CS60021: Scalable Data Mining

Sourangshu Bhattacharya

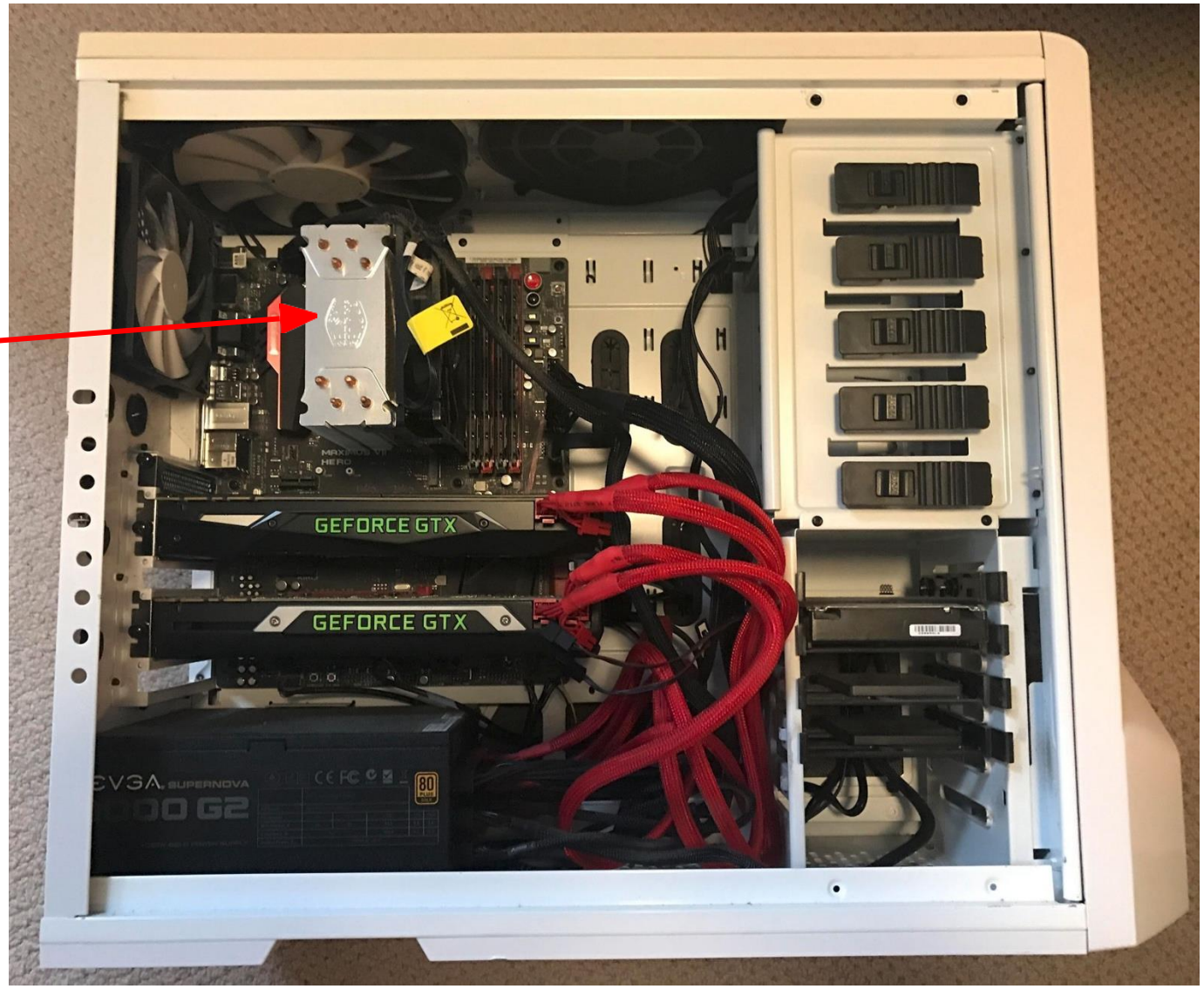
CPU VS GPU

Slides taken from:

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

Spot the CPU!

(central processing unit)



Spot the GPUs!

(graphics processing unit)

