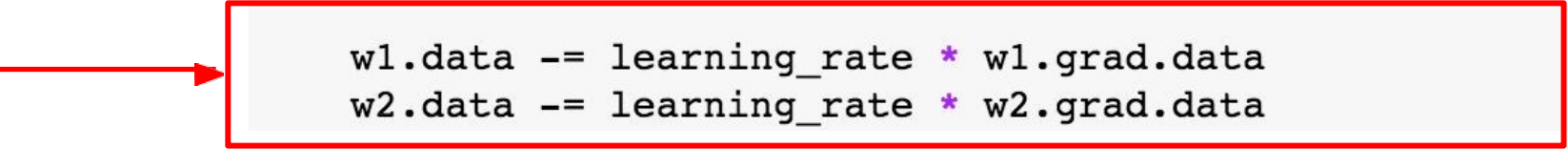
```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()
```

Make gradient
step on weights



```
w1.data -= learning_rate * w1.grad.data
w2.data -= learning_rate * w2.grad.data
```


PyTorch: New Autograd Functions

Define your own autograd functions by writing forward and backward for Tensors

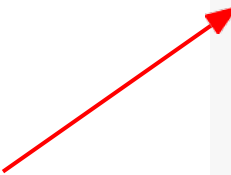
(similar to modular layers in A2)

```
class ReLU(torch.autograd.Function):  
    def forward(self, x):  
        self.save_for_backward(x)  
        return x.clamp(min=0)  
  
    def backward(self, grad_y):  
        x, = self.saved_tensors  
        grad_input = grad_y.clone()  
        grad_input[x < 0] = 0  
        return grad_input
```

PyTorch: New Autograd Functions

```
class ReLU(torch.autograd.Function):  
    def forward(self, x):  
        self.save_for_backward(x)  
        return x.clamp(min=0)  
  
    def backward(self, grad_y):  
        x, = self.saved_tensors  
        grad_input = grad_y.clone()  
        grad_input[x < 0] = 0  
        return grad_input
```

Can use our new autograd function in the forward pass



```
N, D_in, H, D_out = 64, 1000, 100, 10  
  
x = Variable(torch.randn(N, D_in), requires_grad=False)  
y = Variable(torch.randn(N, D_out), requires_grad=False)  
w1 = Variable(torch.randn(D_in, H), requires_grad=True)  
w2 = Variable(torch.randn(H, D_out), requires_grad=True)  
  
learning_rate = 1e-6  
for t in range(500):  
    relu = ReLU()  
    y_pred = relu(x.mm(w1)).mm(w2)  
    loss = (y_pred - y).pow(2).sum()  
  
    if w1.grad: w1.grad.data.zero_()  
    if w2.grad: w2.grad.data.zero_()  
    loss.backward()  
  
    w1.data -= learning_rate * w1.grad.data  
    w2.data -= learning_rate * w2.grad.data
```

PYTORCH NN MODULE

PyTorch: nn

Higher-level wrapper for
working with neural nets

Similar to Keras and friends ...
but only one, and it's good =)

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()

    for param in model.parameters():
        param.data -= learning_rate * param.grad.data
```

PyTorch: nn

Define our model as a sequence of layers

nn also defines common loss functions

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)
```

```
model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)
```

```
learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()

    for param in model.parameters():
        param.data -= learning_rate * param.grad.data
```

PyTorch: nn

Forward pass: feed data to model, and prediction to loss function

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()

    for param in model.parameters():
        param.data -= learning_rate * param.grad.data
```

PyTorch: nn

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()

    for param in model.parameters():
        param.data -= learning_rate * param.grad.data
```

Backward pass:
compute all gradients



PyTorch: nn

```
import torch
from torch.autograd import Variable

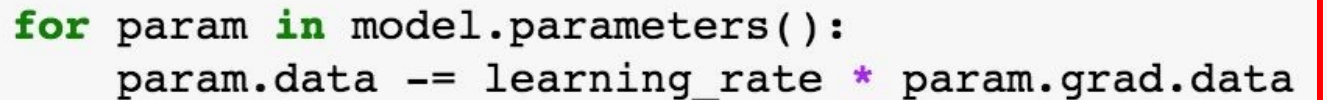
N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    model.zero_grad()
    loss.backward()
```

