Lecture 9:
Hardware and Software

Assignment 3 Released

We released Assignment 3 last night

Modular backprop API
Fully-connected networks
Dropout
Convolutional Networks
Batch Normalization

Due **Monday, October 14, 11:59pm**
Remember to validate your submission

We had a few hotfixes today; check Piazza for details

Deep Learning Hardware

Inside a computer

This image copyright 2017, Justin Johnson

Inside a computer

GPU: "Graphics Processing Unit"

This image is in the public domain

This image copyright 2017, Justin Johnson

Inside a computer

CPU: "Central Processing Unit"

GPU: "Graphics Processing Unit"

NVIDIA vs AMD

NVIDIA vs AMD

GigaFLOPs per Dollar
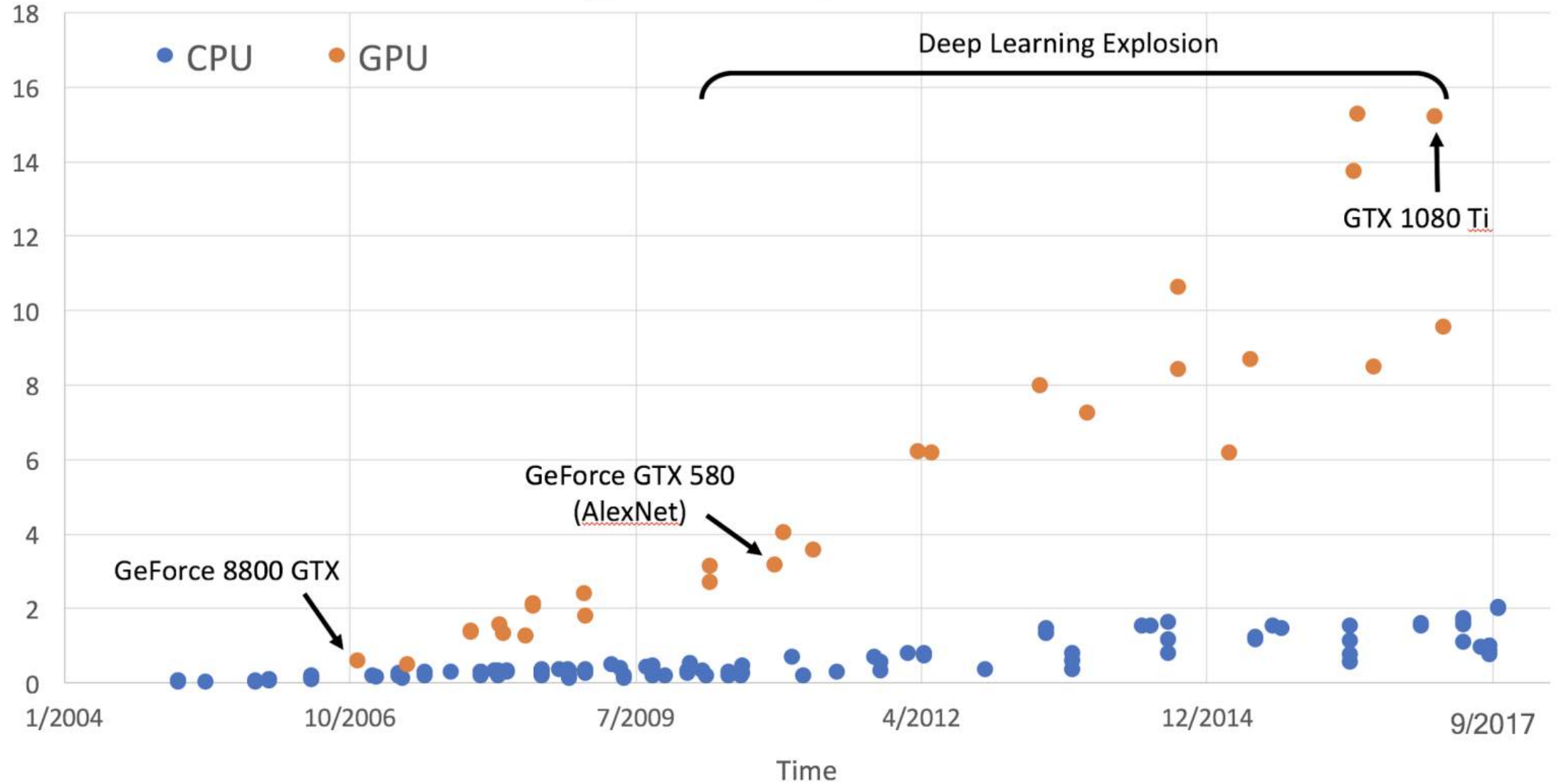
CPU vs GPU

	Cores	Clock Speed (GHz)	Memory	Price	TFLOP/sec
CPU Ryzen 9 3950X	16 (32 threads with hyperthreading)	3.5 (4.7 boost)	System RAM	$749	~4.8 FP32
GPU NVIDIA Titan RTX	4608	1.35 (1.77 boost)	24 GB GDDR6	$2499	~16.3 FP32

CPU: Fewer cores, but each core is much faster and much more capable; great at sequential tasks
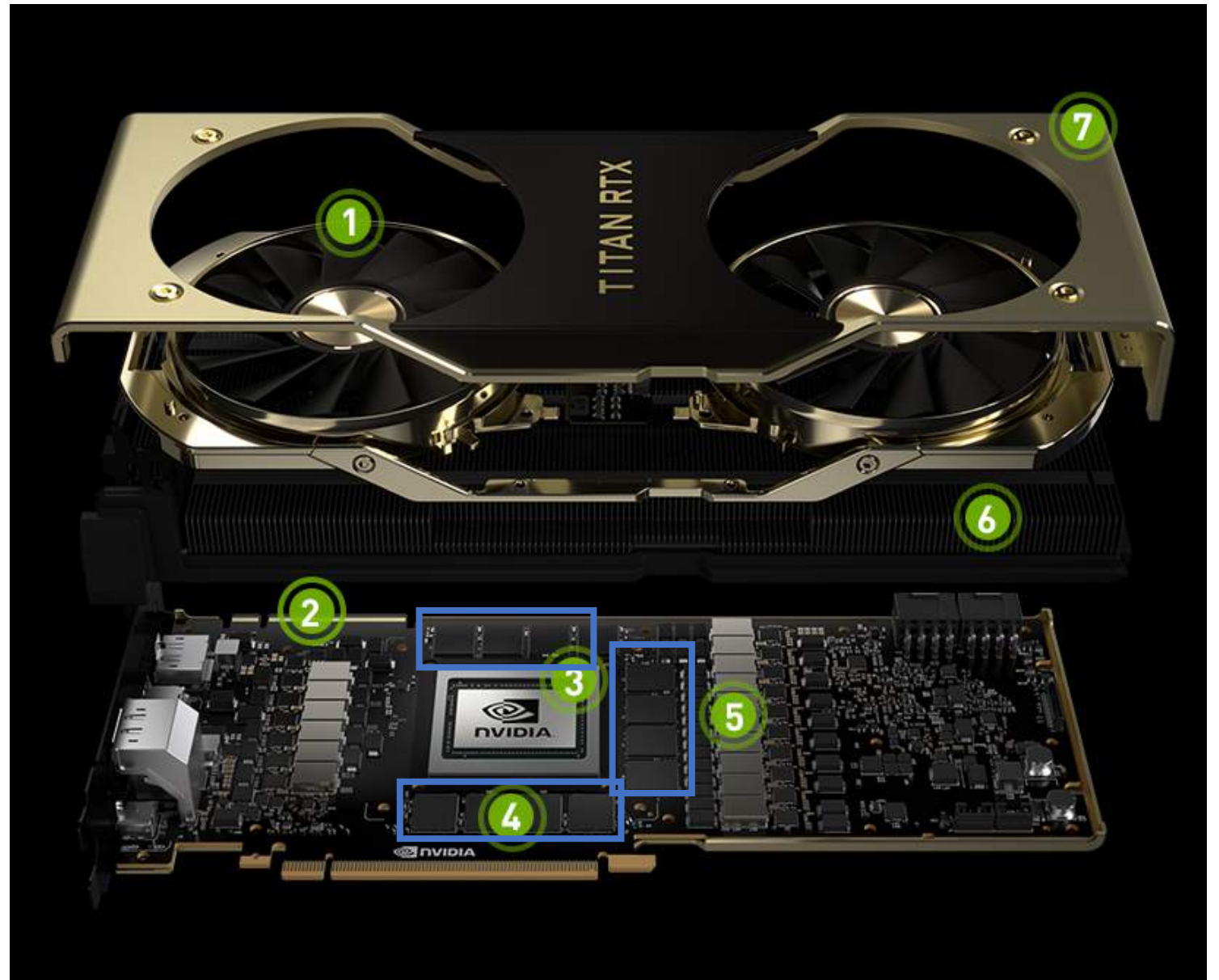
GPU: More cores, but each core is much slower and "dumber"; great for parallel tasks

Inside a GPU:
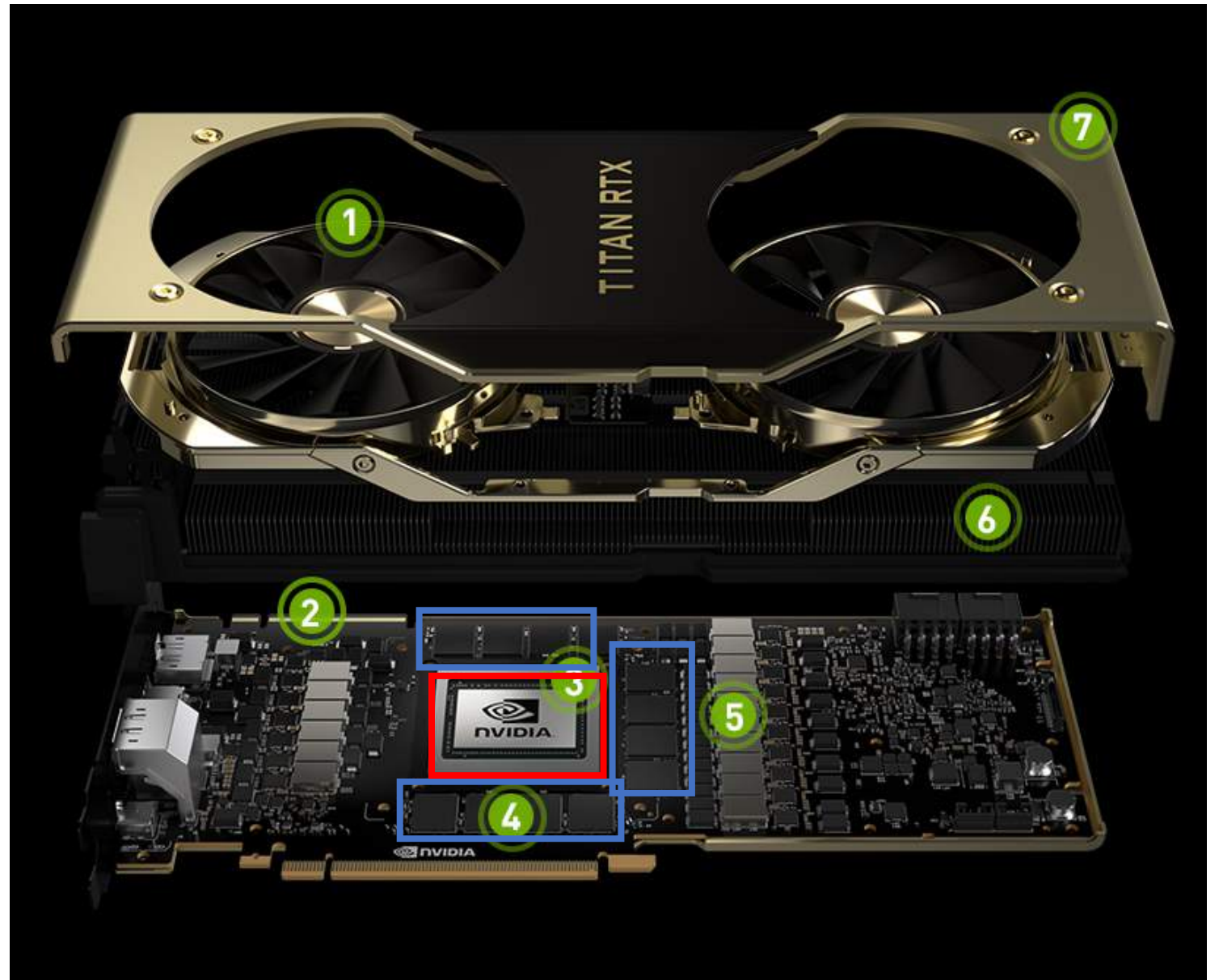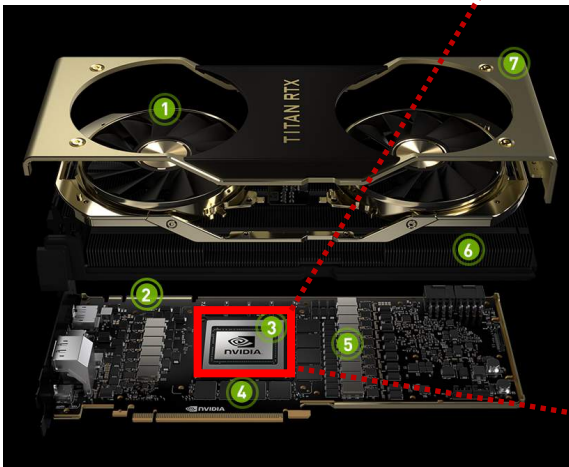# RTX Titan
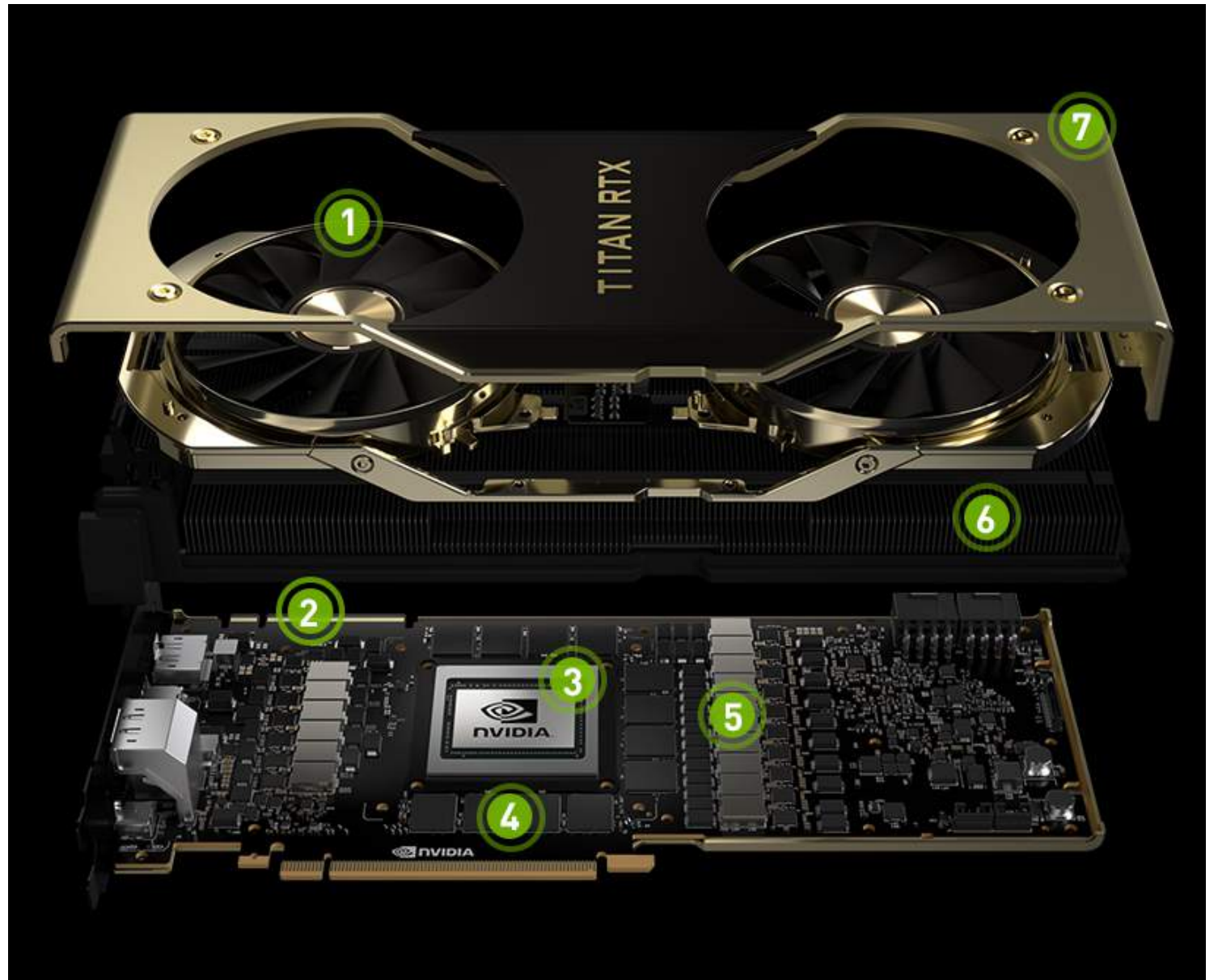
Inside a GPU: RTX Titan

