

CS 4644-DL / 7643-A: LECTURE 13

DANFEI XU

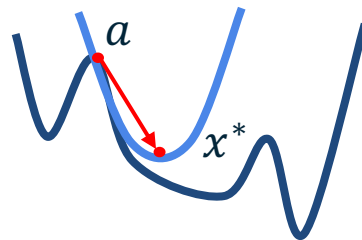
Topics:

- Deep Learning Hardware and Software

Recap: Second-order Optimization

Newton's method for optimization: solving for the critical point we obtain the Newton update rule:

$$\mathbf{x}^* = \mathbf{a} - H^{-1} \nabla f$$



$$\mathbf{H}_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

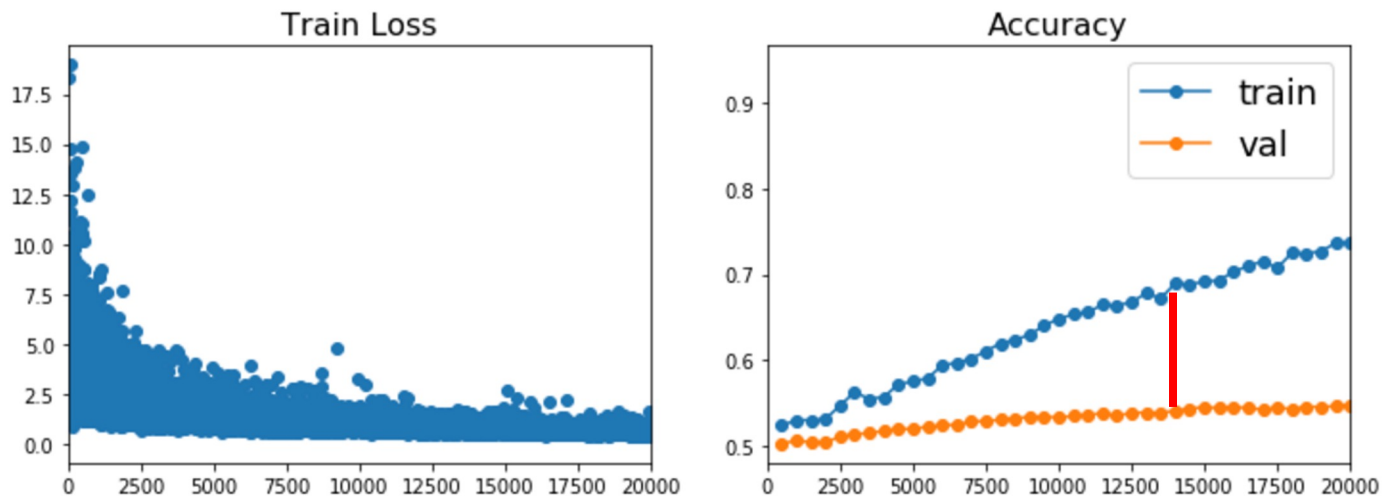
Bad for deep learning! $O(n^3)$ hessian inversion

- Consider BGFS (approximate hessian) or L-BFGS (don't store full hessian in memory)
- L-BFGS works better in full-batch setting.
Disable all stochastic components in training

Administrative

- Reminder: anonymous feedback
- Time to work on the project!

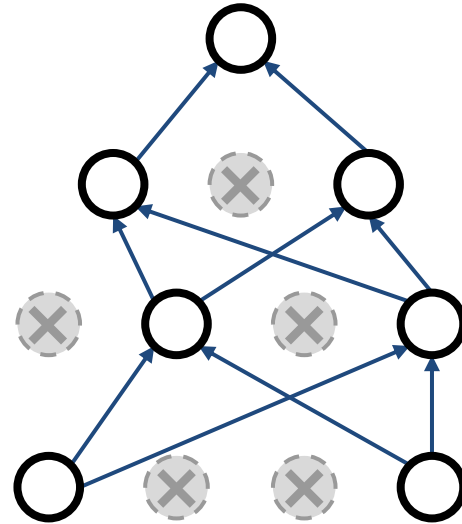
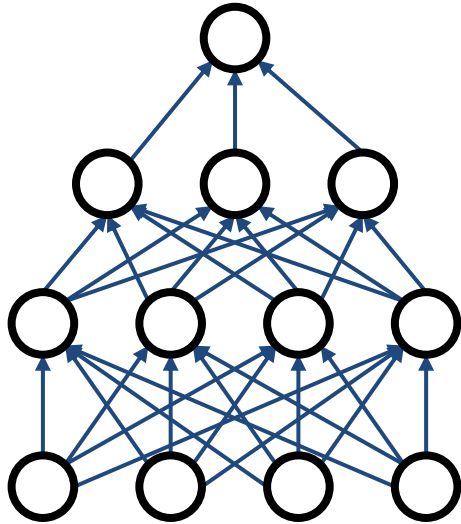
Recap: Test-time performance



Regularization

Recap: Dropout

In each forward pass, randomly set some neurons to zero
Probability of dropping is a hyperparameter; 0.5 is common



Recap: Dropout

```
p = 0.5 # probability of keeping a unit active. higher = less dropout
```

```
def train_step(X):
```

```
    # forward pass for example 3-layer neural network
```

```
    H1 = np.maximum(0, np.dot(W1, X) + b1)
```

```
    U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
```

```
    H1 *= U1 # drop!
```

```
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
```

```
    U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
```

```
    H2 *= U2 # drop!
```

```
    out = np.dot(W3, H2) + b3
```

```
    # backward pass: compute gradients... (not shown)
```

```
    # perform parameter update... (not shown)
```

```
def predict(X):
```

```
    # ensembled forward pass
```

```
    H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
```

```
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
```

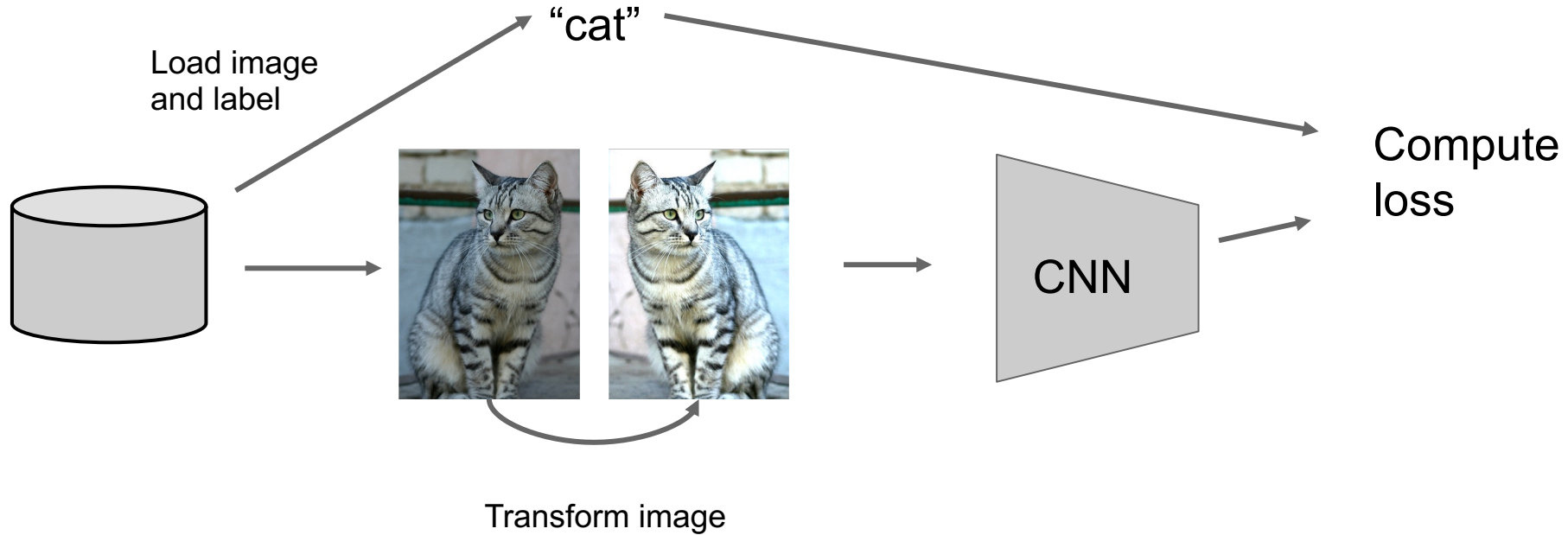
```
    out = np.dot(W3, H2) + b3
```

test time is unchanged!

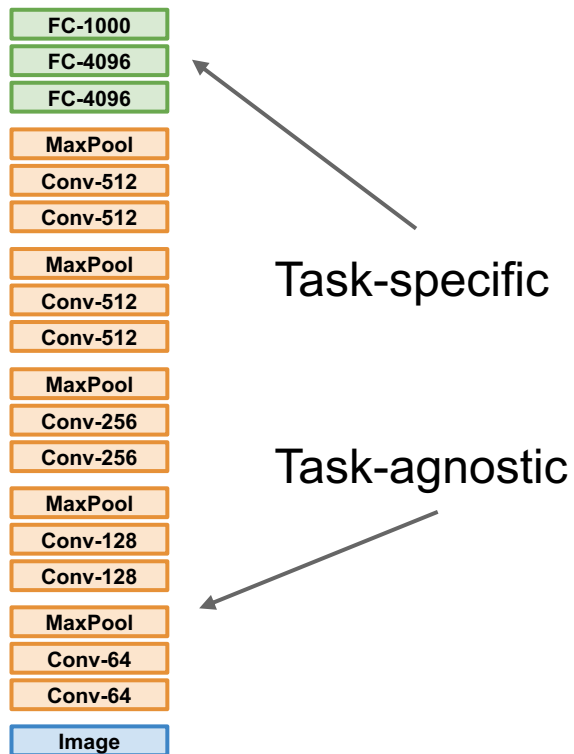


Similar to BatchNorm, different behavior train vs test!

Recap: Data Augmentation



Recap: Transfer Learning



	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	You're in trouble... Try linear classifier from different stages
quite a lot of data	Finetune a few layers	Finetune a larger number of layers

Today

- Deep learning hardware
 - CPU, GPU
- Deep learning software
 - PyTorch and TensorFlow
 - Static and Dynamic computation graphs

Deep Learning Hardware

Inside a computer

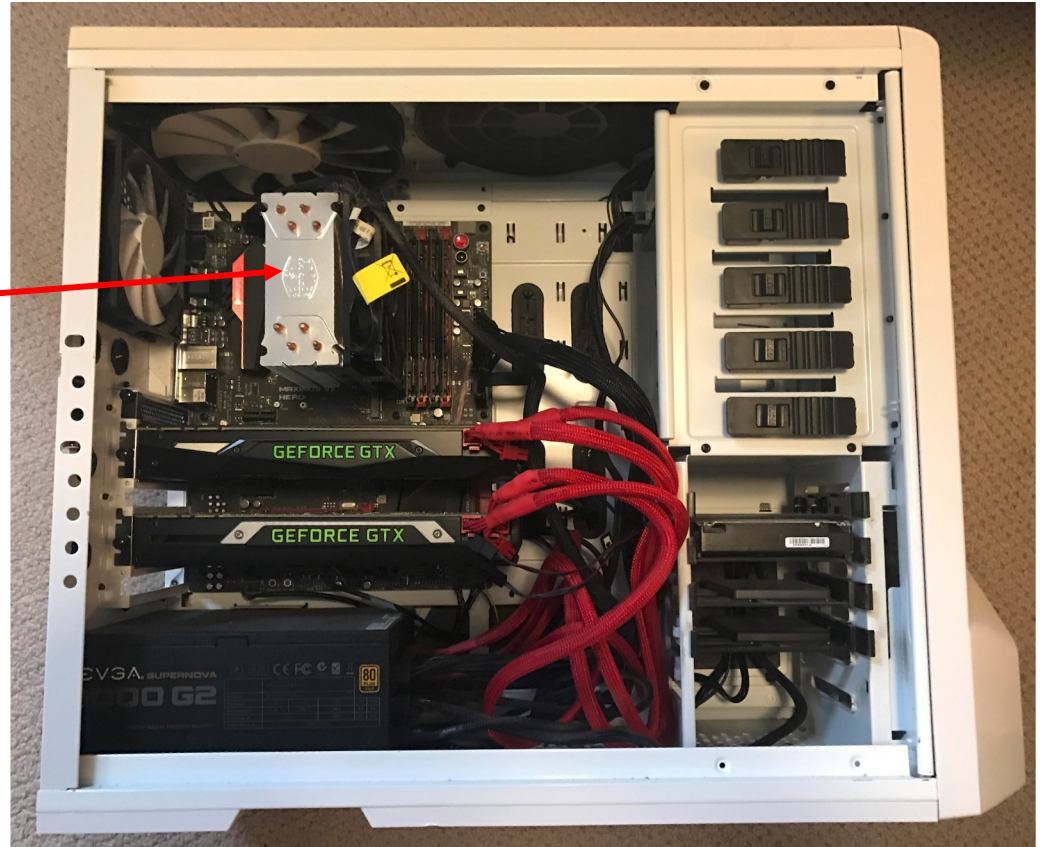


Spot the CPU!