Make gradient step on
each model parameter



```
for param in model.parameters():
    param.data -= learning_rate * param.grad.data
```


PyTorch: optim

Use an **optimizer** for different update rules

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10

x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                              lr=learning_rate)

for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    optimizer.zero_grad()
    loss.backward()

    optimizer.step()
```

PyTorch: optim

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10

x = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = torch.nn.Sequential(
    torch.nn.Linear(D_in, H),
    torch.nn.ReLU(),
    torch.nn.Linear(H, D_out))
loss_fn = torch.nn.MSELoss(size_average=False)

learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                              lr=learning_rate)

for t in range(500):
    y_pred = model(x)
    loss = loss_fn(y_pred, y)

    optimizer.zero_grad()
    loss.backward()

    optimizer.step()
```

Update all parameters
after computing gradients



PyTorch: nn

Define new Modules

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

Modules can contain weights (as Variables) or other Modules

You can define your own Modules using autograd!

```
import torch
from torch.autograd import Variable

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 = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = TwoLayerNet(D_in, H, D_out)

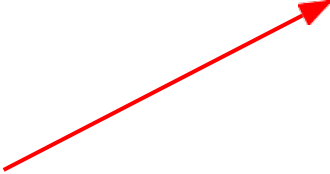
criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

PyTorch: nn

Define new Modules

Define our whole model
as a single Module



```
import torch
from torch.autograd import Variable

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 = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = TwoLayerNet(D_in, H, D_out)

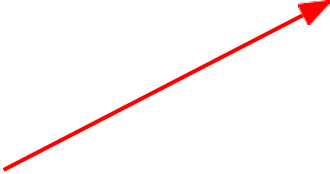
criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

PyTorch: nn

Define new Modules

Initializer sets up two children (Modules can contain modules)



```
import torch
from torch.autograd import Variable

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 = Variable(torch.randn(1, D_in))
y = Variable(torch.randn(1, D_out), requires_grad=False)

model = TwoLayerNet(D_in, H, D_out)

criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

PyTorch: nn

Define new Modules

Define forward pass using
child modules and
autograd ops on Variables

No need to define
backward - autograd will
handle it

```
import torch
from torch.autograd import Variable

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 = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = TwoLayerNet(D_in, H, D_out)


criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

PyTorch: nn

Define new Modules

Construct and train an instance of our model



```
import torch
from torch.autograd import Variable

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 = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)

model = TwoLayerNet(D_in, H, D_out)

criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

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

```
import torch
from torch.autograd import Variable
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)

criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for epoch in range(10):
    for x_batch, y_batch in loader:
        x_var, y_var = Variable(x), Variable(y)
        y_pred = model(x_var)
        loss = criterion(y_pred, y_var)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```


PyTorch: DataLoaders

Iterate over loader to form minibatches

Loader gives Tensors so you need to wrap in Variables

```
import torch
from torch.autograd import Variable
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)

criterion = torch.nn.MSELoss(size_average=False)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
for epoch in range(10):
    for x_batch, y_batch in loader:
        x_var, y_var = Variable(x), Variable(y)
        y_pred = model(x_var)
        loss = criterion(y_pred, y_var)

        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```

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)
```

Static vs Dynamic Graphs

Static vs Dynamic Graphs

TensorFlow: Build graph once, then run many times (**static**)

```
N, D, H = 64, 1000, 100
x = tf.placeholder(tf.float32, shape=(N, D))
y = tf.placeholder(tf.float32, shape=(N, D))
w1 = tf.Variable(tf.random_normal((D, H)))
w2 = tf.Variable(tf.random_normal((H, D)))

h = tf.maximum(tf.matmul(x, w1), 0)
y_pred = tf.matmul(h, w2)
diff = y_pred - y
loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])

learning_rate = 1e-5
new_w1 = w1.assign(w1 - learning_rate * grad_w1)
new_w2 = w2.assign(w2 - learning_rate * grad_w2)
updates = tf.group(new_w1, new_w2)

with tf.Session() as sess:
    sess.run(tf.global_variables_initializer())
    values = {x: np.random.randn(N, D),
              y: np.random.randn(N, D),}
    losses = []
    for t in range(50):
        loss_val, _ = sess.run([loss, updates],
                               feed_dict=values)
```