12x 2GB memory modules

Inside a GPU: RTX Titan

12x 2GB memory modules

Processor

Inside a GPU: RTX Titan
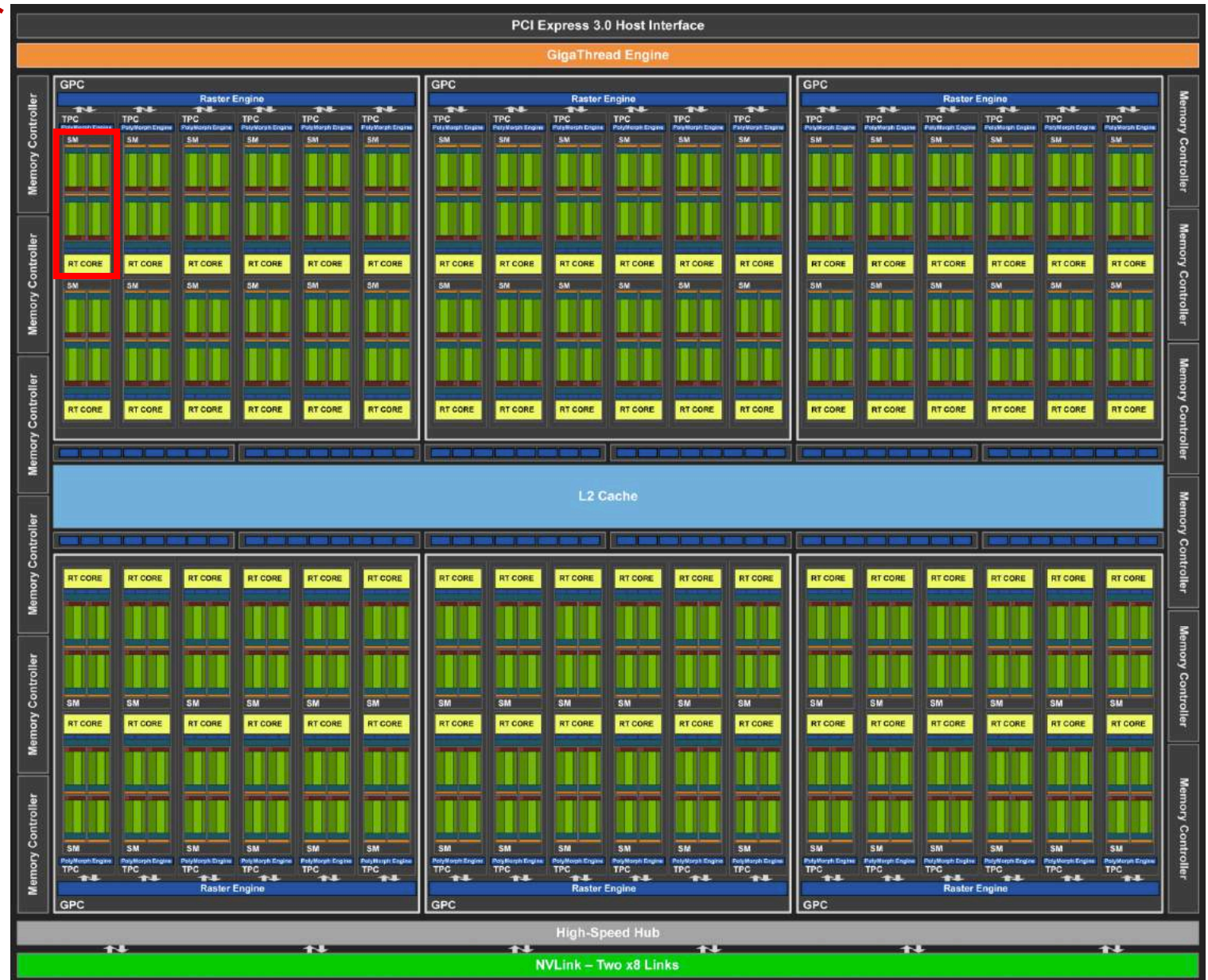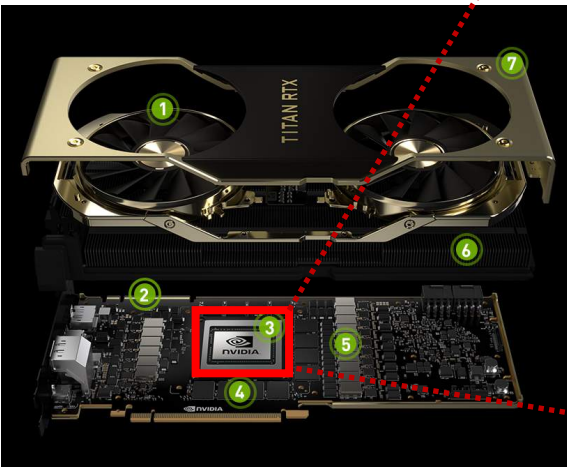
Inside a GPU: RTX Titan

72 Streaming multiprocessors (SMs)

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64 FP32 cores per SM

72 Streaming multiprocessors (SMs)

Inside a GPU: RTX Titan

(72 SM) * (64 FP32 core per SM) * (2 FLOP/cycle)
* (1.77 Gcycle/sec) = **16.3 TFLOP/sec**

64 FP32 cores per SM

72 Streaming multiprocessors (SMs)

Inside a GPU: RTX Titan

(72 SM) * (64 FP32 core per SM) * (2 FLOP/cycle) * (1.77 Gcycle/sec) = **16.3 TFLOP/sec**

Tensor cores use **mixed precision**: Multiplication is done in FP16, and addition is done in FP32

72 Streaming multiprocessors (SMs)

64 FP32 cores per SM

8 Tensor Core per SM

Tensor core: Special hardware!

Let A,B,C be 4x4 matrices; computes AB+C in one clock cycle! (128 FLOP)
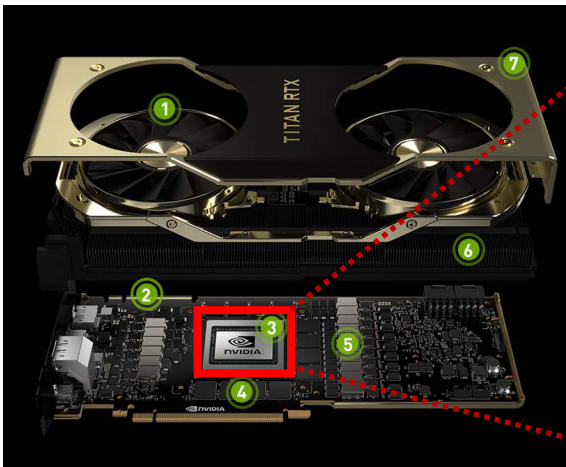
Inside a GPU: RTX Titan

(72 SM) * (64 FP32 core per SM) * (2 FLOP/cycle)
* (1.77 Gcycle/sec) = **16.3 TFLOP/sec**
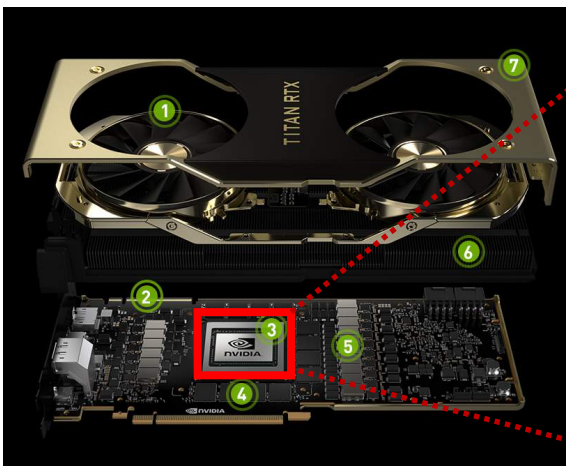
(72 SM) * (8 tensor core per SM)
* (128 FLOP/cycle) * (1.77 Gcycle/sec)
= **130 TFLOP/sec**!

72 Streaming multiprocessors (SMs)

64 FP32 cores per SM

8 Tensor Core per SM

Tensor core: Special hardware!

Let A,B,C be 4x4 matrices; computes AB+C in one clock cycle! (128 FLOP)
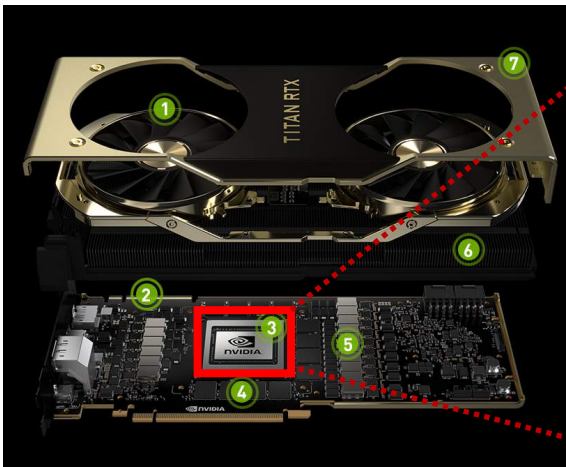
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GPU NVIDIA Titan RTX	4608	1.35 (1.77 boost)	24 GB GDDR6	$2499	~16.3 FP32 ~**130** with Tensor Cores

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

GigaFLOPs per Dollar
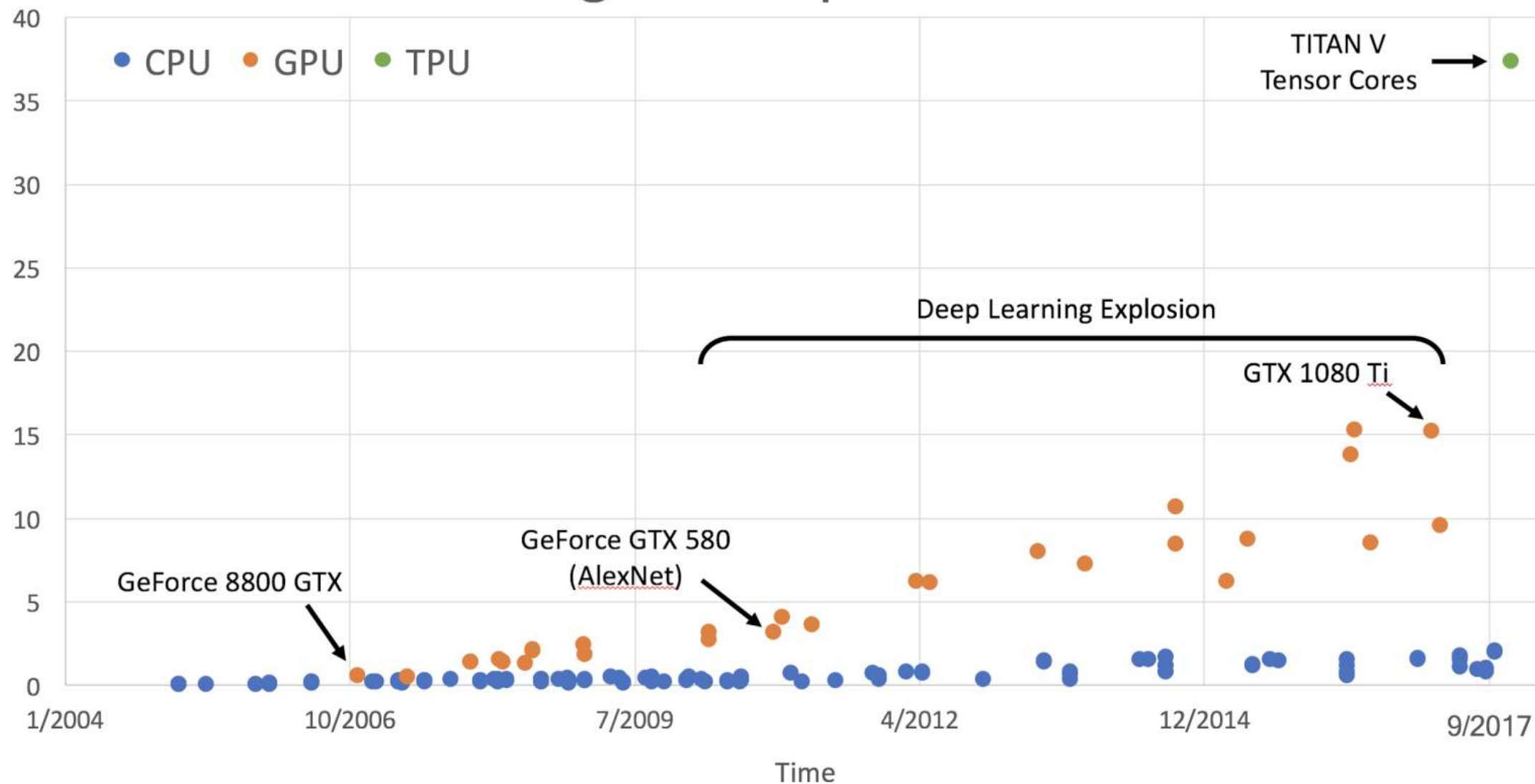
Example: Matrix Multiplication

A x B

B x C
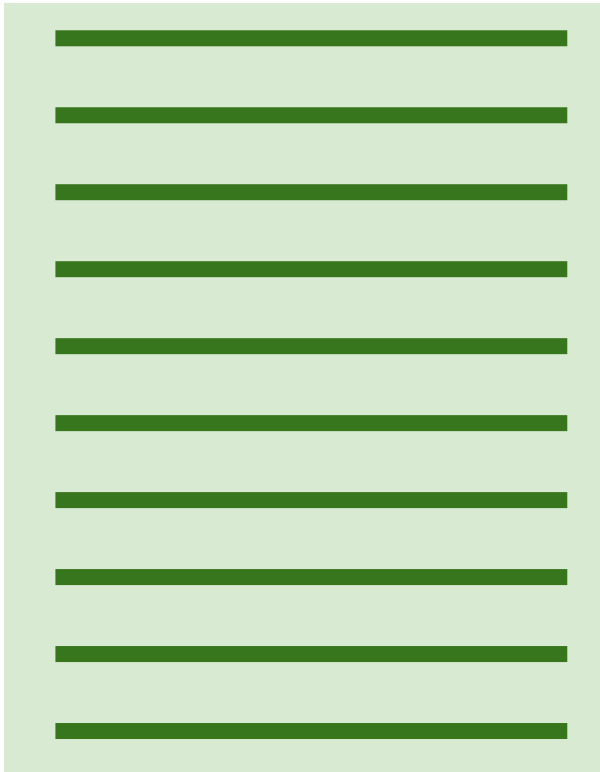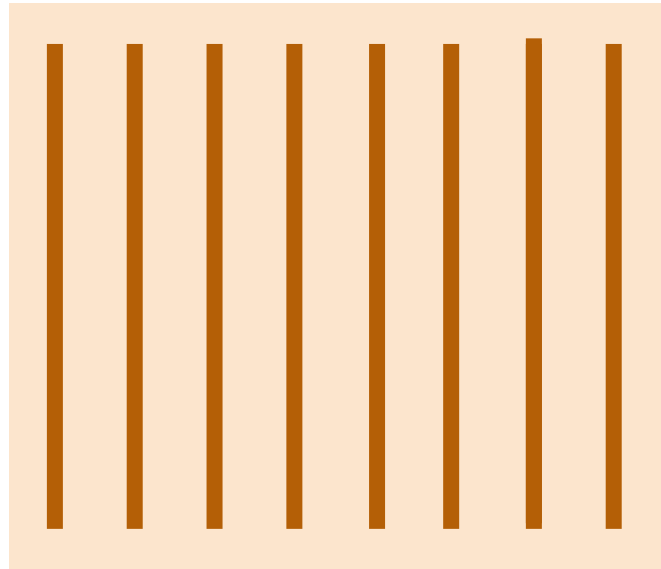
A x C

=
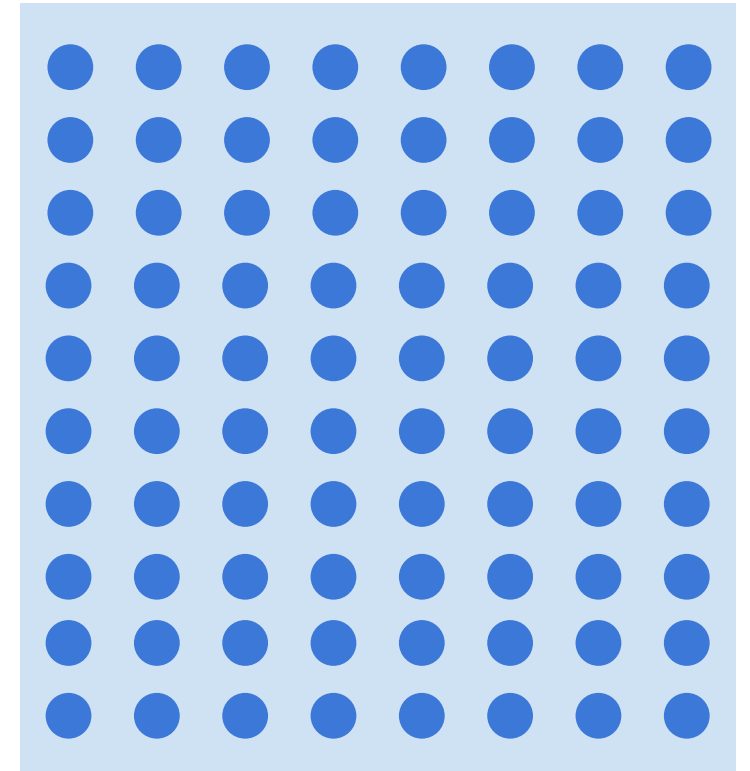
Perfect for GPUs! All output
elements are independent,
can be trivially parallelized

Programming GPUs

- CUDA (NVIDIA only)
  - Write C-like code that runs directly on the GPU
  - NVIDIA provides optimized APIs: cuBLAS, cuFFT, cuDNN, etc
- OpenCL
  - Similar to CUDA, but runs on anything
  - Usually slower on NVIDIA hardware
- EECS 598.009: Applied GPU Programming

Scaling up: Typically 8 GPUs per server

NVIDIA DGX-1: 8x V100 GPUs

Google Tensor Processing Units (TPU)

Special hardware for matrix multiplication, similar to NVIDIA Tensor Cores; also runs in mixed precision (bfloat16)

Cloud TPU v2
180 TFLOPs
64 GB HBM memory
$4.50 / hour
(free on Colab!)