(central processing unit)



[This image](#) is licensed under [CC-BY 2.0](#)

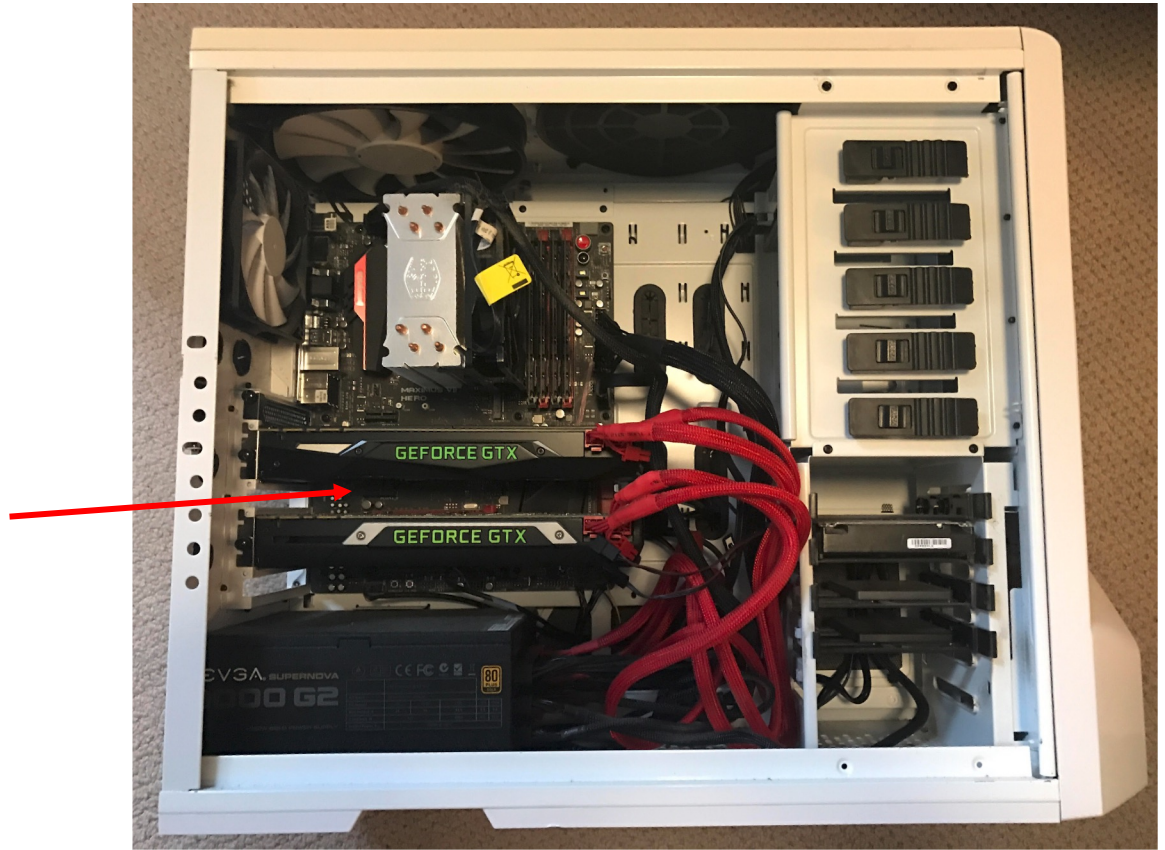


Spot the GPUs!

(graphics processing unit)



This image is licensed under [CC-BY 2.0](https://creativecommons.org/licenses/by/2.0/)



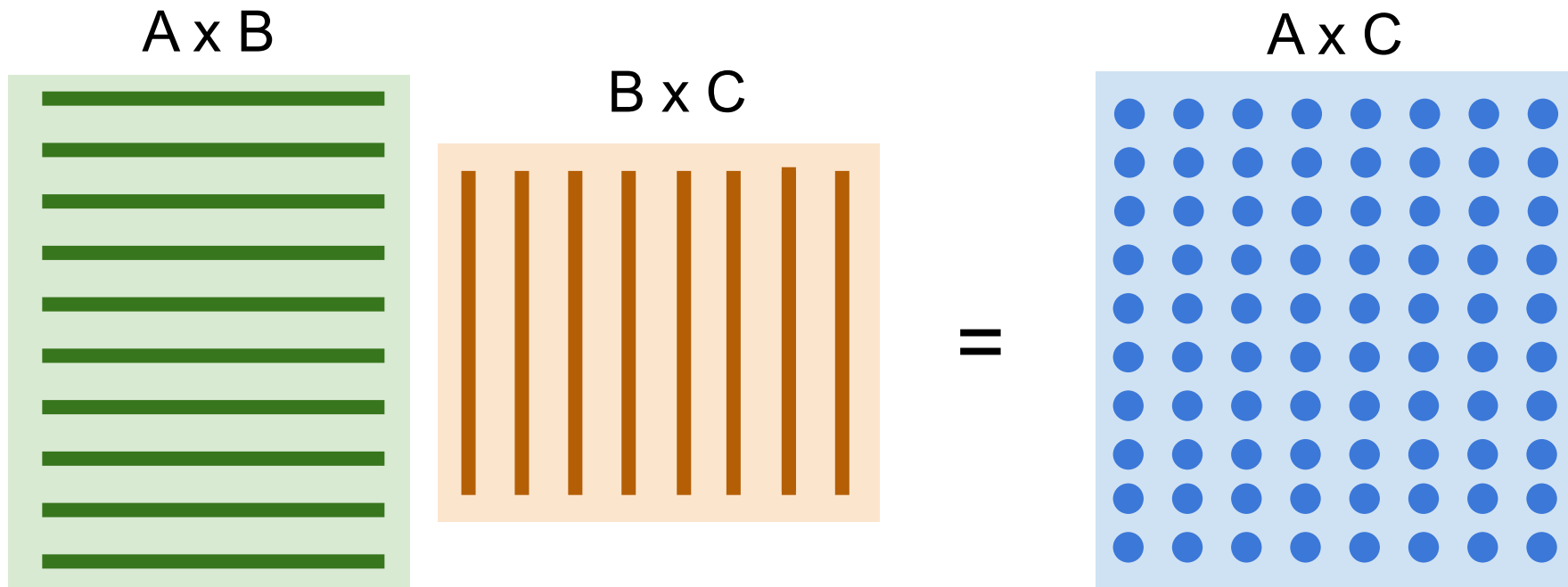
CPU vs GPU

	Cores	Clock Speed	Memory	Price	Speed (throughput)
CPU (Intel Core i9-7900k)	10	4.3 GHz	System RAM	\$385	~640 GFLOPS FP32
GPU (NVIDIA RTX 3090)	10496	1.6 GHz	24 GB GDDR6X	\$1499	~35.6 TFLOPS FP32

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

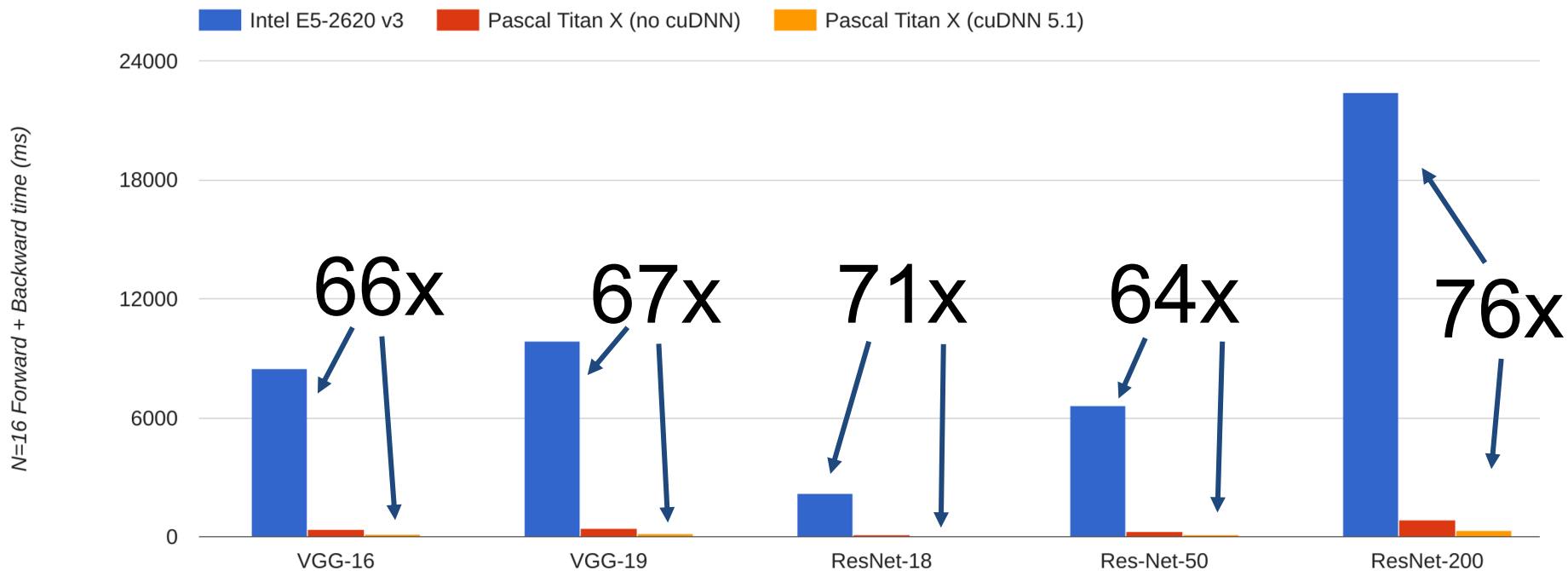
Example: Matrix Multiplication



cuBLAS::GEMM (General Matrix-to-matrix Multiply)