This image is in the public domain

CPU vs GPU

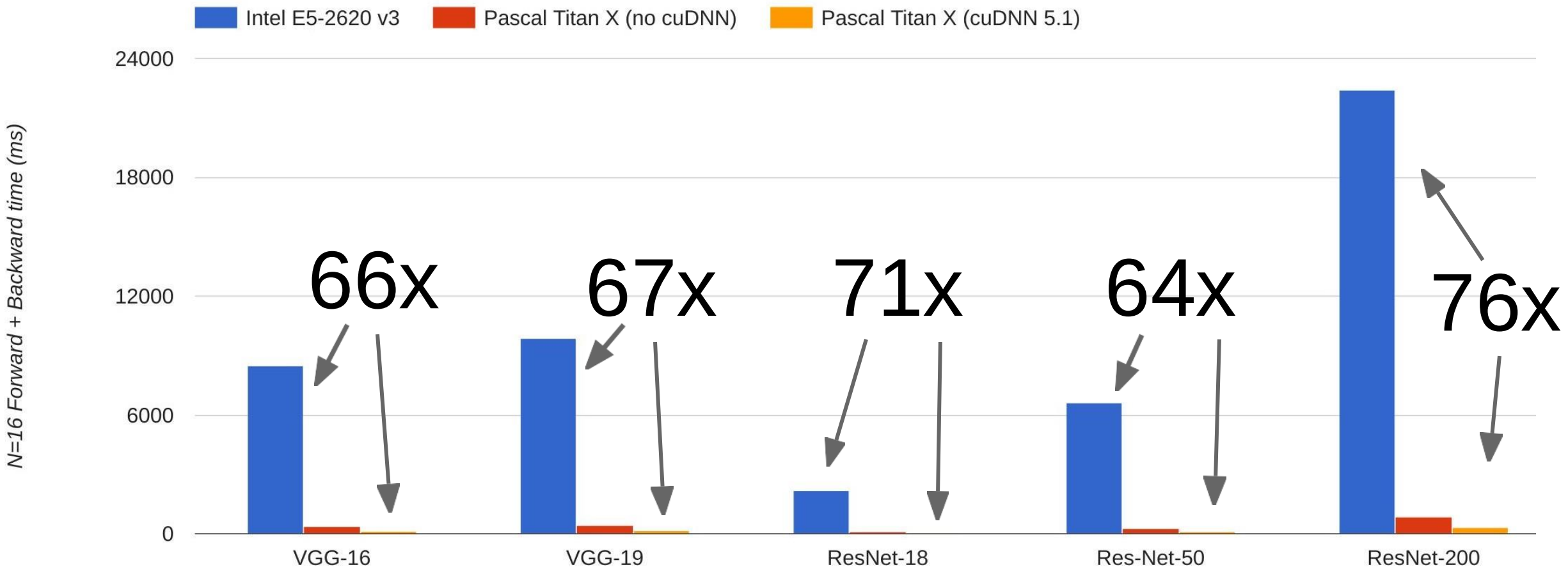
	# Cores	Clock Speed	Memory	Price
CPU (Intel Core i7-7700k)	4 (8 threads with hyperthreading)	4.4 GHz	Shared with system	$339
CPU (Intel Core i7-6950X)	10 (20 threads with hyperthreading)	3.5 GHz	Shared with system	$1723
GPU (NVIDIA Titan Xp)	3840	1.6 GHz	12 GB GDDR5X	$1200
GPU (NVIDIA GTX 1070)	1920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

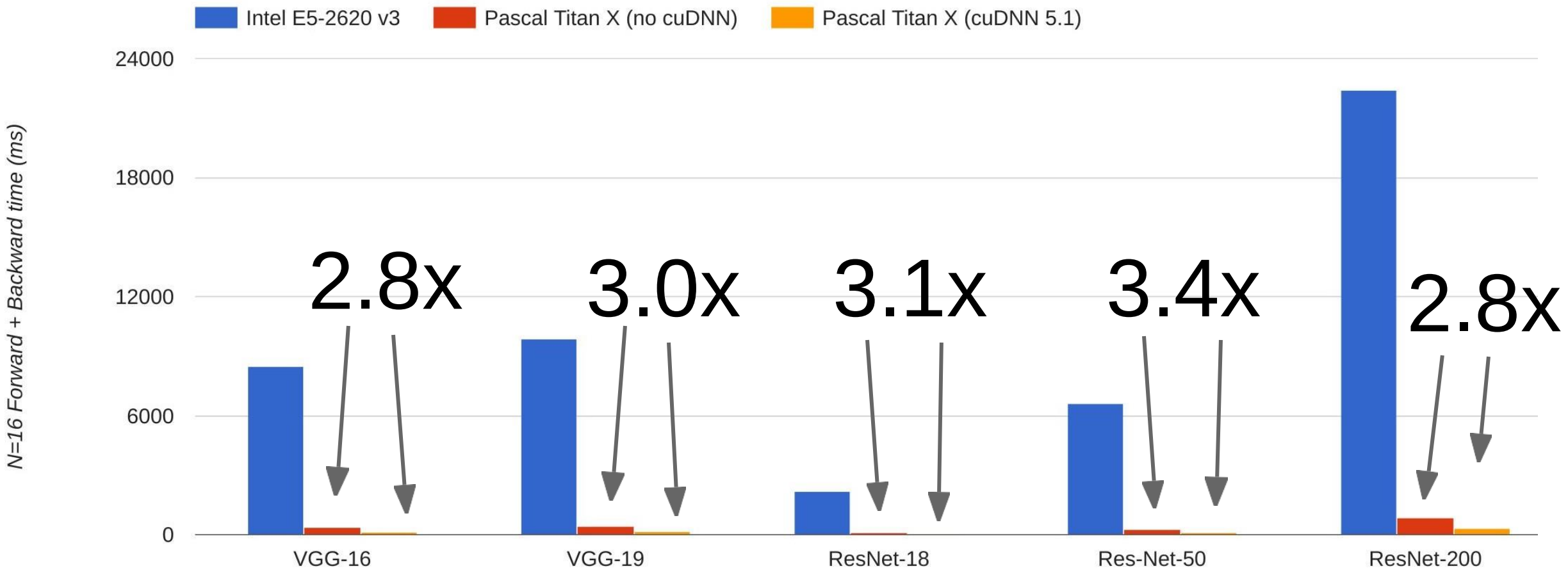
(CPU performance not well-optimized, a little unfair)