Google Tensor Processing Units (TPU)
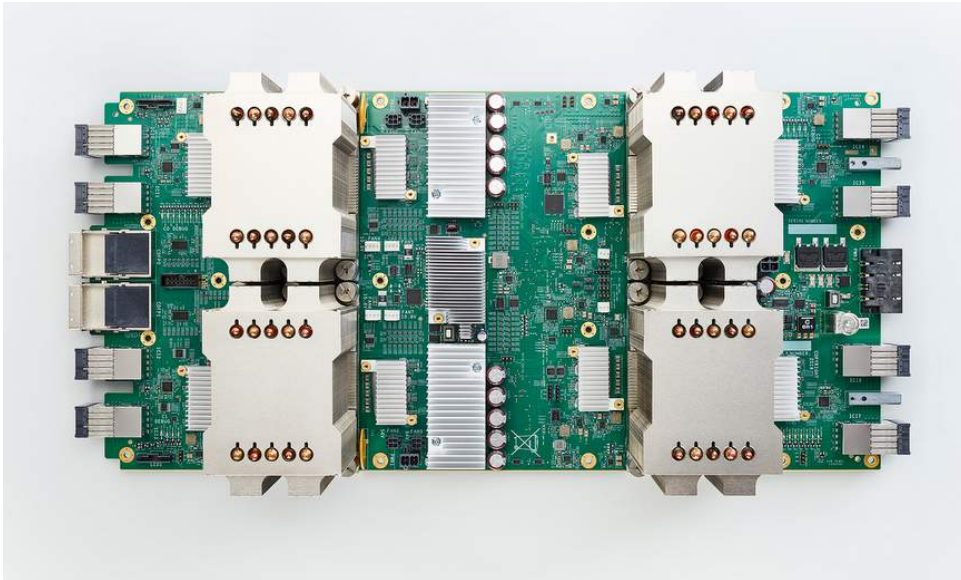
Cloud TPU v2
180 TFLOPs
64 GB HBM memory
$4.50 / hour
(free on Colab!)

Cloud TPU v2 Pod
64 TPU-v2
11.5 PFLOPs
$384 / hour

Google Tensor Processing Units (TPU)
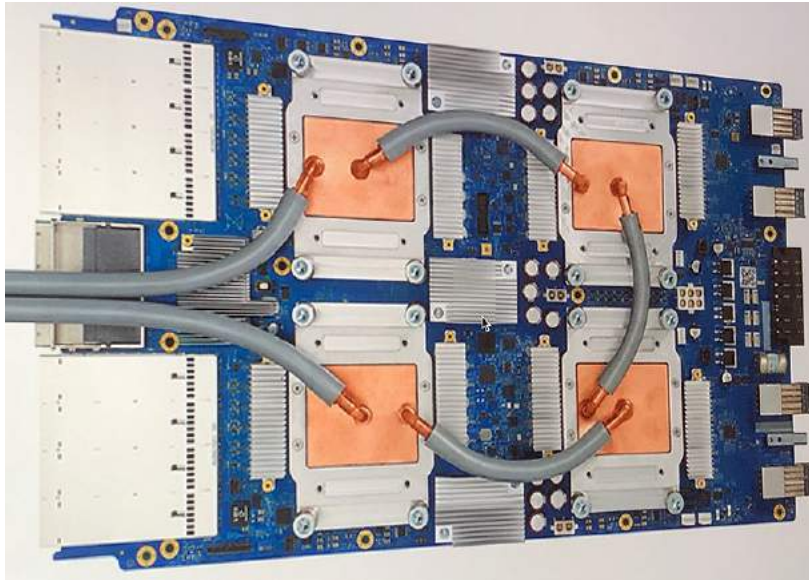
Cloud TPU v3
420 TFLOPs

128 GB HBM memory

$8 / hour

Google Tensor Processing Units (TPU)
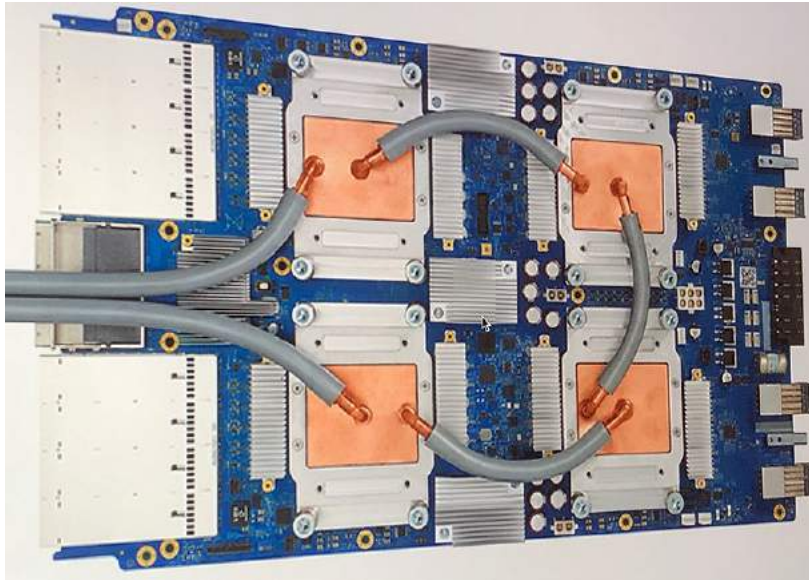
Cloud TPU v3
420 TFLOPs

128 GB HBM memory

$8 / hour

Cloud TPU v3 Pod
256 TPU-v3

107 PFLOPs

Google Tensor Processing Units (TPU)

In order to use TPUs, you have to use TensorFlow

Google Tensor Processing Units (TPU)

In order to use TPUs, you have to use TensorFlow

... For now!

pytorch / pytorch

Watch ▼ 1,329 | ★ Unstar 32,014

<> Code | ⊙ Issues 3,355 | Pull requests 915 | ▶ Actions | Projects 5 | Wiki | Security | Insights
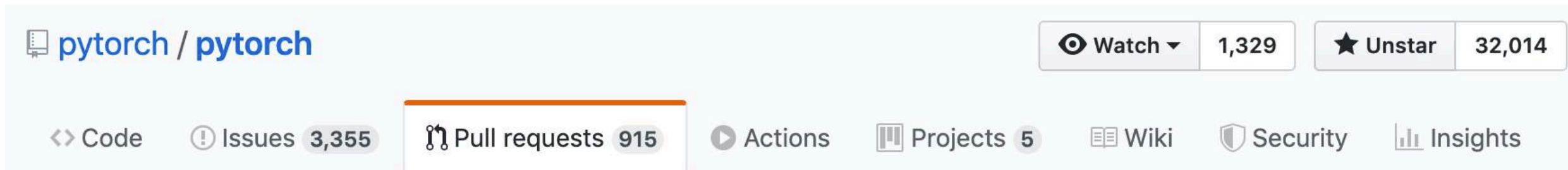
Add XLA / TPU device type, backend type and type id (#16585) #16763

Deep Learning Software

A zoo of frameworks!

PaddlePaddle
(Baidu)

Chainer

Caffe
(UC Berkeley)

→ Caffe2
(Facebook)

MXNet
(Amazon)

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

CNTK
(Microsoft)

Torch
(NYU / Facebook)

→ PyTorch
(Facebook)

JAX
(Google)

Theano
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JAX
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We'll focus on these
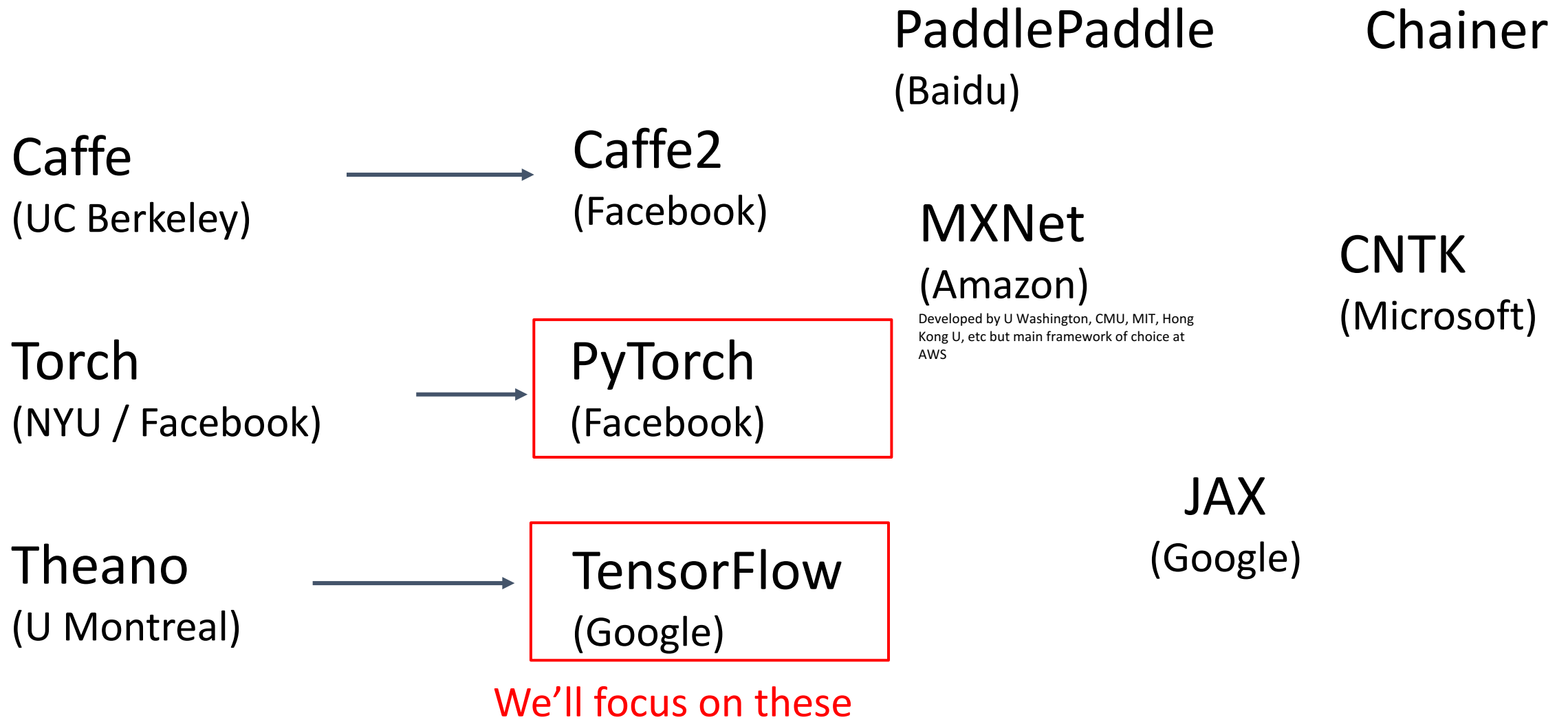
Recall: Computational Graphs

$$f = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

s (scores)

hinge loss

+

L

R

$$R(W)$$
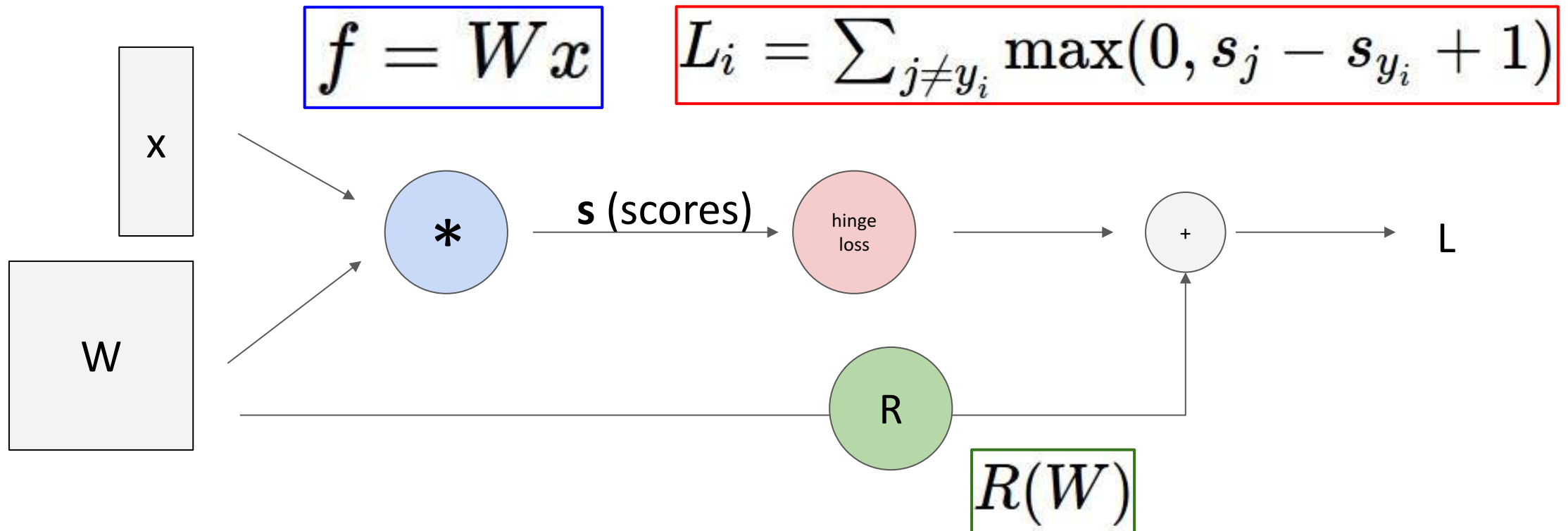
The point of deep learning frameworks

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

PyTorch

PyTorch: Versions

For this class we are using **PyTorch version 1.2** (Released August 2019)

Be careful if you are looking at older PyTorch code – the API changed a lot before 1.0 (0.3 to 0.4 had big changes!)

PyTorch: Fundamental Concepts

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

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

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

PyTorch: Fundamental Concepts

Tensor: Like a numpy array, but can run on GPU   **A1, A2, A3**

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

A4, A5, A6

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

PyTorch: Tensors

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

```python
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

```python
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)
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    grad_w1 = x.t().mm(grad_h)

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    w2 -= learning_rate * grad_w2
```

Forward pass: compute predictions and loss

PyTorch: Tensors

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    grad_h[h < 0] = 0
    grad_w1 = x.t().mm(grad_h)

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

Backward pass: manually compute gradients

PyTorch: Tensors

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    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!

```python
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)
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    w1 -= learning_rate * grad_w1
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```

PyTorch: Autograd

Creating Tensors with **requires_grad=True** enables autograd

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

```python
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

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

Do want gradients with
respect to weights

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import torch

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        w1 -= learning_rate * w1.grad
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        w1.grad.zero_()
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```

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

PyTorch: Autograd

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```

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

PyTorch: Autograd

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```

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

PyTorch: Autograd

x   w1

mm

clamp

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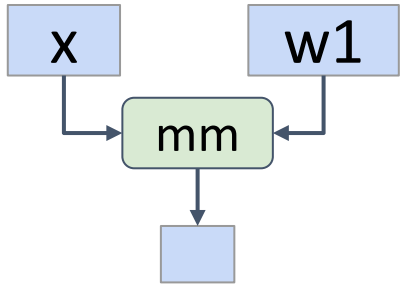requires_grad=True

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```

PyTorch: Autograd

```
x    w1    w2
```

```
x ──┐
    ├─→ mm
w1 ──┘
        │
        ▼
       [ ]
        │
        ▼
     clamp
        │
        ▼
       [ ]
        │
        ├─→ mm ←── w2
        ▼
     y_pred
```
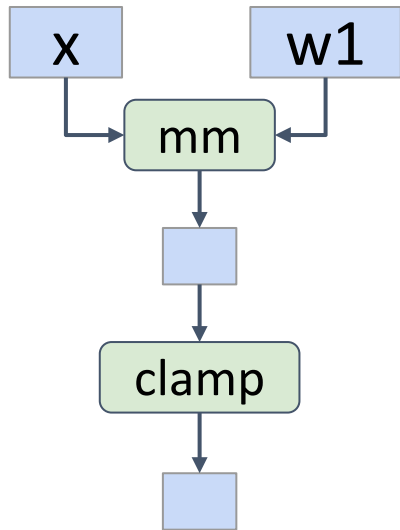
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learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```
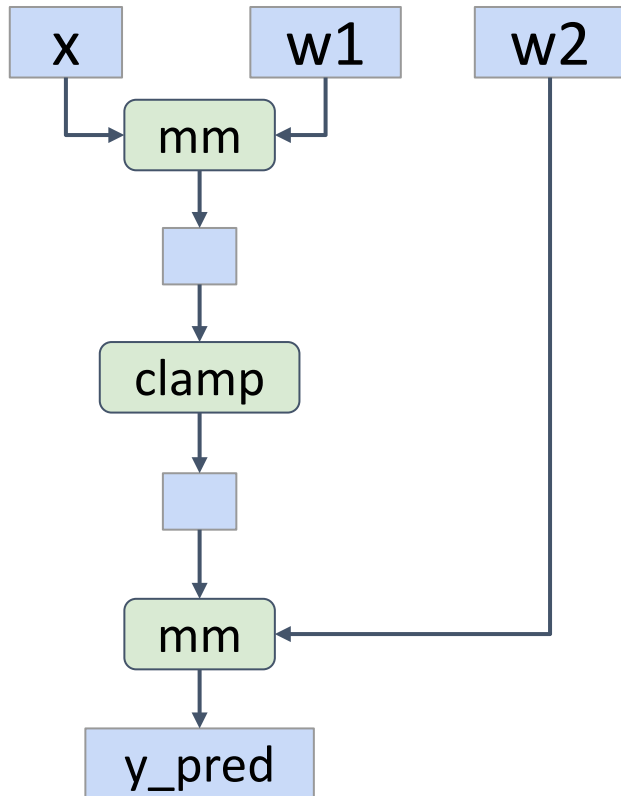
PyTorch: Autograd


