CS 4644-DL / 7643-A: LECTURE 15
DANFEI XU

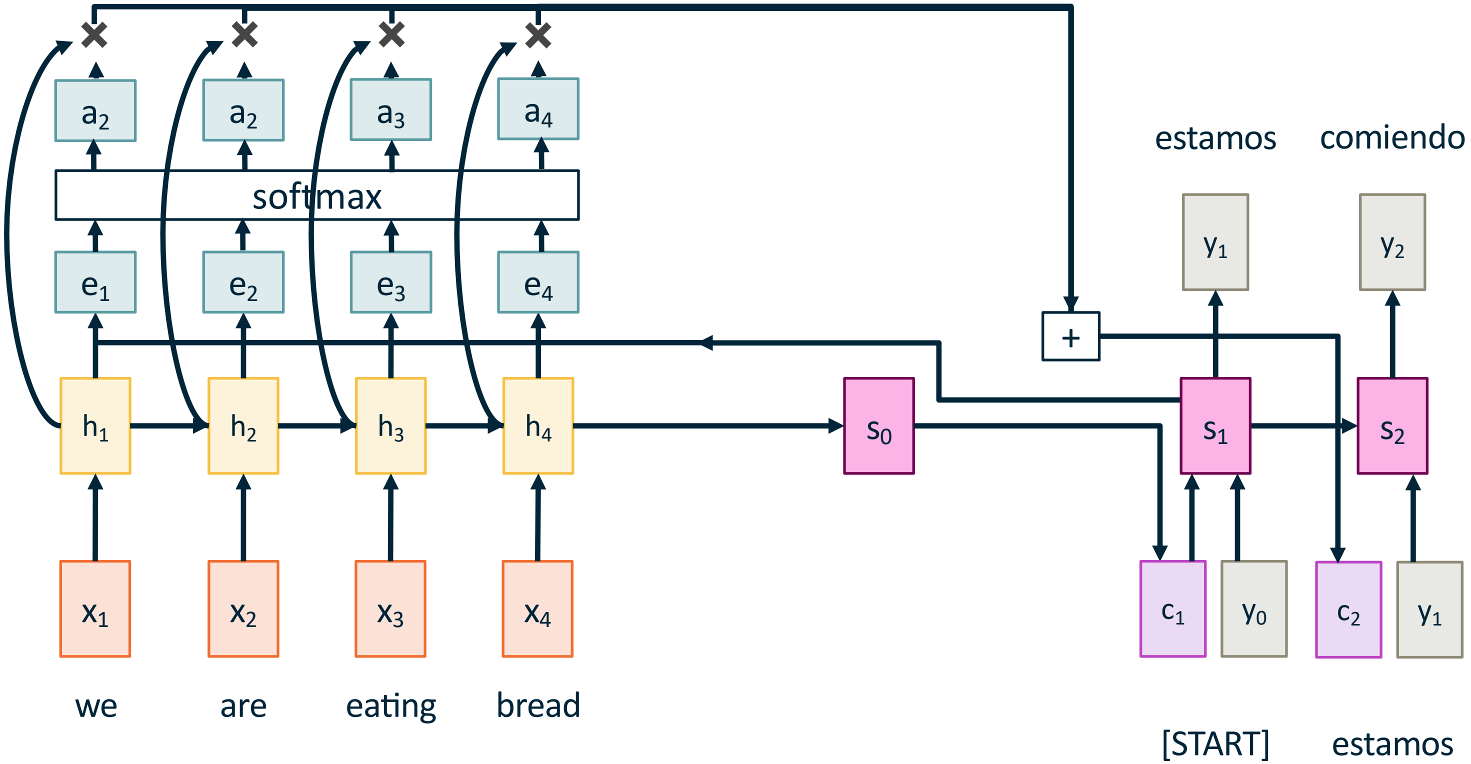
Topics:

- Deep Learning Hardware and Software

Administrative

- Time to work on the project
- We will release the milestone presentation schedule soon
- Start on PS3/HW3 if you haven't
  - Coding: If you passed individual testing cases but are failing end-to-end testing, double check your Multi-Headed Attention. The unit test doesn't catch all errors.
  - DO NOT MODIFY YOUR TEST CODE

Recap: Attention, Transformer, LLMs



Repeat: Use s_1 to compute attention and get the new context vector c_2

Use c_2 to compute s_2, y_2

Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

Recap: Attention, Transformer, LLMs

Example: English to French translation

Input: "The agreement on the European Economic Area was signed in August 1992."

