Lecture 9:
Hardware and Software

Assignment 3 Released

Assignment 3 is released! It covers:

- Fully-connected networks
- Dropout
- Update rules: SGD+Momentum, RMSprop, Adam
- Convolutional networks
- Batch normalization

Due **Friday October 9, 11:59pm**
(Website originally said 10/16 – this was a typo!)

Deep Learning Hardware

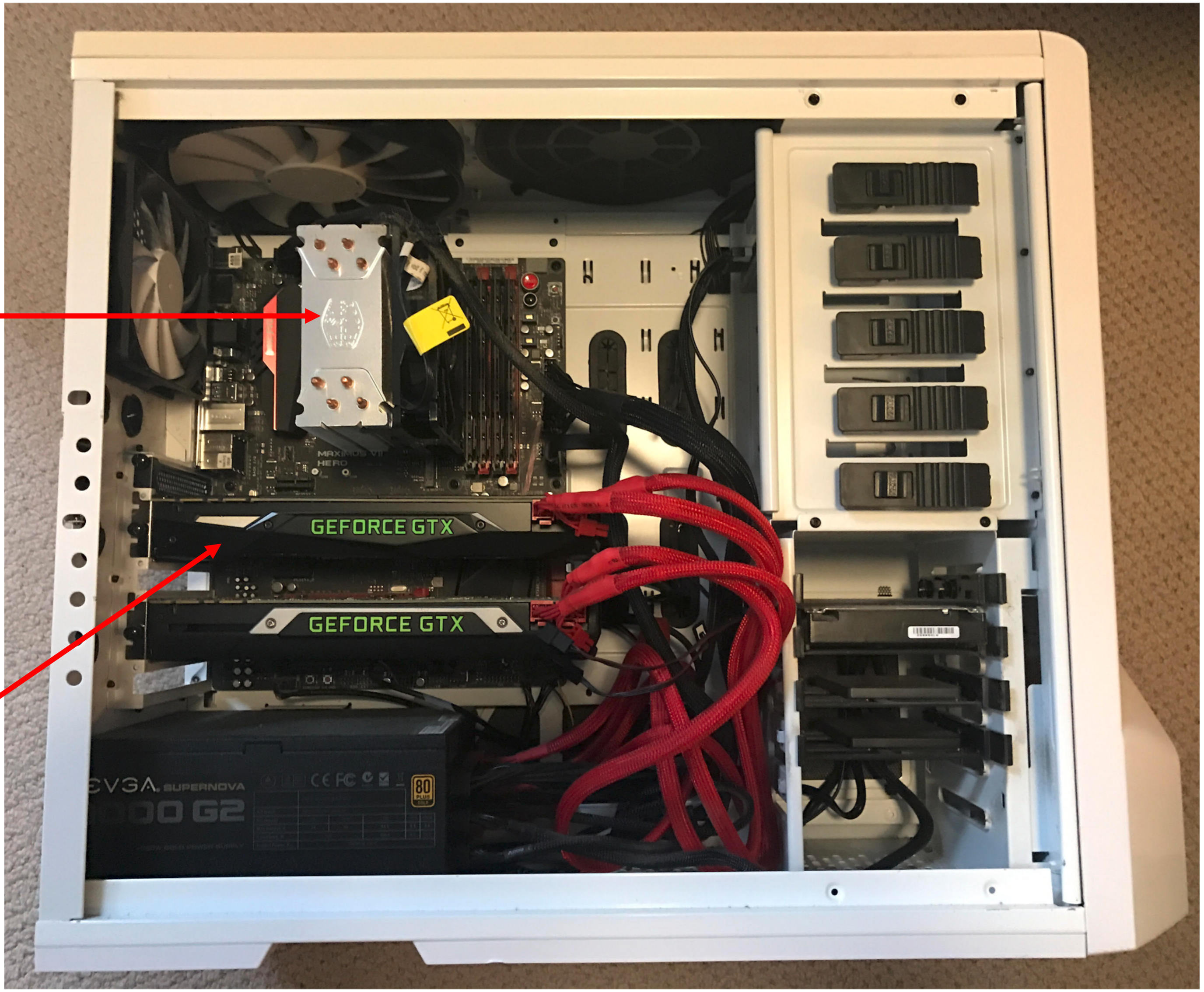
Inside a computer

Inside a computer

GPU: "Graphics Processing Unit"

Inside a computer

CPU: “Central Processing Unit”



GPU: “Graphics Processing Unit”

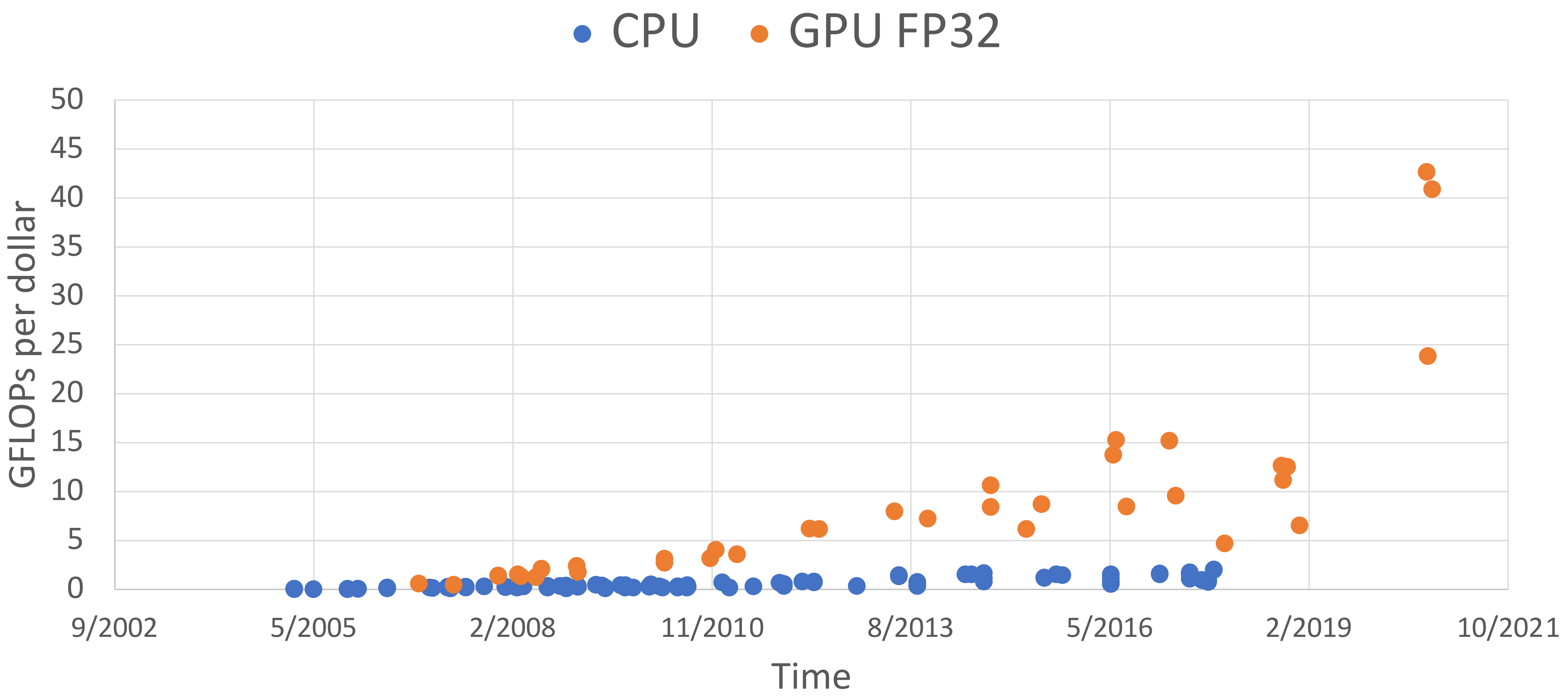
NVIDIA vs AMD

NVIDIA

vs

AMD

GFLOPs per Dollar



CPU vs GPU

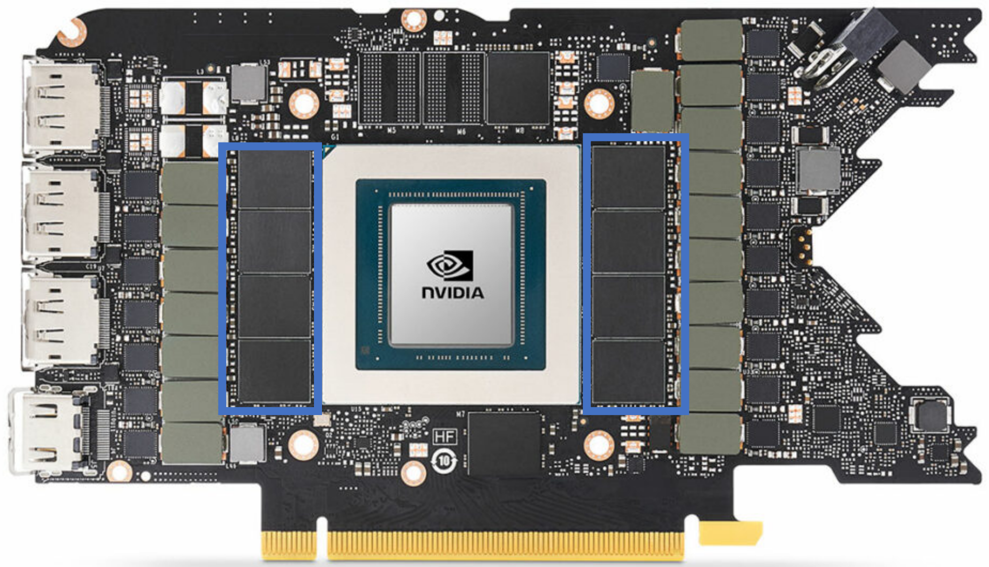
	Cores	Clock Speed (GHz)	Memory	Price	TFLOP/sec
CPU Ryzen Threadripper 3970X	64 (128 threads with hyperthreading)	3.7 (4.5 boost)	System RAM	$1999	~6.9 FP32
GPU NVIDIA RTX 3090	10496	1.4 (1.7 boost)	24 GB GDDR6X	$1499	~35.6 FP32

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

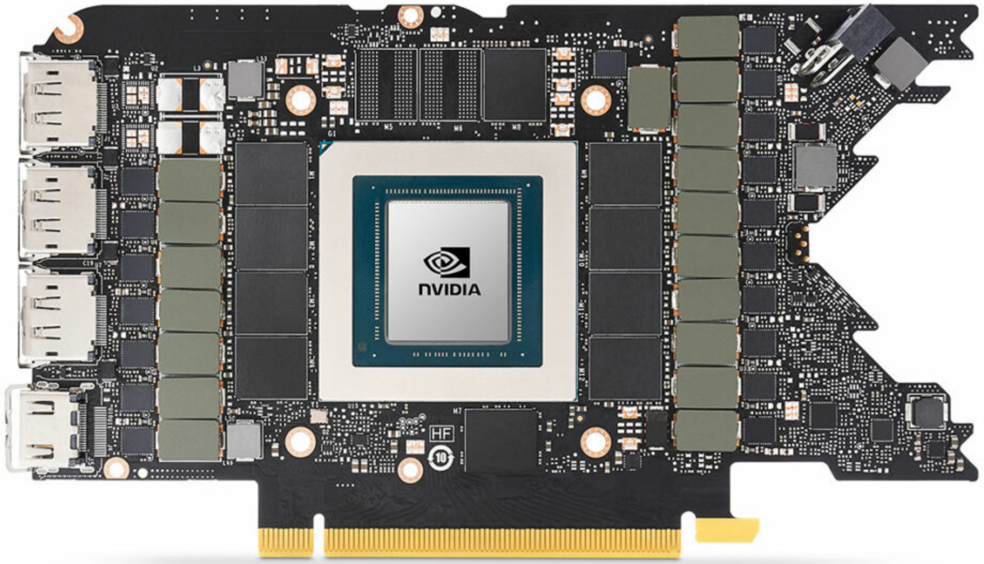
GPU: More cores, but each core is much slower and “dumber”; great for parallel tasks

Inside a GPU: RTX 3090

12x 2GB memory modules



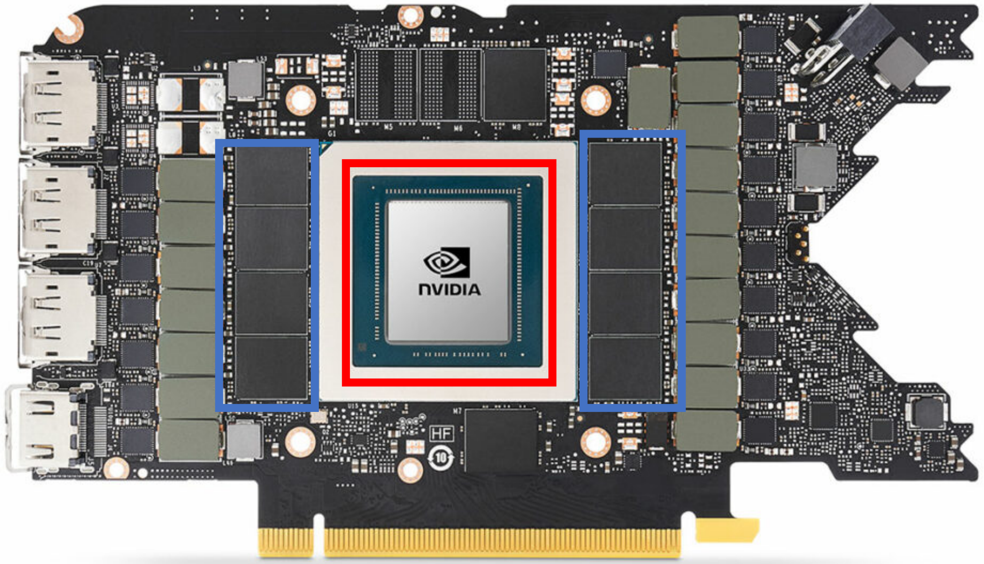
Inside a GPU: RTX 3090



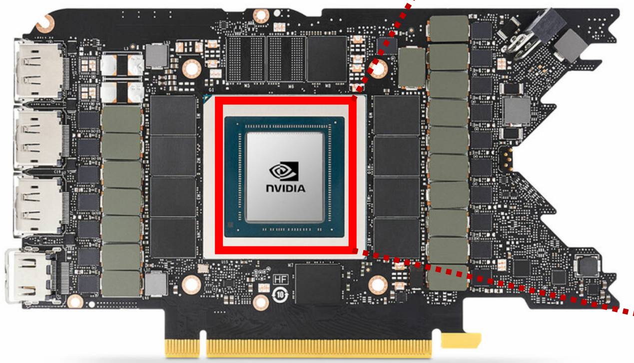
Inside a GPU: RTX 3090

12x 2GB memory modules

Processor

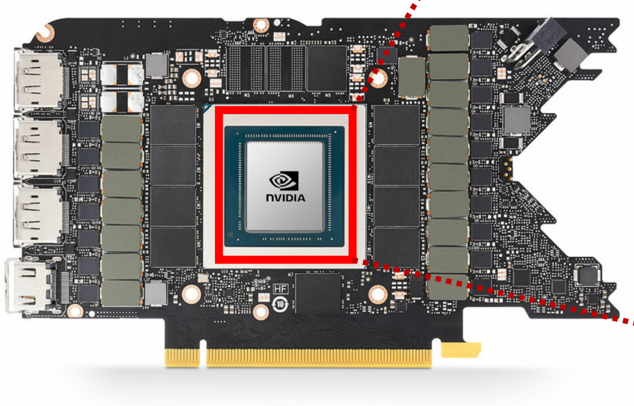


Inside a GPU: RTX 3090

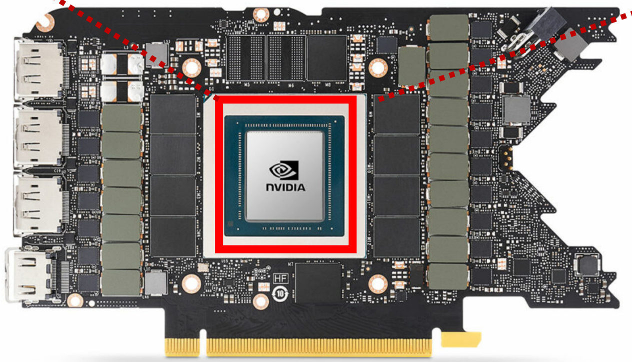


Inside a GPU: RTX 3090

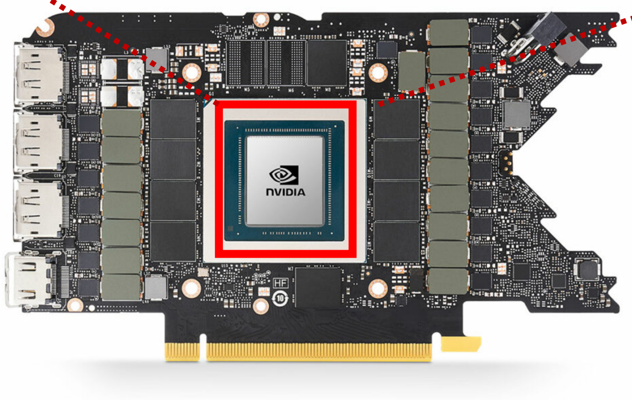
82 Streaming multiprocessors (SMs)