CPU vs GPU in practice

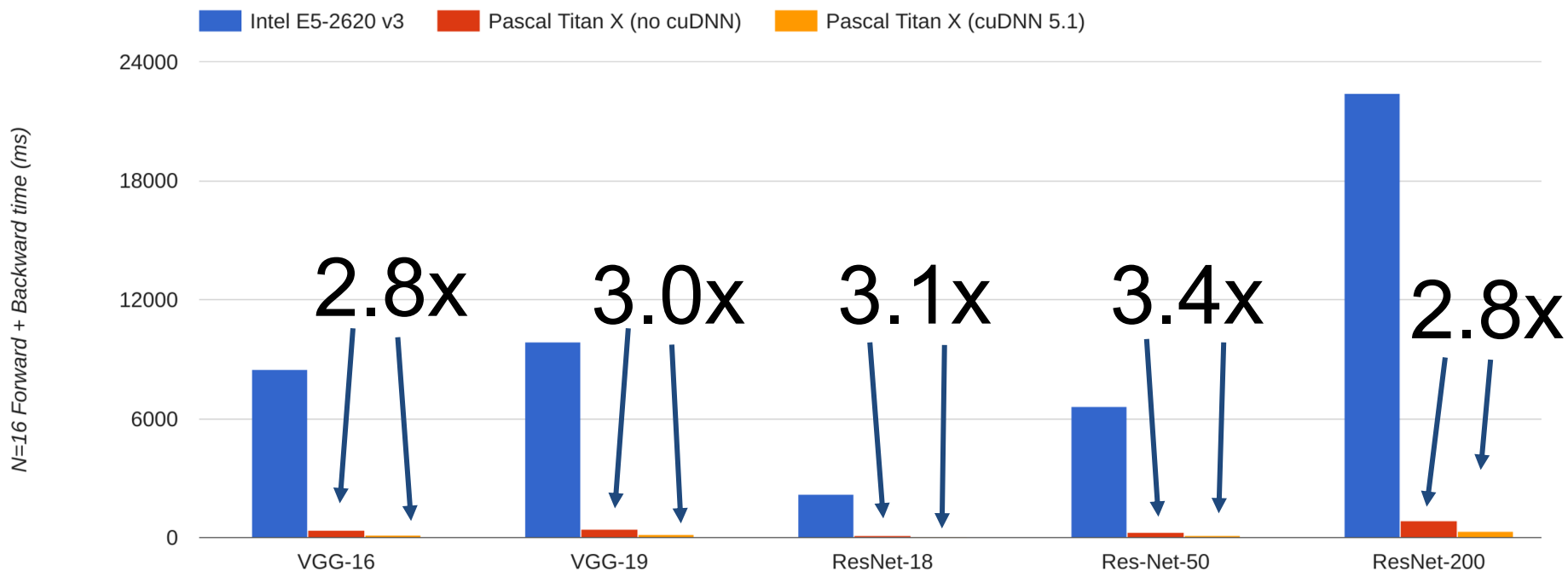
(CPU performance not well-optimized, a little unfair)



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

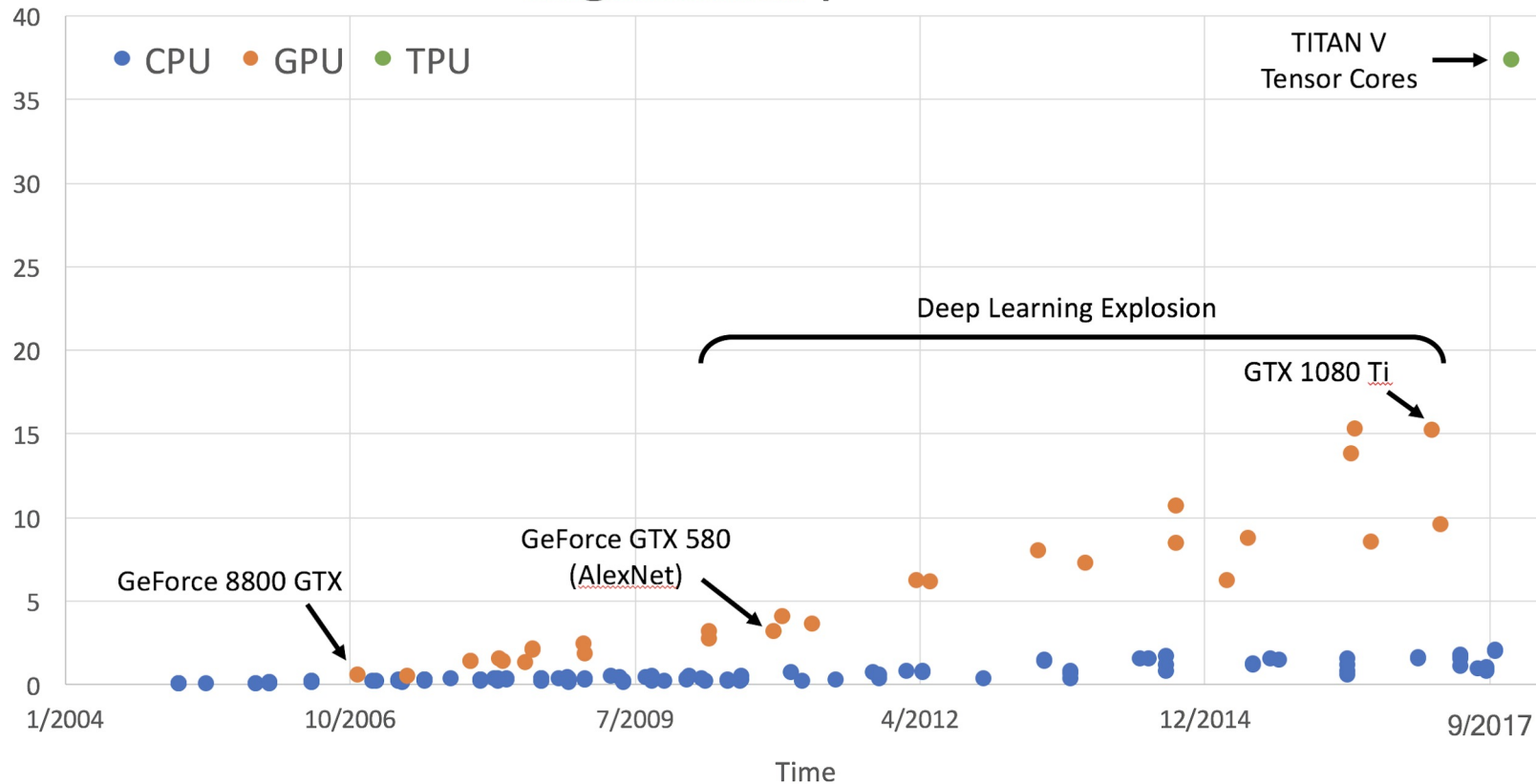
CPU vs GPU in practice

cuDNN much faster than
“unoptimized” CUDA



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

GigaFLOPs per Dollar



NVIDIA

vs

AMD

NVIDIA

vs

AMD

CPU vs GPU

	Cores	Clock Speed	Memory	Price	Speed
CPU (Intel Core i7-7700k)	10	4.3 GHz	System RAM	\$385	~640 GFLOPs FP32
GPU (NVIDIA RTX 3090)	10496	1.6 GHz	24 GB GDDR6X	\$1499	~35.6 TFLOPs FP32
GPU (Data Center) NVIDIA A100	6912 CUDA, 432 Tensor	1.5 GHz	40/80 GB HBM2	\$3/hr (GCP)	~9.7 TFLOPs FP64 ~20 TFLOPs FP32 ~312 TFLOPs FP16
TPU Google Cloud TPUv3	2 Matrix Units (MXUs) per core, 4 cores	?	128 GB HBM	\$8/hr (GCP)	~420 TFLOPs (non-standard FP)

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

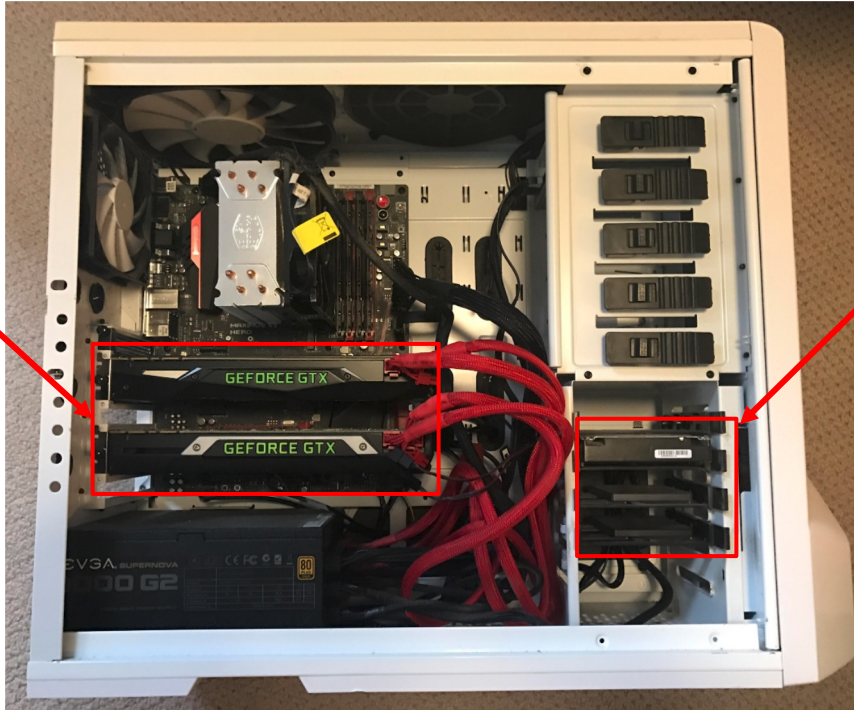
TPU: Specialized hardware for deep learning

Programming GPUs

- CUDA (NVIDIA only)
 - Write C-like code that runs directly on the GPU
 - Optimized APIs: cuBLAS, cuFFT, cuDNN, etc
- OpenCL
 - Similar to CUDA, but runs on anything
 - Usually slower on NVIDIA hardware
- HIP <https://github.com/ROCm-Developer-Tools/HIP>
 - New project that automatically converts CUDA code to something that can run on AMD GPUs
- CS 8803 – GPU at GaTech
 - Taught by Prof. Hyesoon Kim

CPU / GPU Communication

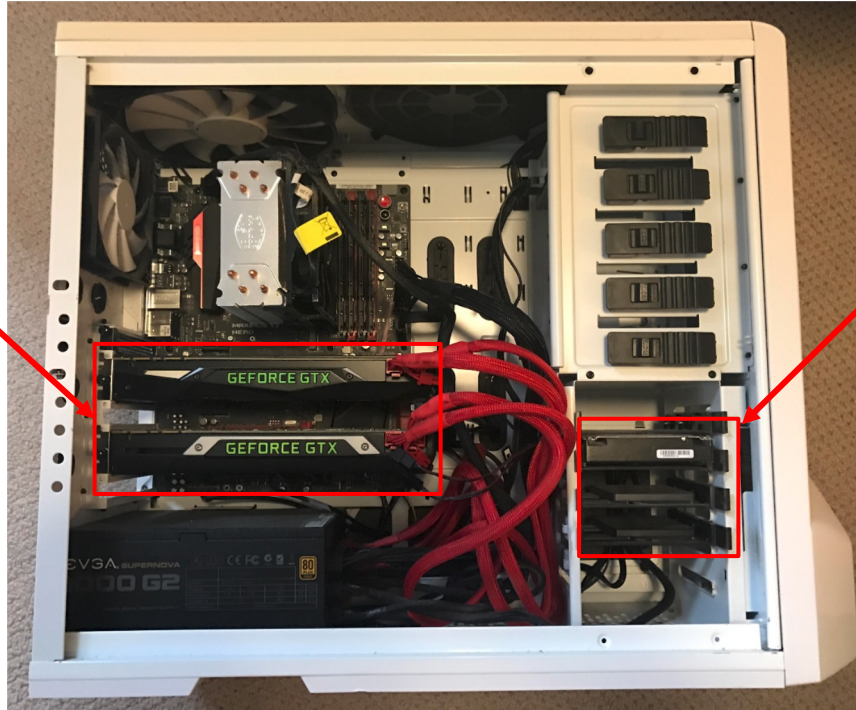
Model
is here



Data is here

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 Software

A zoo of frameworks!

Caffe
(UC Berkeley)



Caffe2
(Facebook)
mostly features absorbed
by PyTorch



Torch
(NYU / Facebook)



PyTorch
(Facebook)

Theano
(U Montreal)



TensorFlow
(Google)

PaddlePaddle
(Baidu)

Chainer
(Preferred Networks)
The company has officially migrated its research
infrastructure to PyTorch

MXNet
(Amazon)

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

CNTK
(Microsoft)

JAX
(Google)

And others...

A zoo of frameworks!