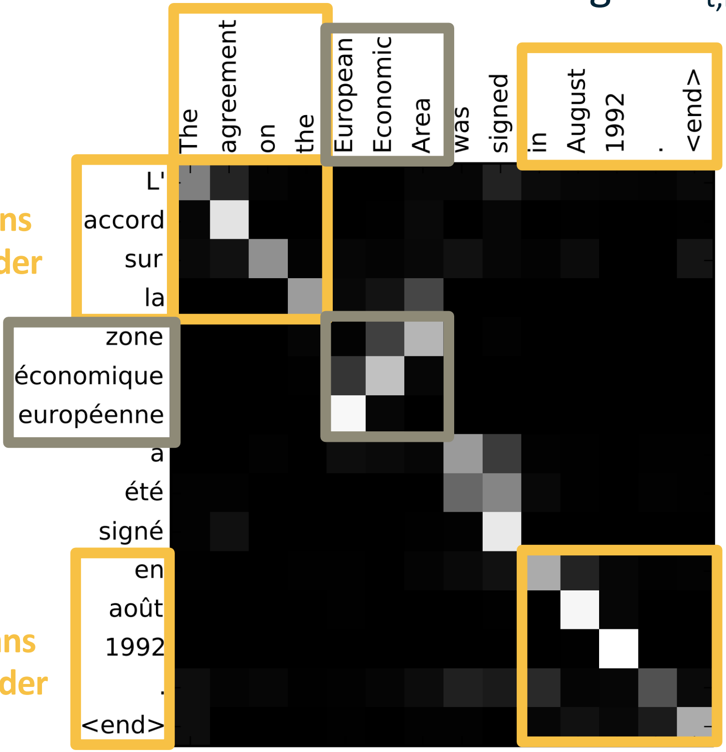
Output: "L'accord sur la zone économique européenne a été signé en août 1992."

Visualize attention weights $a_{t,i}$

Diagonal attention means words correspond in order

Attention figures out different word orders

Diagonal attention means words correspond in order



Bahdanau et al, "Neural machine translation by jointly learning to align and translate", ICLR 2015

Recap: Self-Attention Layer

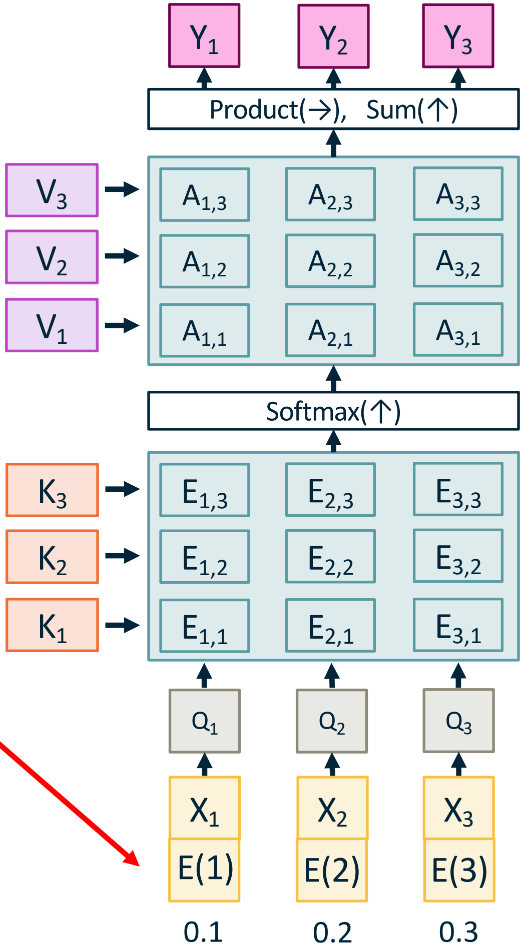
Inputs:
Input vectors: X (Shape: N_X x D_X)
Key matrix: W_K (Shape: D_X x D_Q)
Value matrix: W_V (Shape: D_X x D_V)
Query matrix: W_Q (Shape: D_X x D_Q)

Computation:
Query vectors: $Q = XW_Q$
Key vectors: $K = XW_K$ (Shape: N_X x D_Q)
Value vectors: $V = XW_V$ (Shape: N_X x D_V)
Similarities: $E = QK^T$ (Shape: N_X x N_X) $E_{i,j} = Q_i \cdot K_j / \mathrm{sqrt}(D_Q)$
Attention weights: A = softmax(E, dim=1) (Shape: N_X x N_X)
Output vectors: $Y = AV$ (Shape: N_X x D_V) $Y_i = \sum_j A_{i,j} V_j$

In order to make processing position-aware, concatenate input with **positional encoding E**

E(i) encodes the position of the i-th element in a sequence

E() can be a simple function (e.g., linear or sin functions) or a learned lookup table.