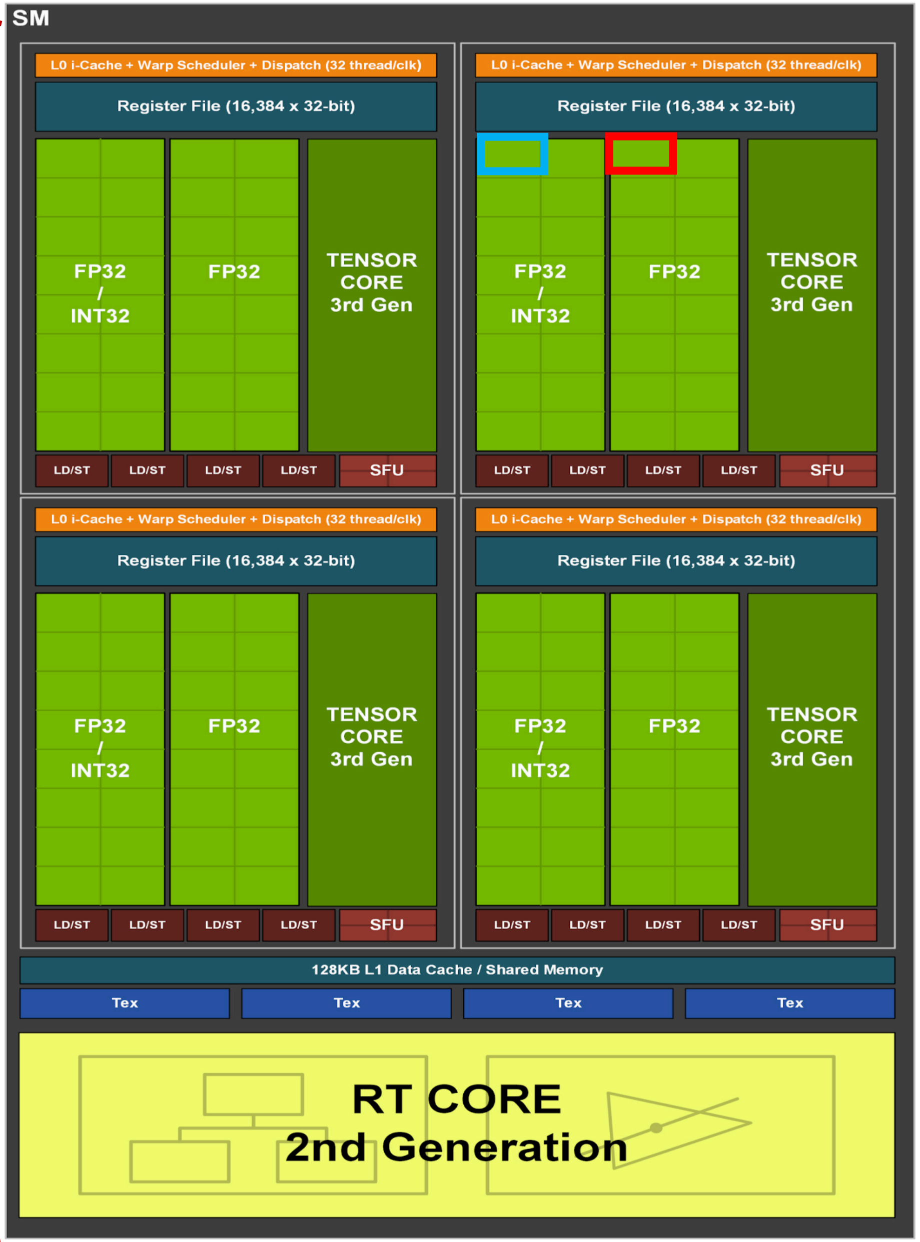


Inside a GPU: RTX 3090



Inside a GPU: RTX 3090

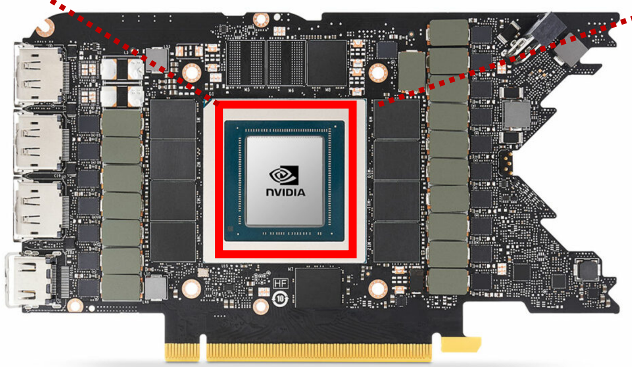


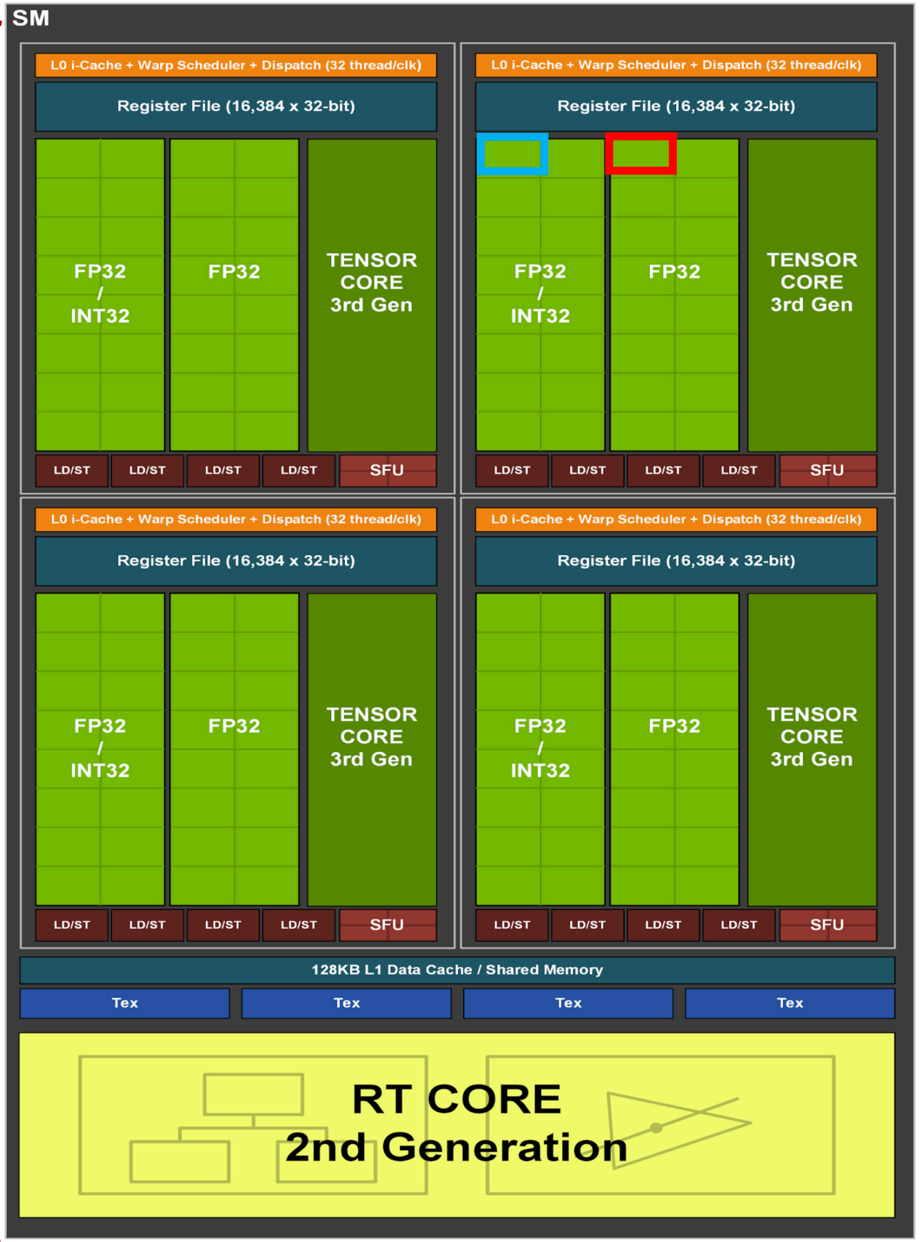


64 FP32 cores per SM

64 INT32/FP32 cores per SM

Inside a GPU: RTX 3090





64 FP32 cores per SM

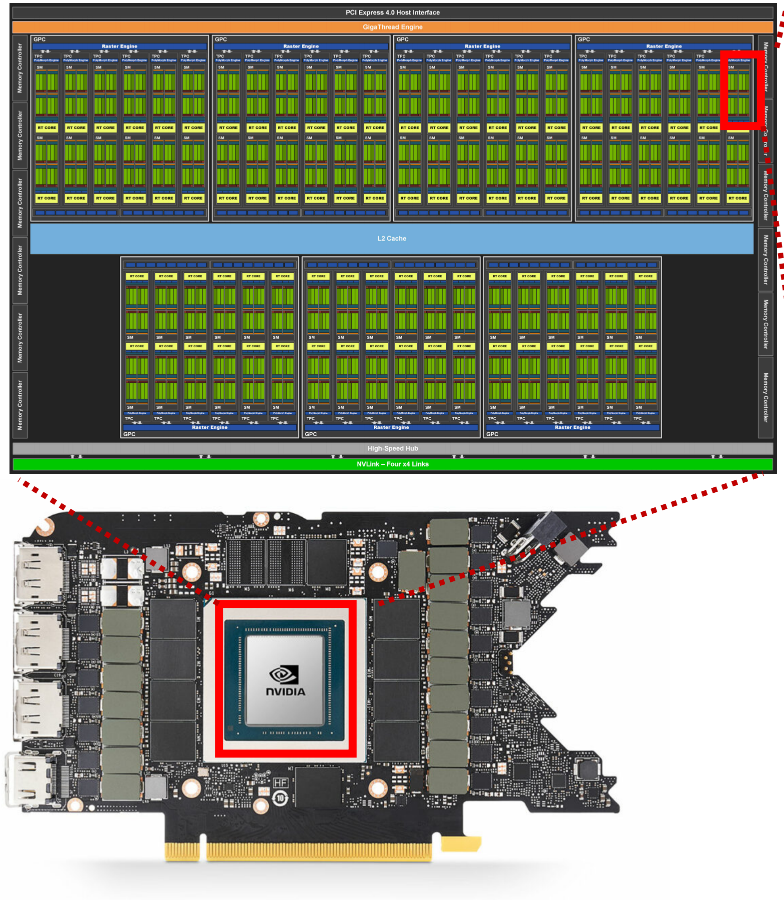
64 INT32/FP32 cores per SM

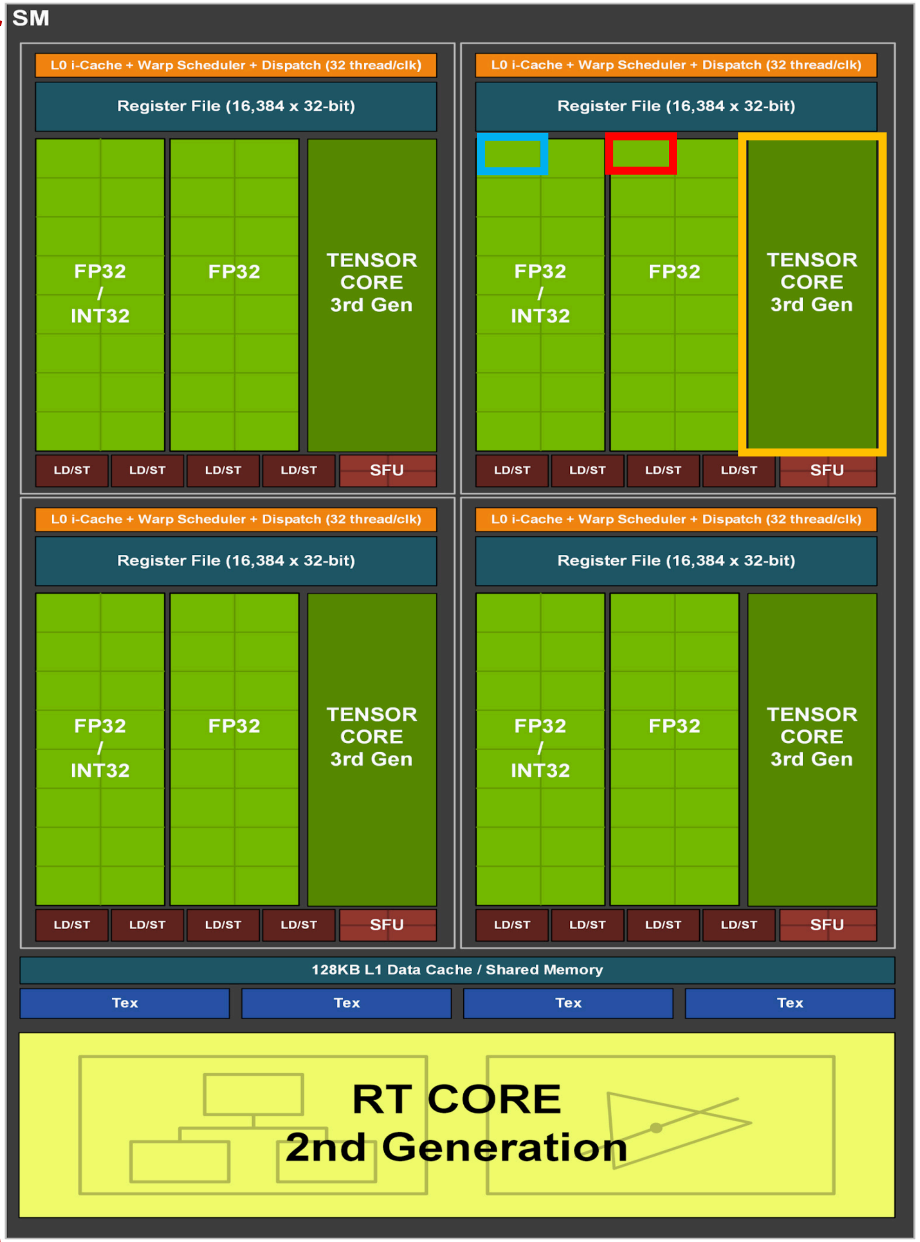
35.6 FP32 TFLOP/sec

Multiply:
- 82 SM
- 128 FP32 core/SM
- 2 FLOP/cycle
- 1.7 GCycle / sec

= 35.6 TFLOP/sec

Inside a GPU: RTX 3090





64 FP32 cores per SM

64 INT32/FP32 cores per SM

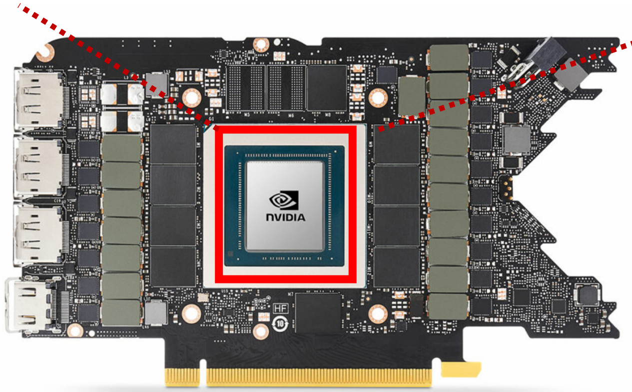
35.6 FP32 TFLOP/sec

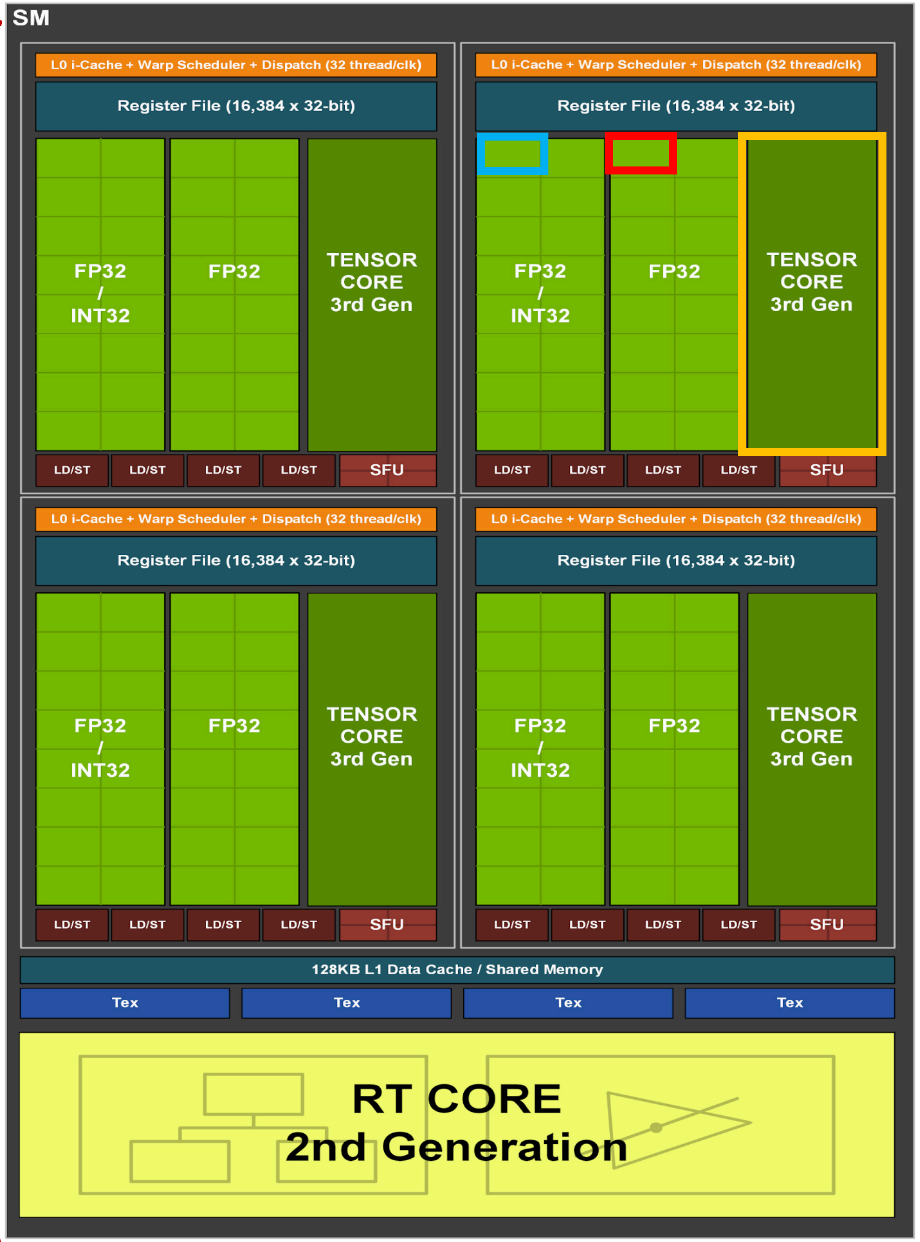
4 Tensor Core per SM

Special hardware!

Let A, B, C be matrices (A 4x4, B,C 4x8). Compute AB+C in one clock cycle (256 FLOP)

Inside a GPU: RTX 3090





64 FP32 cores per SM

64 INT32/FP32 cores per SM

35.6 FP32 TFLOP/sec

4 Tensor Core per SM

35.6 FP32 TFLOP/sec

Multiply:
- 82 SM
- 4 Tensor Core/SM
- 256 FLOP/cycle
- 1.7 GCycle / sec

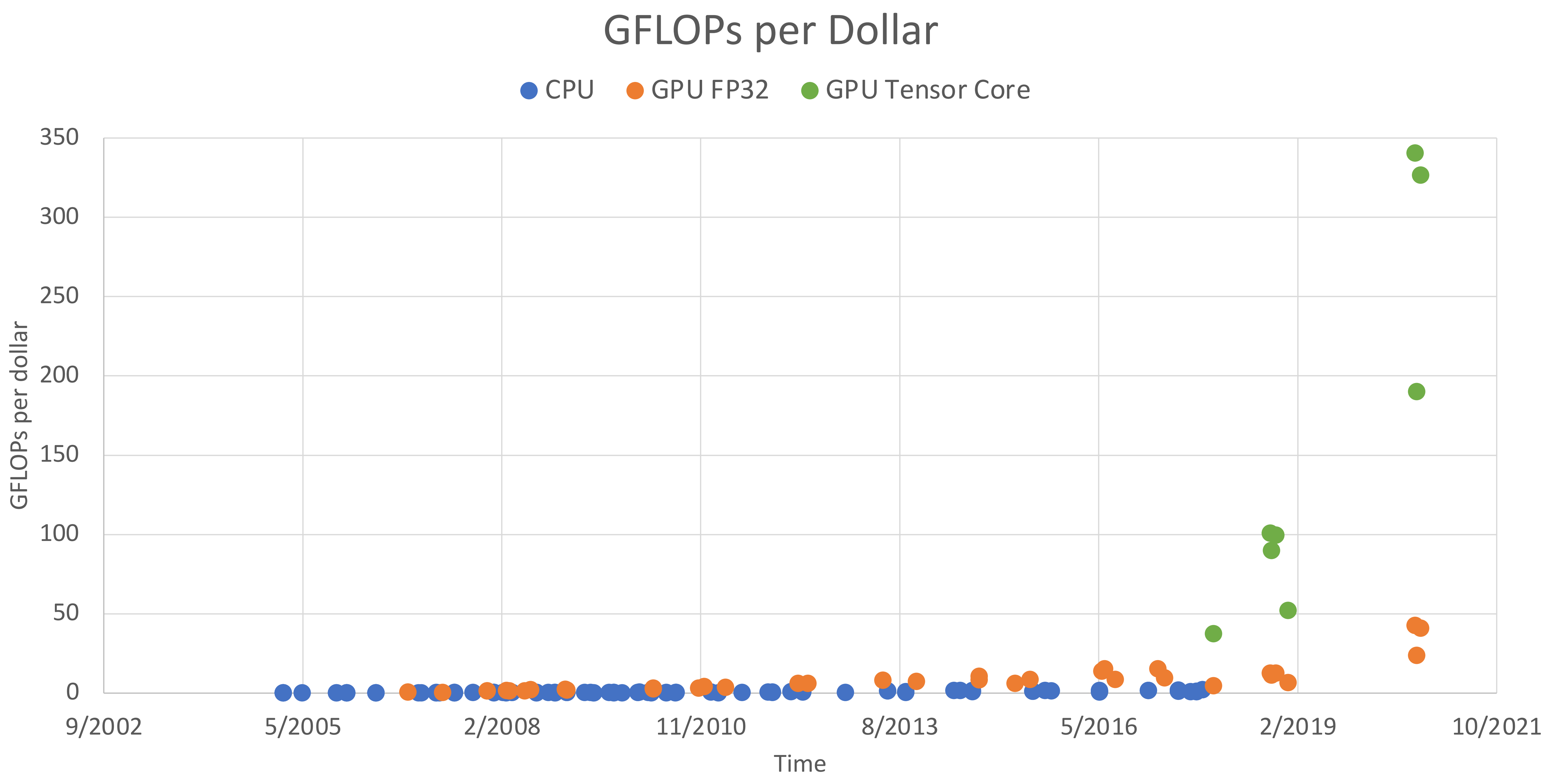
= 142 TFLOP/sec

CPU vs GPU