Build graph

Run each iteration

PyTorch: Each forward pass defines a new graph (**dynamic**)

```
import torch
from torch.autograd import Variable

N, D_in, H, D_out = 64, 1000, 100, 10
x = Variable(torch.randn(N, D_in), requires_grad=False)
y = Variable(torch.randn(N, D_out), requires_grad=False)
w1 = Variable(torch.randn(D_in, H), requires_grad=True)
w2 = Variable(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()

    if w1.grad: w1.grad.data.zero_()
    if w2.grad: w2.grad.data.zero_()
    loss.backward()

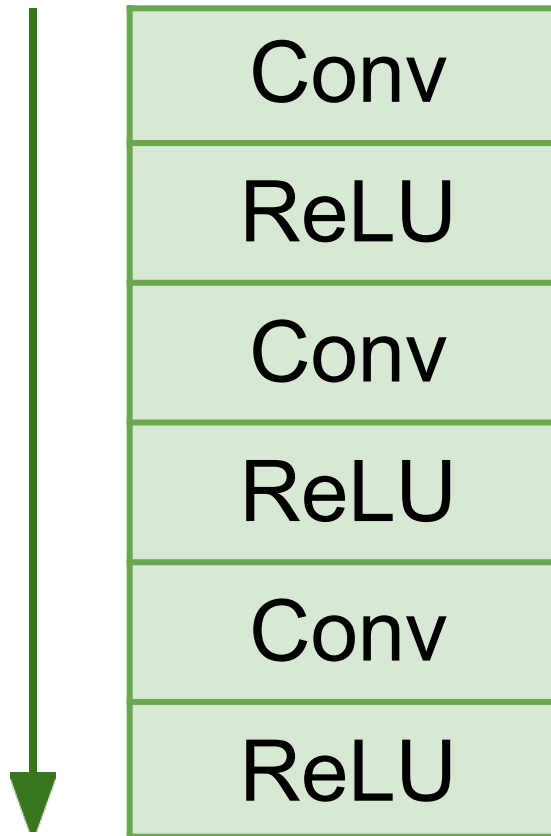
    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

New graph each iteration

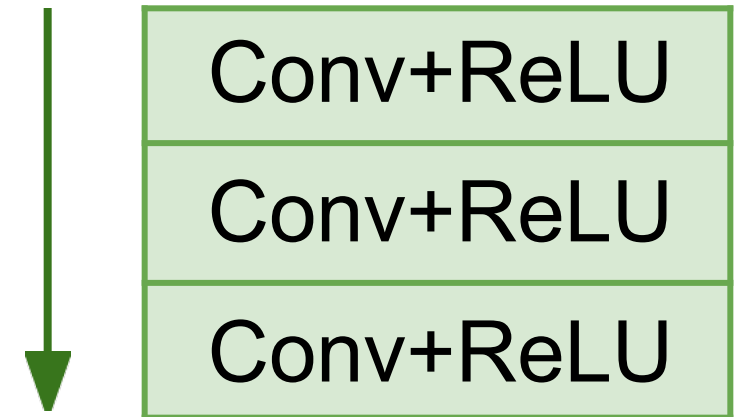
Static vs Dynamic: Optimization

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

The graph you wrote



Equivalent graph with **fused operations**



Static vs Dynamic: Serialization

Static

Once graph is built,
can **serialize** it and
run it without the code
that built the graph!

Dynamic

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

Static vs Dynamic: Conditional

$$y = \begin{cases} w1 * x & \text{if } z > 0 \\ w2 * x & \text{otherwise} \end{cases}$$

Static vs Dynamic: Conditional

$$y = \begin{cases} w1 * x & \text{if } z > 0 \\ w2 * x & \text{otherwise} \end{cases}$$

PyTorch: Normal Python