Caffe
(UC Berkeley)



Caffe2
(Facebook)
mostly features absorbed
by PyTorch



Torch
(NYU / Facebook)



PyTorch
(Facebook)

Theano
(U Montreal)



TensorFlow
(Google)

We'll focus on these

PaddlePaddle
(Baidu)

Chainer
(Preferred Networks)
The company has officially migrated its research
infrastructure to PyTorch

MXNet
(Amazon)

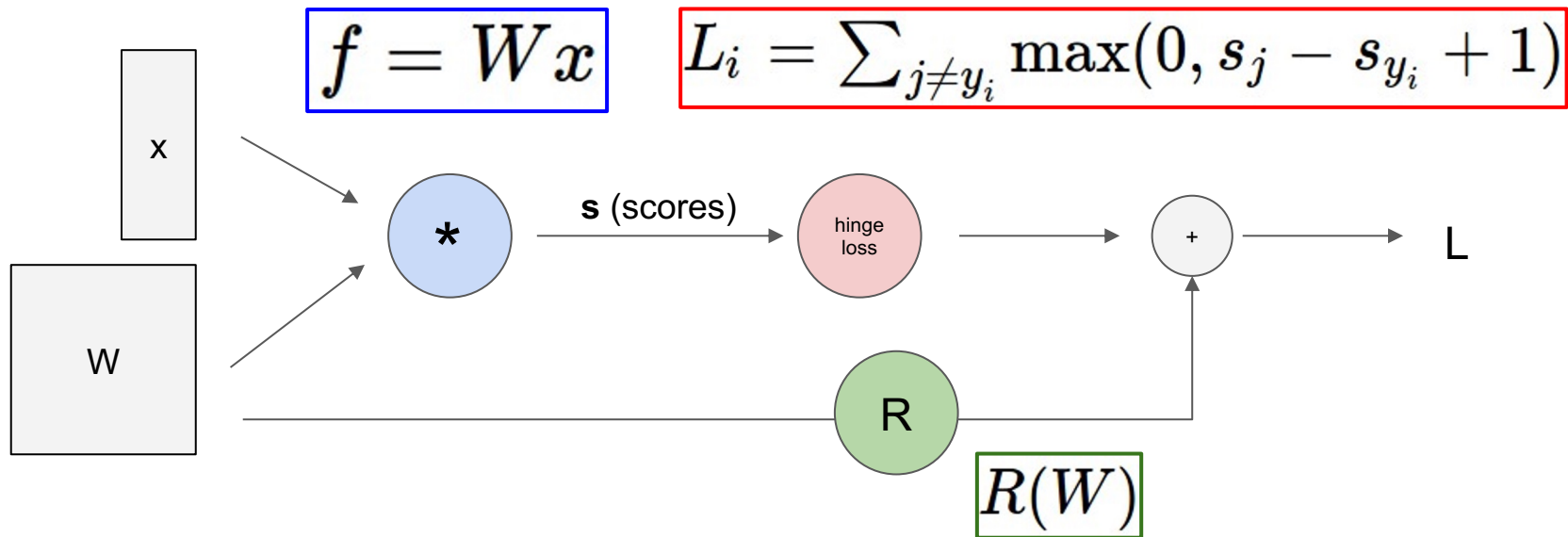
Developed by U Washington, CMU, MIT,
Hong Kong U, etc but main framework of
choice at AWS

CNTK
(Microsoft)

JAX
(Google)

And others...

Recall: Computational Graphs



Recall: Computational Graphs

input image

weights

loss

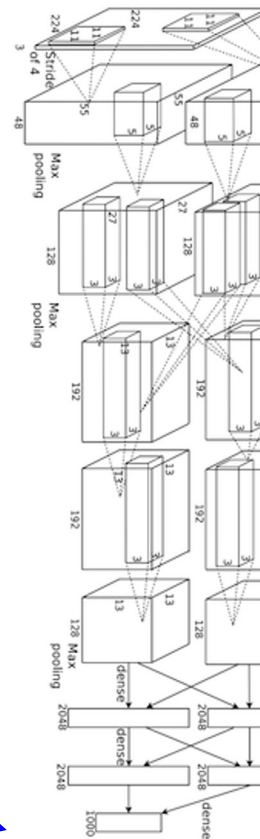


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Recall: Computational Graphs

input image

loss

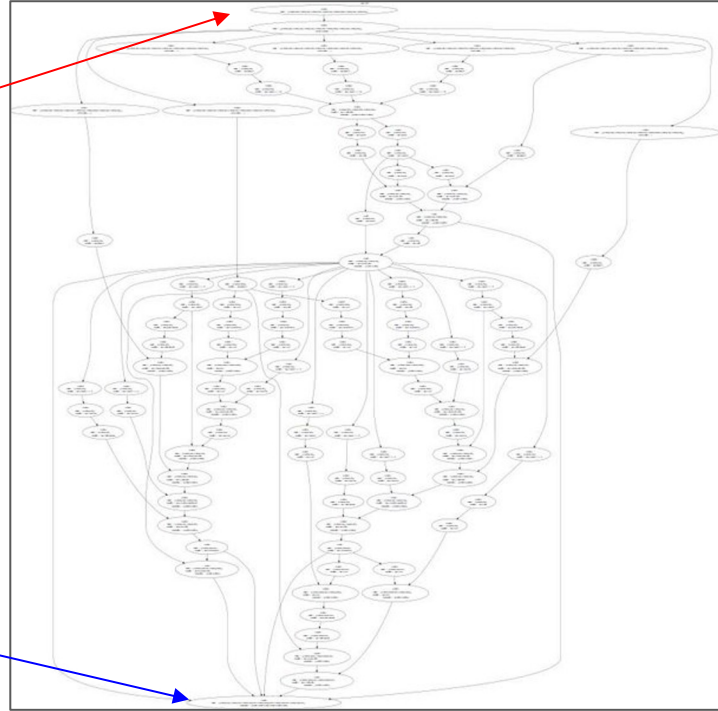


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

The point of deep learning frameworks

- (1) Quick to develop and test new ideas
- (2) Automatically compute gradients
- (3) Run it all efficiently on GPU (wrap cuDNN, cuBLAS, OpenCL, etc)

Computational Graphs

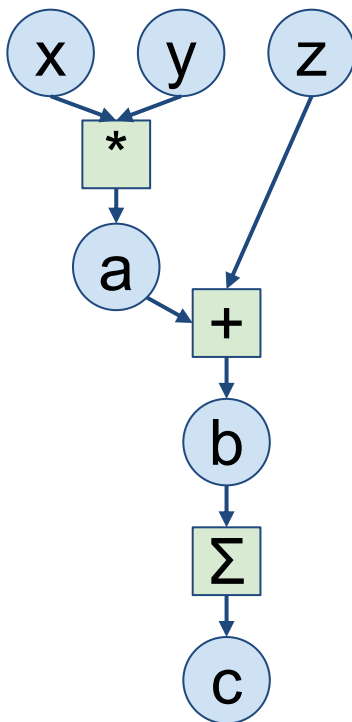
Numpy

```
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)
```



Computational Graphs

Numpy

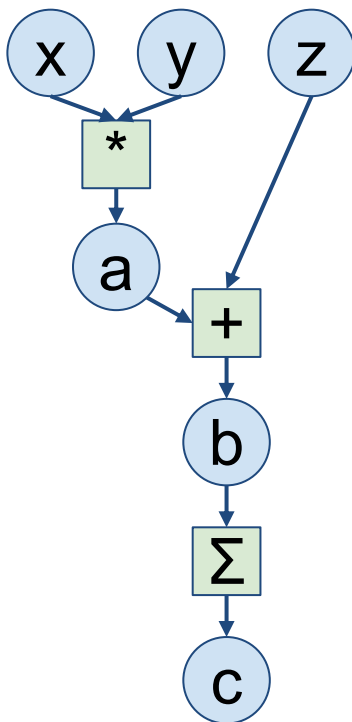
```
import numpy as np
np.random.seed(0)

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
```



Computational Graphs

Numpy

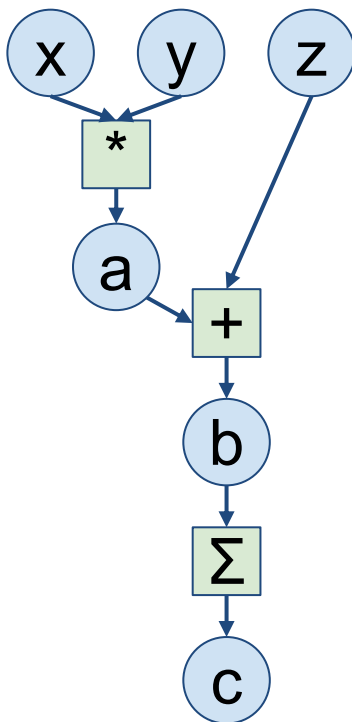
```
import numpy as np
np.random.seed(0)

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
```



Good:

Clean API, easy to write numeric code

Bad:

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

Computational Graphs

Numpy

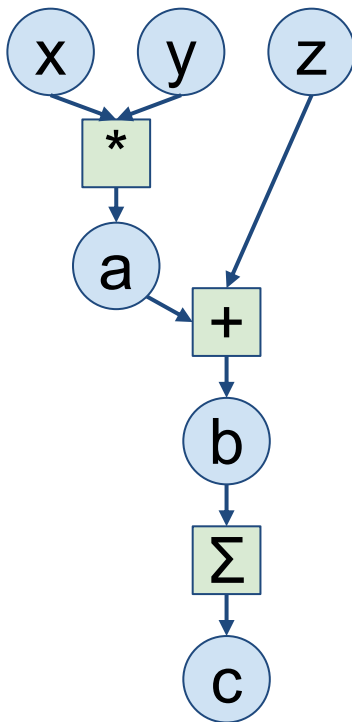
```
import numpy as np
np.random.seed(0)

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
```



PyTorch

```
import torch

N, D = 3, 4
x = torch.randn(N, D)
y = torch.randn(N, D)
z = torch.randn(N, D)

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

Looks exactly like numpy!

Computational Graphs

Numpy

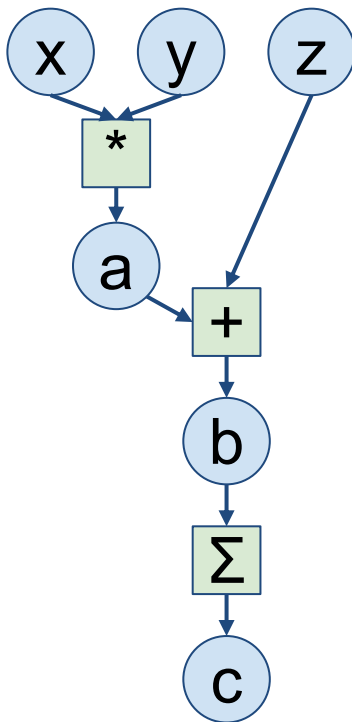
```
import numpy as np
np.random.seed(0)

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
```



PyTorch

```
import torch

N, D = 3, 4
x = torch.randn(N, D, requires_grad=True)
y = torch.randn(N, D)
z = torch.randn(N, D)

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

c.backward()
print(x.grad)
```

PyTorch handles gradients for us!

Computational Graphs

Numpy

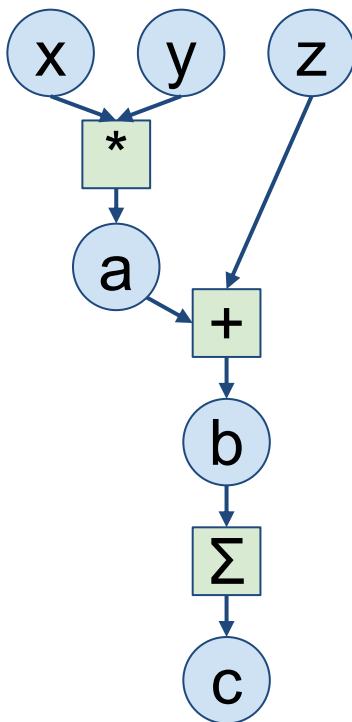
```
import numpy as np
np.random.seed(0)