	Cores	Clock Speed (GHz)	Memory	Price	TFLOP/sec
CPU Ryzen Threadripper 3970X	64 (128 threads with hyperthreading)	3.7 (4.5 boost)	System RAM	$1999	~6.9 FP32
GPU NVIDIA RTX 3090	10496	1.4 (1.7 boost)	24 GB GDDR6X	$1499	~35.6 FP32 ~142 TFLOP with Tensor core

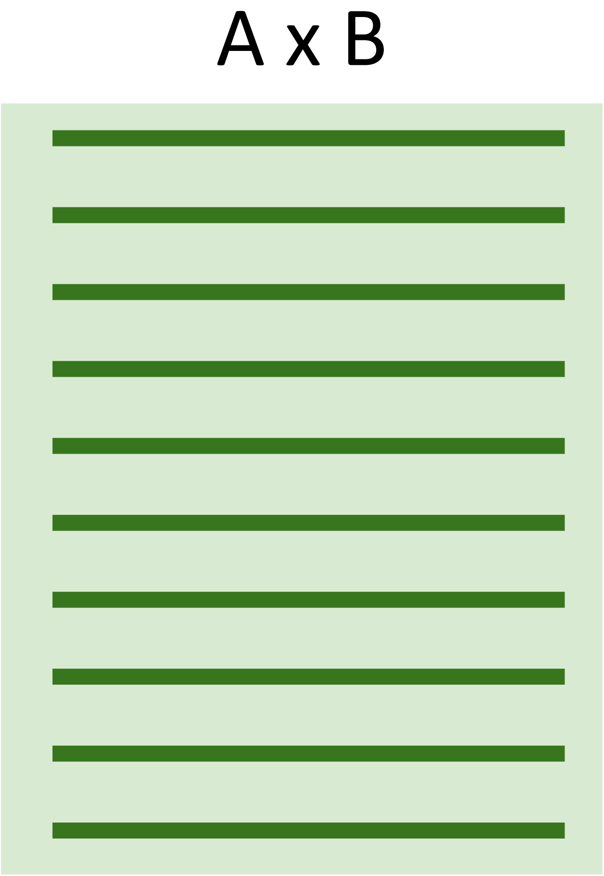
CPU: Fewer cores, but each core is much faster and much more capable; great at sequential tasks

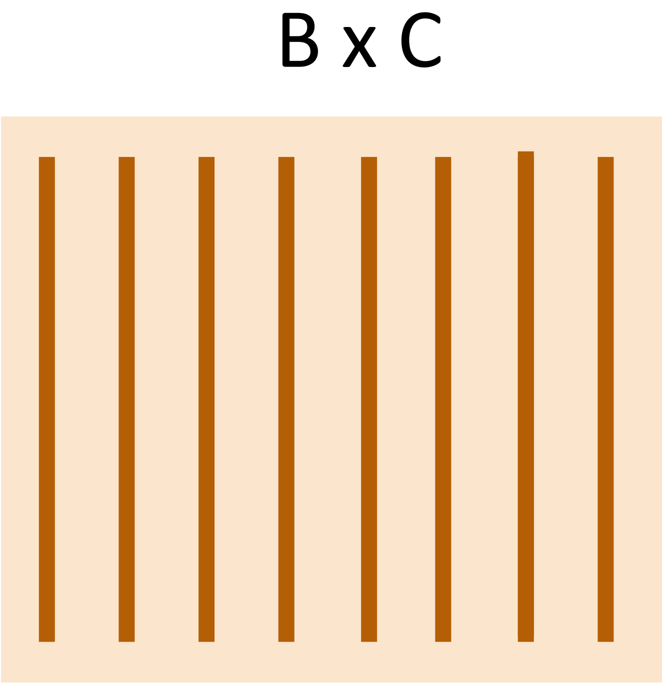
GPU: More cores, but each core is much slower and "dumber"; great for parallel tasks



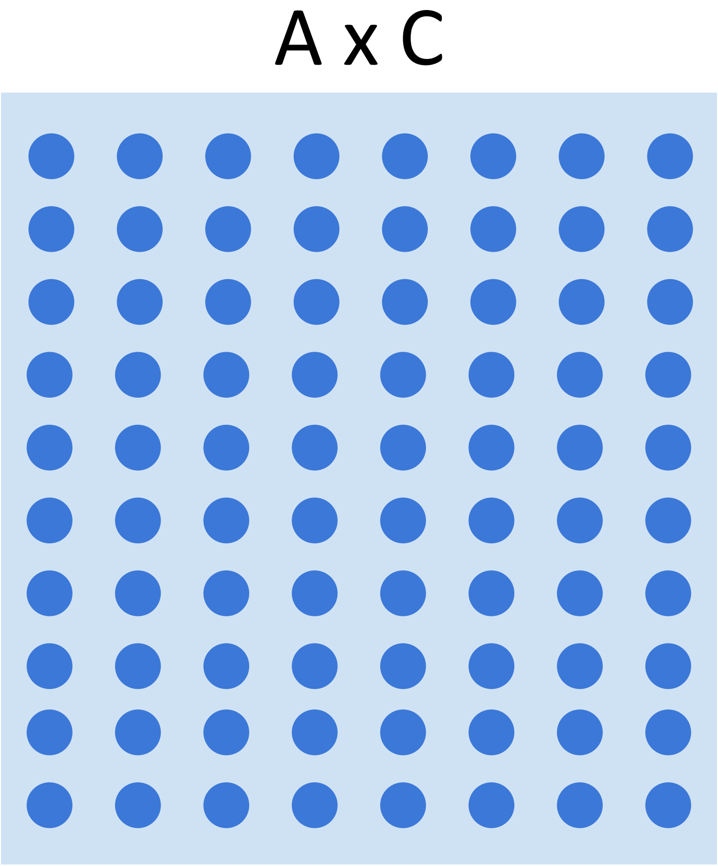
GFLOPs per Dollar
CPU
GPU FP32
GPU Tensor Core
350
300
250
200
150
100
50
0
GFLOPs per dollar
9/2002
5/2005
2/2008
11/2010
8/2013
5/2016
2/2019
10/2021
Time

Example: Matrix Multiplication





=



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

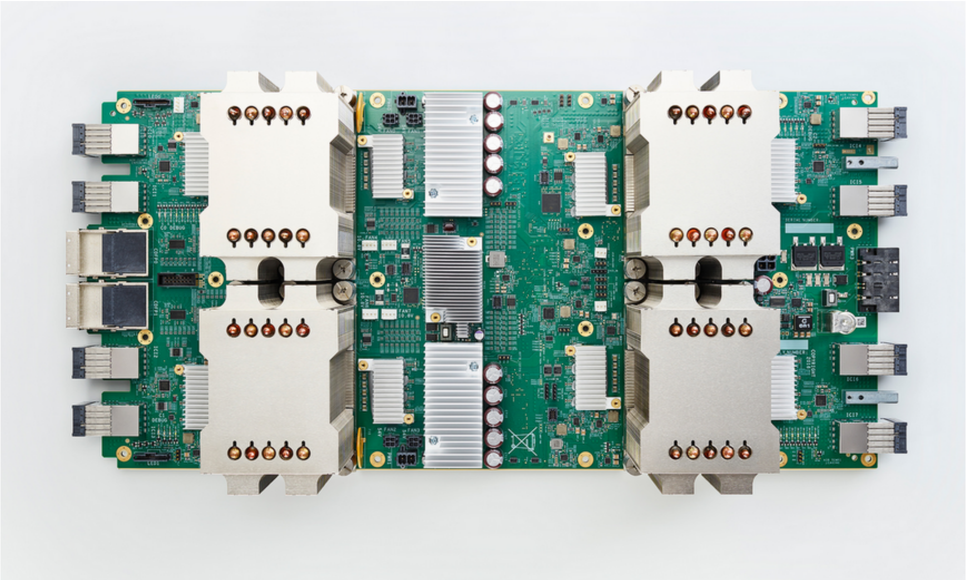
Programming GPUs

- 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

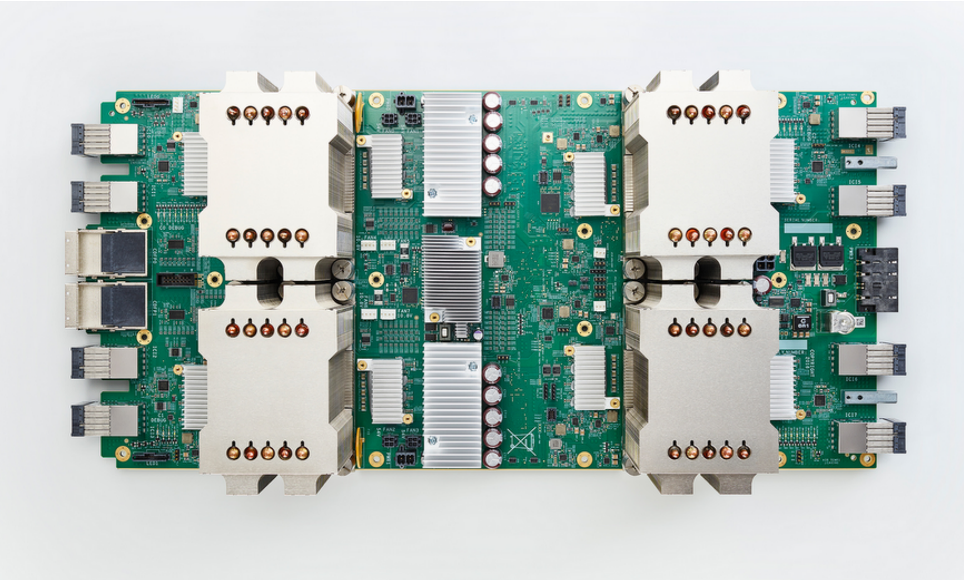
Google Tensor Processing Units (TPU)



Cloud TPU v2-8
180 TFLOP/sec
64 GB HBM memory
$6 / hour
(free on Colab!)