Data from https://github.com/jcjohnson/cnn-benchmarks

CPU vs GPU in practice

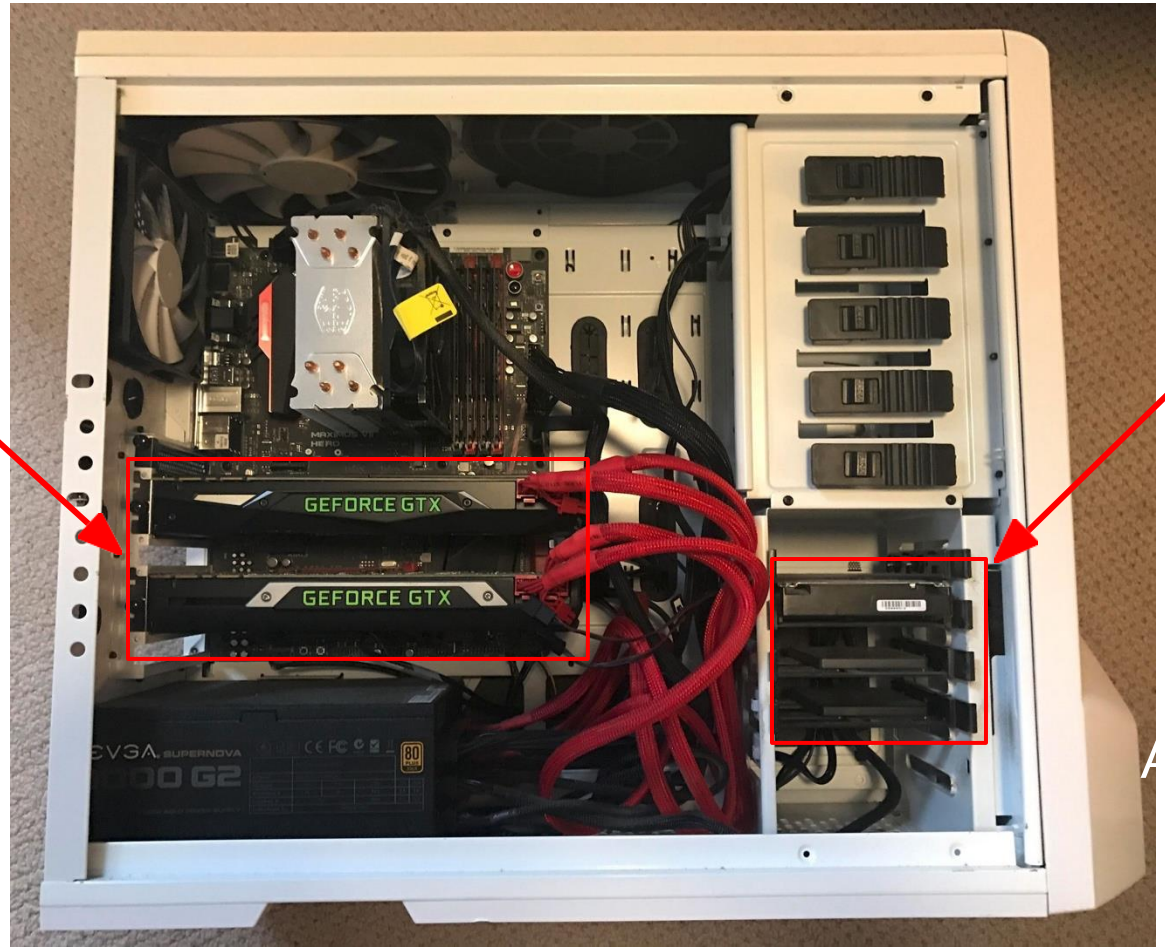
cuDNN much faster than "unoptimized" CUDA