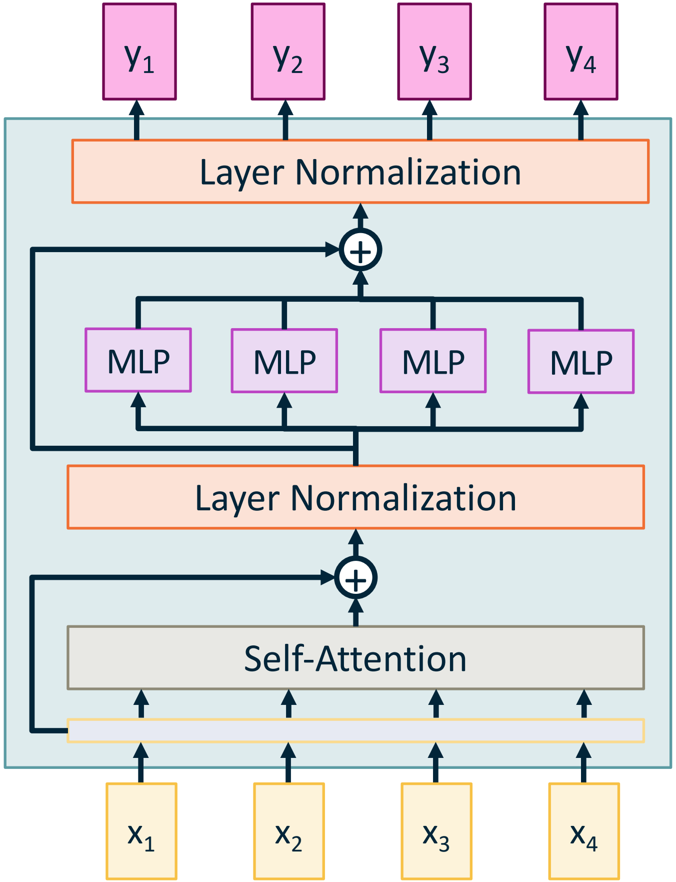
Recap: Transformer Block

Transformer Block:
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction among vectors!

Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable



Recap: The Transformer

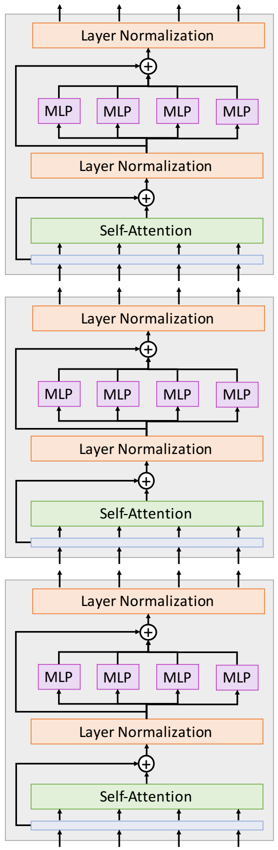
<u>Transformer Block</u>:
Input: Set of vectors x
Output: Set of vectors y

Self-attention is the only interaction among vectors!

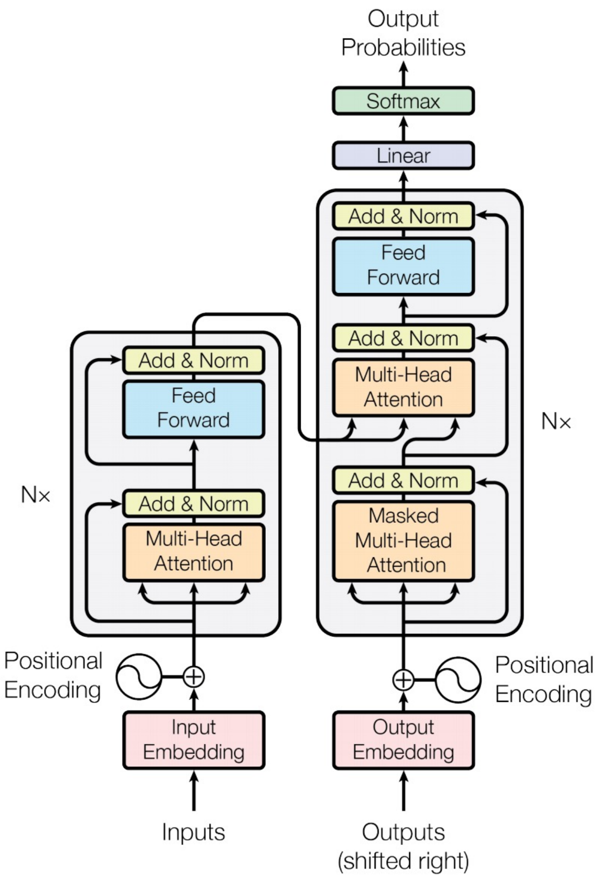
Layer norm and MLP work independently per vector