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

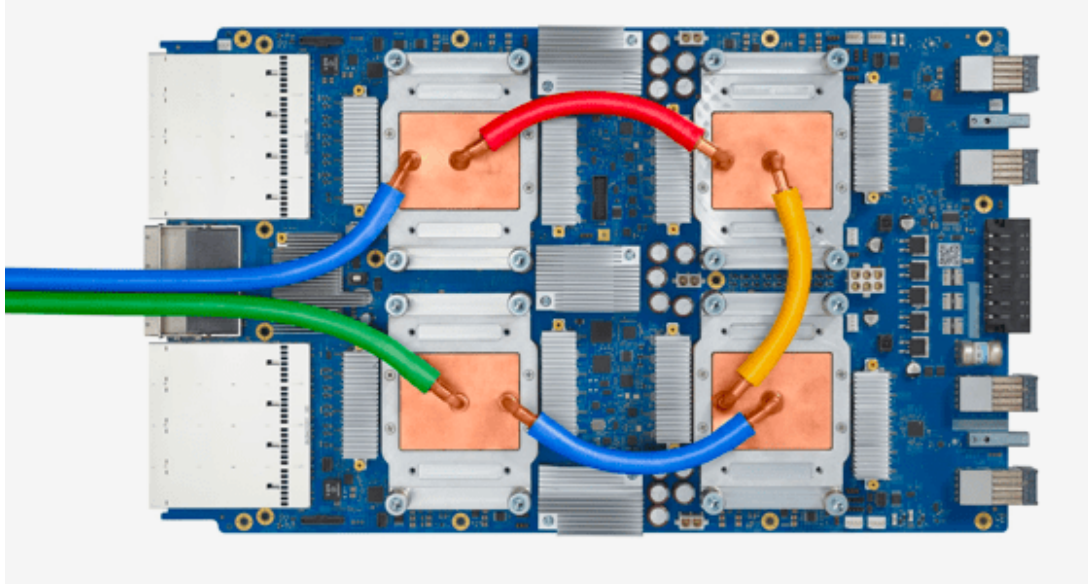
Google Tensor Processing Units (TPU)



Cloud TPU v2-8
180 TFLOP/sec
64 GB HBM memory
$6 / hour
(free on Colab!)

Cloud TPU v2 Pod
16x TPU-v2-8
11.5 PFLOPs
$384 / hour

Google Tensor Processing Units (TPU)



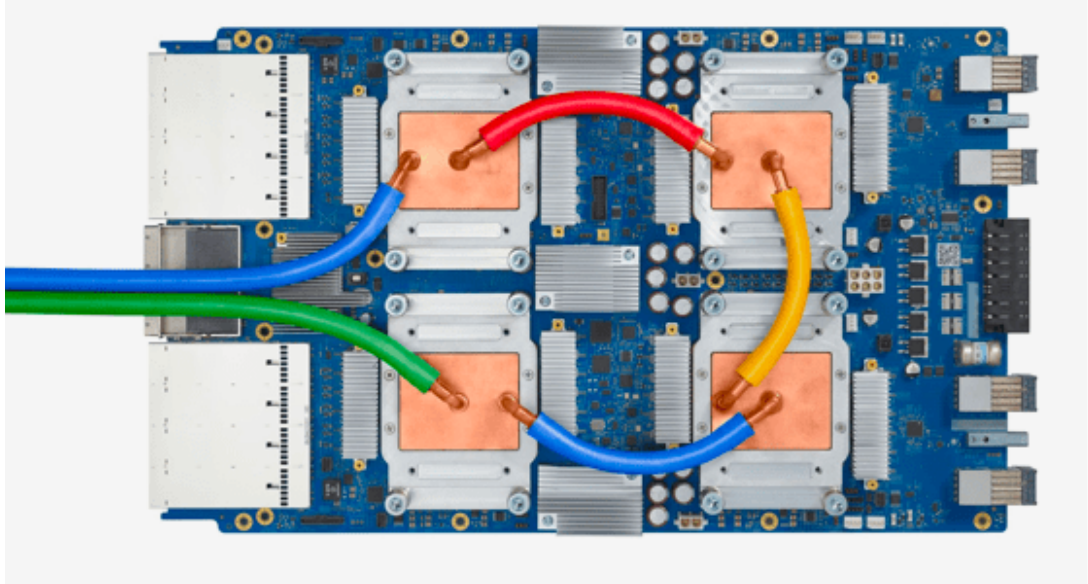
Cloud TPU v3-8

420 TFLOP/sec

128 GB HBM memory

$8 / hour

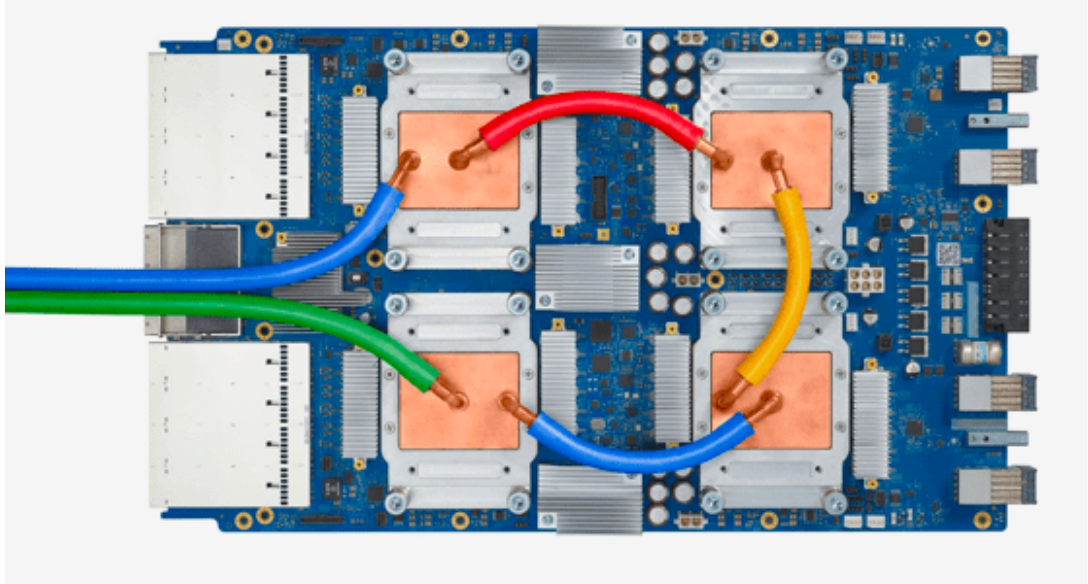
Google Tensor Processing Units (TPU)



Cloud TPU v3-8
420 TFLOP/sec
128 GB HBM memory
$8 / hour

Cloud TPU v3 Pod
256 TPU-v3
107 PFLOPs

Google Tensor Processing Units (TPU)



<u>Cloud TPU v3-8</u>

420 TFLOP/sec

128 GB HBM memory

$8 / hour

<u>Cloud TPU v3 Pod</u>

256 TPU-v3

107 PFLOPs

Contact sales rep for pricing

Deep Learning Software

A zoo of frameworks!

Caffe
(UC Berkeley)

→

Caffe2
(Facebook)

Torch
(NYU / Facebook)

→

PyTorch
(Facebook)

Theano
(U Montreal)

→

TensorFlow
(Google)

PaddlePaddle
(Baidu)

Chainer

MXNet
(Amazon)

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

CNTK
(Microsoft)

JAX
(Google)

A zoo of frameworks!

Caffe
(UC Berkeley)

Caffe2
(Facebook)

Torch
(NYU / Facebook)

PyTorch
(Facebook)

Theano
(U Montreal)

TensorFlow
(Google)

We'll focus on these

PaddlePaddle
(Baidu)

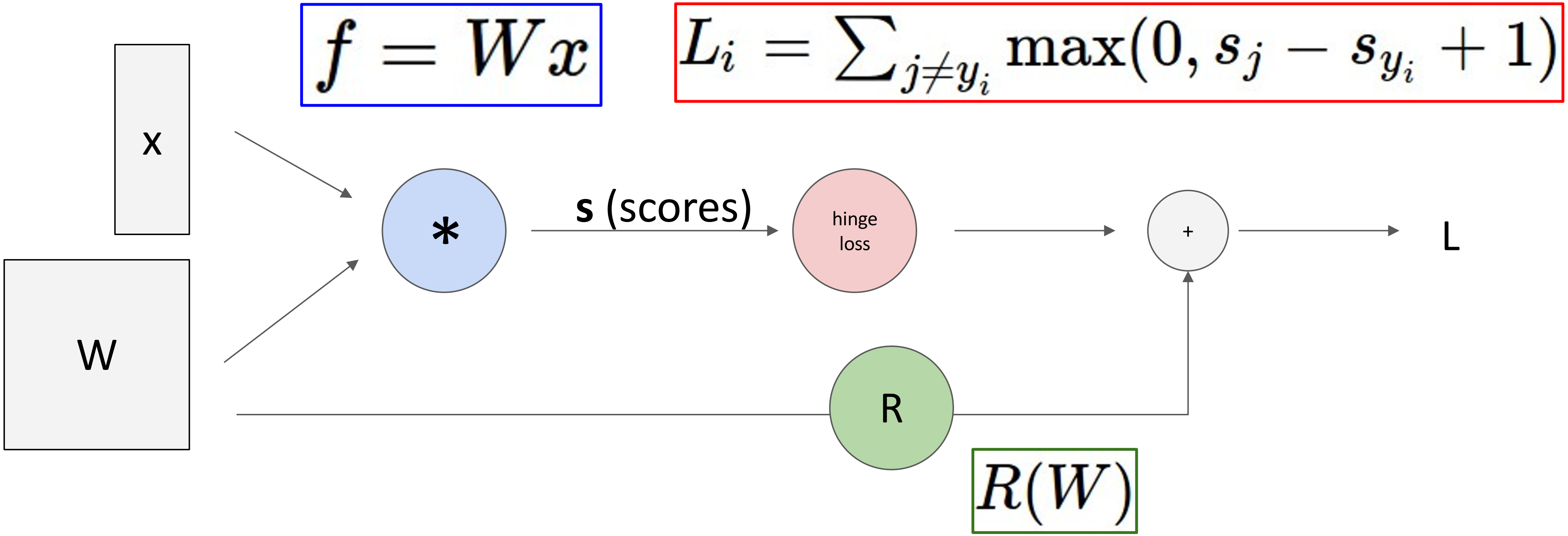
Chainer

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

CNTK
(Microsoft)

JAX
(Google)

Recall: Computational Graphs



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 1.6** (Released July 2020)

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

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

A4, A5, A6

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)
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    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):
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    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

```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

```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):
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    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)
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    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

```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

```
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

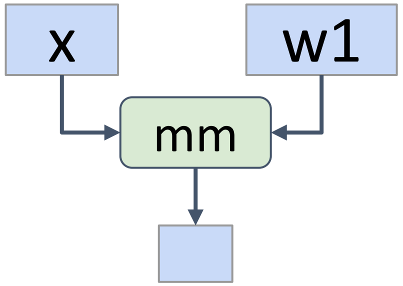
```
import torch

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

```
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_()
```

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

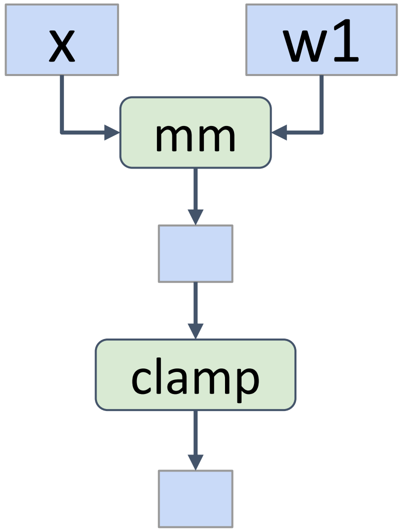
PyTorch: Autograd



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

```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_()
```

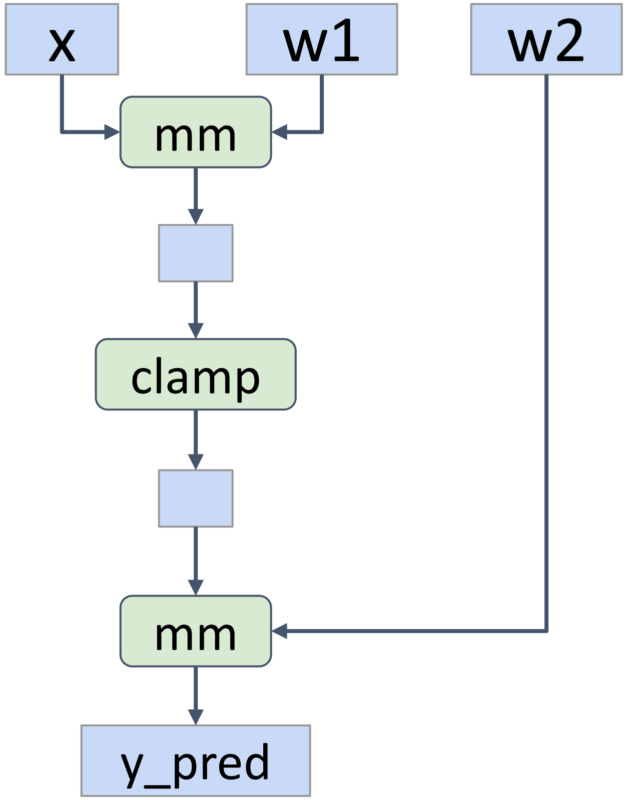
PyTorch: Autograd



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

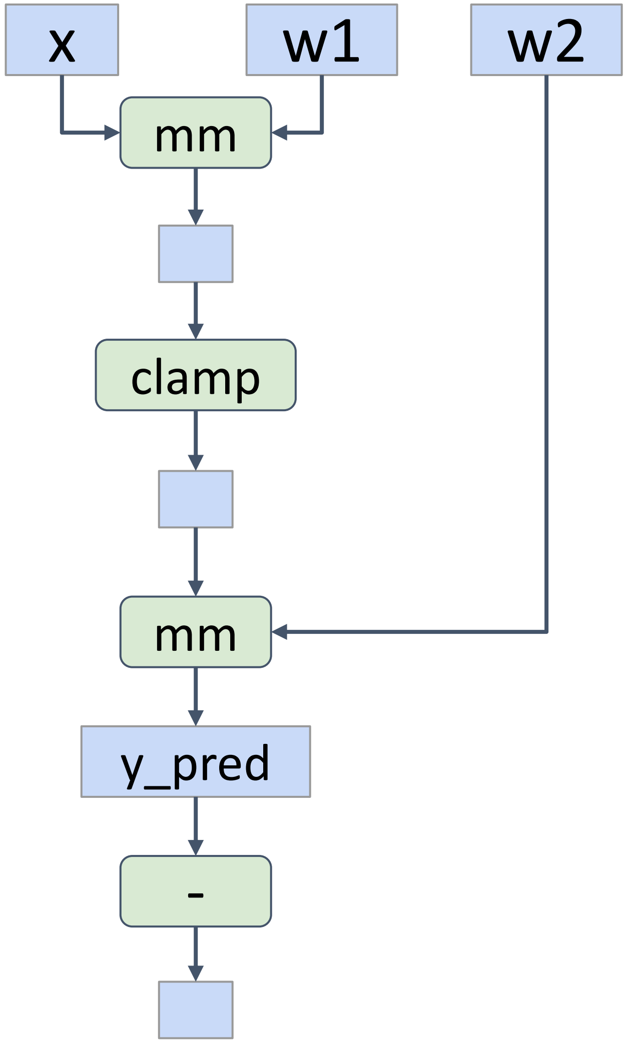
```
import torch

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

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

    loss.backward()