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
```



PyTorch

```
import torch
device = 'cuda:0'
N, D = 3, 4
x = torch.randn(N, D, requires_grad=True,
                device=device)
y = torch.randn(N, D, device=device)
z = torch.randn(N, D, device=device)

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

c.backward()
print(x.grad)
```

Trivial to run on GPU - just construct arrays on a different device!

PyTorch

(More details)

PyTorch: Fundamental Concepts

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

torch.autograd: Package for building computational graphs out of Tensors, and automatically computing gradients

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

PyTorch: Versions

For this class we are using **PyTorch version ≥ 1.10**
(newest is 1.12)

Major API change in release 1.0

Be careful if you are looking at older PyTorch code (<1.0)!

PyTorch: Tensors

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
```

PyTorch: Tensors

Create random tensors
for data and 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
```

PyTorch: Tensors

Forward pass: compute predictions and 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
```

PyTorch: Tensors

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
```

PyTorch: Tensors

```
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



PyTorch: Tensors

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
```

PyTorch: Autograd

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_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_()
```

PyTorch: Autograd

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
        w1.grad.zero_()
        w2.grad.zero_()
```


PyTorch: Autograd

Compute gradient of loss
with respect to w1 and w2

```
import torch

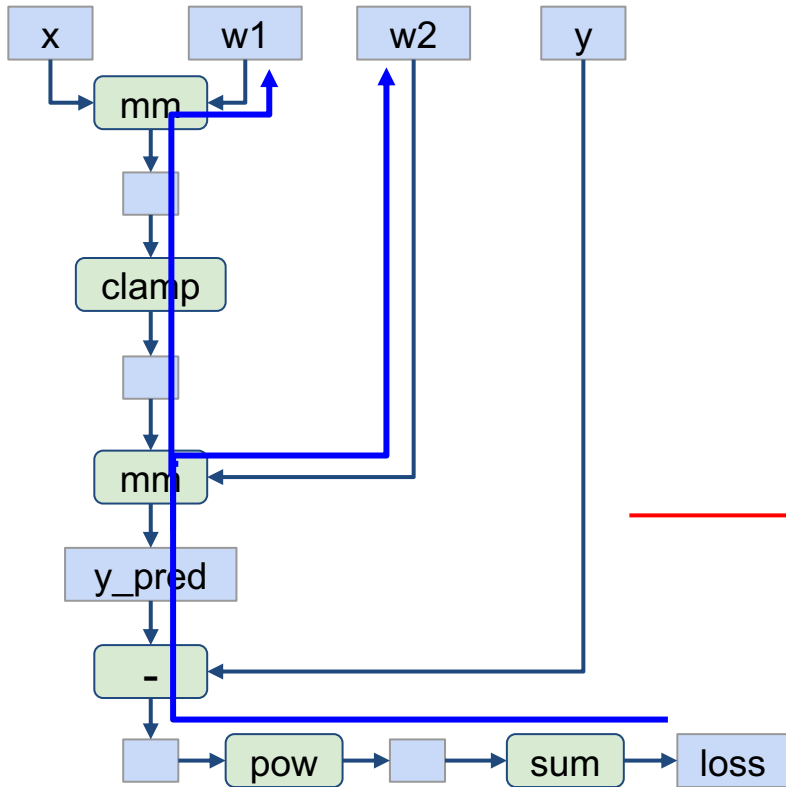
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

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
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: 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)
```

```
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
```

```
        w1.grad.zero_()
```

```
        w2.grad.zero_()
```

PyTorch: 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)
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
        w1.grad.zero_()
        w2.grad.zero_()
```

Make gradient step on weights, then zero them. Torch.no_grad means “don’t build a computational graph for this part”

PyTorch: Autograd

PyTorch methods that end in underscore modify the Tensor in-place; methods that don't return a new Tensor

```
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
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: New Autograd Functions

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

Use ctx object to “cache” values for the backward pass

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

PyTorch: New Autograd Functions

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

Use ctx object to “cache” values for the backward pass

Define a helper function to make it easy to use the new function

```
class MyReLU(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        ctx.save_for_backward(x)
        return x.clamp(min=0)

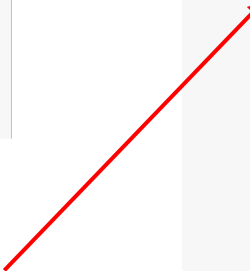
    @staticmethod
    def backward(ctx, grad_y):
        x, = ctx.saved_tensors
        grad_input = grad_y.clone()
        grad_input[x < 0] = 0
        return grad_input

def my_relu(x):
    return MyReLU.apply(x)
```

PyTorch: New Autograd Functions

```
class MyReLU(torch.autograd.Function):  
    @staticmethod  
    def forward(ctx, x):  
        ctx.save_for_backward(x)  
        return x.clamp(min=0)  
  
    @staticmethod  
    def backward(ctx, grad_y):  
        x, = ctx.saved_tensors  
        grad_input = grad_y.clone()  
        grad_input[x < 0] = 0  
        return grad_input  
  
def my_relu(x):  
    return MyReLU.apply(x)
```

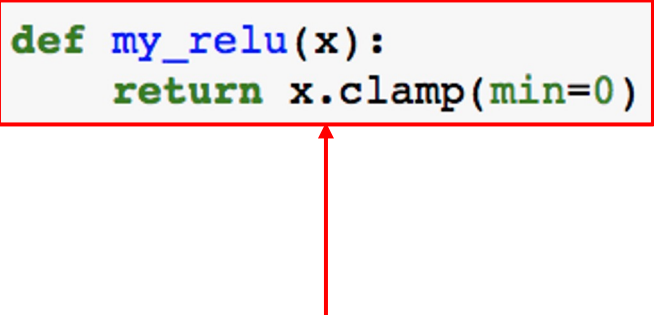
Can use our new autograd
function in the forward pass



```
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 = my_relu(x.mm(w1)).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_()
```

PyTorch: New Autograd Functions

```
def my_relu(x):  
    return x.clamp(min=0)
```



In practice you almost never need to define new autograd functions! Only do it when you need custom backward. In this case we can just use a normal PyTorch function

```
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 = my_relu(x.mm(w1)).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_()
```


PyTorch: nn

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()
```

PyTorch: nn

Define our model as a sequence of layers; each layer is an object that holds learnable 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)
```

```
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()
```

PyTorch: nn

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()
```

PyTorch: nn

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()
```

PyTorch: nn

Backward pass: compute gradient with respect to all model weights (they 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)

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()
```

PyTorch: nn

```
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()
```

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

```
with torch.no_grad():
    for param in model.parameters():
        param -= learning_rate * param.grad
    model.zero_grad()
```

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 params
and zero gradients



PyTorch: nn

Define new Modules

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

Modules can contain weights or other modules

You can define your own Modules using autograd!

```
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()
```

PyTorch: nn

Define new Modules

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()
```

PyTorch: nn

Define new Modules

Initializer sets up two children (Modules can contain 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()
```

PyTorch: nn

Define new Modules

Define forward pass using
child modules

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()
```

PyTorch: nn

Define new 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)
```

Construct and train an
instance of our model



```
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()
```

PyTorch: nn

Define new Modules

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()
```

PyTorch: nn

Define new Modules

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)

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: nn

Define new Modules

Stack multiple instances of the component in a sequential



```
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: 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)
```

PyTorch: Computational Graphs

input image

loss

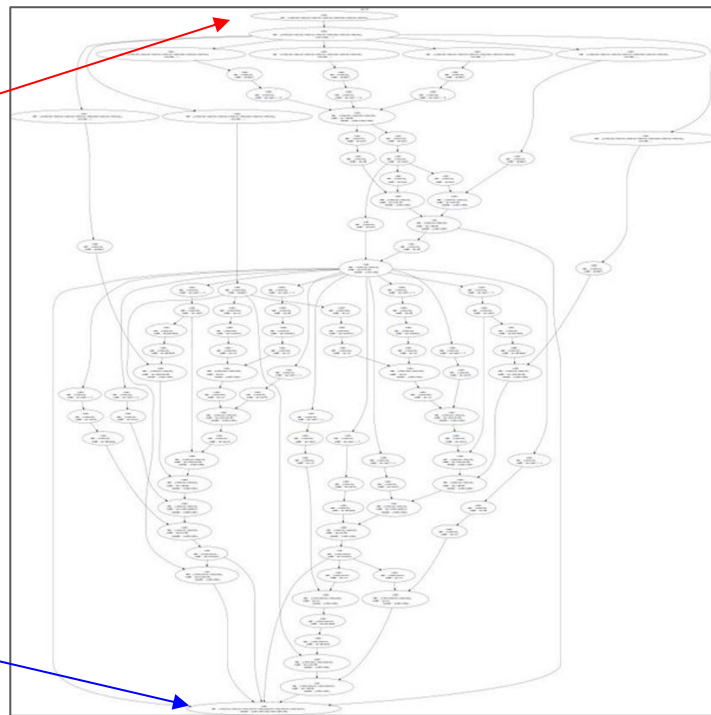


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

PyTorch: Dynamic Computation Graphs

```
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()
```

PyTorch: Dynamic Computation Graphs

x

w1

w2

y

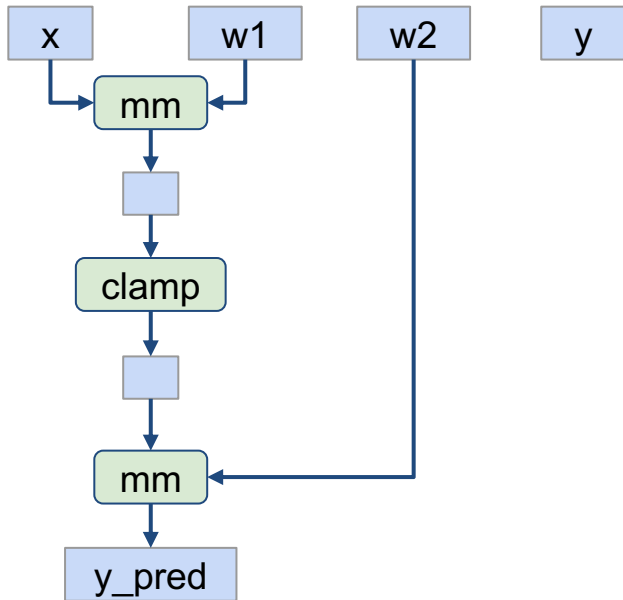
```
import torch
```

```
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_pred = x.mm(w1).clamp(min=0).mm(w2)  
    loss = (y_pred - y).pow(2).sum()  
  
    loss.backward()
```

Create Tensor objects

PyTorch: Dynamic Computation Graphs



```
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):
```

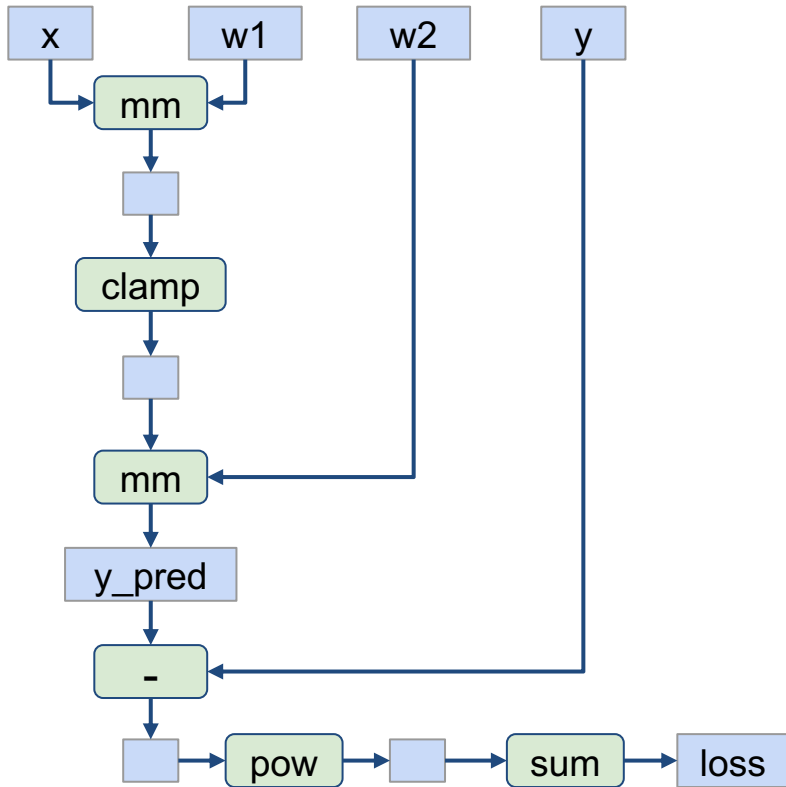
```
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
```