```python
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


```python
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_()
```

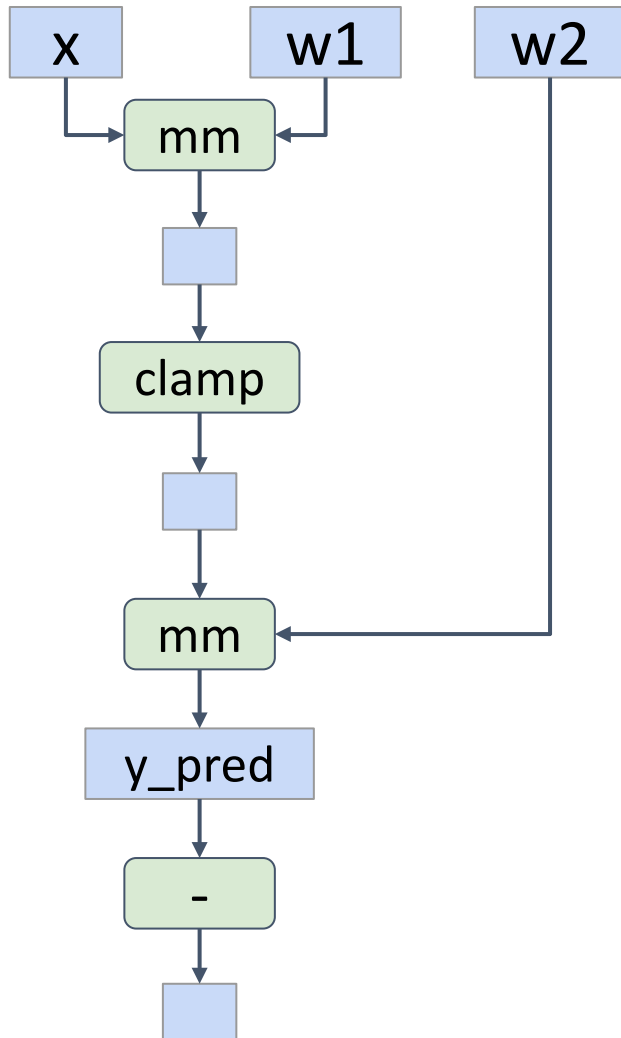# PyTorch: Autograd


```python
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 leaf nodes.

Backprop to all inputs that require grad
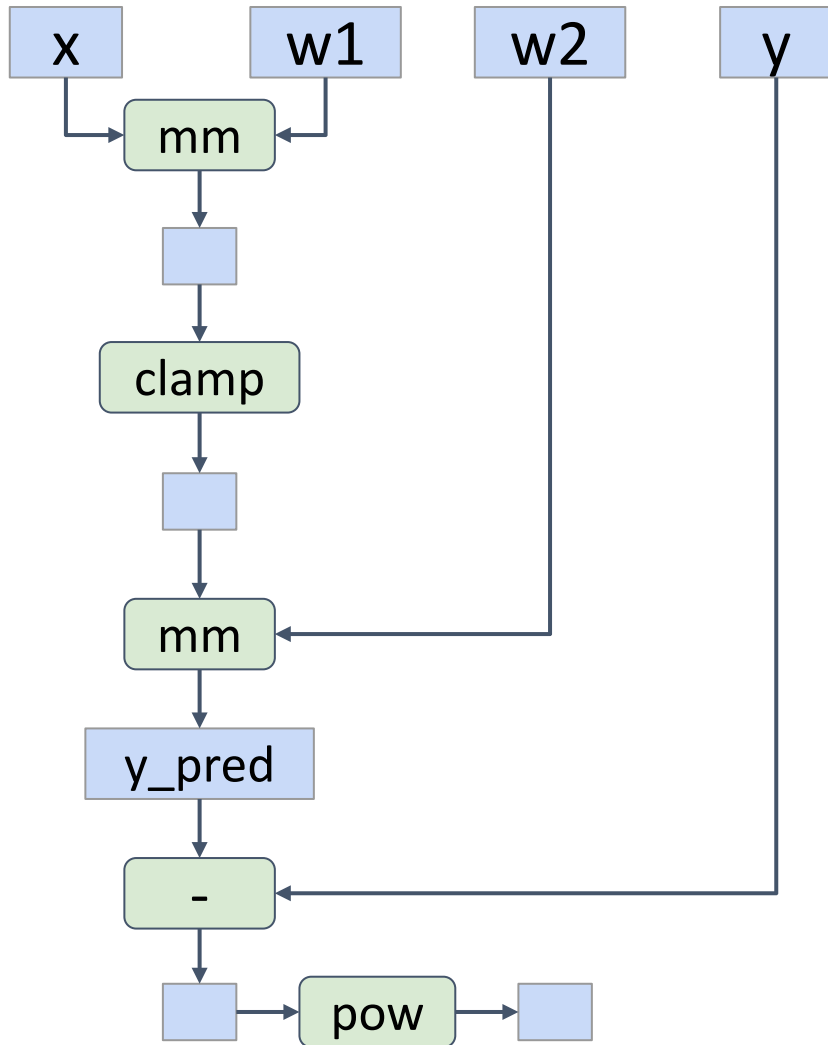
```python
import torch

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_()
```

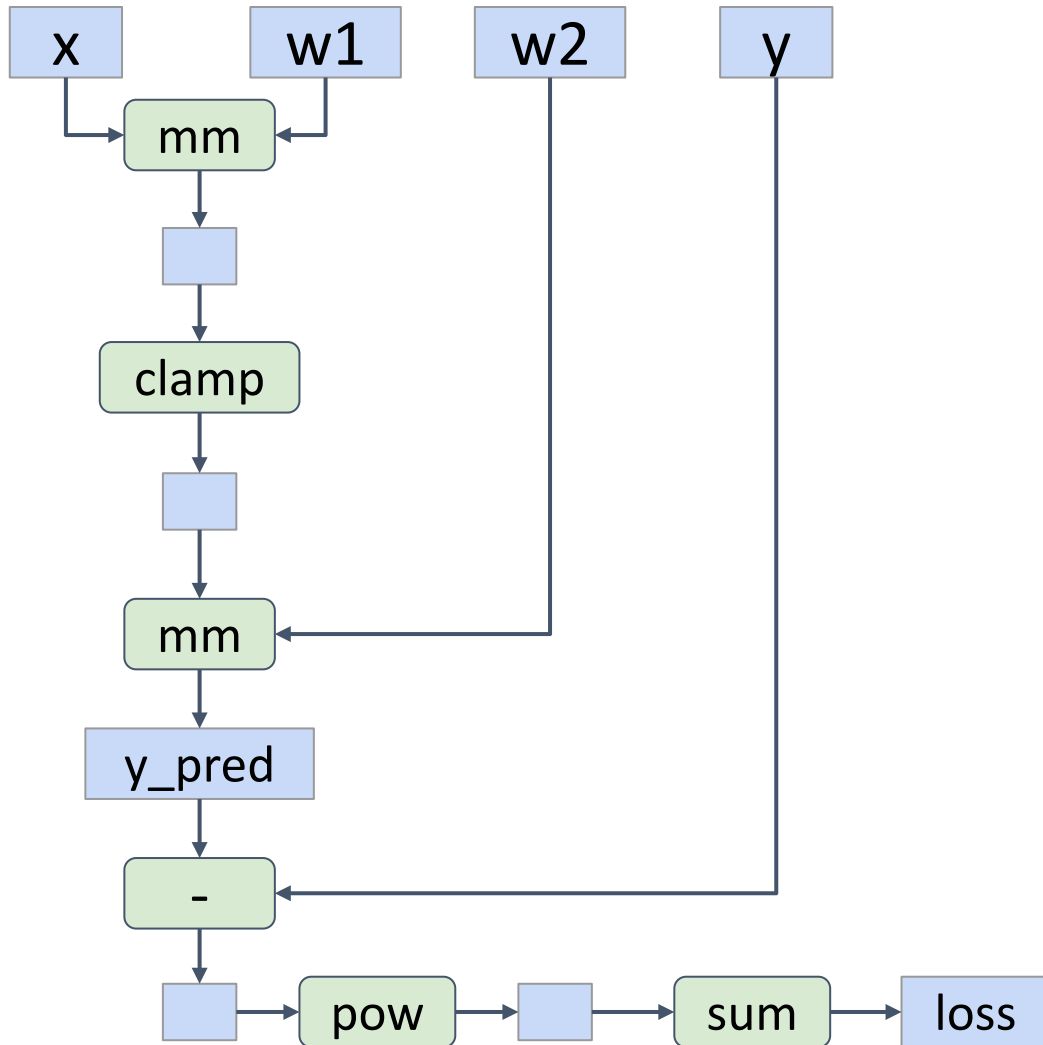# PyTorch: Autograd

x   w1   w2   y

```python
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_()
```

→ ReLU (handwritten annotation pointing to `clamp(min=0)`)

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

PyTorch: Autograd

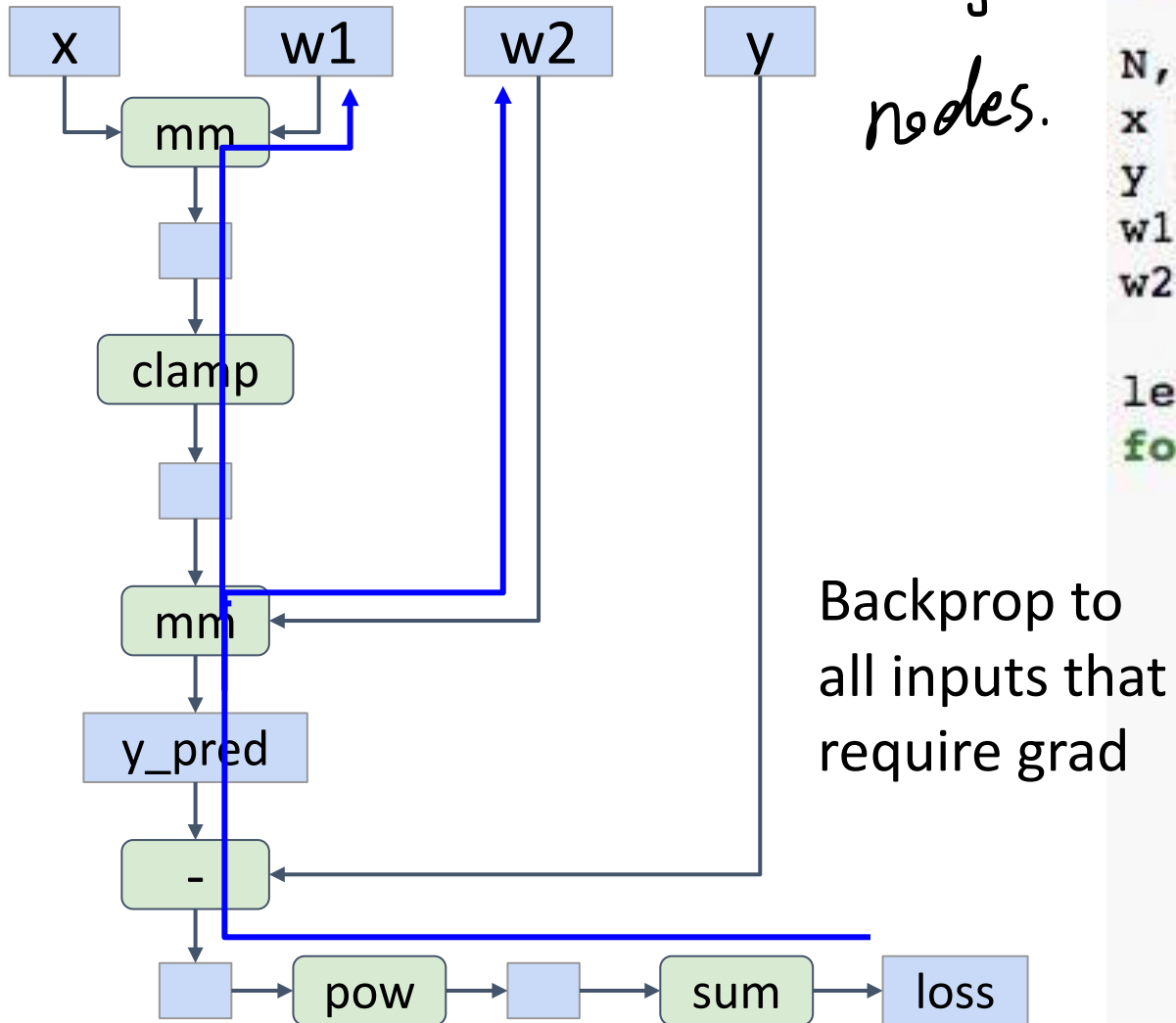x   w1   w2   y

```python
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_()
```

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

Make gradient step on weights

PyTorch: Autograd

x   w1   w2   y

```python
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_()
```

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

Set gradients to zero – forgetting this is a common bug!

PyTorch: Autograd

| 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()

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```
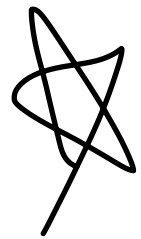
After backward finishes, gradients are **accumulated** into w1.grad and w2.grad and the graph is destroyed

Tell PyTorch not to build a graph for these operations

manager

PyTorch: New functions

Can define new operations
using Python functions

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

```python
import torch

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

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

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

    loss.backward()
    if t % 50 == 0:
        print(t, loss.item())

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: New functions

Can define new operations
using Python functions

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


When our function runs,
it will add to the graph

Gradients computed
with autograd

just add more nodes.

```python
import torch

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

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

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

    loss.backward()
    if t % 50 == 0:
        print(t, loss.item())

    with torch.no_grad():
        w1 -= learning_rate * w1.grad
        w2 -= learning_rate * w2.grad
        w1.grad.zero_()
        w2.grad.zero_()
```

PyTorch: New functions

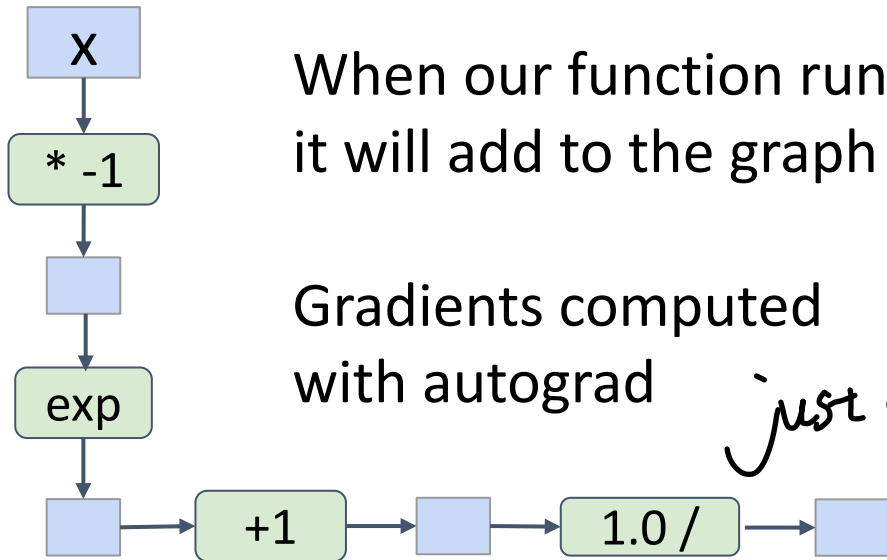Can define new operations
using Python functions

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


When our function runs,
it will add to the graph

Gradients computed
with autograd

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

```python
class Sigmoid(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        y = 1.0 / (1.0 + (-x).exp())
        ctx.save_for_backward(y)
        return y

    @staticmethod
    def backward(ctx, grad_y):
        y, = ctx.saved_tensors
        grad_x = grad_y * y * (1.0 - y)
        return grad_x

def sigmoid(x):
    return Sigmoid.apply(x)
```

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

PyTorch: New functions

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

Can define new operations using Python functions

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


When our function runs, it will add to the graph

Gradients computed with autograd

```python
class Sigmoid(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        y = 1.0 / (1.0 + (-x).exp())
        ctx.save_for_backward(y)
        return y

    @staticmethod
    def backward(ctx, grad_y):
        y, = ctx.saved_tensors
        grad_x = grad_y * y * (1.0 - y)
        return grad_x

def sigmoid(x):
    return Sigmoid.apply(x)
```

single node

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

PyTorch: New functions

Can define new operations
using Python functions

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

When our function runs,
it will add to the graph

Gradients computed
with autograd

```
x
|
* -1
|
[ ]
|
exp
|
[ ] → +1 → [ ] → 1.0 / → [ ]
```

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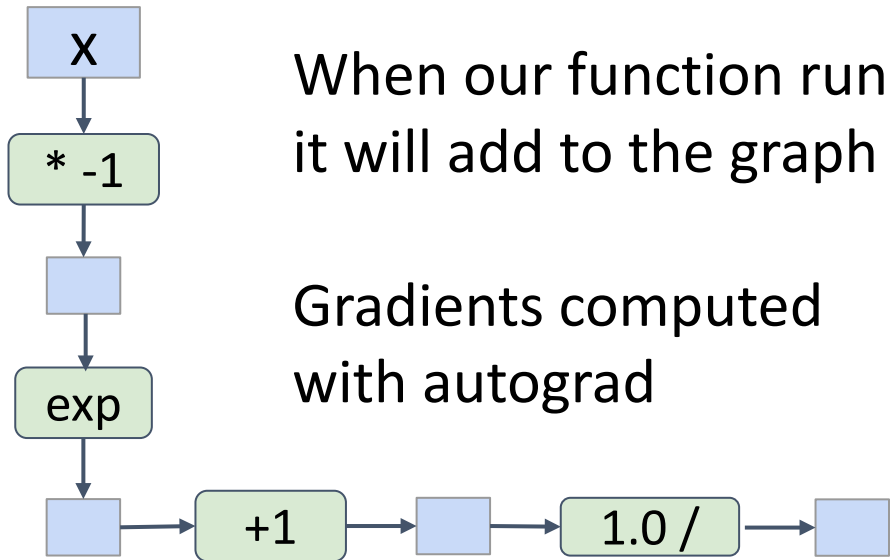forward and backward

```python
class Sigmoid(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x):
        y = 1.0 / (1.0 + (-x).exp())
        ctx.save_for_backward(y)
        return y

    @staticmethod
    def backward(ctx, grad_y):
        y, = ctx.saved_tensors
        grad_x = grad_y * y * (1.0 - y)
        return grad_x

def sigmoid(x):
    return Sigmoid.apply(x)
```

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

PyTorch: nn

Higher-level wrapper for working with neural nets

Use this! It will make your life easier

```python
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

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

```python
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

```python
import torch

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

model = torch.nn.Sequential(
            torch.nn.Linear(D_in, H),
            torch.nn.ReLU(),
            torch.nn.Linear(H, D_out))

learning_rate = 1e-2
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

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

Forward pass: Feed data to model and compute loss

PyTorch: nn

```python
import torch

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

model = torch.nn.Sequential(
            torch.nn.Linear(D_in, H),
            torch.nn.ReLU(),
            torch.nn.Linear(H, D_out))

learning_rate = 1e-2
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

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

Forward pass: Feed data to model and compute loss

torch.nn.functional has useful helpers like loss functions

Criterion.