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

PyTorch: Autograd



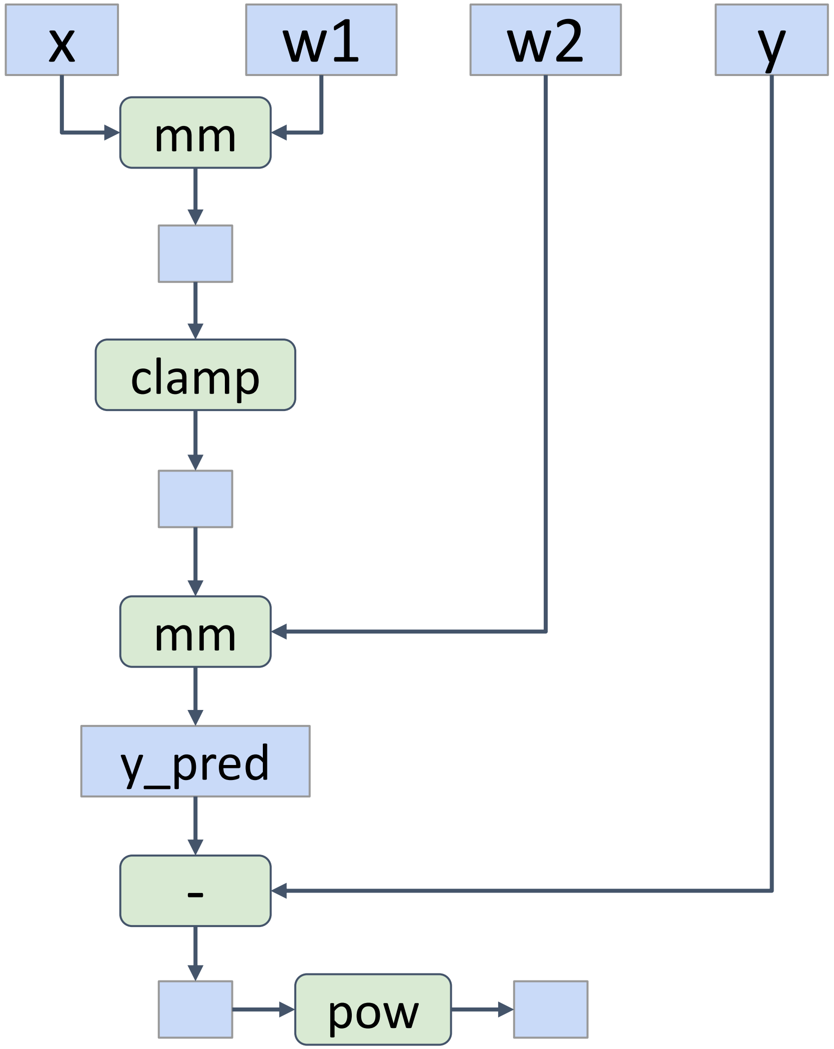

```
import torch

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



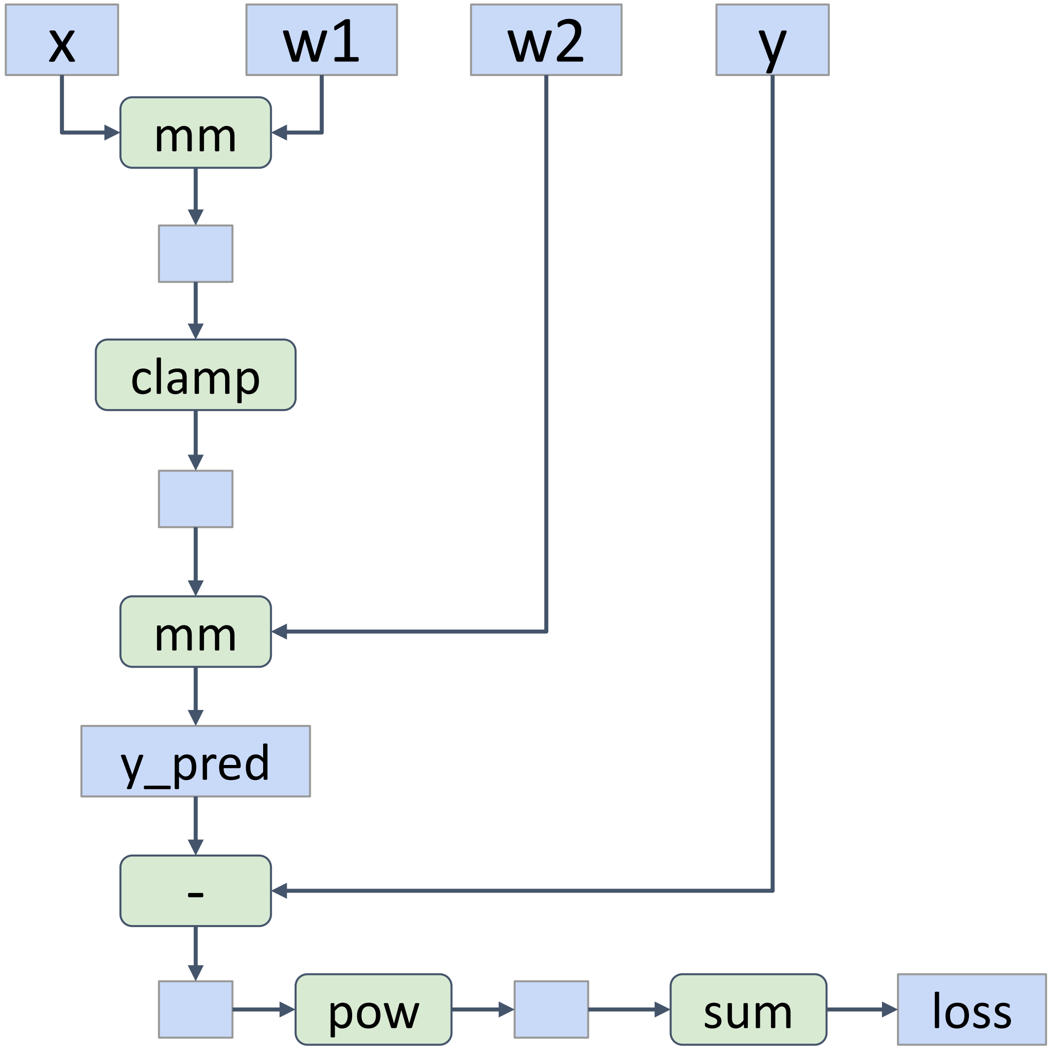

```python
import torch

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



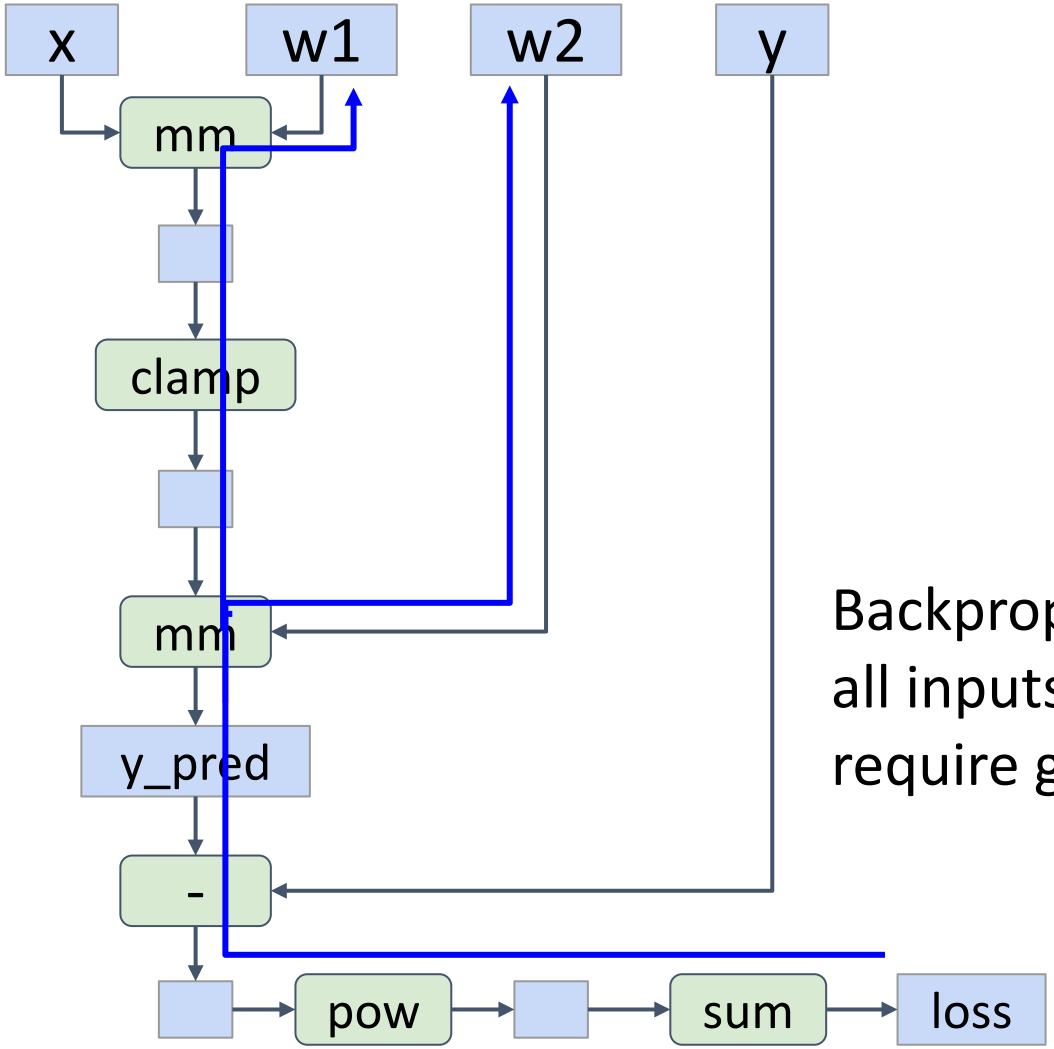

```python
import torch

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



Backprop to all inputs that require grad

```
import torch

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

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

```
import torch

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

learning_rate = 1e-6
for t in range(500):
    y_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

```
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

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!

```
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_()
```

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

PyTorch: New functions

Can define new operations using Python functions

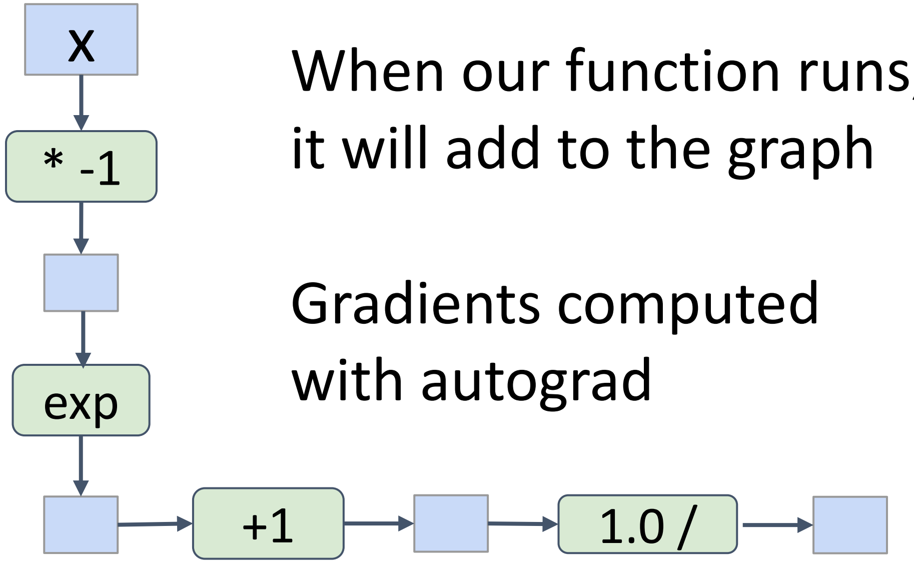
```
def sigmoid(x):
  return 1.0 / (1.0 + (-x).exp())
```

```
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

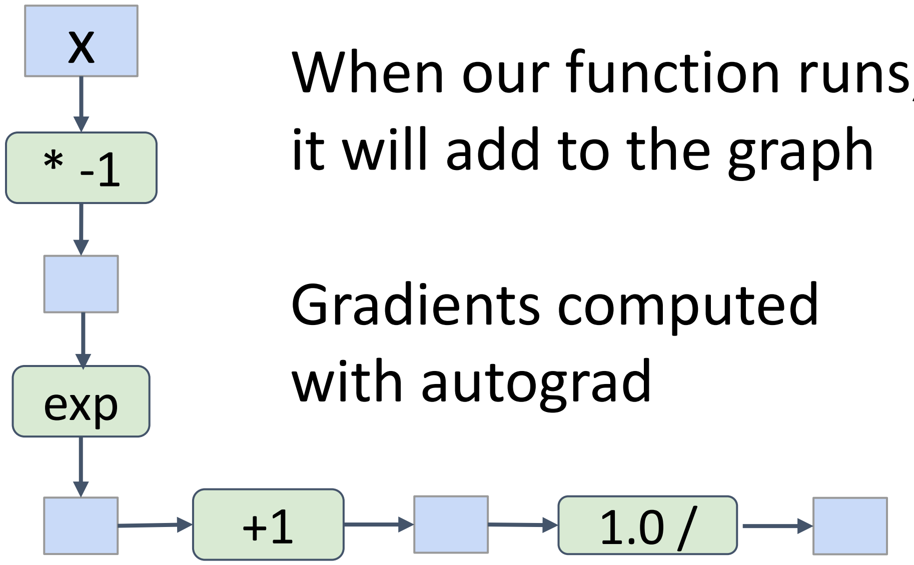
Gradients computed with autograd

```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

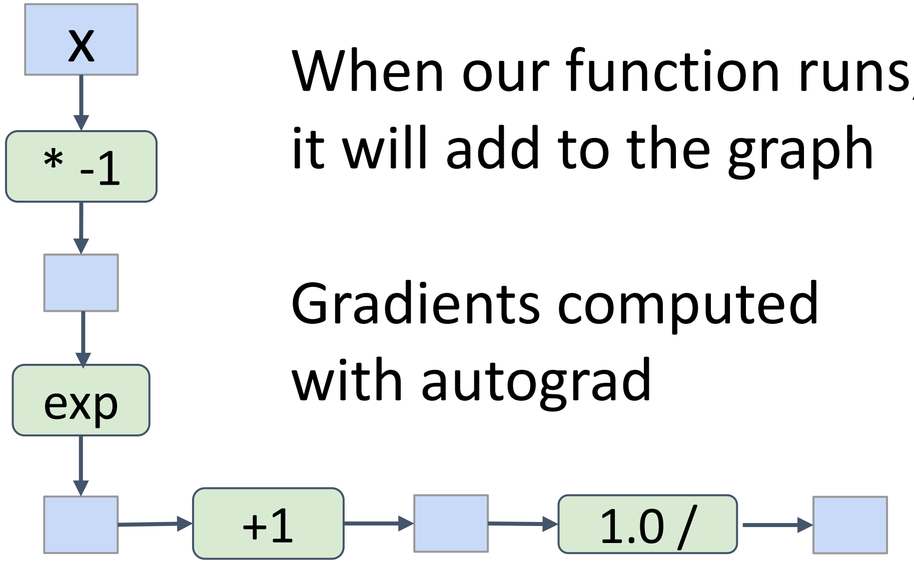
```python
class Sigmoid(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x):
    y = 1.0 / (1.0 + (-x).exp())
    ctx.save_for_backward(y)
    return y

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

PyTorch: New functions

Can define new operations using Python functions

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



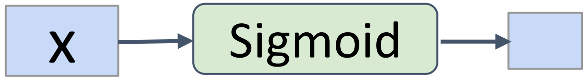
When our function runs, it will add to the graph

Gradients computed with autograd

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

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

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

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

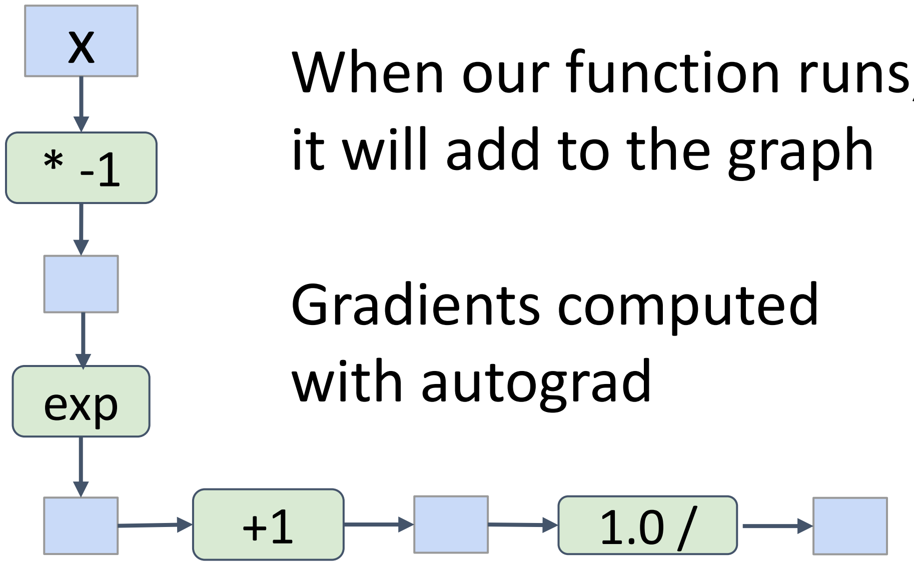
Now when our function runs, it adds one node to the graph!



PyTorch: New functions

Can define new operations using Python functions

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



When our function runs, it will add to the graph

Gradients computed with autograd

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

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

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

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

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