```
N, D, H = 3, 4, 5

x = Variable(torch.randn(N, D))
w1 = Variable(torch.randn(D, H))
w2 = Variable(torch.randn(D, H))

z = 10
if z > 0:
    y = x.mm(w1)
else:
    y = x.mm(w2)
```


Static vs Dynamic: Conditional

$$y = \begin{cases} w1 * x & \text{if } z > 0 \\ w2 * x & \text{otherwise} \end{cases}$$

PyTorch: Normal Python

```
N, D, H = 3, 4, 5

x = Variable(torch.randn(N, D))
w1 = Variable(torch.randn(D, H))
w2 = Variable(torch.randn(D, H))

z = 10
if z > 0:
    y = x.mm(w1)
else:
    y = x.mm(w2)
```

TensorFlow: Special TF control flow operator!

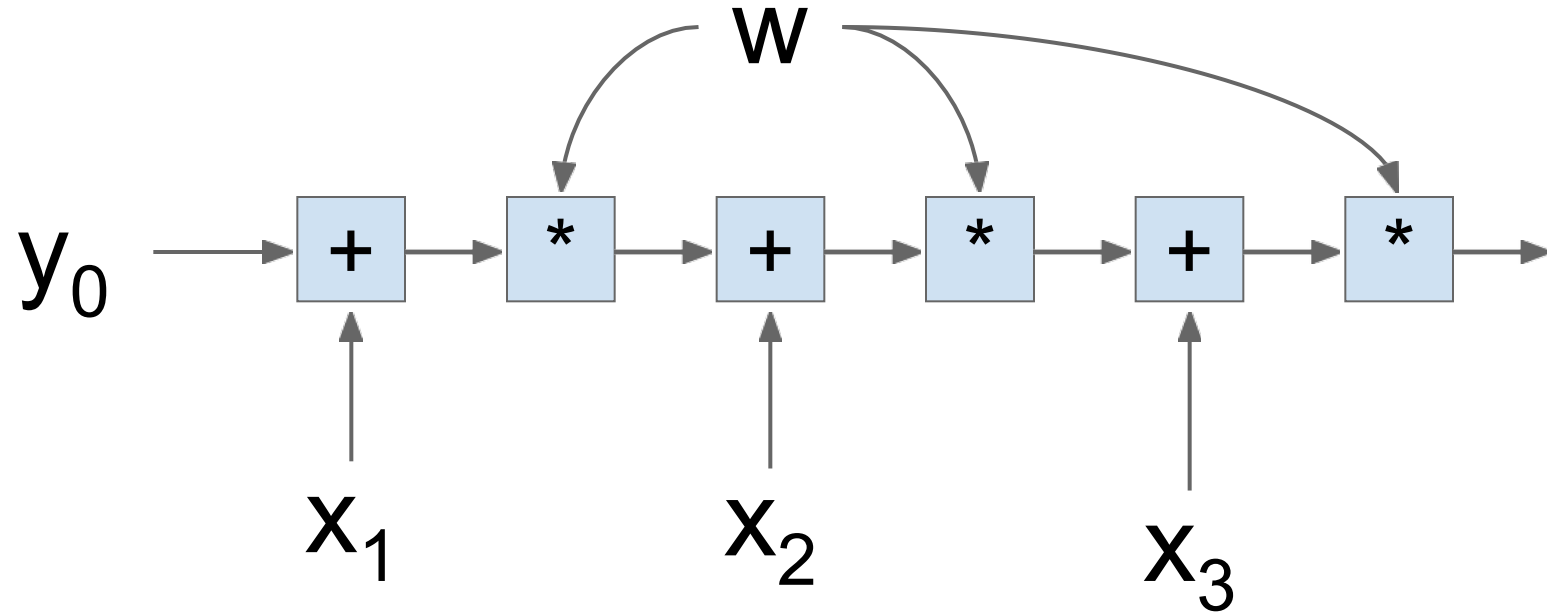
```
N, D, H = 3, 4, 5
x = tf.placeholder(tf.float32, shape=(N, D))
z = tf.placeholder(tf.float32, shape=None)
w1 = tf.placeholder(tf.float32, shape=(D, H))
w2 = tf.placeholder(tf.float32, shape=(D, H))