Data from https://github.com/jcjohnson/cnn-benchmarks

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

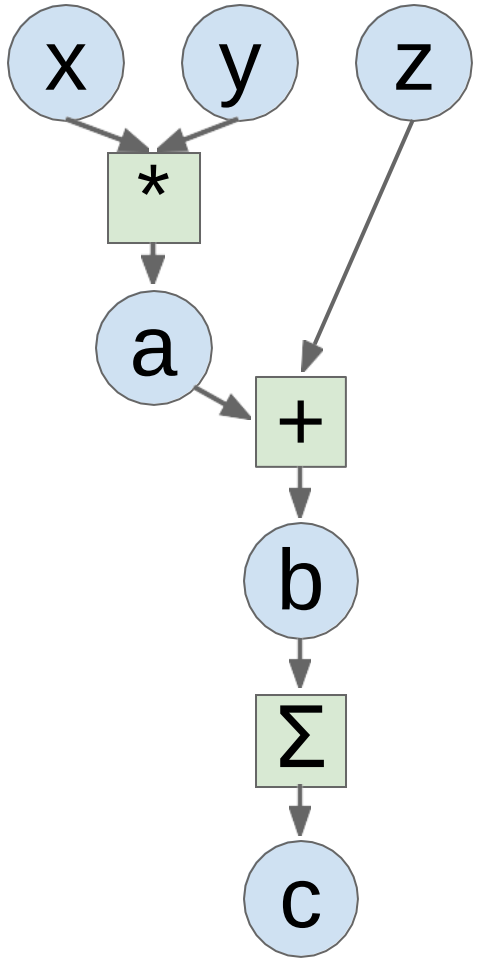
```
import numpy as np
np.random.seed(0)

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)

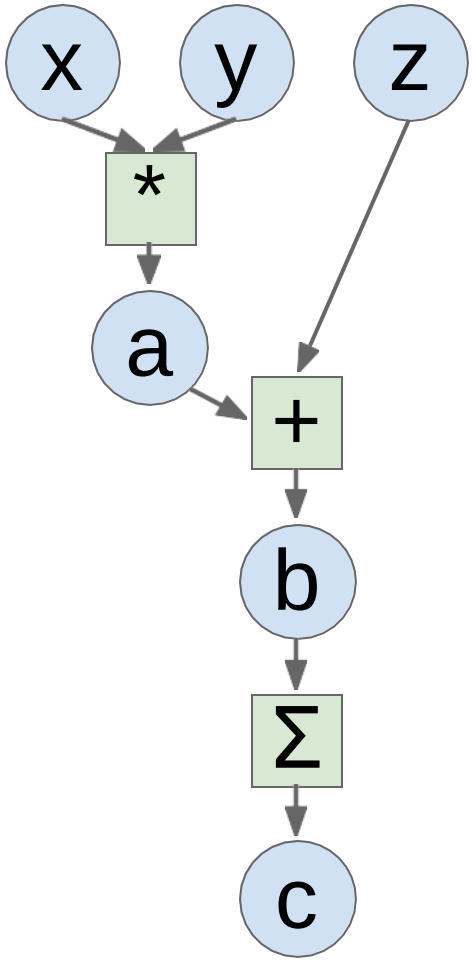
grad_c = 1.0
grad_b = grad_c * np.ones((N, D))
grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```



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

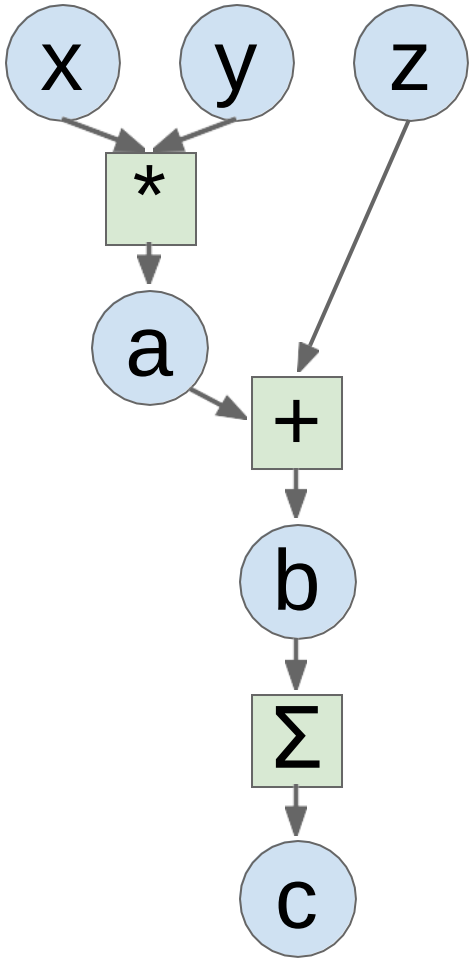
x = Variable(torch.randn(N, D),
             requires_grad=True)
y = Variable(torch.randn(N, D),
             requires_grad=True)
z = Variable(torch.randn(N, D),
             requires_grad=True)

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

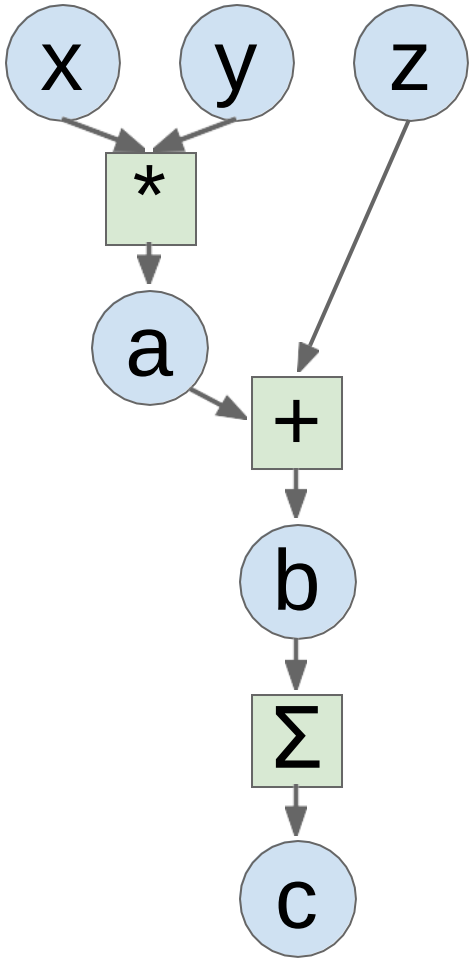
x = Variable(torch.randn(N, D),
             requires_grad=True)
y = Variable(torch.randn(N, D),
             requires_grad=True)
z = Variable(torch.randn(N, D),
             requires_grad=True)

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

```
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N, D = 3, 4

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y = Variable(torch.randn(N, D),
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a = x * y
b = a + z
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c.backward()