PyTorch: nn

```python
import torch

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

model = torch.nn.Sequential(
        torch.nn.Linear(D_in, H),
        torch.nn.ReLU(),
        torch.nn.Linear(H, D_out))

learning_rate = 1e-2
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

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

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

PyTorch: nn

```python
import torch

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

model = torch.nn.Sequential(
            torch.nn.Linear(D_in, H),
            torch.nn.ReLU(),
            torch.nn.Linear(H, D_out))

learning_rate = 1e-2
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

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

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

PyTorch: optim

Use an **optimizer** for different update rules

```python
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

```python
import torch

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

model = torch.nn.Sequential(
            torch.nn.Linear(D_in, H),
            torch.nn.ReLU(),
            torch.nn.Linear(H, D_out))

learning_rate = 1e-4
optimizer = torch.optim.Adam(model.parameters(),
                                lr=learning_rate)
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)

    loss.backward()

    optimizer.step()
    optimizer.zero_grad()
```

After computing gradients, use optimizer to update and zero gradients

PyTorch: nn Defining Modules

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

Modules can contain weights or other modules

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

```python
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
Defining Modules

Define our whole model as
a single Module

```python
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
Defining Modules

Initializer sets up two children (Modules can contain modules)

```python
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
Defining Modules

Define forward pass using child modules and tensor operations

No need to define backward - autograd will handle it

```python
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
Defining Modules

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

build residual blocks.

```python
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()
```
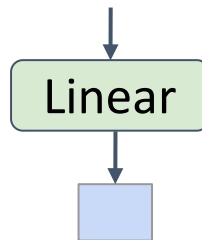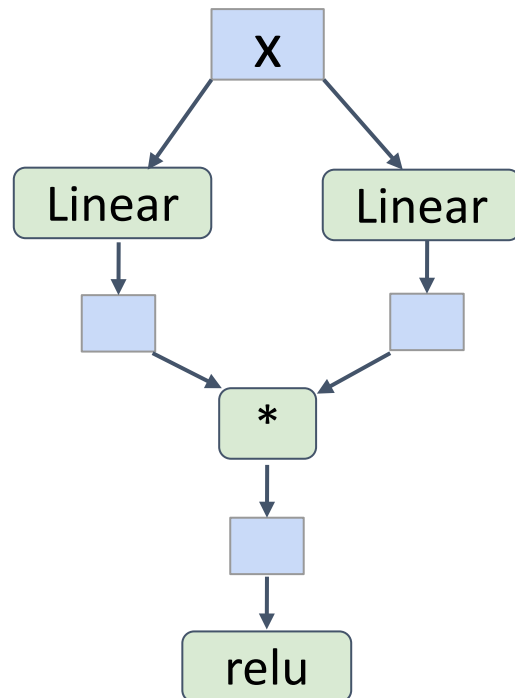
PyTorch: nn
Defining Modules

Define network component
as a Module subclass

```python
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()
```
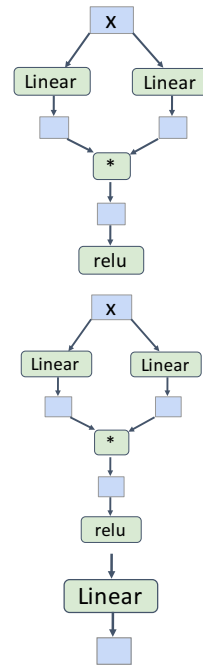
PyTorch: nn
Defining Modules

Stack multiple instances of the component in a sequential

Very easy to quickly build complex network architectures!

```python
import torch

class ParallelBlock(torch.nn.Module):
    def __init__(self, D_in, D_out):
        super(ParallelBlock, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, D_out)
        self.linear2 = torch.nn.Linear(D_in, D_out)
    def forward(self, x):
        h1 = self.linear1(x)
        h2 = self.linear2(x)
        return (h1 * h2).clamp(min=0)

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

model = torch.nn.Sequential(
            ParallelBlock(D_in, H),
            ParallelBlock(H, H),
            torch.nn.Linear(H, D_out))

optimizer = torch.optim.Adam(model.parameters(), lr=1e-4)
for t in range(500):
    y_pred = model(x)
    loss = torch.nn.functional.mse_loss(y_pred, y)
    loss.backward()
    optimizer.step()
    optimizer.zero_grad()
```

PyTorch: DataLoaders

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

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

```python
import torch
from torch.utils.data import TensorDataset, DataLoader

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

loader = DataLoader(TensorDataset(x, y), batch_size=8)
model = TwoLayerNet(D_in, H, D_out)

optimizer = torch.optim.SGD(model.parameters(), lr=1e-2)
for epoch in range(20):
    for x_batch, y_batch in loader:
        y_pred = model(x_batch)
        loss = torch.nn.functional.mse_loss(y_pred, y_batch)

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

PyTorch: DataLoaders

```python
import torch
from torch.utils.data import TensorDataset, DataLoader

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


loader = DataLoader(TensorDataset(x, y), batch_size=8)
model = TwoLayerNet(D_in, H, D_out)


optimizer = torch.optim.SGD(model.parameters(), lr=1e-2)
for epoch in range(20):
    for x_batch, y_batch in loader:
        y_pred = model(x_batch)
        loss = torch.nn.functional.mse_loss(y_pred, y_batch)

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

Iterate over loader to form minibatches

PyTorch: DataLoaders

```python
import torch
from torch.utils.data import TensorDataset, DataLoader

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

loader = DataLoader(TensorDataset(x, y), batch_size=8)
model = TwoLayerNet(D_in, H, D_out)

optimizer = torch.optim.SGD(model.parameters(), lr=1e-2)
for epoch in range(20):
    for x_batch, y_batch in loader:
        y_pred = model(x_batch)
        loss = torch.nn.functional.mse_loss(y_pred, y_batch)

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

Iterate over loader to form minibatches

PyTorch: Pretrained Models

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

```python
import torch
import torchvision

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

PyTorch: **Dynamic Computation Graphs**

```python
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
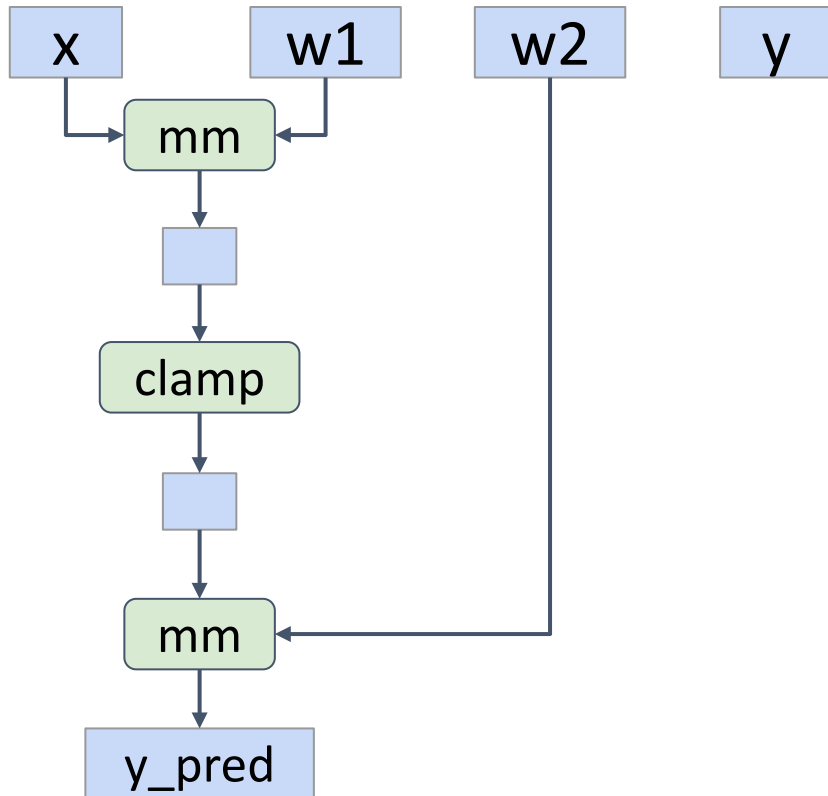
| x | | w1 | w2 | | y |

```python
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
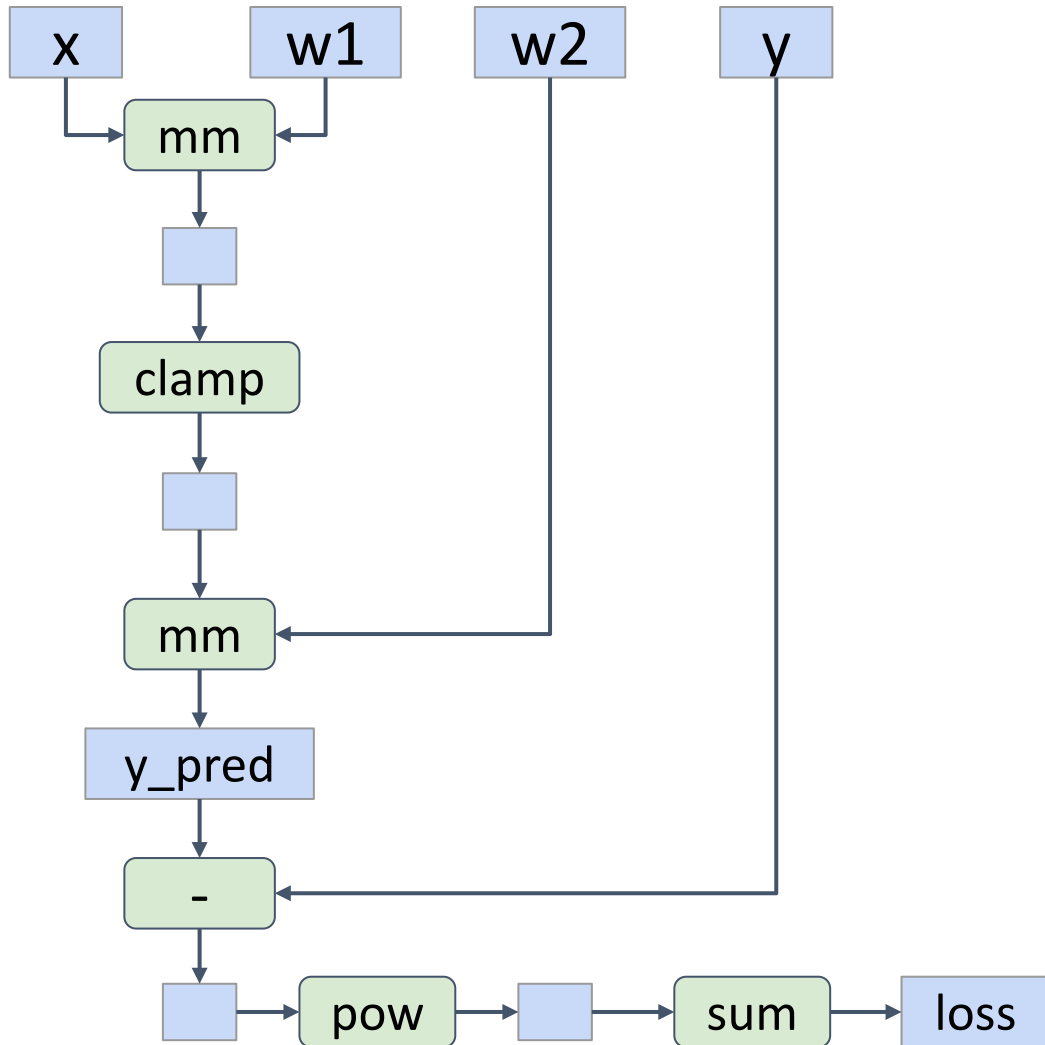


```
import torch

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
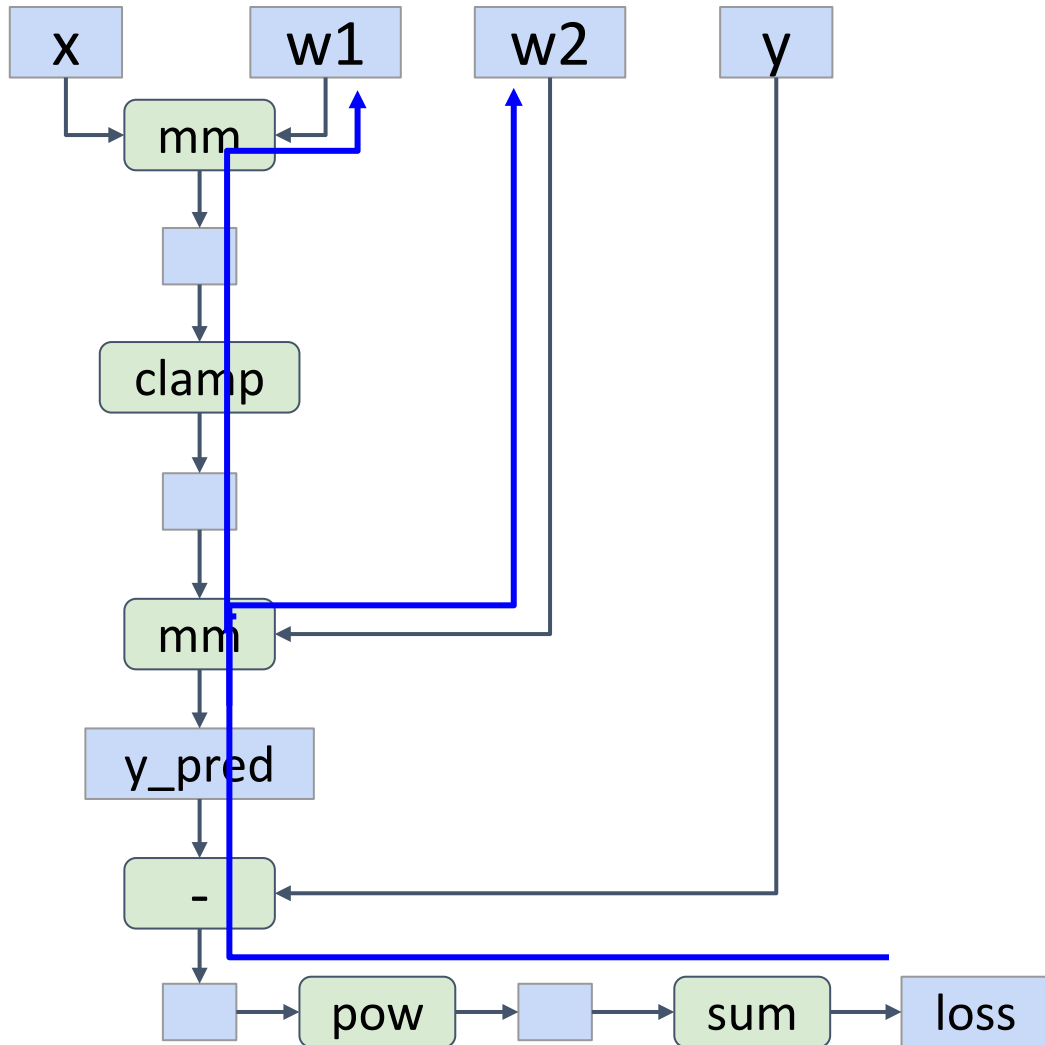
PyTorch: Dynamic Computation Graphs


```
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()
```