def f1(): return tf.matmul(x, w1)
def f2(): return tf.matmul(x, w2)
y = tf.cond(tf.less(z, 0), f1, f2)

with tf.Session() as sess:
    values = {
        x: np.random.randn(N, D),
        z: 10,
        w1: np.random.randn(D, H),
        w2: np.random.randn(D, H),
    }
    y_val = sess.run(y, feed_dict=values)
```

Static vs Dynamic: Loops

$$y_t = (y_{t-1} + x_t) * w$$



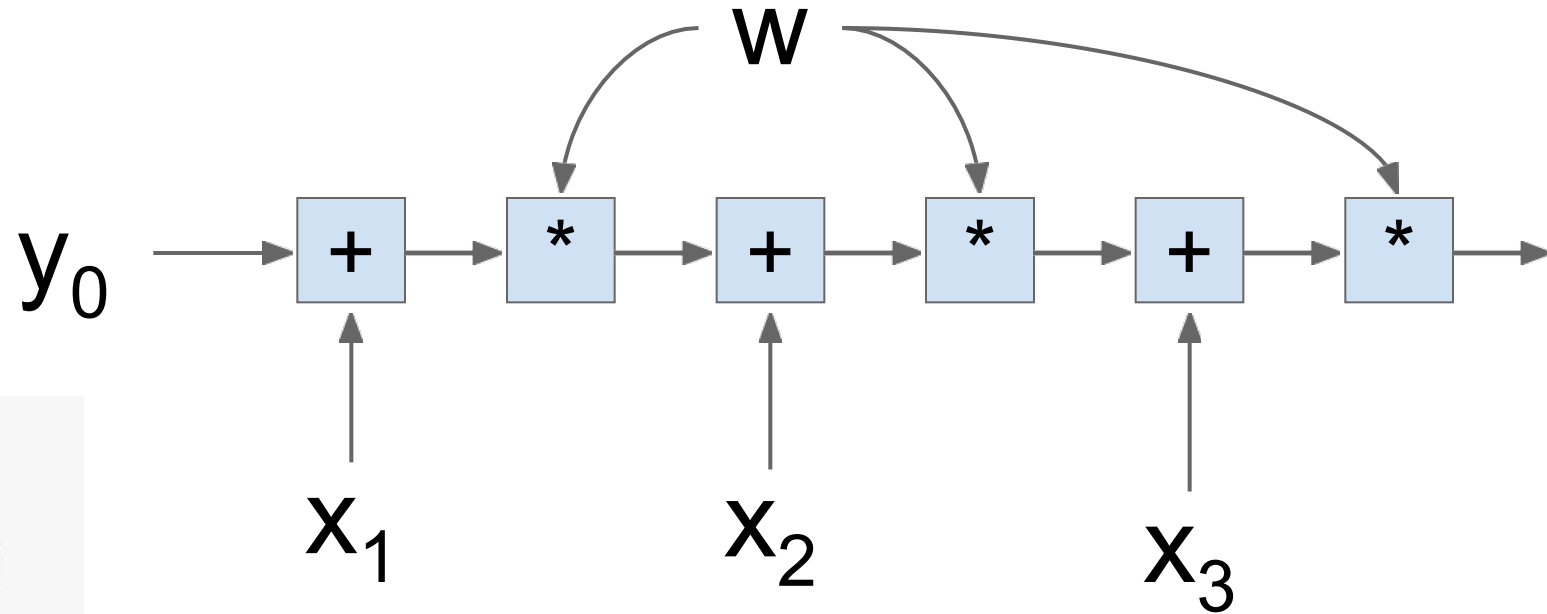
Static vs Dynamic: Loops

$$y_t = (y_{t-1} + x_t) * w$$

PyTorch: Normal Python