```
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

```
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

```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

```
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

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()

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

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

PyTorch: optim

Use an **optimizer** for different update rules

```
import torch

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

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

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

    loss.backward()

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

PyTorch: optim

```
import torch

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

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

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

    loss.backward()

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

After computing gradients, use optimizer to update and zero gradients

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

```
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)

```
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()
```

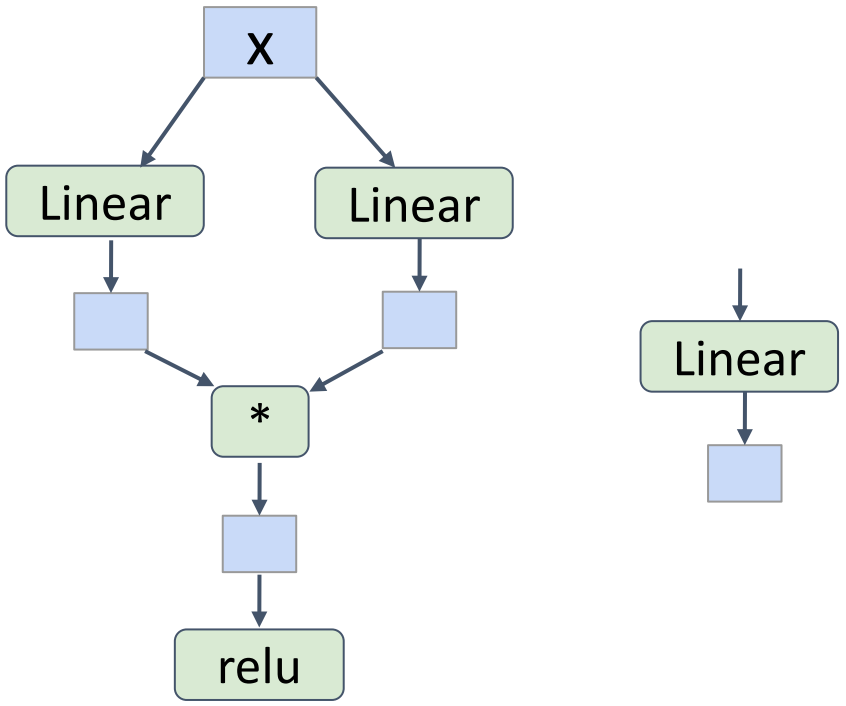
PyTorch: nn Defining Modules

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

```
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

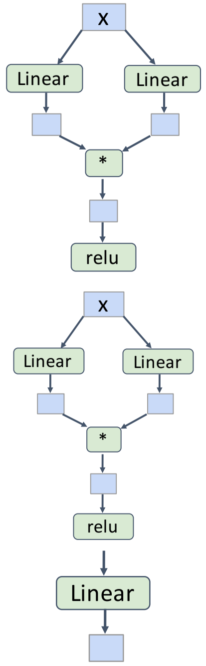
Define network component as a Module subclass




```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

```
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

Iterate over loader to form minibatches

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

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

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

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

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

PyTorch: DataLoaders

Iterate over loader to form minibatches

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

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

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

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

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

PyTorch: 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: 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()
```

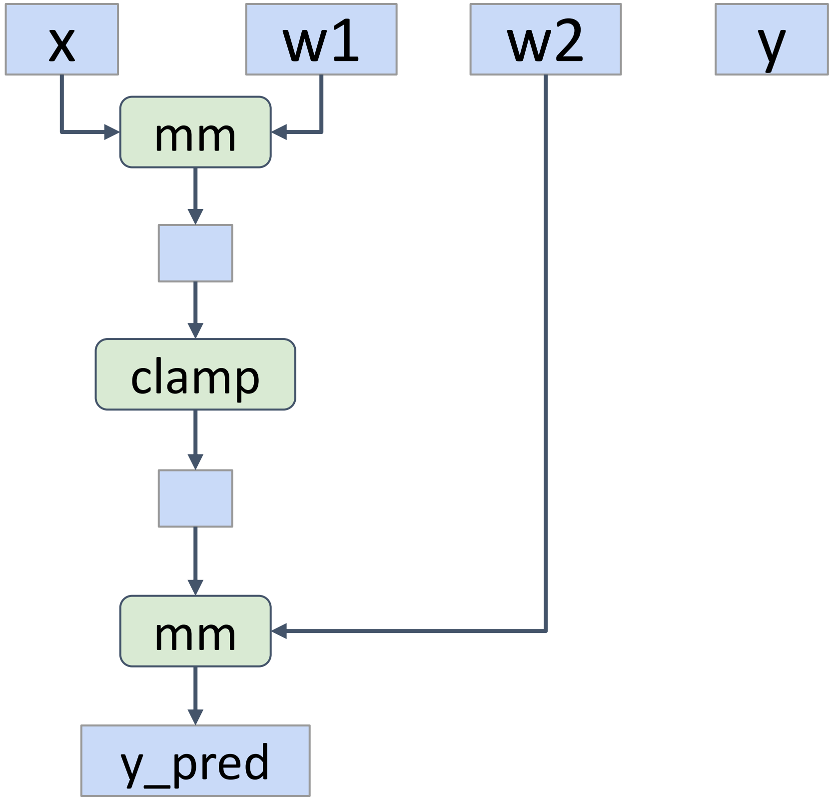
PyTorch: **Dynamic Computation Graphs**

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

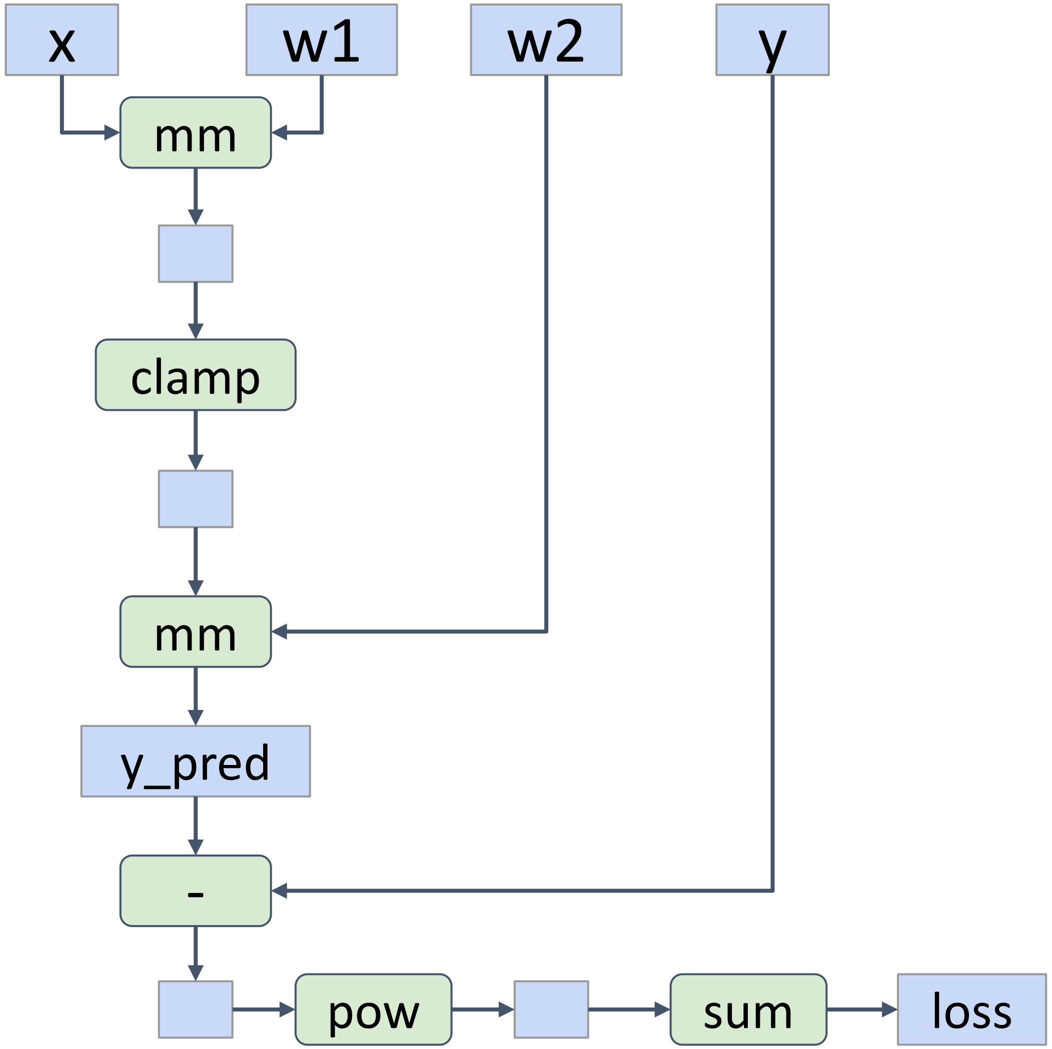
PyTorch: Dynamic Computation Graphs




```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

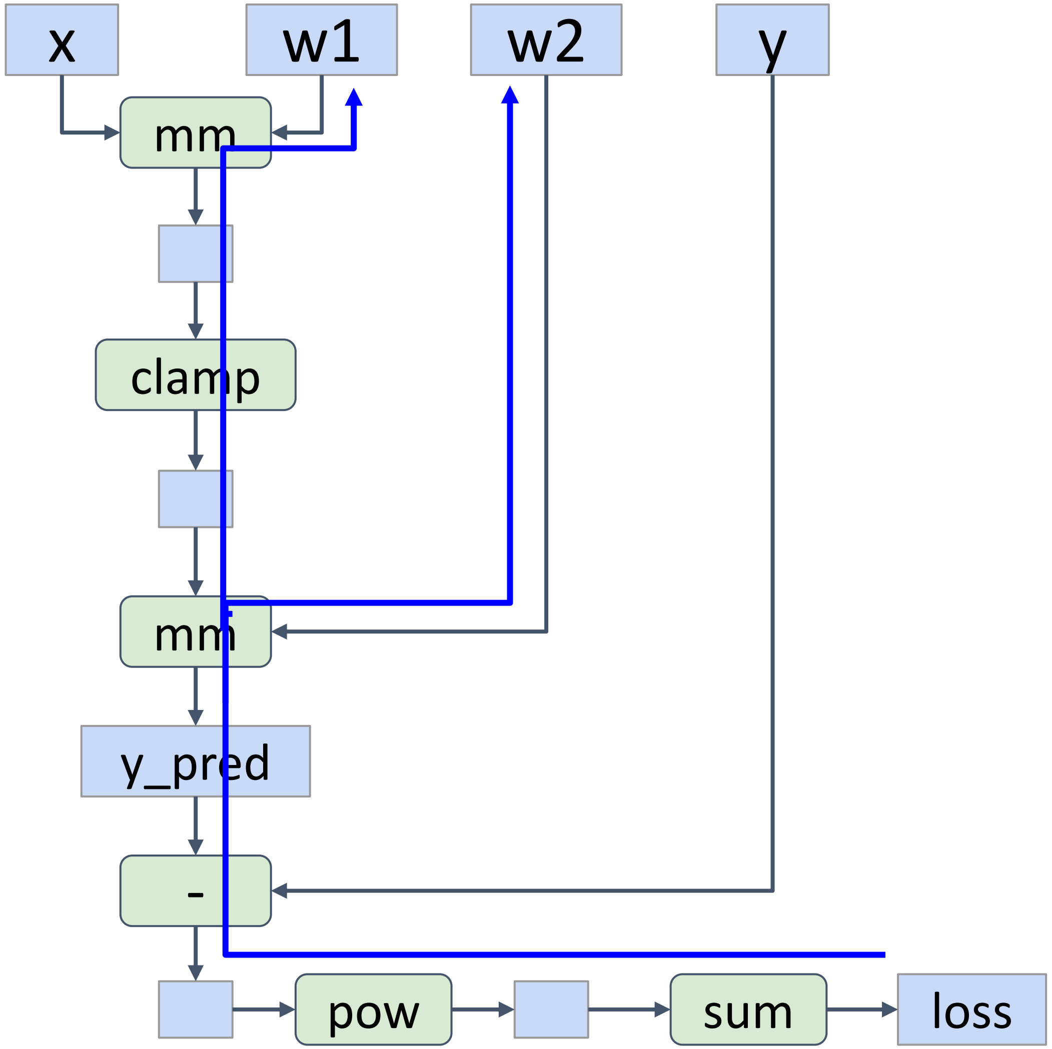
PyTorch: **Dynamic Computation Graphs**




```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()
```

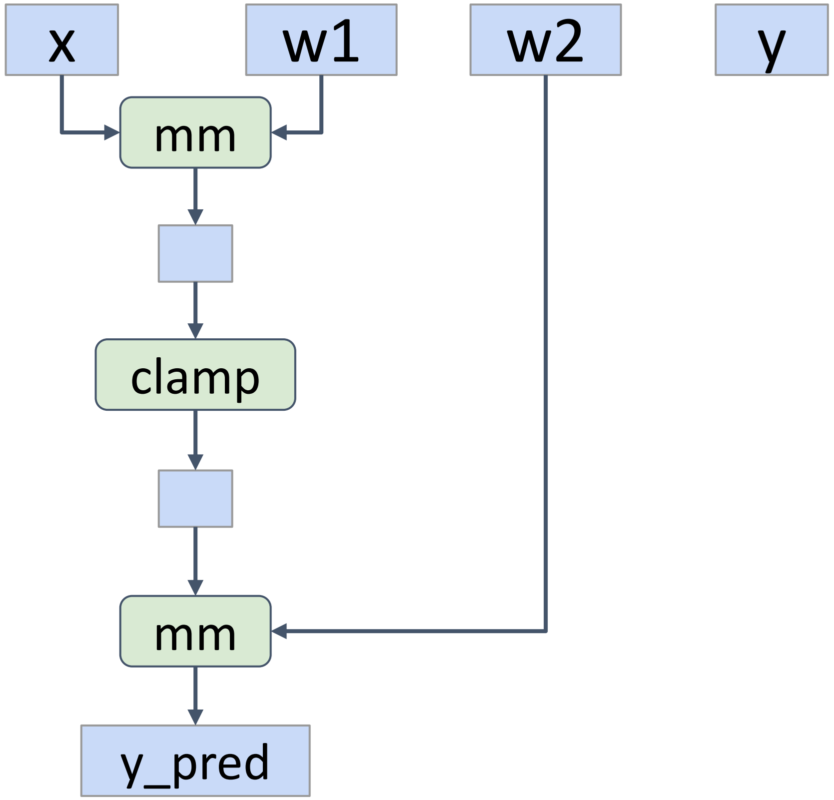
Perform backprop, throw away graph

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()
```