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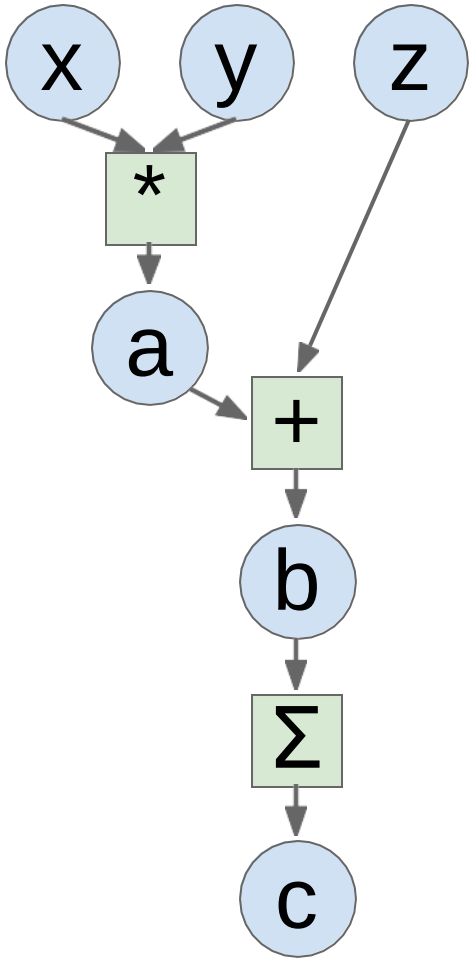
```

Computational Graphs



Calling c.backward()
computes all gradients

PyTorch

```
import torch
from torch.autograd import Variable

N, D = 3, 4

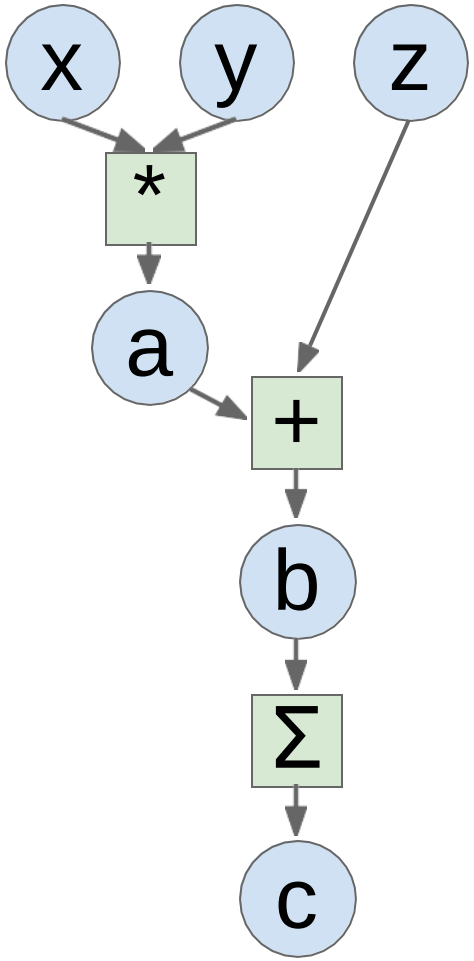
x = Variable(torch.randn(N, D),
             requires_grad=True)
y = Variable(torch.randn(N, D),
             requires_grad=True)
z = Variable(torch.randn(N, D),
             requires_grad=True)

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

- **Tensor**: Imperative ndarray, but runs on GPU
- **Variable**: Node in a computational graph; stores data and gradient
- **Module**: A neural network layer; may store state or learnable weights

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

```
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()

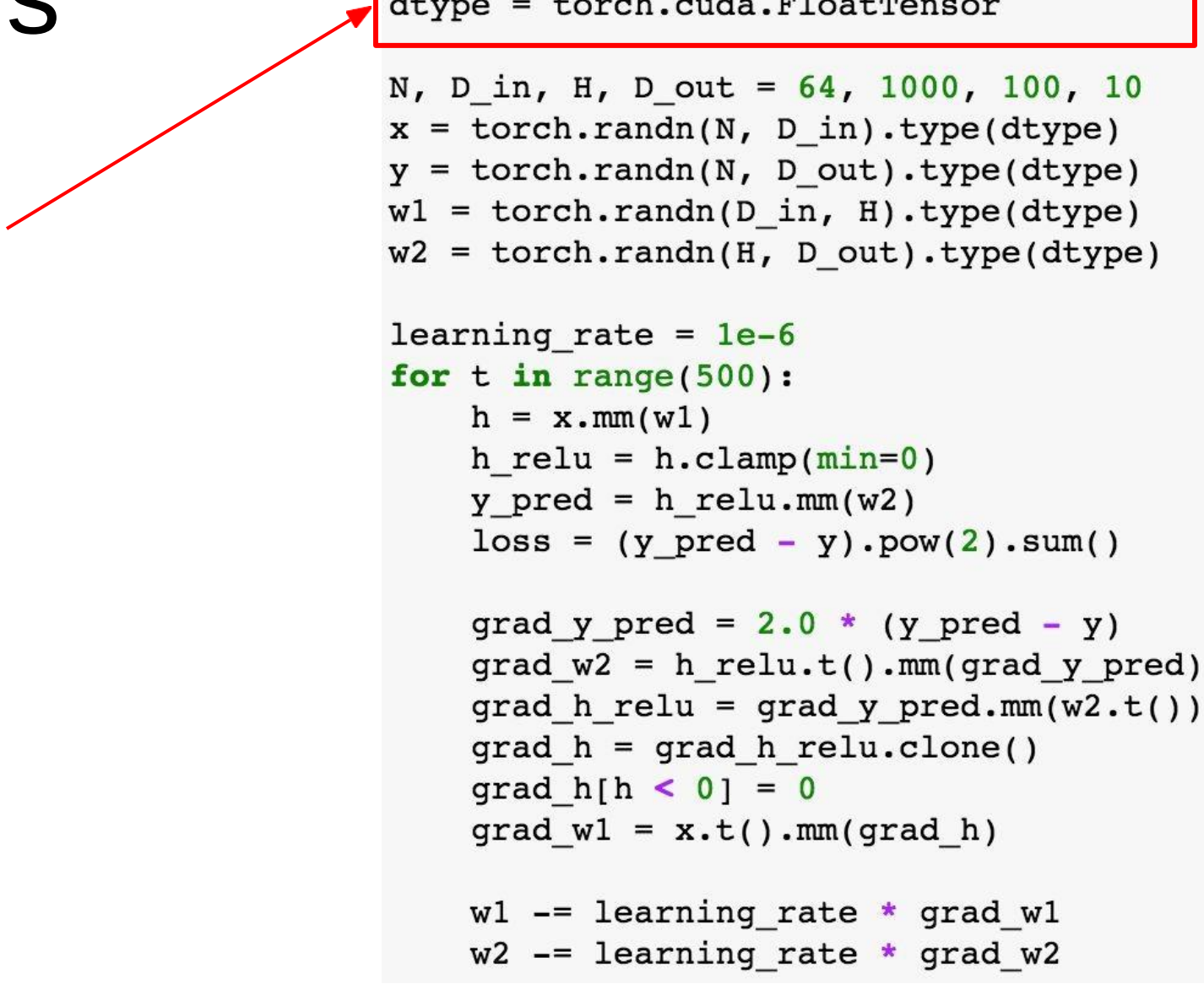
    grad_y_pred = 2.0 * (y_pred - y)
    grad_w2 = h_relu.t().mm(grad_y_pred)
    grad_h_relu = grad_y_pred.mm(w2.t())
    grad_h = grad_h_relu.clone()
    grad_h[h < 0] = 0
    grad_w1 = x.t().mm(grad_h)

    w1 -= learning_rate * grad_w1
    w2 -= learning_rate * grad_w2
```