```
T, D = 3, 4
y0 = Variable(torch.randn(D))
x = Variable(torch.randn(T, D))
w = Variable(torch.randn(D))

y = [y0]
for t in range(T):
    prev_y = y[-1]
    next_y = (prev_y + x[t]) * w
    y.append(next_y)
```



Static vs Dynamic: Loops

$$y_t = (y_{t-1} + x_t) * w$$

PyTorch: Normal Python

```
T, D = 3, 4
y0 = Variable(torch.randn(D))
x = Variable(torch.randn(T, D))
w = Variable(torch.randn(D))

y = [y0]
for t in range(T):
    prev_y = y[-1]
    next_y = (prev_y + x[t]) * w
    y.append(next_y)
```

TensorFlow: Special TF control flow

```
T, N, D = 3, 4, 5
x = tf.placeholder(tf.float32, shape=(T, D))
y0 = tf.placeholder(tf.float32, shape=(D,))
w = tf.placeholder(tf.float32, shape=(D,))

def f(prev_y, cur_x):
    return (prev_y + cur_x) * w

y = tf.foldl(f, x, y0)

with tf.Session() as sess:
    values = {
        x: np.random.randn(T, D),
        y0: np.random.randn(D),
        w: np.random.randn(D),
    }
    y_val = sess.run(y, feed_dict=values)
```

Dynamic Graphs in TensorFlow

TensorFlow Fold make dynamic graphs easier in TensorFlow through **dynamic batching**

Tensorboard

Visualizing pytorch graphs

```
for t in range(500):
    y_pred = model(x)
    loss = criterion(y_pred, y)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

x_input = Variable(torch.randn((1, D_in)))

writer = SummaryWriter('runs/exp1')

writer.add_graph(model, x_input)
writer.close()
```

```
import torch
from torch.autograd import Variable
from torch.utils.tensorboard import SummaryWriter

class TwoLayerNet(torch.nn.Module):
    def __init__(self, D_in, 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 = Variable(torch.randn(N, D_in))
y = Variable(torch.randn(N, D_out), requires_grad=False)
model = TwoLayerNet(D_in, D_out)
optimizer = torch.optim.SGD(model.parameters(), lr=1e-4)
criterion = torch.nn.MSELoss(reduction='mean')
```

Visualizing pytorch graphs

TensorBoard

GRAPHS UPLOAD Settings Refresh Settings Help

TwoLayerNet
Subgraph: 7 nodes

Search nodes (regex)

Fit to screen
Download PNG
Upload file

Run (1) exp1
Tag (2) Default

Graph type
 Op graph
 Conceptual graph
 Profile

Legend

- colors
- same substructure
- unique substructure (* = expandable)
- Namespace* ?
- OpNode ?
- Unconnected series* ?
- Connected series* ?
- Constant ?
- Summary ?
- Dataflow edge ?
- Control dependency edge ?

```
graph BT; input[input] -- "1x1000" --> linear1[Linear[linear1]]; linear1 -- "1x1000" --> input2[input]; input2 -- "1x10" --> linear2[Linear[linear2]]; linear2 -- "1x10" --> output[output];
```


ONNX EXPORT

ONNX

- Open neural network exchange
- Provides an open format for saving DL models in files
- Models can be saved from various tools
 - Pytorch, Tensorflow, Scikit-learn
- Models saved in ONNX format can be executed in various platforms:
 - Caffe2 – Python
 - <https://onnxruntime.ai/>

Exporting Pytorch module to ONNX

```
import torch
import torchvision

dummy_input = torch.randn(10, 3, 224, 224, device='cuda')
model = torchvision.models.alexnet(pretrained=True).cuda()