Perform backprop,
throw away graph

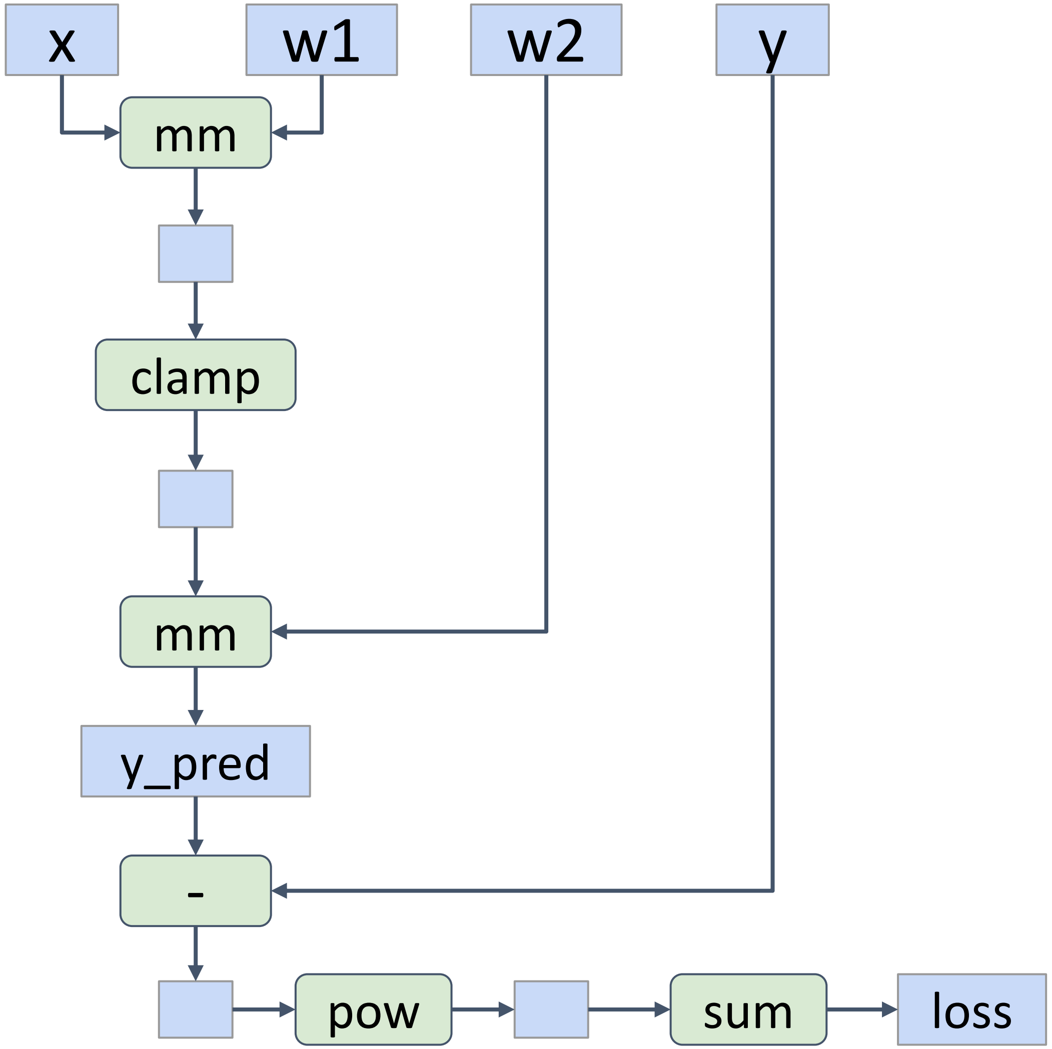
PyTorch: Dynamic Computation Graphs




```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

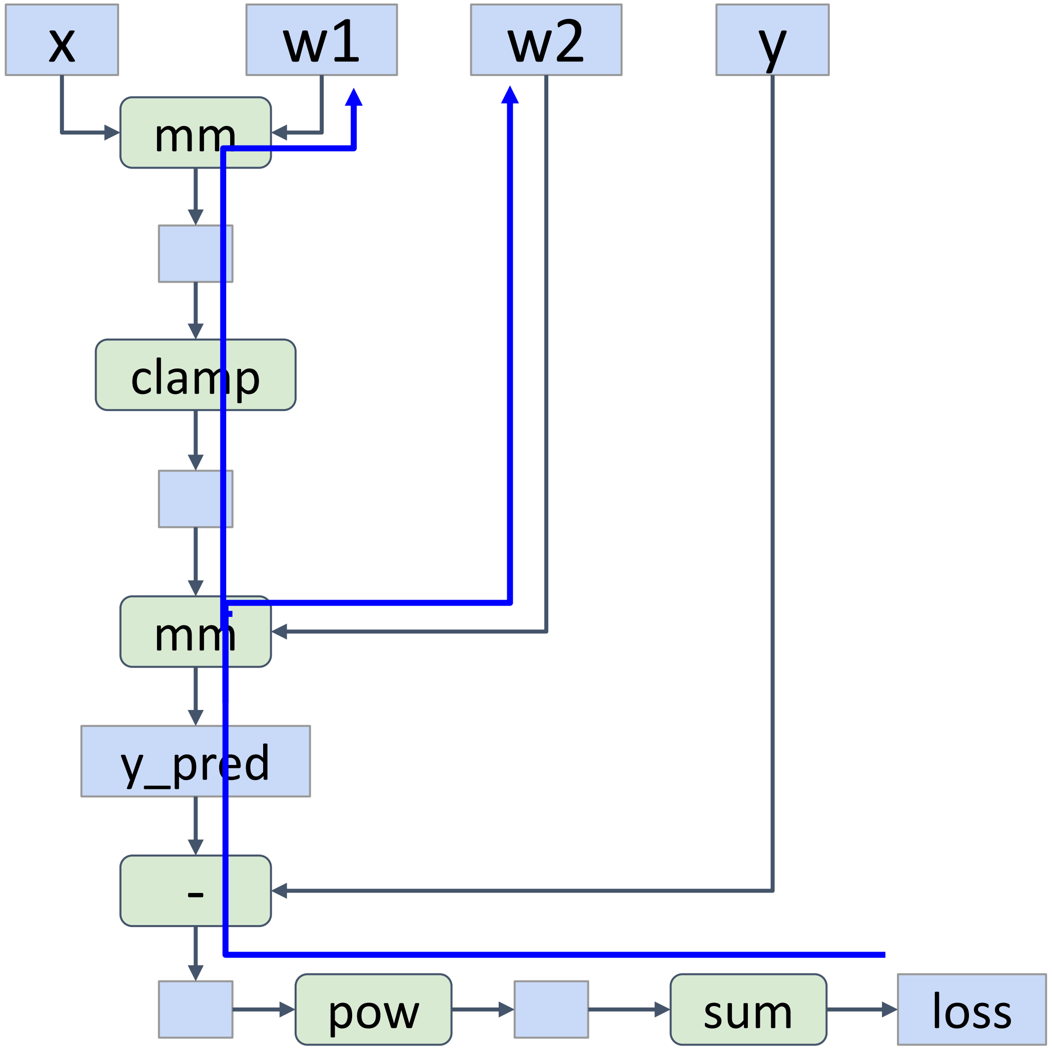
PyTorch: **Dynamic Computation Graphs**




```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




```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**

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

```
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

```
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!

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)

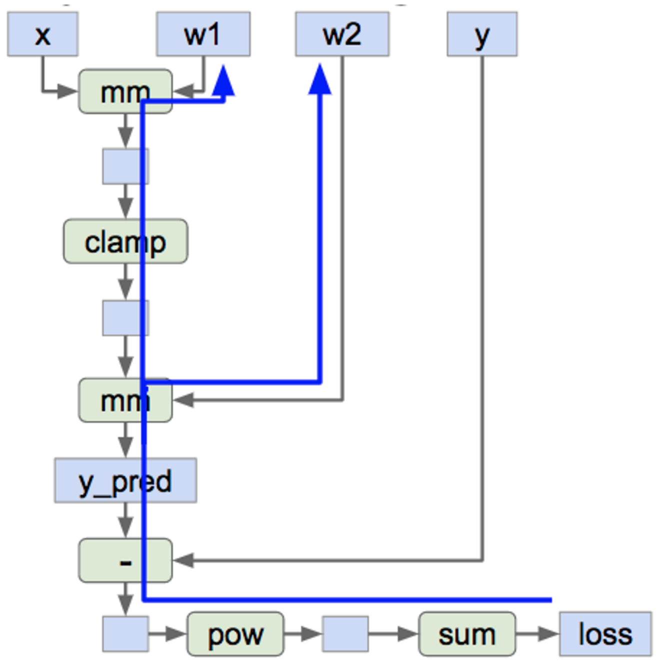
```
import torch

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()
```

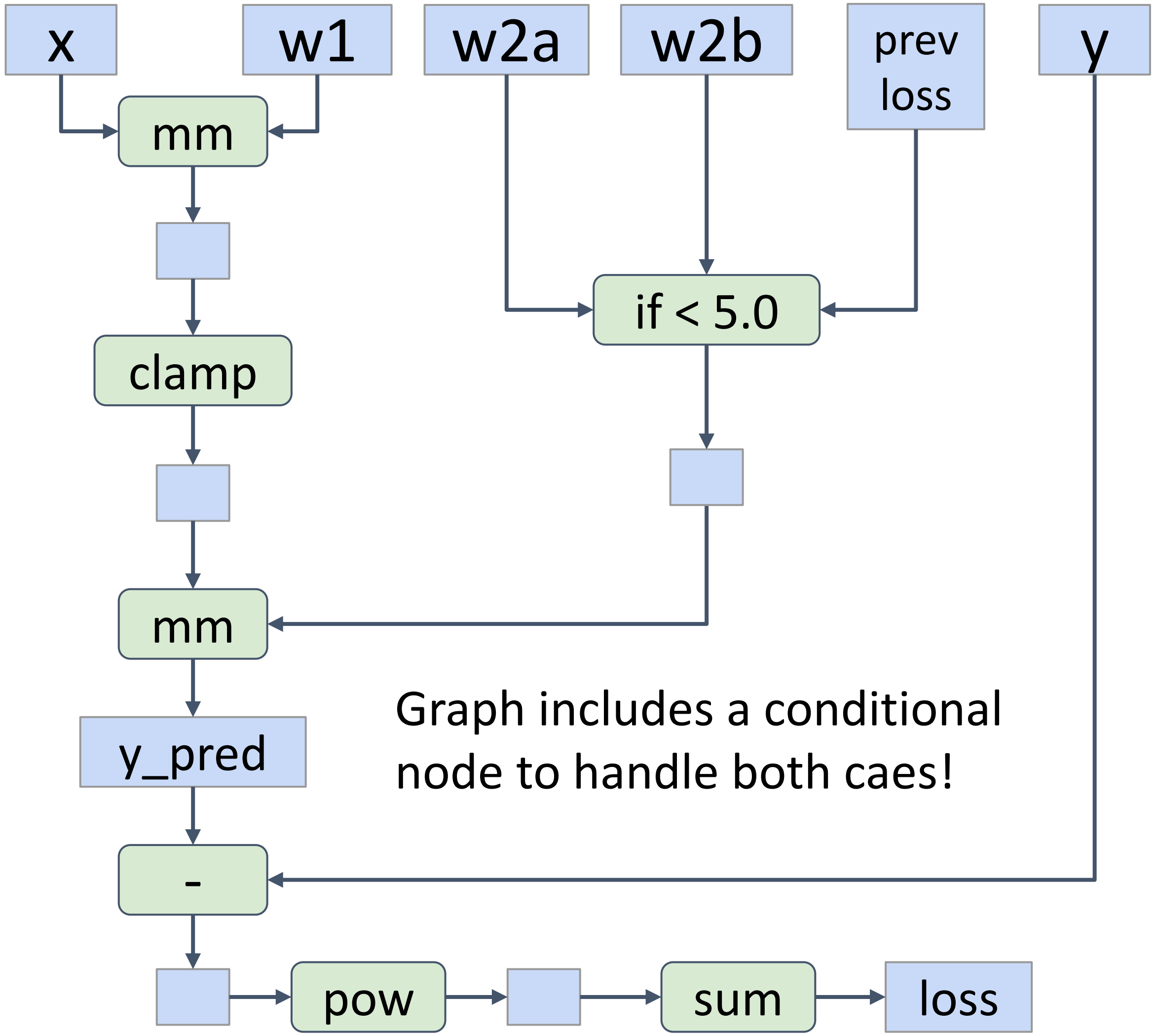
PyTorch: Static Graphs with JIT

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

Lots of magic here!

```
import torch

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

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

graph = torch.jit.script(model)

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

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

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

```
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

```
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++

Dynamic

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

Static vs Dynamic Graphs: Debugging

Static

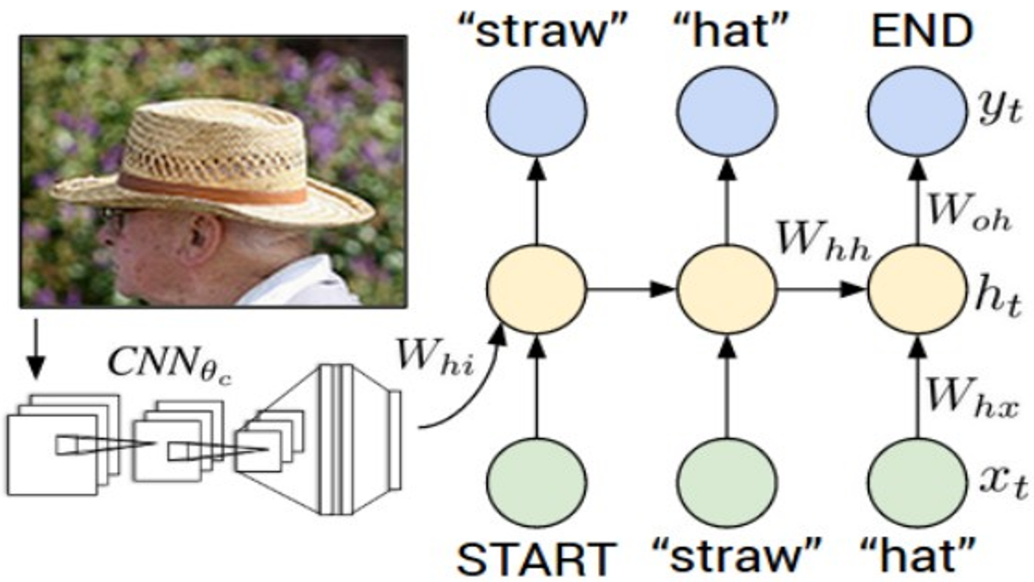
Lots of indirection between the code you write and the code that runs – can be hard to debug, benchmark, etc

Dynamic

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

Dynamic Graph Applications

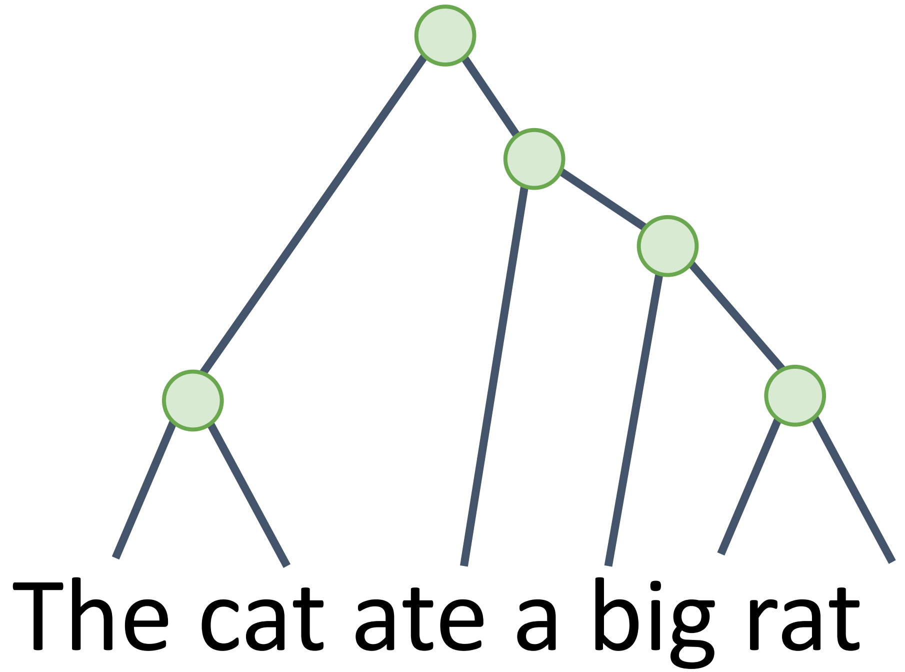
Model structure depends on the input:
- Recurrent Networks