```
    loss = (y_pred - y).pow(2).sum()
```

```
    loss.backward()
```

Build graph data structure AND
perform computation

PyTorch: Dynamic Computation Graphs



```
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):
```

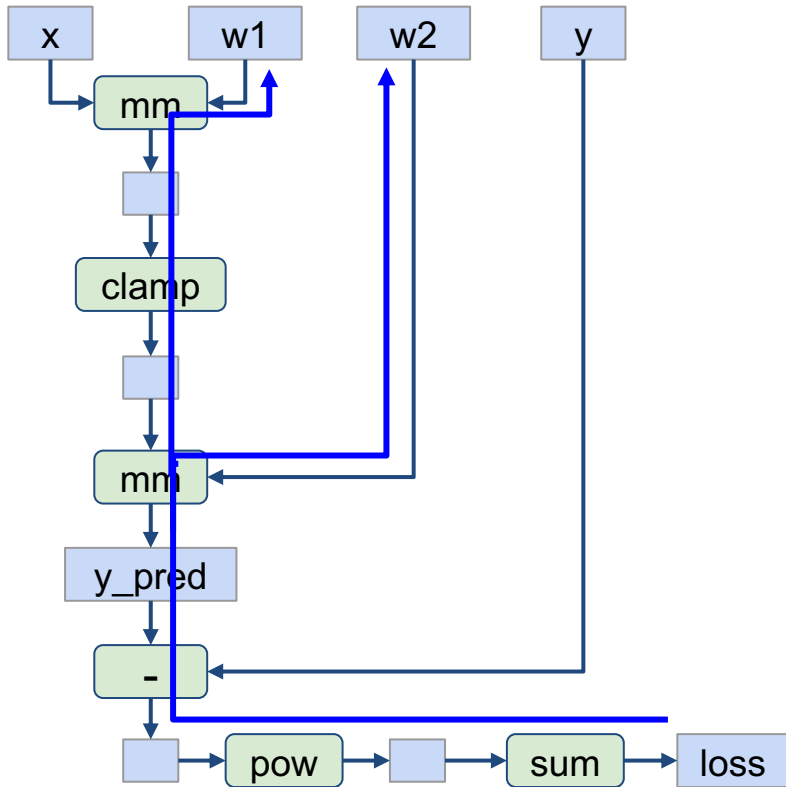
```
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
```

```
    loss = (y_pred - y).pow(2).sum()
```

```
    loss.backward()
```

Build graph data structure AND
perform computation

PyTorch: Dynamic Computation Graphs



```
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()
```

Search for path between loss and `w1`, `w2`
(for backprop) AND perform computation

PyTorch: Dynamic Computation Graphs

x

w1

w2

y

```
import torch

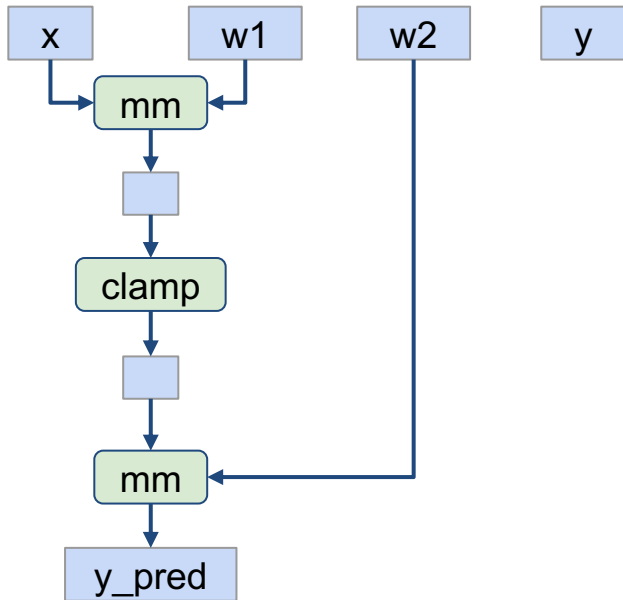
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

Throw away the graph, backprop path, and rebuild it from scratch on every iteration

PyTorch: Dynamic Computation Graphs



```
import torch

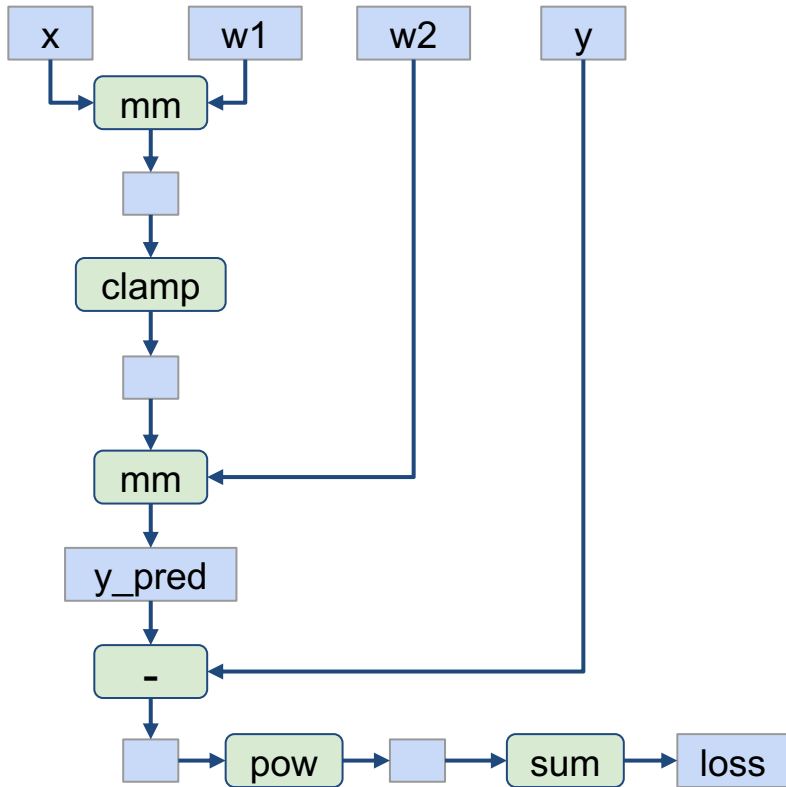
N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2 = torch.randn(H, D_out, requires_grad=True)

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

PyTorch: Dynamic Computation Graphs



```
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):
```

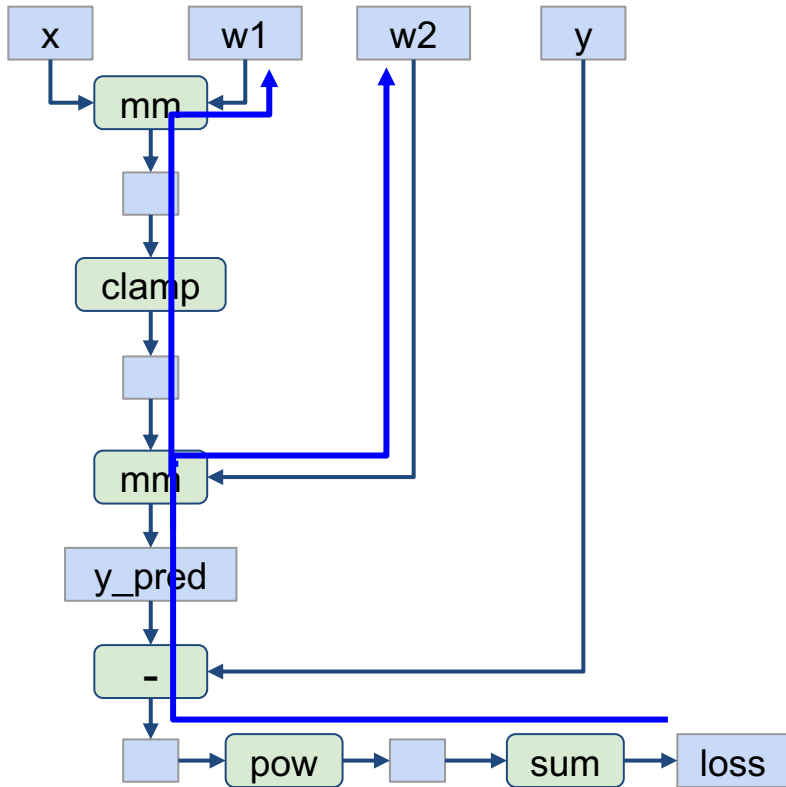
```
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
```

```
    loss = (y_pred - y).pow(2).sum()
```

```
    loss.backward()
```

Build graph data structure AND
perform computation

PyTorch: Dynamic Computation Graphs



```
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()
```

Search for path between loss and `w1`, `w2`
(for backprop) AND perform computation

PyTorch: Dynamic Computation Graphs

Building the graph and **computing** the graph happen at the same time.

Seems inefficient, especially if we are building the same graph over and over again...

```
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()

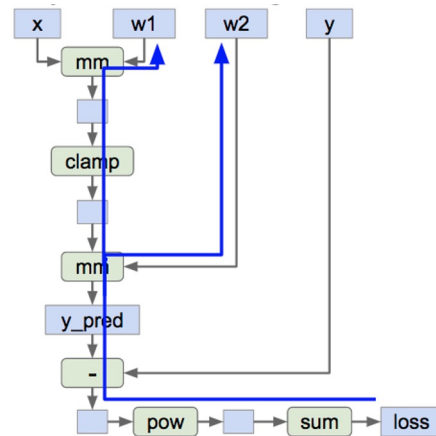
    loss.backward()
```

Static Computation Graphs

Alternative: **Static** graphs

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

Step 2: Reuse the same graph on every iteration



```
graph = build_graph()
```

```
for x_batch, y_batch in loader:  
    run_graph(graph, x=x_batch, y=y_batch)
```

TensorFlow

TensorFlow Versions

Pre-2.0 (1.14 latest)

Default static graph,
optionally dynamic
graph (eager mode).

2.0+

Default dynamic graph,
optionally static graph.
We use 2.4 in this class.

TensorFlow: Neural Net (Pre-2.0)

```
import numpy as np
import tensorflow as tf
```

(Assume imports at the top of each snippet)

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

with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              y: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                    feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```


TensorFlow: Neural Net (Pre-2.0)

First **define**
computational graph



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

Then **run** the graph
many times



```
with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              y: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                    feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```

TensorFlow: 2.0+ vs. pre-2.0

```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

with tf.GradientTape() as tape:
    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))
    gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:
“Eager” Mode by default

```
assert(tf.executing_eagerly())
```

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

with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              y: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                    feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```

Tensorflow 1.13

TensorFlow: 2.0+ vs. pre-2.0

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

with tf.GradientTape() as tape:
    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))
    gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:
“Eager” Mode by default
`assert(tf.executing_eagerly())`

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

with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              v: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                    feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```

Tensorflow 1.13

TensorFlow: 2.0+ vs. pre-2.0

```
N, D, H = 64, 1000, 100
```

```
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
with tf.GradientTape() as tape:
    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))
    gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:

“Eager” Mode by default

```
assert(tf.executing_eagerly())
```

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

```
with tf.Session() as sess:
    values = {x: np.random.randn(N, D),
              w1: np.random.randn(D, H),
              w2: np.random.randn(H, D),
              y: np.random.randn(N, D),}
    out = sess.run([loss, grad_w1, grad_w2],
                    feed_dict=values)
    loss_val, grad_w1_val, grad_w2_val = out
```

Tensorflow 1.13

TensorFlow: Neural Net

Convert input numpy
arrays to TF **tensors**.
Create weights as
tf.Variable

```
N, D, H = 64, 1000, 100
```

```
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)  
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)  
w1 = tf.Variable(tf.random.uniform((D, H))) # weights  
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
with tf.GradientTape() as tape:  
    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))  
gradients = tape.gradient(loss, [w1, w2].)
```

TensorFlow: Neural Net

Use `tf.GradientTape()`
context to build
dynamic computation
graph.

```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

with tf.GradientTape() as tape:
    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))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net

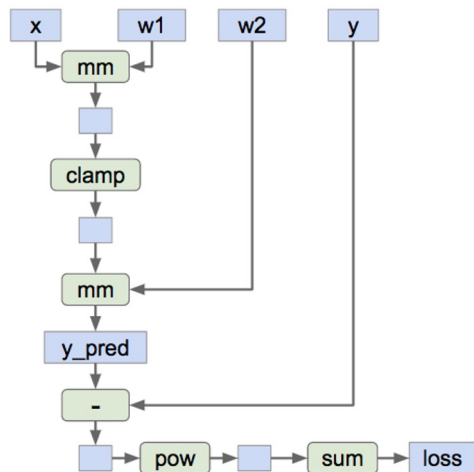
All forward-pass operations in the contexts (including function calls) gets traced for computing gradient later.