Perform backprop,
throw away graph

PyTorch: Dynamic Computation Graphs

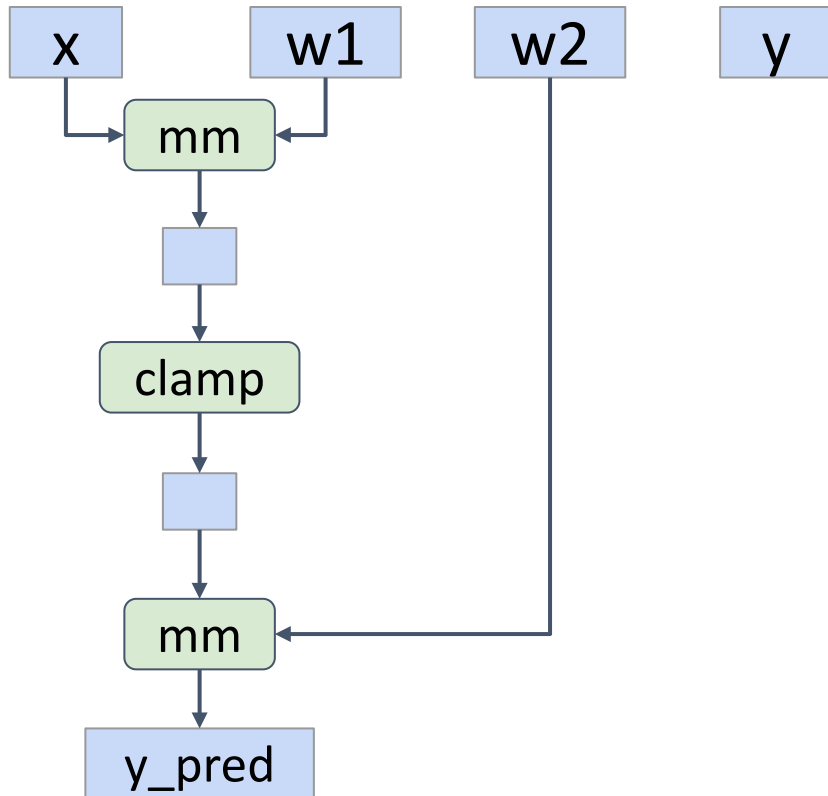| x | | w1 | | w2 | | y |

```python
import torch

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

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

    loss.backward()
```

Perform backprop,
throw away graph

PyTorch: Dynamic Computation Graphs
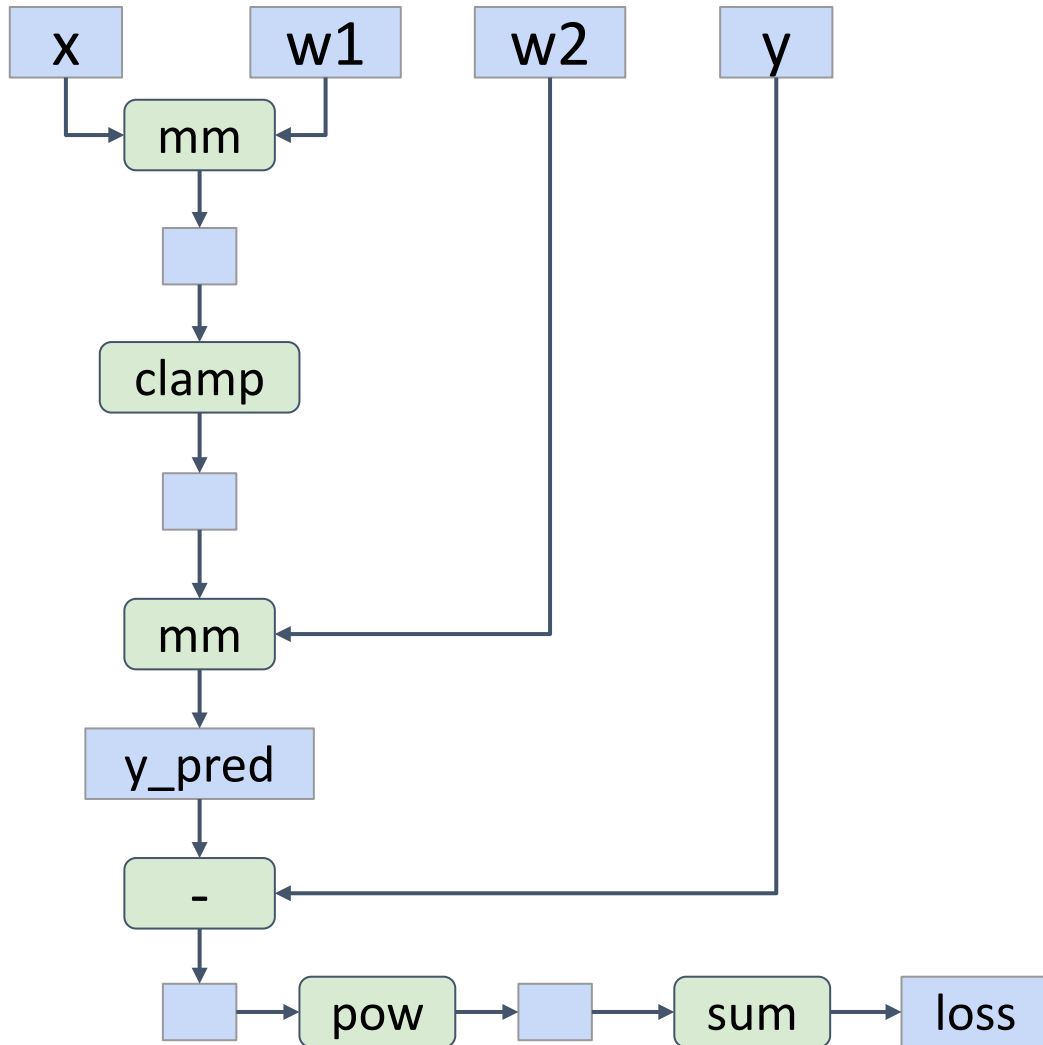


```python
import torch

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

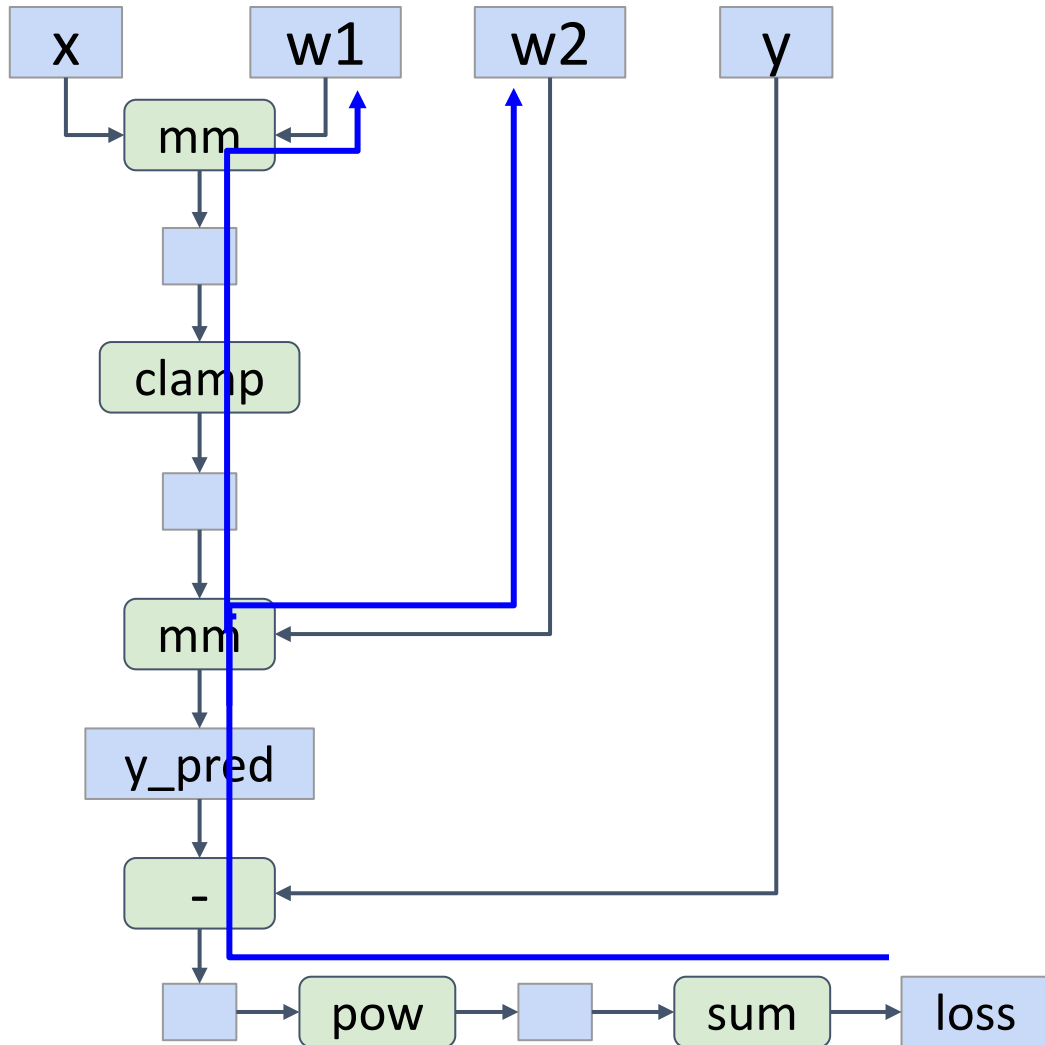# PyTorch: Dynamic Computation Graphs


```
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()
```

Perform backprop,
throw away graph

PyTorch: Dynamic Computation Graphs

Dynamic graphs let you use regular Python control flow during the forward pass!

```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
prev_loss = 5.0
for t in range(500):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
    prev_loss = loss.item()
```
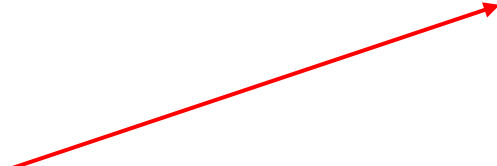
PyTorch: **Dynamic Computation Graphs**

Dynamic graphs let you use regular Python control flow during the forward pass!

Initialize two different weight matrices for second layer

```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
prev_loss = 5.0
for t in range(500):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
    prev_loss = loss.item()
```

PyTorch: Dynamic Computation Graphs

benefit

Dynamic graphs let you use regular Python control flow during the forward pass!

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

(this model doesn't makes sense! Just a simple dynamic example)

```python
import torch

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

learning_rate = 1e-6
prev_loss = 5.0
for t in range(500):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
    prev_loss = loss.item()
```
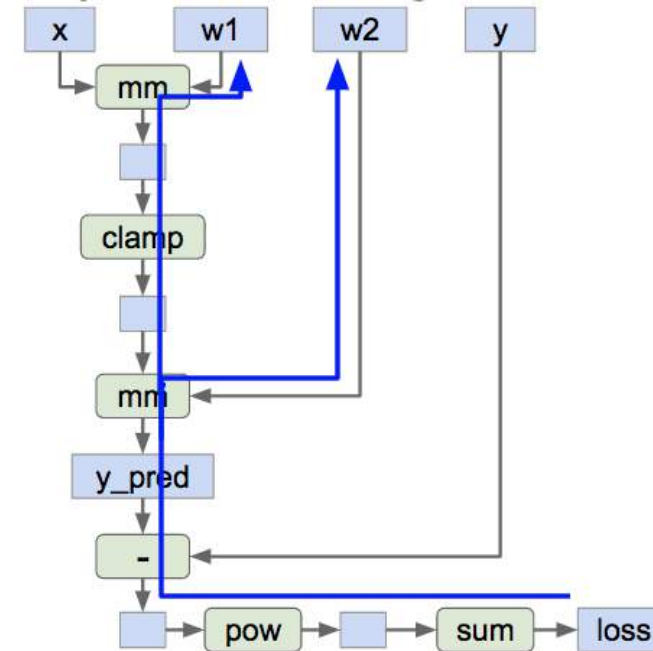
Alternative: Static Computation Graphs

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)
```

PyTorch: Static Graphs with JIT

Define model as a
Python function

```python
import torch

def model(x, y, w1, w2a, w2b, prev_loss):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    return loss

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

graph = torch.jit.script(model)

prev_loss = 5.0
learning_rate = 1e-6
for t in range(500):
    loss = graph(x, y, w1, w2a, w2b, prev_loss)

    loss.backward()
    prev_loss = loss.item()
```

PyTorch: Static Graphs with JIT

```python
import torch

def model(x, y, w1, w2a, w2b, prev_loss):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    return loss


N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

graph = torch.jit.script(model)

prev_loss = 5.0
learning_rate = 1e-6
for t in range(500):
    loss = graph(x, y, w1, w2a, w2b, prev_loss)

    loss.backward()
    prev_loss = loss.item()
```
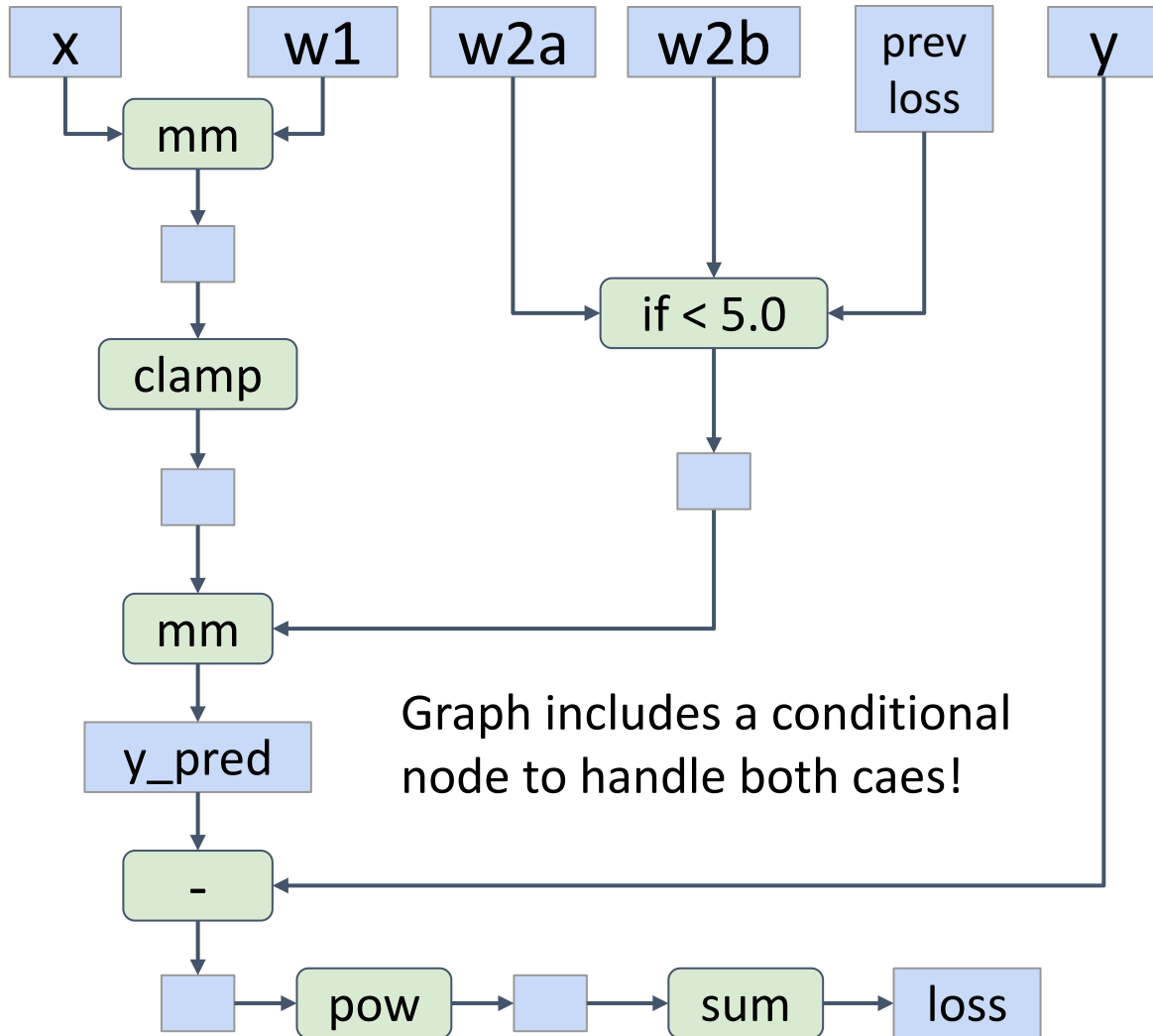
Just-In-Time compilation:
Introspect the source code
of the function, **compile** it
into a graph object.

Lots of magic here!

PyTorch: Static Graphs with JIT

Graph includes a conditional node to handle both caes!

```python
import torch

def model(x, y, w1, w2a, w2b, prev_loss):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    return loss


N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

graph = torch.jit.script(model)

prev_loss = 5.0
learning_rate = 1e-6
for t in range(500):
    loss = graph(x, y, w1, w2a, w2b, prev_loss)

    loss.backward()
    prev_loss = loss.item()
```

PyTorch: Static Graphs with JIT

```python
import torch

def model(x, y, w1, w2a, w2b, prev_loss):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    return loss


N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

graph = torch.jit.script(model)

prev_loss = 5.0
learning_rate = 1e-6
for t in range(500):
    loss = graph(x, y, w1, w2a, w2b, prev_loss)

    loss.backward()
    prev_loss = loss.item()
```

Use our compiled graph object at each forward pass

PyTorch: Static Graphs with JIT

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

Calling function uses graph

```python
import torch

@torch.jit.script
def model(x, y, w1, w2a, w2b, prev_loss):
    w2 = w2a if prev_loss < 5.0 else w2b
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()
    return loss

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in)
y = torch.randn(N, D_out)
w1 = torch.randn(D_in, H, requires_grad=True)
w2a = torch.randn(H, D_out, requires_grad=True)
w2b = torch.randn(H, D_out, requires_grad=True)

prev_loss = 5.0
learning_rate = 1e-6
for t in range(500):
    loss = model(x, y, w1, w2a, w2b, prev_loss)

    loss.backward()
    prev_loss = loss.item()
```
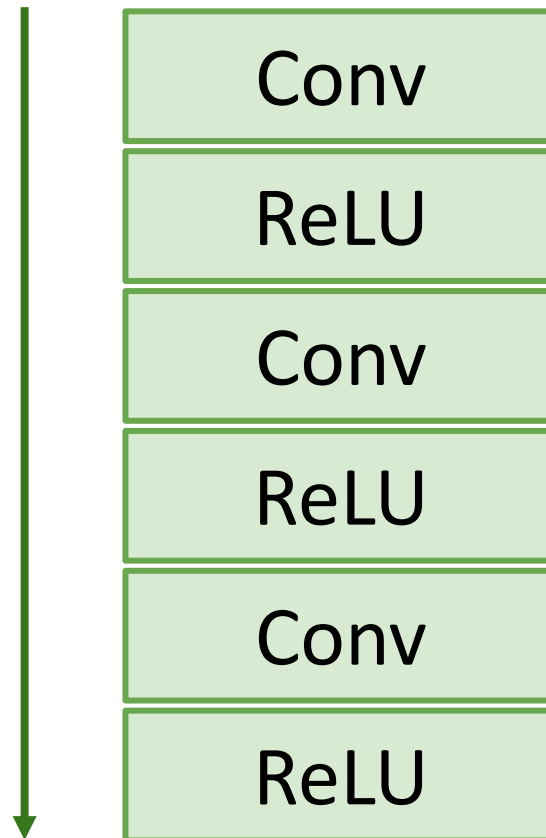
Static vs Dynamic Graphs: Optimization

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

The graph you wrote

Conv

ReLU

Conv

ReLU

Conv

ReLU

Equivalent graph with **fused operations**

Conv+ReLU

Conv+ReLU

Conv+ReLU

Static vs Dynamic Graphs: Serialization

Static

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

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

Can run in
C++ without python.