# Providing input and output names sets the display names for values
# within the model's graph. Setting these does not change the semantics
# of the graph; it is only for readability.
#
# The inputs to the network consist of the flat list of inputs (i.e.
# the values you would pass to the forward() method) followed by the
# flat list of parameters. You can partially specify names, i.e. provide
# a list here shorter than the number of inputs to the model, and we will
# only set that subset of names, starting from the beginning.
input_names = [ "actual_input_1" ] + [ "learned_%d" % i for i in range(16) ]
output_names = [ "output1" ]

torch.onnx.export(model, dummy_input, "alexnet.onnx", verbose=True,
input_names=input_names, output_names=output_names)
```

ONNX File format

```
# These are the inputs and parameters to the network, which have taken on  
# the names we specified earlier.  
graph(%actual_input_1 : Float(10, 3, 224, 224)  
      %learned_0 : Float(64, 3, 11, 11)  
      %learned_1 : Float(64)  
      %learned_2 : Float(192, 64, 5, 5)  
      %learned_3 : Float(192)  
      # ---- omitted for brevity ----  
      %learned_14 : Float(1000, 4096)  
      %learned_15 : Float(1000)) {  
  # Every statement consists of some output tensors (and their types),  
  # the operator to be run (with its attributes, e.g., kernels, strides,  
  # etc.), its input tensors (%actual_input_1, %learned_0, %learned_1)  
  %17 : Float(10, 64, 55, 55) = onnx::Conv[dilations=[1, 1], group=1, kernel_shape=  
[11, 11], pads=[2, 2, 2, 2], strides=[4, 4]](%actual_input_1, %learned_0,  
%learned_1), scope: AlexNet/Sequential[features]/Conv2d[0]  
  %18 : Float(10, 64, 55, 55) = onnx::Relu(%17), scope:  
AlexNet/Sequential[features]/ReLU[1]
```

ONNX File format

```
%19 : Float(10, 64, 27, 27) = onnx::MaxPool[kernel_shape=[3, 3], pads=[0, 0, 0, 0], strides=[2, 2]](%18), scope: AlexNet/Sequential[features]/MaxPool2d[2]
# ---- omitted for brevity ----
%29 : Float(10, 256, 6, 6) = onnx::MaxPool[kernel_shape=[3, 3], pads=[0, 0, 0, 0], strides=[2, 2]](%28), scope: AlexNet/Sequential[features]/MaxPool2d[12]
# Dynamic means that the shape is not known. This may be because of a
# limitation of our implementation (which we would like to fix in a
# future release) or shapes which are truly dynamic.
%30 : Dynamic = onnx::Shape(%29), scope: AlexNet
%31 : Dynamic = onnx::Slice[axes=[0], ends=[1], starts=[0]](%30), scope: AlexNet
%32 : Long() = onnx::Squeeze[axes=[0]](%31), scope: AlexNet
%33 : Long() = onnx::Constant[value={9216}](), scope: AlexNet
# ---- omitted for brevity ----
%output1 : Float(10, 1000) = onnx::Gemm[alpha=1, beta=1, broadcast=1, transB=1]
(%45, %learned_14, %learned_15), scope: AlexNet/Sequential[classifier]/Linear[6]
return (%output1);
}
```

Running ONNX models

```
# ...continuing from above
import caffe2.python.onnx.backend as backend
import numpy as np

rep = backend.prepare(model, device="CUDA:0") # or "CPU"
# For the Caffe2 backend:
# rep.predict_net is the Caffe2 protobuf for the network
# rep.workspace is the Caffe2 workspace for the network
# (see the class caffe2.python.onnx.backend.Workspace)
outputs = rep.run(np.random.randn(10, 3, 224, 224).astype(np.float32))
# To run networks with more than one input, pass a tuple
# rather than a single numpy ndarray.
print(outputs[0])
```

References

- Deep Learning with Pytorch. Eli Stevens, Luca Antiga, Thomas Viehman, Manning publishers.
- Exporting a model from pytorch to ONNX and running using ONNX runtime:
https://pytorch.org/tutorials/advanced/super_resolution_with_onnxruntime.html
- Tensorboard tutorial:
https://pytorch.org/tutorials/intermediate/tensorboard_tutorial.html