```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

with tf.GradientTape() as tape:
    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))
gradients = tape.gradient(loss, [w1, w2]).
```

TensorFlow: Neural Net



Forward pass

```
N, D, H = 64, 1000, 100
```

```
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
with tf.GradientTape() as tape:
```

```
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))
gradients = tape.gradient(loss, [w1, w2].)
```


TensorFlow: Neural Net

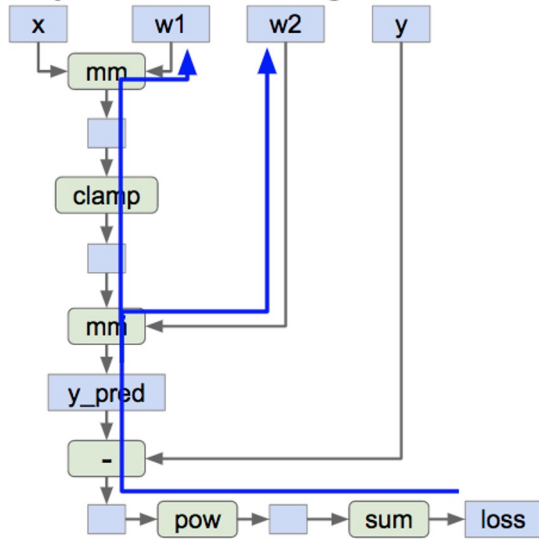
tape.gradient() uses the
traced computation
graph to compute
gradient for the weights

```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

with tf.GradientTape() as tape:
    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))
    gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net



Backward pass

```
N, D, H = 64, 1000, 100
```

```
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
with tf.GradientTape() as tape:
    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))
    gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net

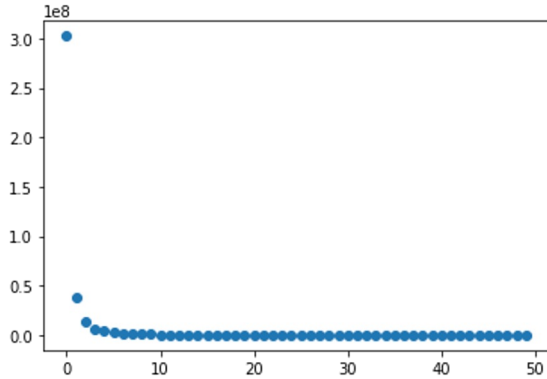
```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
learning_rate = 1e-6
for t in range(50):
    with tf.GradientTape() as tape:
        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))
        gradients = tape.gradient(loss, [w1, w2])
        w1.assign(w1 - learning_rate * gradients[0])
        w2.assign(w2 - learning_rate * gradients[1])
```

Train the network: Run the training step over and over, use gradient to update weights

TensorFlow: Neural Net



Train the network: Run the training step over and over, use gradient to update weights

```
N, D, H = 64, 1000, 100
```

```
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights
```

```
learning_rate = 1e-6
for t in range(50):
    with tf.GradientTape() as tape:
        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))
        gradients = tape.gradient(loss, [w1, w2])
        w1.assign(w1 - learning_rate * gradients[0])
        w2.assign(w2 - learning_rate * gradients[1])
```

TensorFlow: Optimizer

Can use an **optimizer** to compute gradients and update weights

```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

optimizer = tf.optimizers.SGD(1e-6)

learning_rate = 1e-6
for t in range(50):
    with tf.GradientTape() as tape:
        h = 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))
        gradients = tape.gradient(loss, [w1, w2])
    optimizer.apply_gradients(zip(gradients, [w1, w2])).
```

TensorFlow: Loss

Use predefined
loss functions



```
N, D, H = 64, 1000, 100

x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
w1 = tf.Variable(tf.random.uniform((D, H))) # weights
w2 = tf.Variable(tf.random.uniform((H, D))) # weights

optimizer = tf.optimizers.SGD(1e-6)

for t in range(50):
    with tf.GradientTape() as tape:
        h = tf.maximum(tf.matmul(x, w1), 0)
        y_pred = tf.matmul(h, w2)
        diff = y_pred - y
        loss = tf.losses.MeanSquaredError()(y_pred, y)
    gradients = tape.gradient(loss, [w1, w2])
    optimizer.apply_gradients(zip(gradients, [w1, w2]))
```

TensorFlow: High-Level Wrappers

Keras (<https://keras.io/>)

tf.keras (https://www.tensorflow.org/api_docs/python/tf/keras)

tf.estimator (https://www.tensorflow.org/api_docs/python/tf/estimator)

Sonnet (<https://github.com/deepmind/sonnet>)


TFLearn (<http://tflearn.org/>)

TensorLayer (<http://tensorlayer.readthedocs.io/en/latest/>)

@tf.function: compile static graph

tf.function decorator
(implicitly) compiles
python functions to
static graph for better
performance

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,),
                                activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)
```



```
@tf.function
def model_func(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)
    return y_pred, loss

for t in range(50):
    with tf.GradientTape() as tape:
        y_pred, loss = model_func(x, y)
    gradients = tape.gradient(
        loss, model.trainable_variables)
    optimizer.apply_gradients(
        zip(gradients, model.trainable_variables))
```


@tf.function: compile static graph

Here we compare the forward-pass time of the same model under dynamic graph mode and static graph mode

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)
```

```
@tf.function
def model_static(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)
    return y_pred, loss

def model_dynamic(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)
```

```
print("dynamic graph: ", timeit.timeit(lambda: model_dynamic(x, y), number=10))
print("static graph: ", timeit.timeit(lambda: model_static(x, y), number=10))
```

```
dynamic graph: 0.02520249200000535
static graph: 0.03932226699998864
```

@tf.function: compile static graph

Static graph is *in theory* faster than dynamic graph, but the performance gain depends on the type of model / layer / computation graph.

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)
```

```
@tf.function
def model_static(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)
    return y_pred, loss
```

```
def model_dynamic(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)

print("dynamic graph: ", timeit.timeit(lambda: model_dynamic(x, y), number=10))
print("static graph: ", timeit.timeit(lambda: model_static(x, y), number=10))
```

```
dynamic graph: 0.02520249200000535
static graph: 0.03932226699998864
```

@tf.function: compile static graph

Static graph is *in theory* faster than dynamic graph, but the performance gain depends on the type of model / layer / computation graph.

```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer = tf.optimizers.SGD(1e-1)
```

```
@tf.function
def model_static(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)
    return y_pred, loss
```

```
def model_dynamic(x, y):
    y_pred = model(x)
    loss = tf.losses.MeanSquaredError()(y_pred, y)

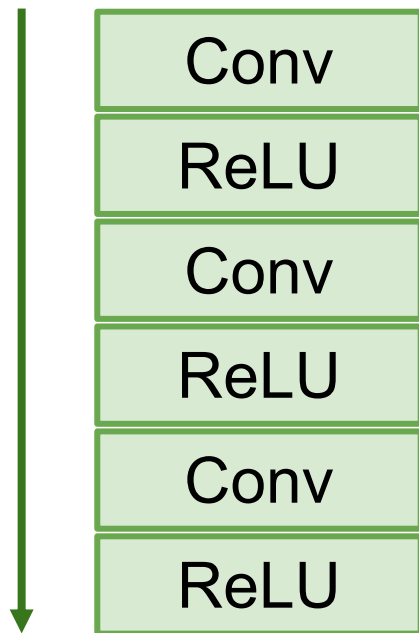
print("dynamic graph:", timeit.timeit(lambda: model_dynamic(x, y), number=1000))
print("static graph:", timeit.timeit(lambda: model_static(x, y), number=1000))
```

```
dynamic graph: 2.3648411540000325
static graph: 1.1723986679999143
```

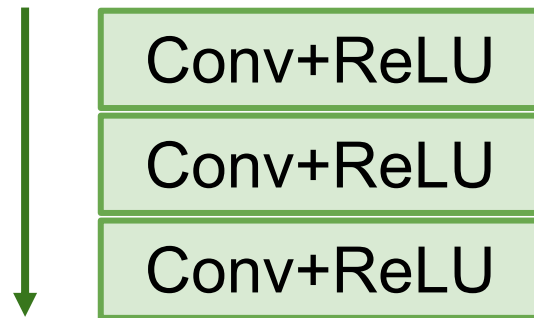
Static vs Dynamic: Optimization

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

The graph you wrote



Equivalent graph with **fused operations**



Static PyTorch: TorchScript

```
graph(%self.1 :
  __torch__.torch.nn.modules.module.__torch_mangle_4.Module,
    %input : Float(3, 4),
    %h : Float(3, 4)):
  %19 :
  __torch__.torch.nn.modules.module.__torch_mangle_3.Module =
  prim::GetAttr[name="linear"](%self.1)
  %21 : Tensor =
  prim::CallMethod[name="forward"](%19, %input)
  %12 : int = prim::Constant[value=1]() #
  <ipython-input-40-26946221023e>:7:0
  %13 : Float(3, 4) = aten::add(%21, %h, %12) #
  <ipython-input-40-26946221023e>:7:0
  %14 : Float(3, 4) = aten::tanh(%13) #
  <ipython-input-40-26946221023e>:7:0
  %15 : (Float(3, 4), Float(3, 4)) =
  prim::TupleConstruct(%14, %14)
  return (%15)
```

```
class MyCell(torch.nn.Module):
    def __init__(self):
        super(MyCell, self).__init__()
        self.linear = torch.nn.Linear(4, 4)

    def forward(self, x, h):
        new_h = torch.tanh(self.linear(x) + h)
        return new_h, new_h

my_cell = MyCell()
x, h = torch.rand(3, 4), torch.rand(3, 4)
traced_cell = torch.jit.trace(my_cell, (x, h))
print(traced_cell.graph)
traced_cell(x, h)
```

Build static graph with `torch.jit.trace`

PyTorch vs TensorFlow, Static vs Dynamic

PyTorch

Dynamic Graphs

Static: TorchScript

TensorFlow

Dynamic: Eager

Static: @tf.function

Static vs Dynamic: Serialization

Static

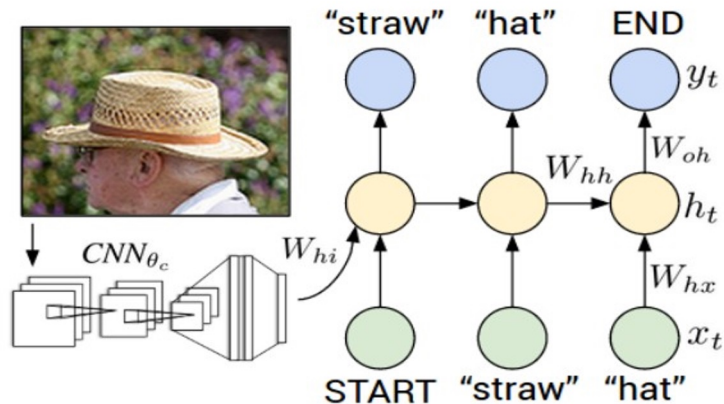
Once graph is built, can **serialize** it and run it without the code that built the graph!