Dynamic

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

need python interpreter every time
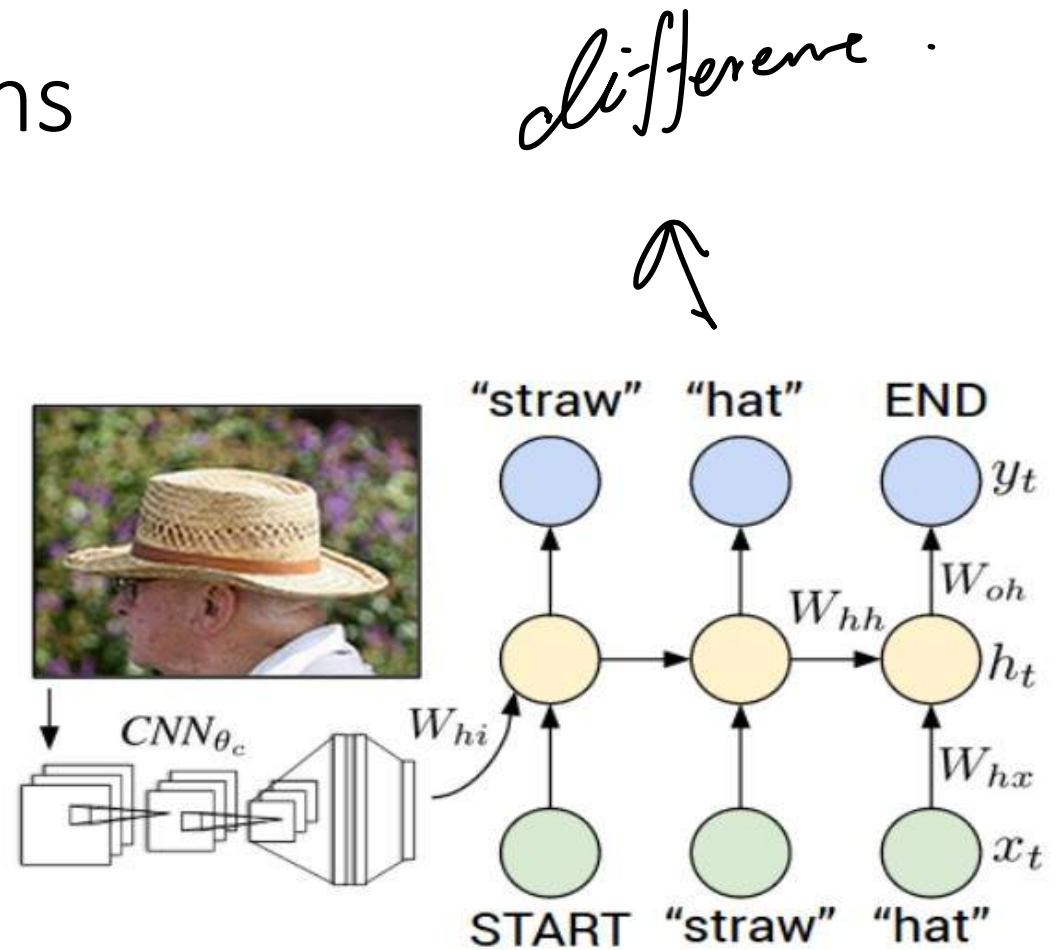
Static vs <u>Dynamic Graphs</u>: Debugging

Static

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

Dynamic

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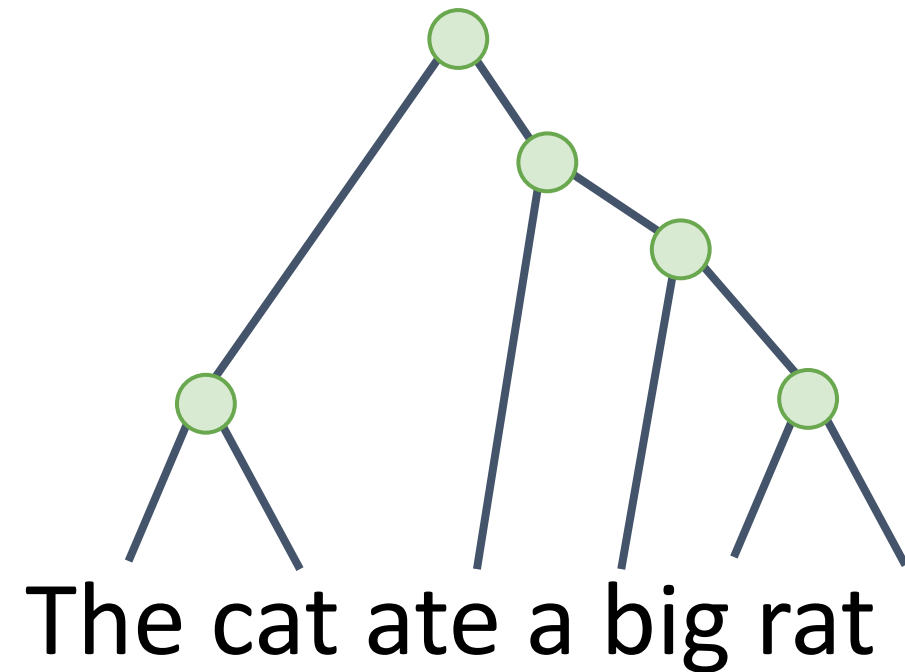
Dynamic Graph Applications

difference

Model structure
depends on the input:
- Recurrent Networks

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015

Dynamic Graph Applications

Model structure
depends on the input:
- Recurrent Networks
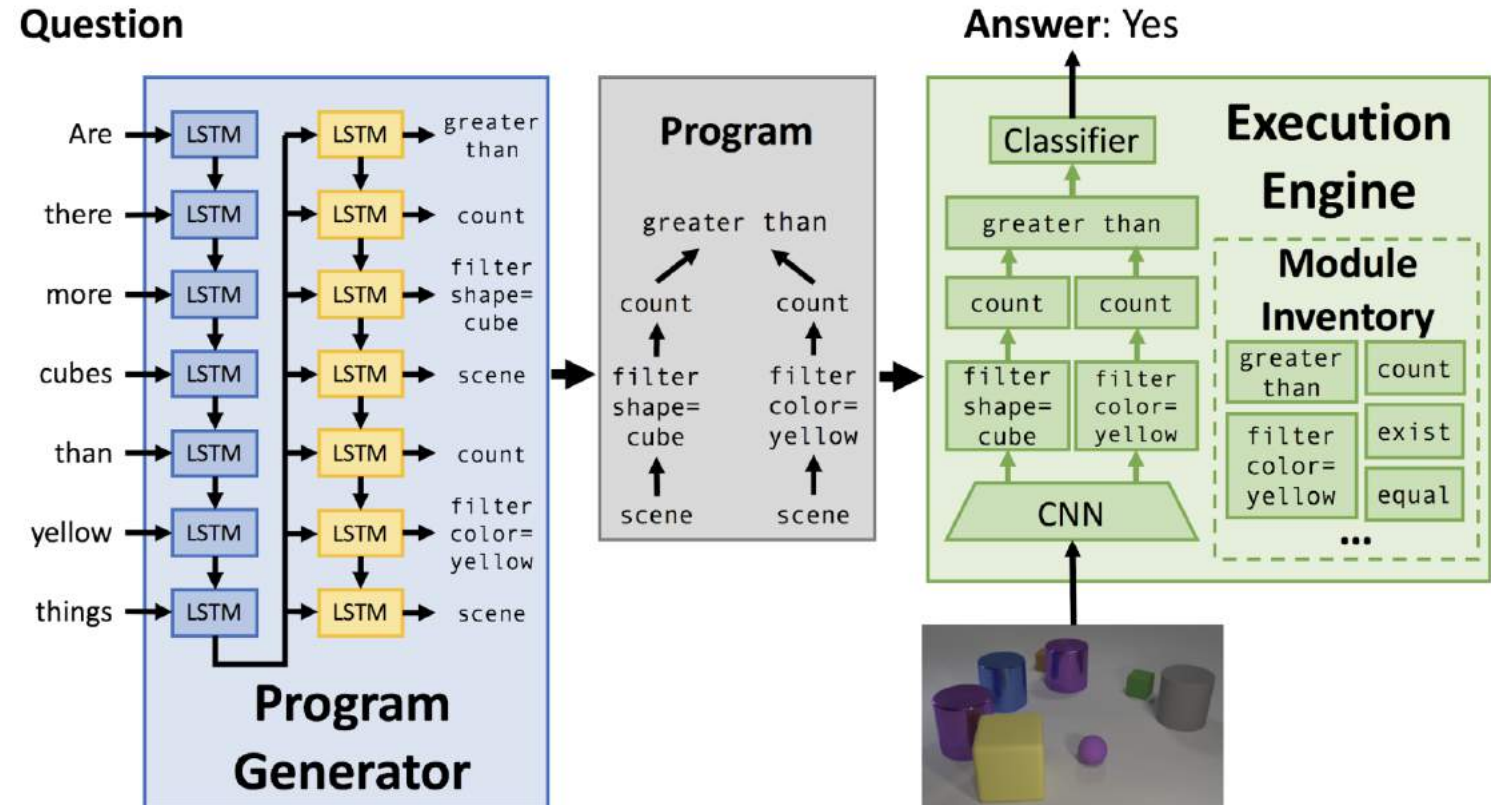- Recursive Networks

The cat ate a big rat

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments
for Generating Image Descriptions", CVPR 2015

Dynamic Graph Applications

Model structure depends on the input:
- Recurrent Networks
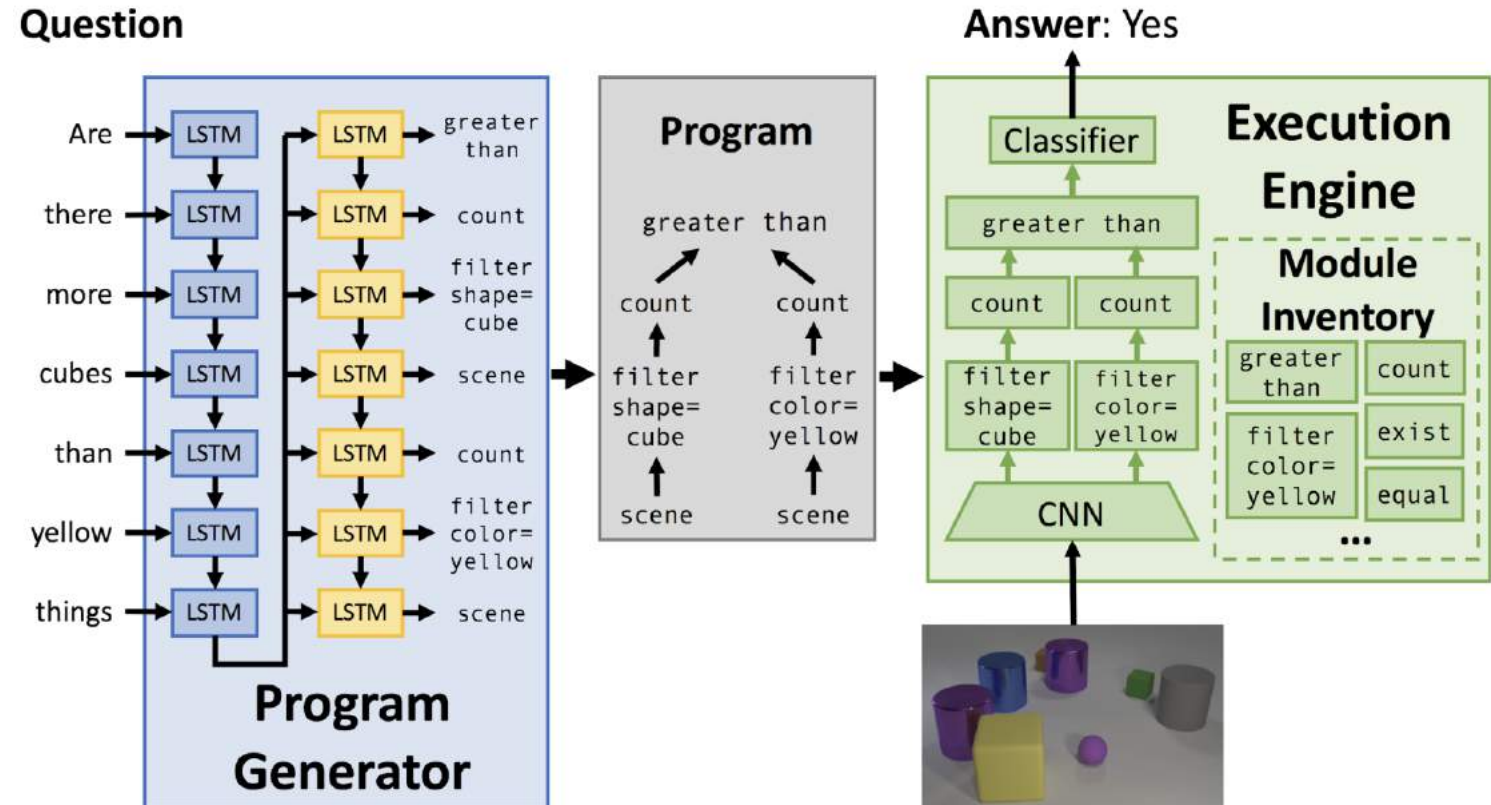- Recursive Networks
- Modular Networks

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

Model structure depends on the input:
- Recurrent Networks
- Recursive Networks
- Modular Networks
- (Your idea here!)

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

TensorFlow

TensorFlow Versions

TensorFlow 1.0

- Final release: 1.15.0-rc2
  - Released yesterday!
- Default: **static graphs**
- Optional: dynamic graphs (eager mode)

TensorFlow 2.0

- Released Monday 9/30!
- Default: **dynamic graphs**
- Optional: static graphs

TensorFlow 1.0: Static Graphs

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

(Assume imports at the top of each snippet)

```python
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 1.0: Static Graphs

```python
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])
```

First **define** computational graph

```python
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
```

Then **run** the graph many times

TensorFlow 2.0:
Dynamic Graphs

```python
import tensorflow as tf

N, Din, H, Dout = 16, 1000, 100, 10

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))
w1 = tf.Variable(tf.random.normal((Din, H)))
w2 = tf.Variable(tf.random.normal((H, Dout)))

learning_rate = 1e-6
for t in range(1000):
    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))

    grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

    w1.assign(w1 - learning_rate * grad_w1)
    w2.assign(w2 - learning_rate * grad_w2)
```

Create TensorFlow Tenssors for data and weights

Weights need to be wrapped in tf.Variable so we can mutate them

TensorFlow 2.0: Dynamic Graphs

```python
import tensorflow as tf

N, Din, H, Dout = 16, 1000, 100, 10

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))
w1 = tf.Variable(tf.random.normal((Din, H)))
w2 = tf.Variable(tf.random.normal((H, Dout)))

learning_rate = 1e-6
for t in range(1000):
    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))

    grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

    w1.assign(w1 - learning_rate * grad_w1)
    w2.assign(w2 - learning_rate * grad_w2)
```

Scope forward pass under a GradientTape to tell TensorFlow to start building a graph

TensorFlow 2.0: Dynamic Graphs

```python
import tensorflow as tf

N, Din, H, Dout = 16, 1000, 100, 10

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))
w1 = tf.Variable(tf.random.normal((Din, H)))
w2 = tf.Variable(tf.random.normal((H, Dout)))

learning_rate = 1e-6
for t in range(1000):
  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))

  grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

  w1.assign(w1 - learning_rate * grad_w1)
  w2.assign(w2 - learning_rate * grad_w2)
```

Ask the tape to compute gradients

TensorFlow 2.0:
Dynamic Graphs

```python
import tensorflow as tf

N, Din, H, Dout = 16, 1000, 100, 10

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))
w1 = tf.Variable(tf.random.normal((Din, H)))
w2 = tf.Variable(tf.random.normal((H, Dout)))

learning_rate = 1e-6
for t in range(1000):
  with tf.GradientTape() as tape:
    h = tf.maximum(tf.matmul(x, w1), 0)
    y_pred = tf.matmul(h, w2)
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  grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