Gradient descent step on weights

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

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w1 = Variable(torch.randn(D_in, H), requires_grad=True)
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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
```

Make gradient step on weights

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

Backward pass:
compute all 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))
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
```

Make gradient step on each model parameter

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)

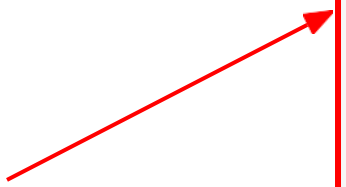
model = TwoLayerNet(D_in, H, D_out)

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(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 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

```
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()
```

Construct and train an instance of our model

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()

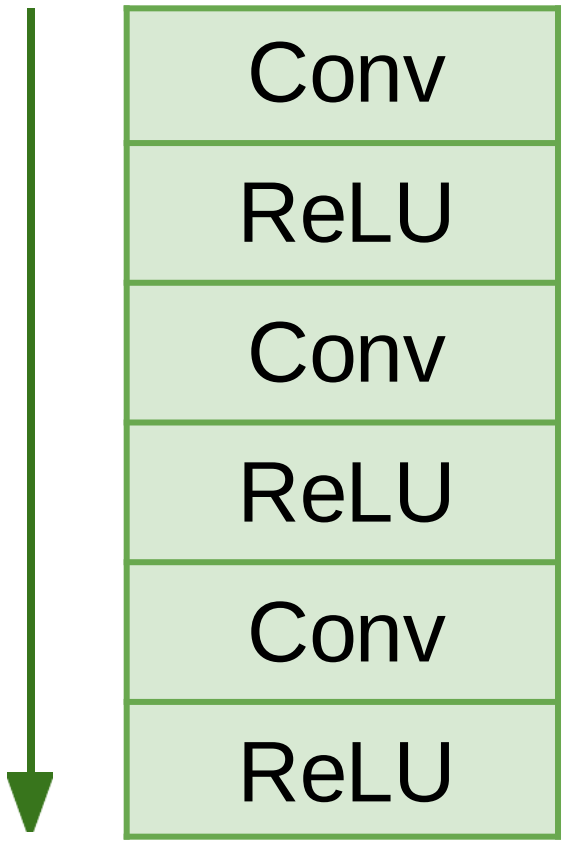
    w1.data -= learning_rate * w1.grad.data
    w2.data -= learning_rate * w2.grad.data
```

New graph each iteration

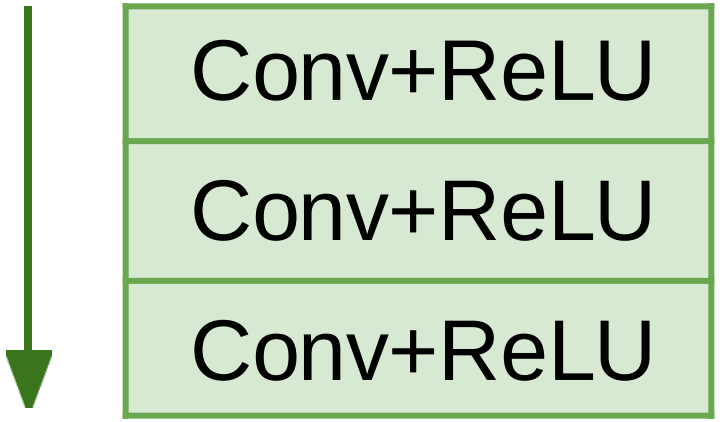
Static vs Dynamic: Optimization

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!

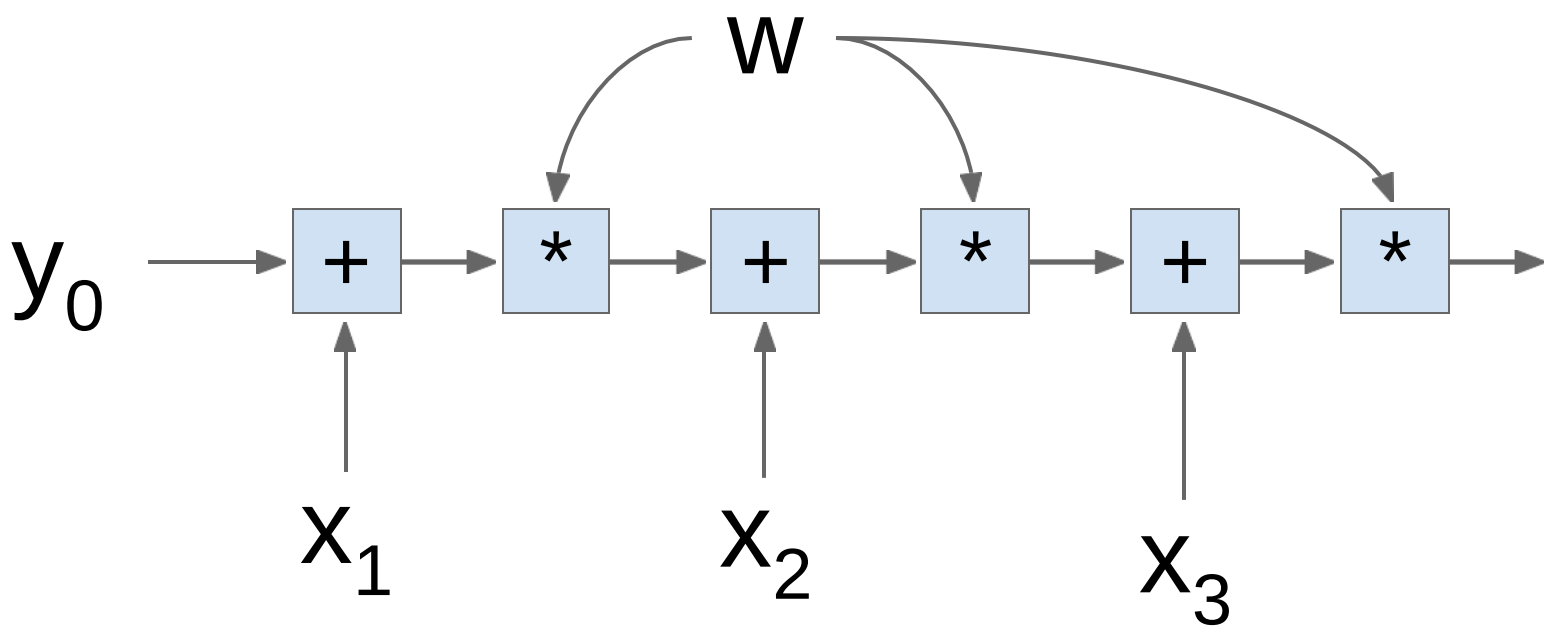
```
N, D, H = 3, 4, 5
x = tf.placeholder(tf.float32, shape=(N, D))
z = tf.placeholder(tf.float32, shape=None)
w1 = tf.placeholder(tf.float32, shape=(D, H))
w2 = tf.placeholder(tf.float32, shape=(D, H))

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)
```

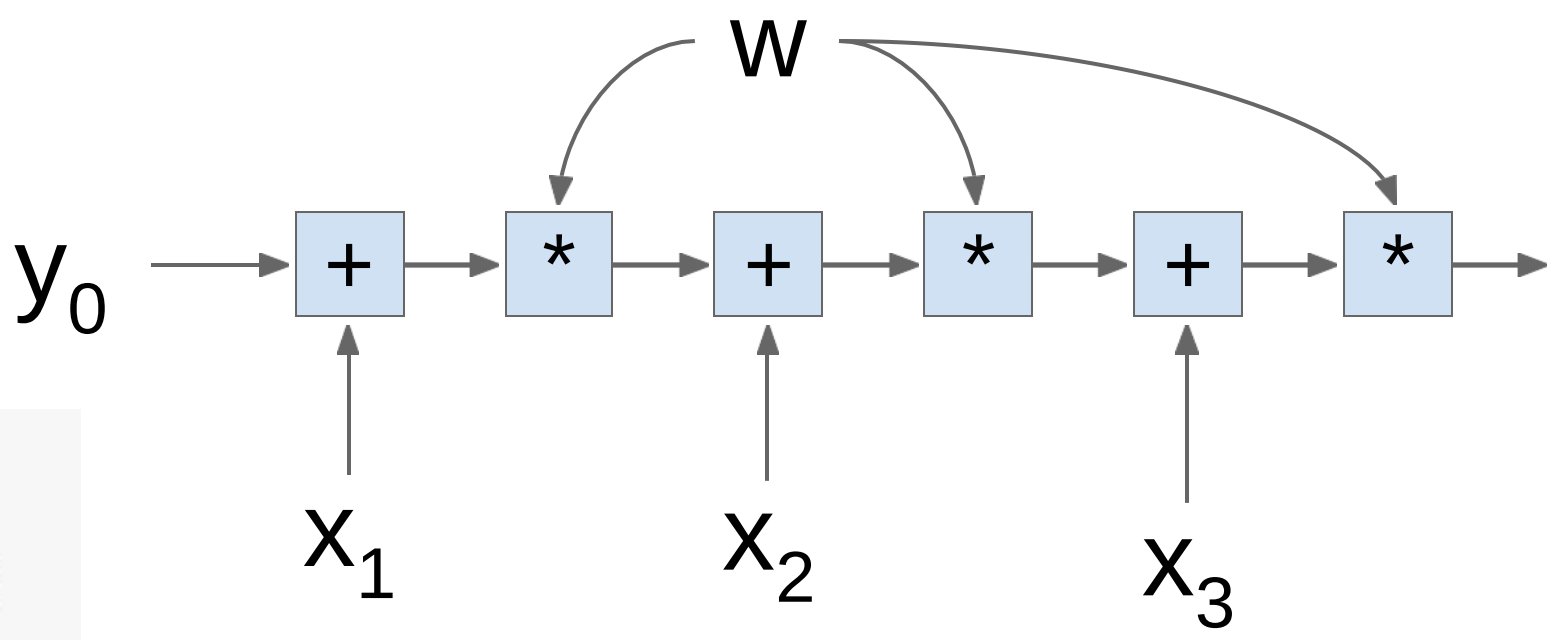
Static vs Dynamic: Loops

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



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)
```