Dynamic

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

Dynamic Graph Applications

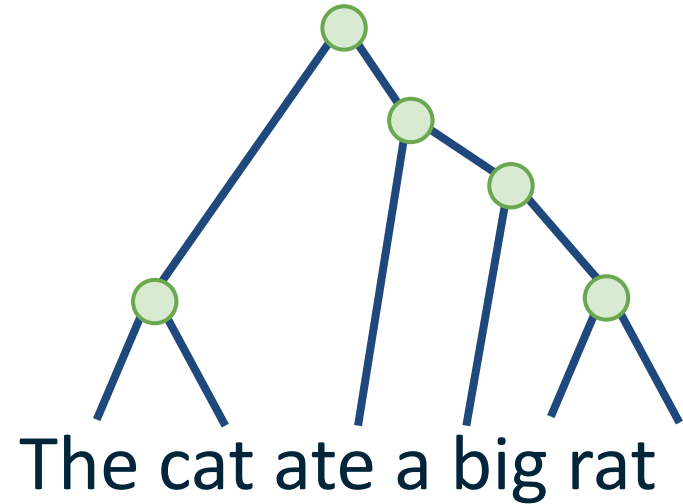
- Recurrent networks



Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015
Figure copyright IEEE, 2015. Reproduced for educational purposes.

Dynamic Graph Applications

- Recurrent networks
- Recursive networks



Dynamic Graph Applications

- Recurrent networks
- Recursive networks
- Modular networks

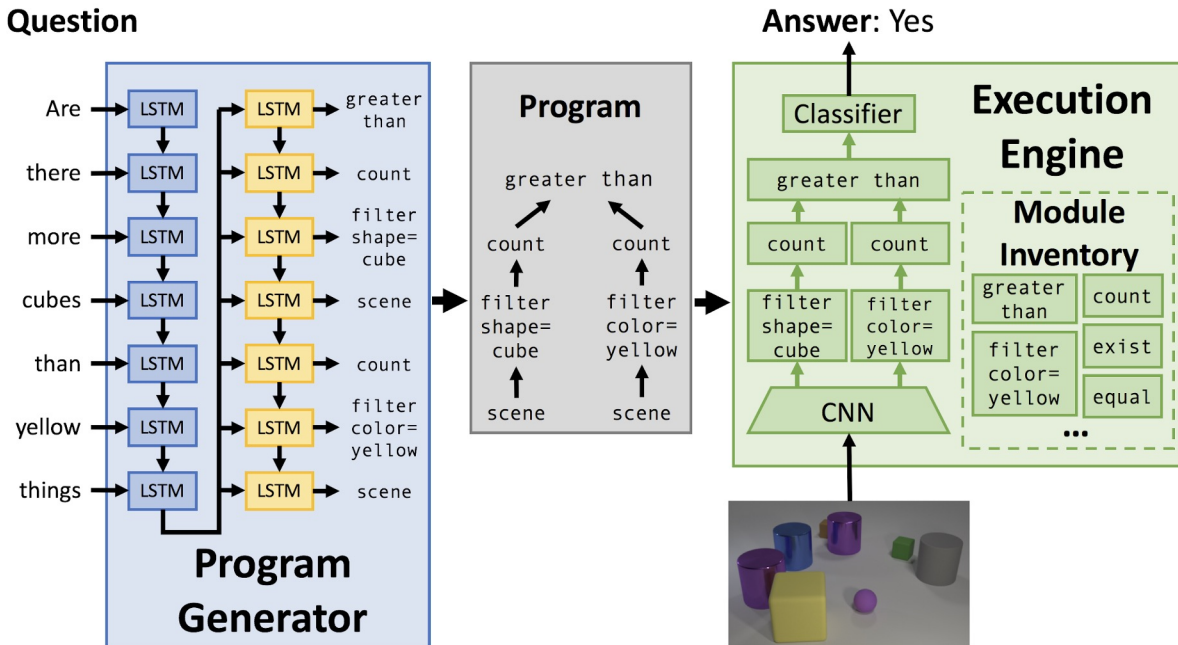


Figure copyright Justin Johnson, 2017. Reproduced with permission.

Andreas et al, "Neural Module Networks", CVPR 2016

Andreas et al, "Learning to Compose Neural Networks for Question Answering", NAACL 2016

Johnson et al, "Inferring and Executing Programs for Visual Reasoning", ICCV 2017

Dynamic Graph Applications

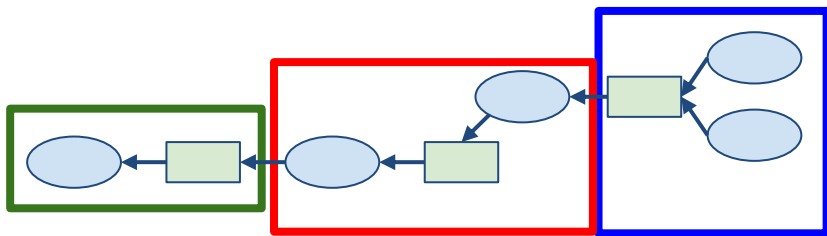
- Recurrent networks
- Recursive networks
- Modular Networks
- (Your creative idea here)

Model Parallel vs. Data Parallel

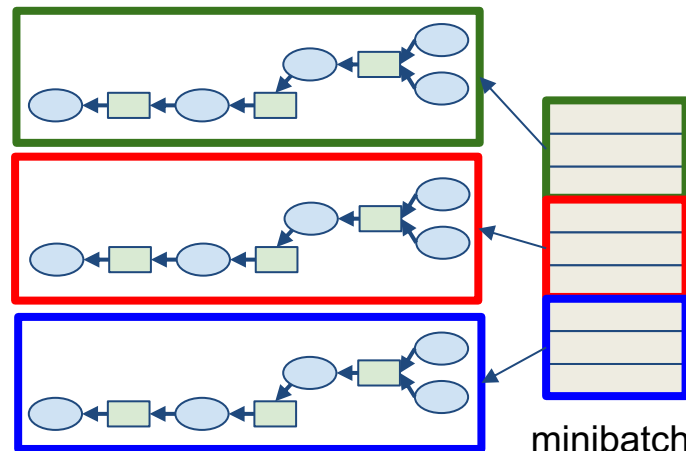
Model parallelism:
split computation
graph into parts &
distribute to GPUs/
nodes



Data parallelism: split
minibatch into chunks &
distribute to GPUs/ nodes



Model Parallel



Data Parallel

PyTorch: Data Parallel

`nn.DataParallel`

Pro: Easy to use (just wrap the model and run training script as normal)

Con: Single process & single node. Can be bottlenecked by CPU with large number of GPUs (8+).

`nn.DistributedDataParallel`

Pro: Multi-nodes & multi-process training

Con: Need to hand-designate device and manually launch training script for each process / nodes.

Horovod (<https://github.com/horovod/horovod>): Supports both PyTorch and TensorFlow

<https://pytorch.org/docs/stable/nn.html#dataparallel-layers-multi-gpu-distributed>

TensorFlow: Data Parallel

[tf.distributed.Strategy](#)

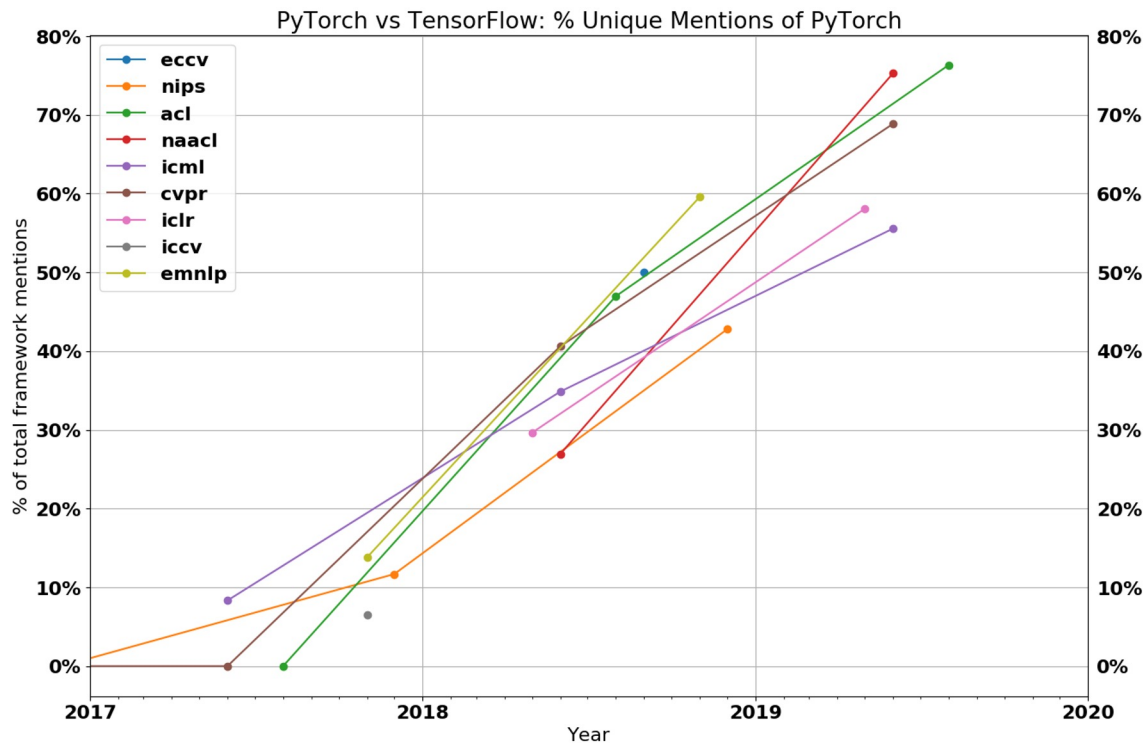
```
strategy = tf.distribute.MirroredStrategy()

with strategy.scope():
    model = tf.keras.Sequential([
        tf.keras.layers.Conv2D(32, 3, activation='relu', input_shape=(28, 28, 1)),
        tf.keras.layers.MaxPooling2D(),
        tf.keras.layers.Flatten(),
        tf.keras.layers.Dense(64, activation='relu'),
        tf.keras.layers.Dense(10)
    ])

    model.compile(loss=tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True),
                  optimizer=tf.keras.optimizers.Adam(),
                  metrics=['accuracy'])
```

<https://www.tensorflow.org/tutorials/distribute/keras>

PyTorch vs. TensorFlow: Academia



<https://thegradient.pub/state-of-ml-frameworks-2019-pytorch-dominates-research-tensorflow-dominates-industry/>

PyTorch vs. TensorFlow: Academia

CONFERENCE	PT 2018	PT 2019	PT GROWTH	TF 2018	TF 2019	TF GROWTH
CVPR	82	280	240%	116	125	7.7%
NAACL	12	66	450%	34	21	-38.2%
ACL	26	103	296%	34	33	-2.9%
ICLR	24	70	192%	54	53	-1.9%
ICML	23	69	200%	40	53	32.5%

<https://thegradient.pub/state-of-ml-frameworks-2019-pytorch-dominates-research-tensorflow-dominates-industry/>

My Advice:

PyTorch is my personal favorite. Clean API, native dynamic graphs make it very easy to develop and debug. Can build model using the default API then compile static graph using JIT. Almost all academic research uses PyTorch

TensorFlow's syntax became a lot more intuitive after 2.0. Not perfect but has huge community and wide usage. Can use same framework for research and production. Probably use a higher-level wrapper (Keras, Sonnet, etc.).