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```

Gradient descent
step, update weights

TensorFlow 2.0: Static Graphs

Define a function that implements forward, backward, and update

Annotating with tf.function will compile the function into a graph! (similar to torch.jit.script)

```python
@tf.function
def step(x, y, w1, w2):
    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))

    grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

    w1.assign(w1 - learning_rate * grad_w1)
    w2.assign(w2 - learning_rate * grad_w2)
    return loss

N, Din, H, Dout = 16, 1000, 100, 10

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))
w1 = tf.Variable(tf.random.normal((Din, H)))
w2 = tf.Variable(tf.random.normal((H, Dout)))

learning_rate = 1e-6
for t in range(1000):
    loss = step(x, y, w1, w2)
```

TensorFlow 2.0: Static Graphs

Define a function that implements forward, backward, and update

Annotating with tf.function will compile the function into a graph! (similar to torch.jit.script)

(note TF graph can include gradient computation and update, unlike PyTorch)

```python
@tf.function
def step(x, y, w1, w2):
    with tf.GradientTape() as tape:
        h = tf.maximum(tf.matmul(x, w1), 0)
        y_pred = tf.matmul(h, w2)
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        loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))

    grad_w1, grad_w2 = tape.gradient(loss, [w1, w2])

    w1.assign(w1 - learning_rate * grad_w1)
    w2.assign(w2 - learning_rate * grad_w2)
    return loss

N, Din, H, Dout = 16, 1000, 100, 10

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learning_rate = 1e-6
for t in range(1000):
    loss = step(x, y, w1, w2)
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TensorFlow 2.0: Static Graphs

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learning_rate = 1e-6
for t in range(1000):
    loss = step(x, y, w1, w2)
```

Call the compiled step function in the training loop

Keras: High-level API

```python
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import InputLayer, Dense

N, Din, H, Dout = 16, 1000, 100, 10

model = Sequential()
model.add(InputLayer(input_shape=(Din,)))
model.add(Dense(units=H, activation='relu'))
model.add(Dense(units=Dout))
params = model.trainable_variables

loss_fn = tf.keras.losses.MeanSquaredError()
opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))

for t in range(1000):
  with tf.GradientTape() as tape:
    y_pred = model(x)
    loss = loss_fn(y_pred, y)
  grads = tape.gradient(loss, params)
  opt.apply_gradients(zip(grads, params))
```

Keras: High-level API

Object-oriented API:
build the model as a
stack of layers

```python
import tensorflow as tf
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```

Keras: High-level API

Keras gives you common loss functions and optimization algorithms

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opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

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for t in range(1000):
    with tf.GradientTape() as tape:
        y_pred = model(x)
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opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

x = tf.random.normal((N, Din))
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for t in range(1000):
    with tf.GradientTape() as tape:
        y_pred = model(x)
        loss = loss_fn(y_pred, y)
    grads = tape.gradient(loss, params)
    opt.apply_gradients(zip(grads, params))
```

Forward pass:
Compute loss,
build graph

Backward pass:
compute gradients

Keras: High-level API

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N, Din, H, Dout = 16, 1000, 100, 10

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opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))

for t in range(1000):
    with tf.GradientTape() as tape:
        y_pred = model(x)
        loss = loss_fn(y_pred, y)
    grads = tape.gradient(loss, params)
    opt.apply_gradients(zip(grads, params))
```

Optimizer object
updates parameters

Keras: High-level API

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N, Din, H, Dout = 16, 1000, 100, 10

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model.add(Dense(units=Dout))

params = model.trainable_variables

loss_fn = tf.keras.losses.MeanSquaredError()
opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))

def step():
  y_pred = model(x)
  loss = loss_fn(y_pred, y)
  return loss

for t in range(1000):
  opt.minimize(step, params)
```

Define a function
that returns the loss

Keras: High-level API

```python
import tensorflow as tf
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import InputLayer, Dense

N, Din, H, Dout = 16, 1000, 100, 10

model = Sequential()
model.add(InputLayer(input_shape=(Din,)))
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params = model.trainable_variables

loss_fn = tf.keras.losses.MeanSquaredError()
opt = tf.keras.optimizers.SGD(learning_rate=1e-6)

x = tf.random.normal((N, Din))
y = tf.random.normal((N, Dout))

def step():
    y_pred = model(x)
    loss = loss_fn(y_pred, y)
    return loss

for t in range(1000):
    opt.minimize(step, params)
```
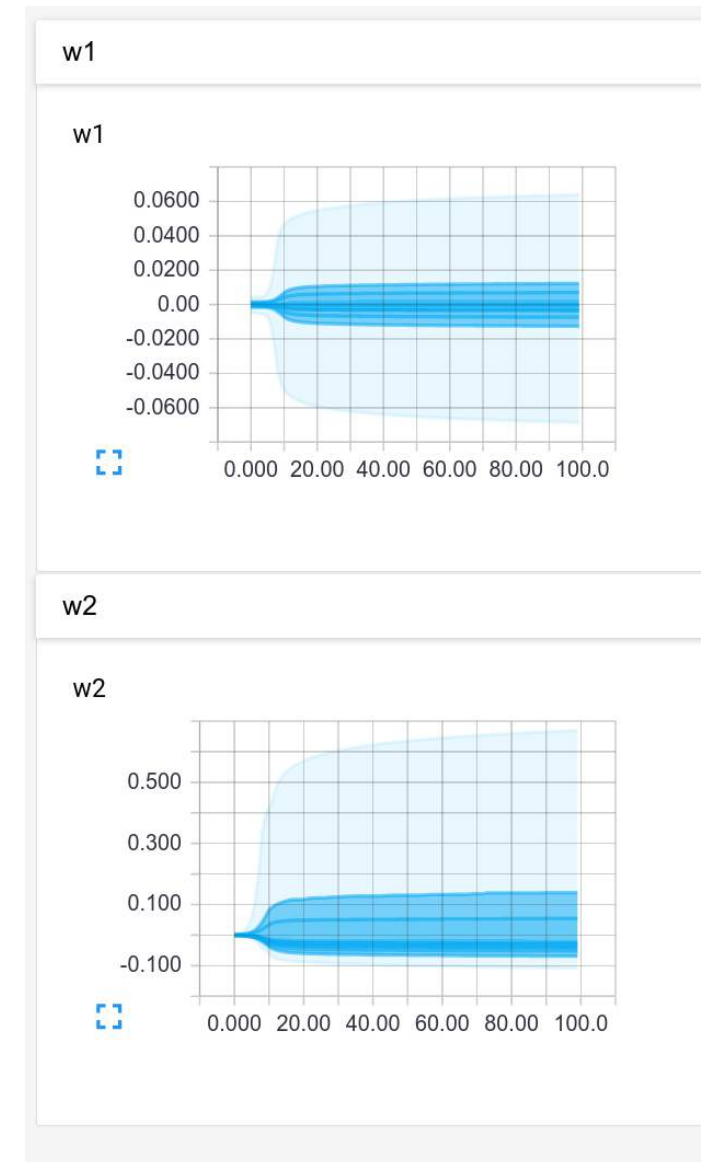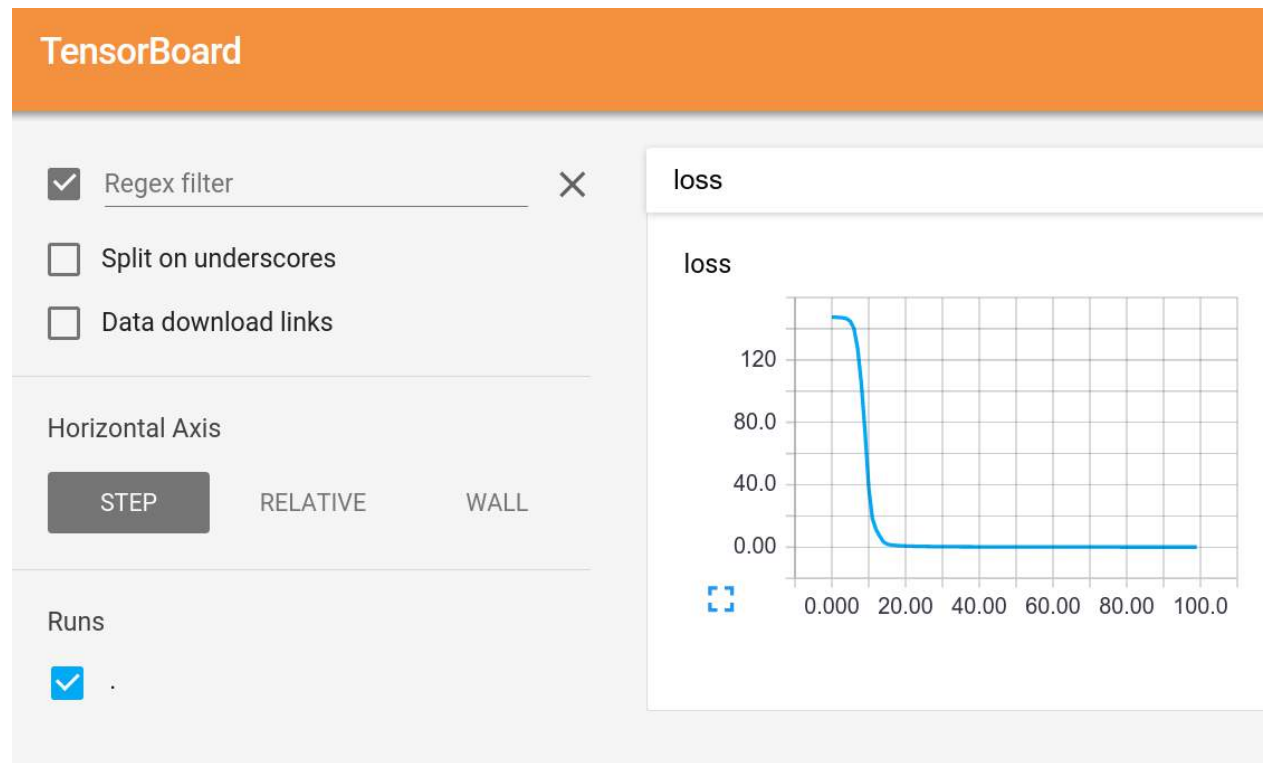
Optimizer computes gradients and updates parameters

TensorBoard

Add logging to code to record loss, stats, etc
Run server and get pretty graphs!
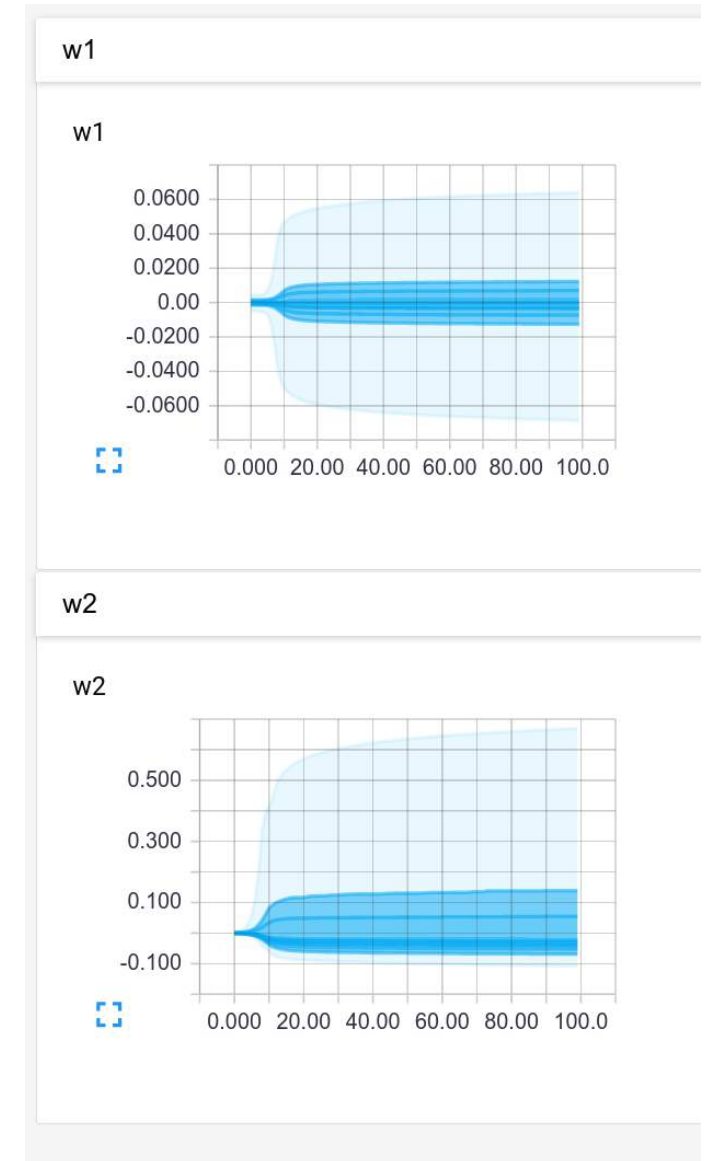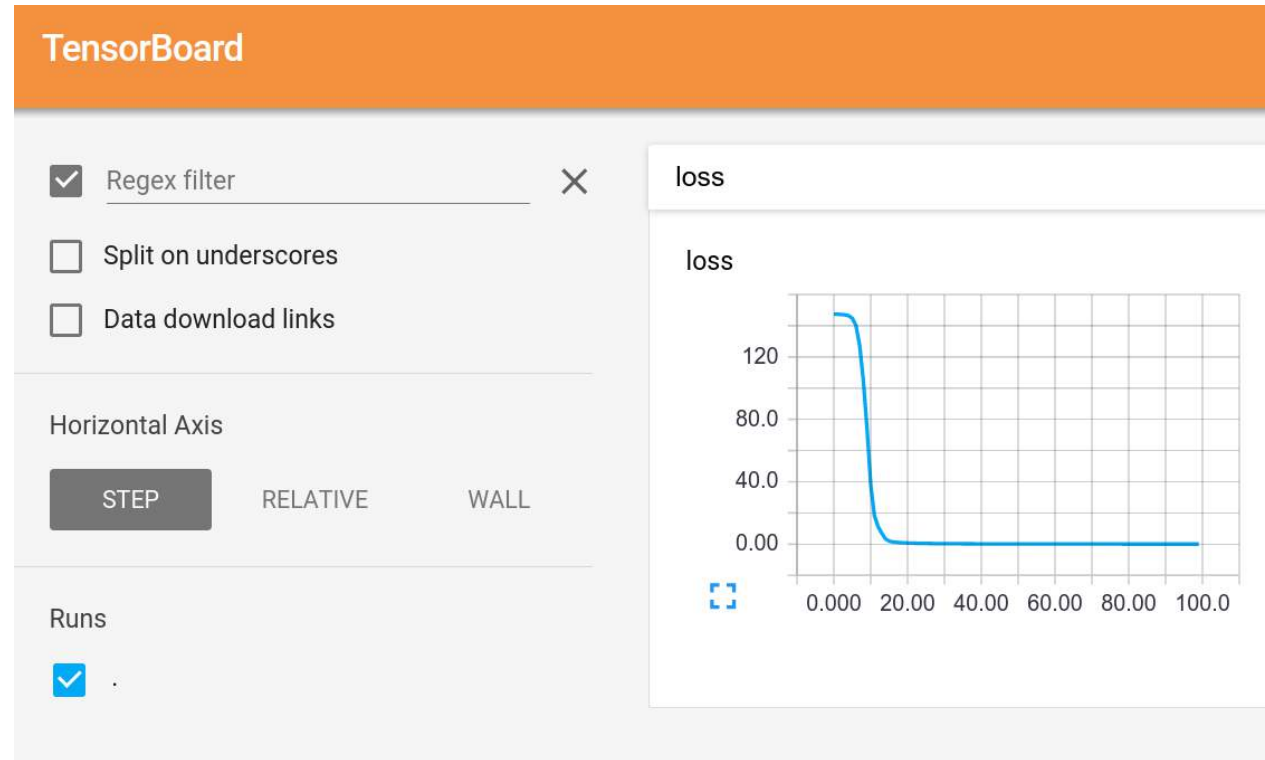
TensorBoard

Also works with PyTorch: torch.utils.tensorboard

PyTorch vs TensorFlow

PyTorch
- My personal favorite
- Clean, imperative API
- Easy dynamic graphs for debugging
- JIT allows static graphs for production
- Cannot use TPUs
- Not easy to deploy on mobile

TensorFlow 1.0
- Static graphs by default
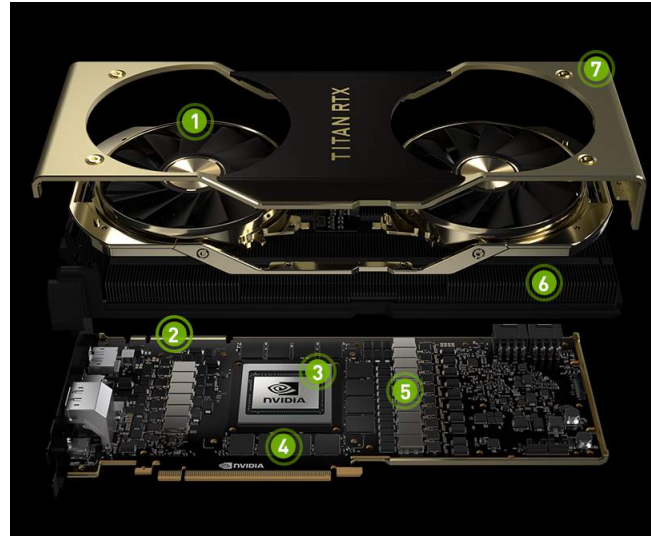- Can be confusing to debug
- API a bit messy

TensorFlow 2.0
- Dynamic by default
- Standardized on Keras API
- Just came out, no consensus yet

Summary: Hardware

Summary: Software

Static Graphs vs **Dynamic Graphs**

PyTorch vs **TensorFlow**

Next time:
Training Neural Networks