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')

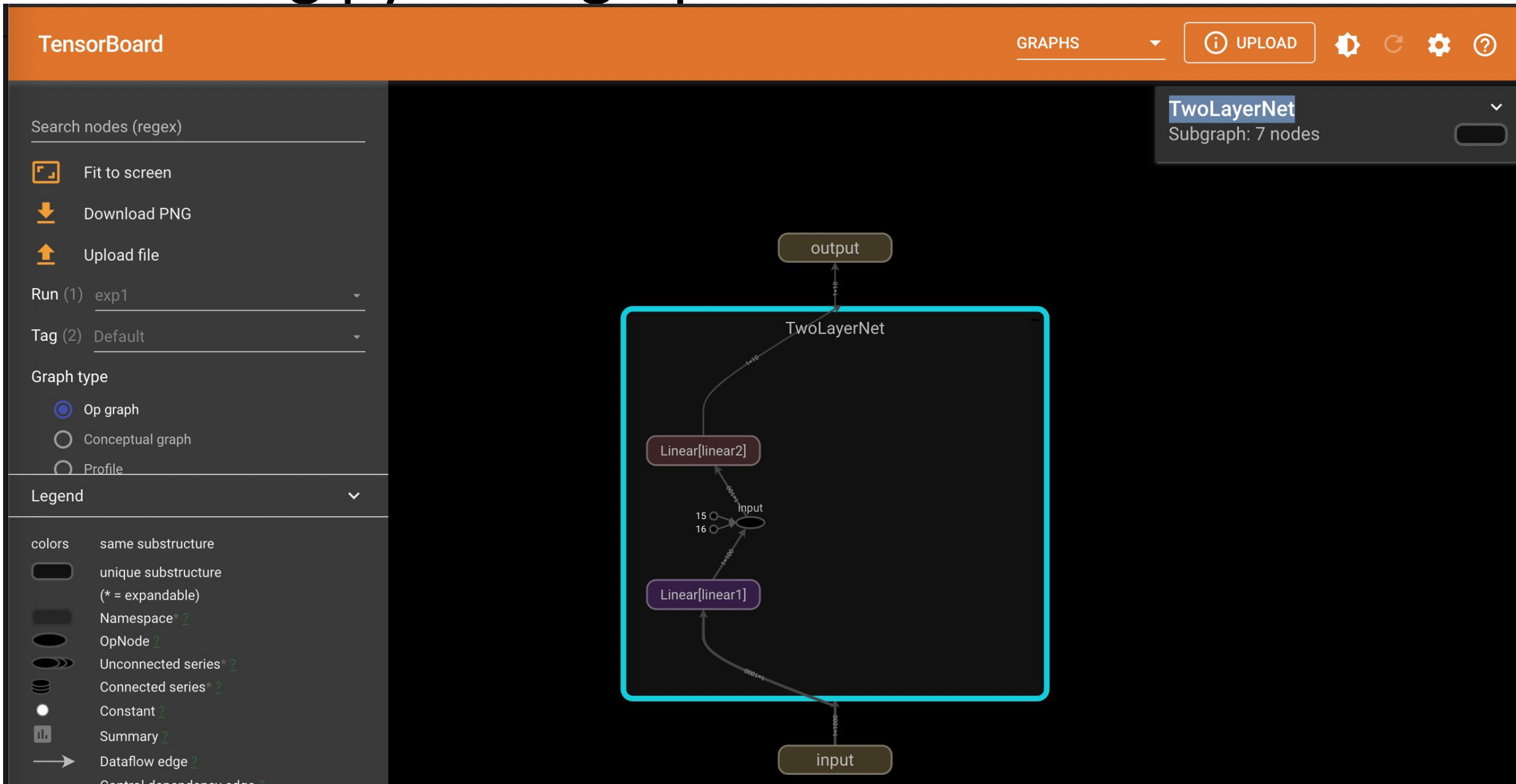
writer.add_graph(model,x_input)
writer.close()
```

```
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



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