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

Dynamic Graph Applications

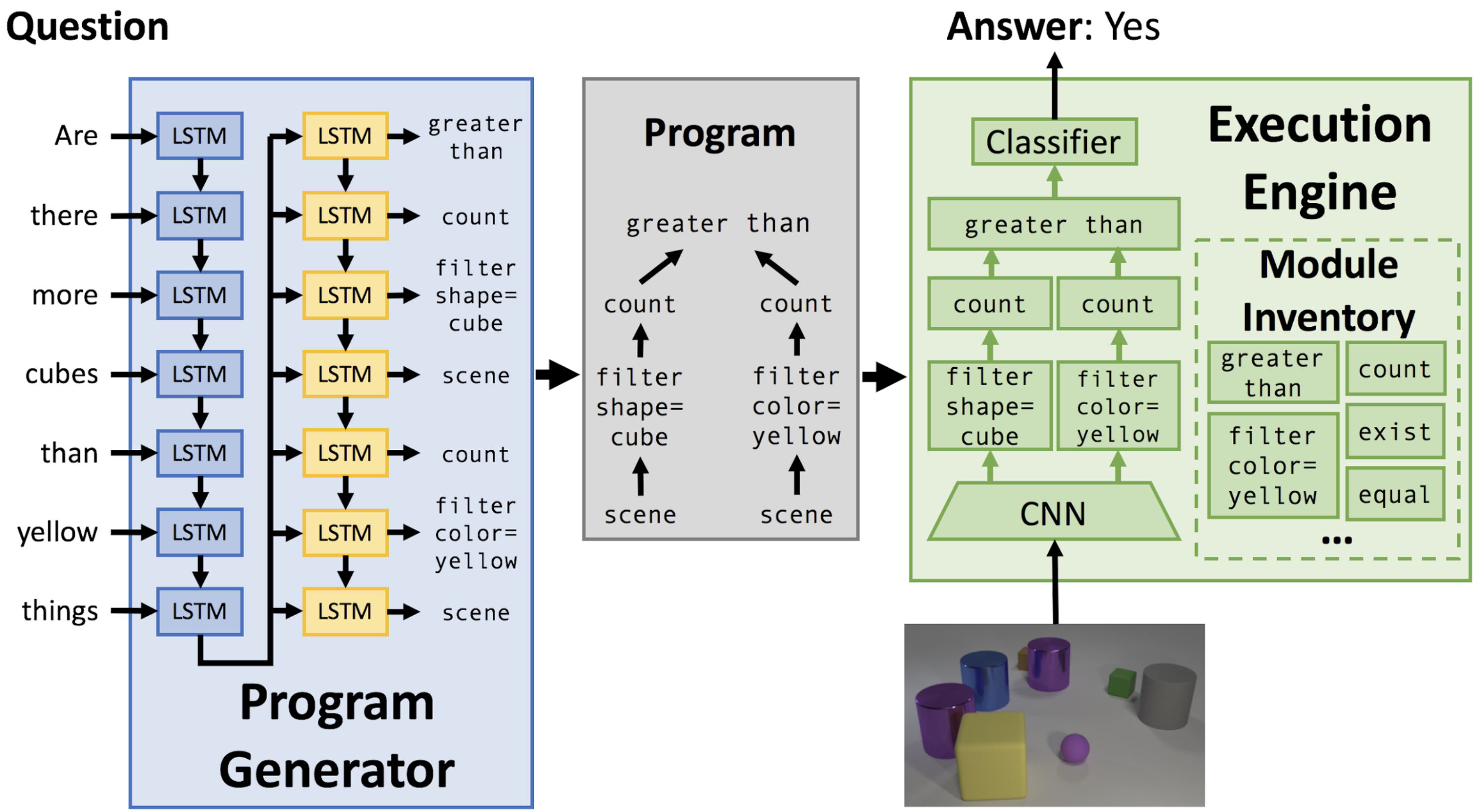
Model structure depends on the input:
- Recurrent Networks
- Recursive Networks



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

Dynamic Graph Applications

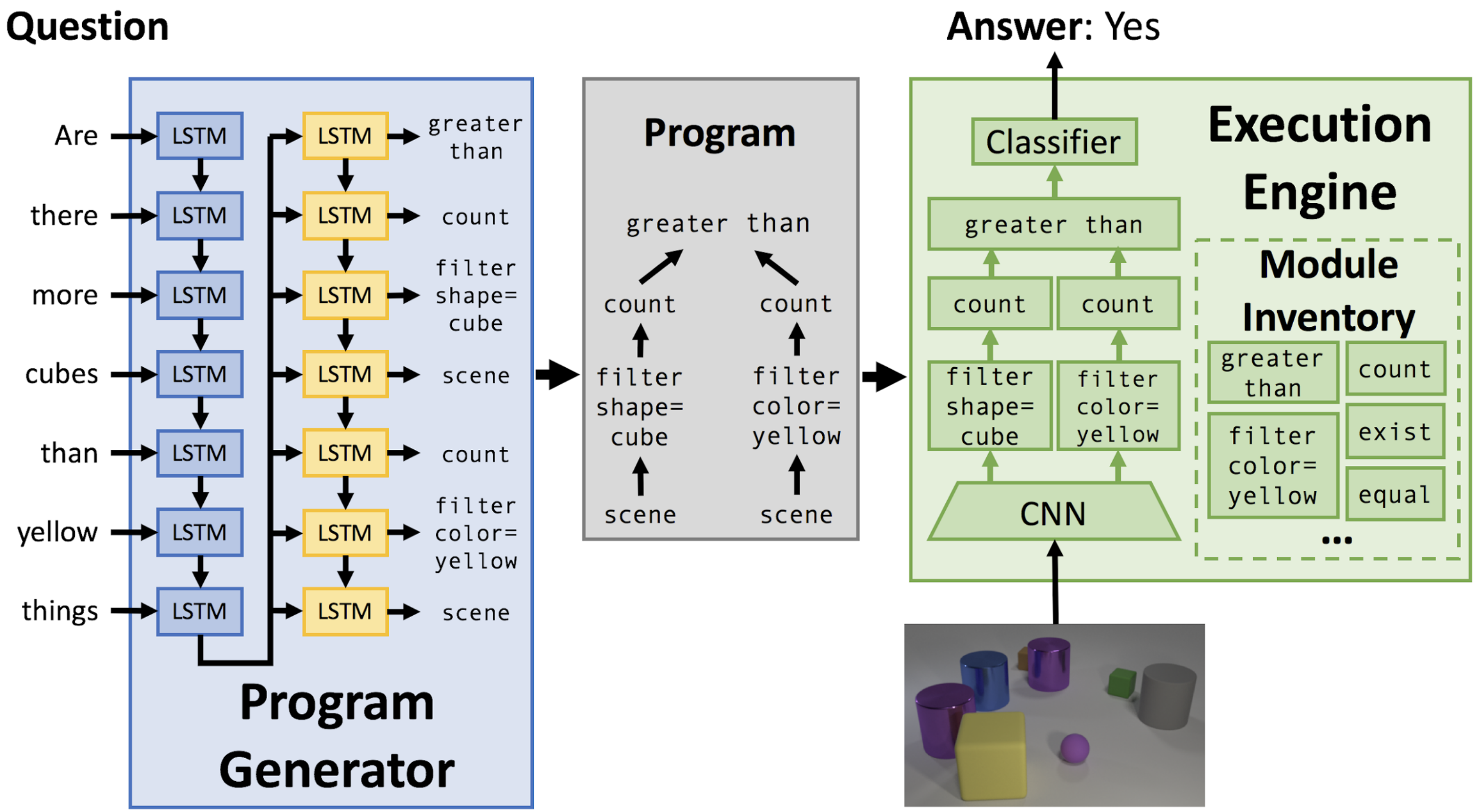
Model structure depends on the input:
- Recurrent Networks
- Recursive Networks
- Modular Networks



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

TensorFlow

TensorFlow Versions

TensorFlow 1.0

- Final release: 1.15.3
- Default: **static graphs**
- Optional: dynamic graphs (eager mode)

TensorFlow 2.0

- Current release: 2.3.1
  - Released 9/24
- 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

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: **Dynamic Graphs**

Create TensorFlow Tensors for data and weights

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

```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)
```

TensorFlow 2.0: Dynamic Graphs

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

```
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)
```

TensorFlow 2.0: **Dynamic Graphs**

```
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

```
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)
```

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)

```
@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)

```
@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

```
@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)
```

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

```
import tensorflow as tf
from tensorflow.keras.models import Sequential
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N, Din, H, Dout = 16, 1000, 100, 10

model = Sequential()
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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

Keras gives you common loss functions and optimization algorithms

```
import tensorflow as tf
from tensorflow.keras.models import Sequential
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N, Din, H, Dout = 16, 1000, 100, 10

model = Sequential()
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loss_fn = tf.keras.losses.MeanSquaredError()
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)
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Keras: High-level API

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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

```
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))
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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

```python
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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))

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()
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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)
```
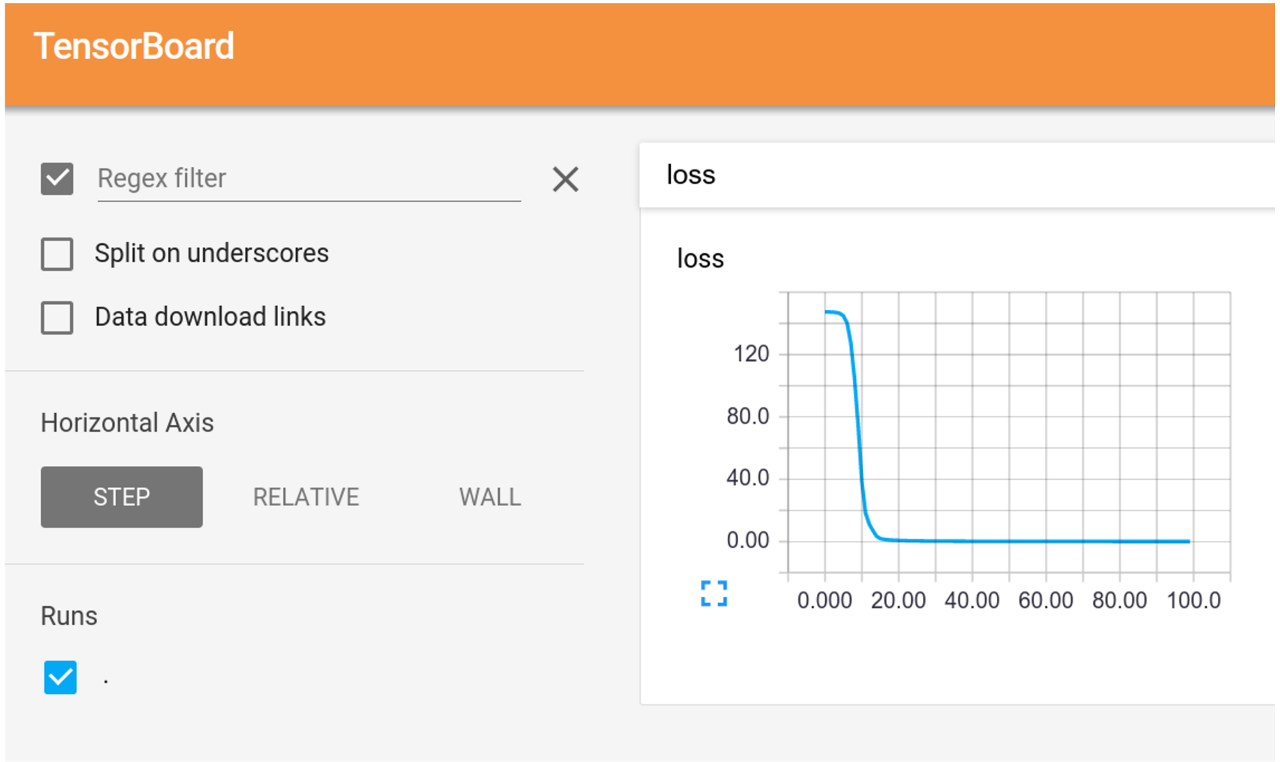

Optimizer computes gradients and updates parameters

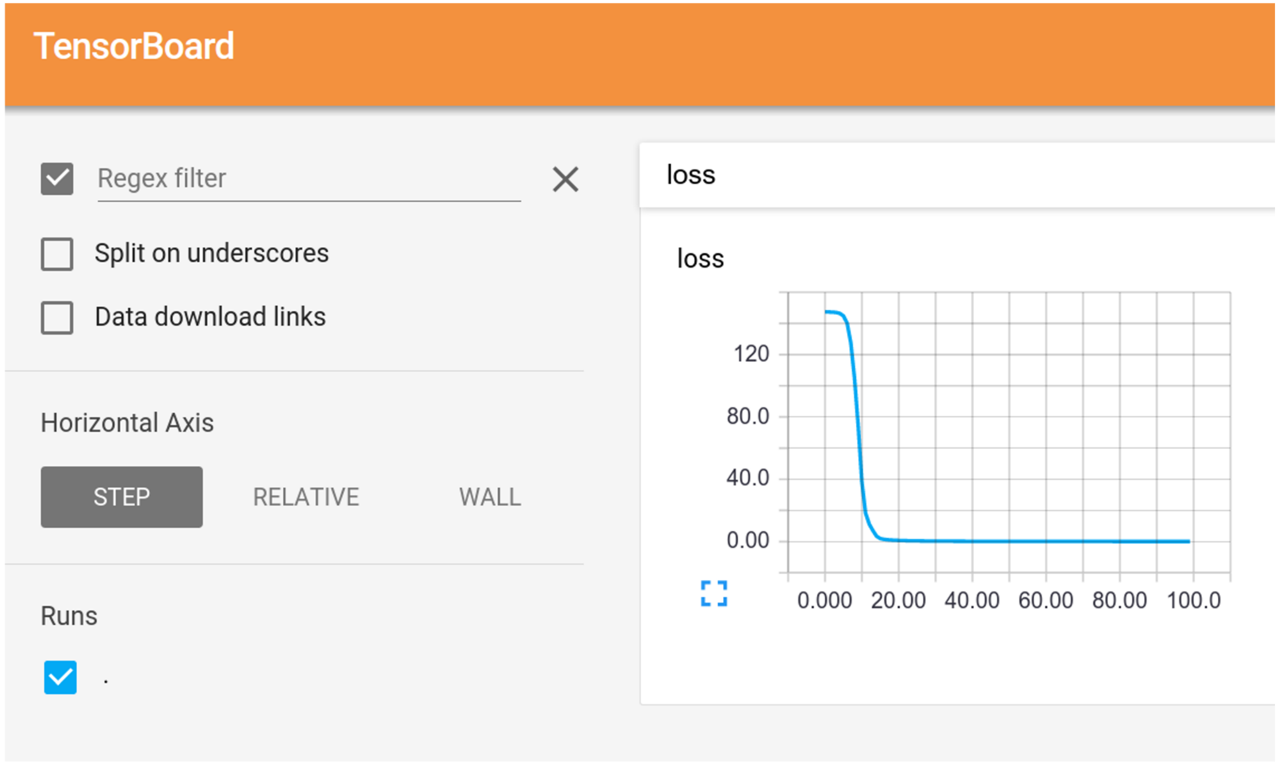
TensorBoard

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

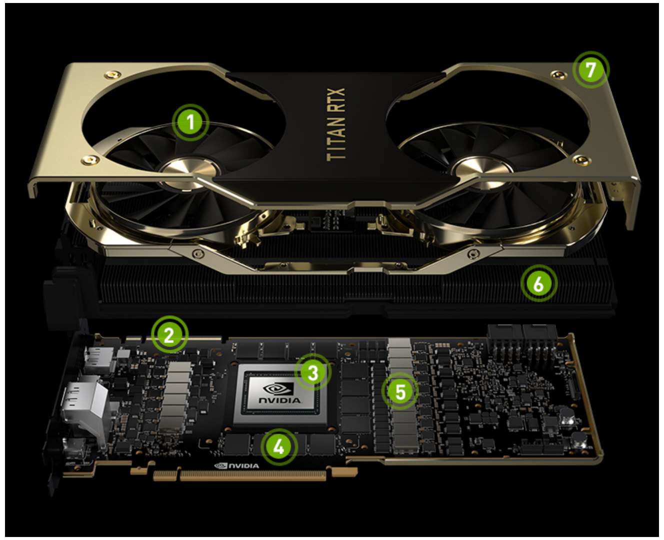
TensorFlow 1.0
- Static graphs by default
- Can be confusing to debug
- API a bit messy

TensorFlow 2.0
- Dynamic by default
- Standardized on Keras API
- API still confusing

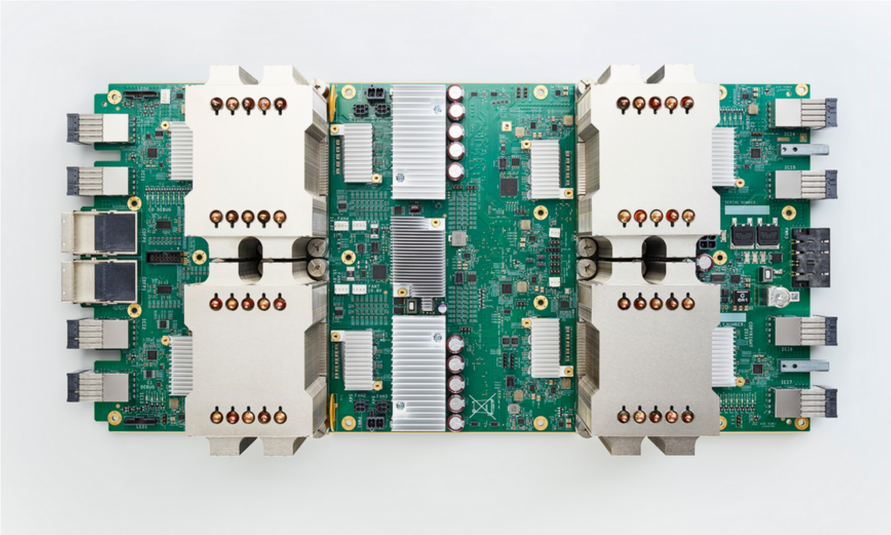
Summary: Hardware

CPU

GPU



TPU



Summary: Software

Static Graphs vs **Dynamic Graphs**

PyTorch vs **TensorFlow**

Next time:
Training Neural Networks