Highly scalable, highly parallelizable

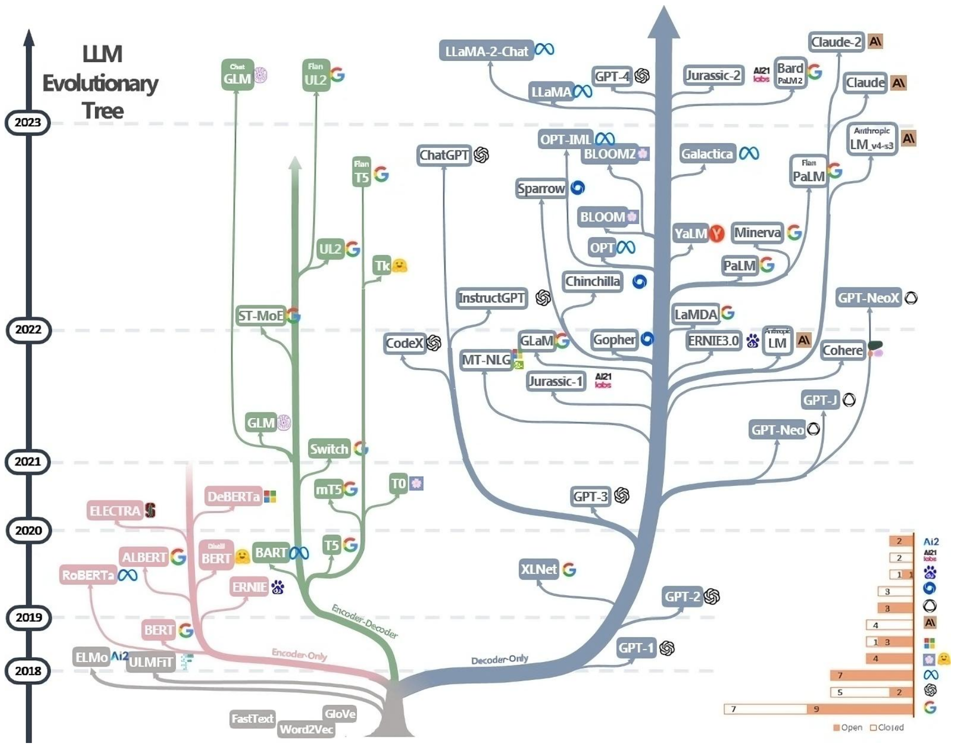
A **Transformer** is a sequence of transformer blocks



Recap: Encoder-Decoder Transformer



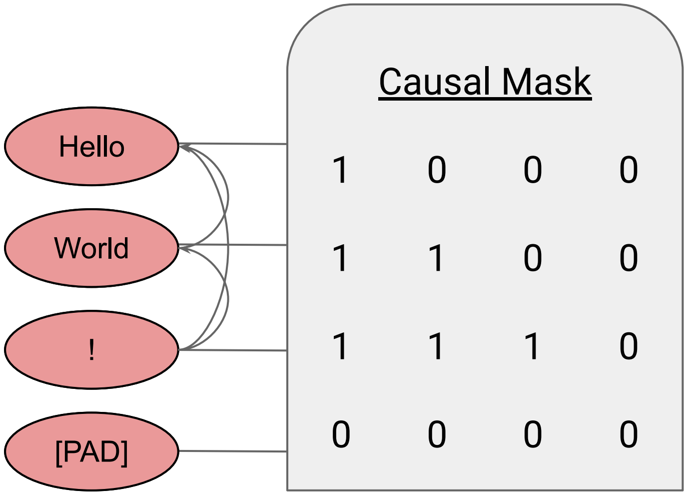
Recap: LLMs



LLM Evolutionary Tree
2023
2022
2021
2020
2019
2018
Chat GLM
Flan UL2
Flan T5
UL2
Tk
ST-MoE
GLM
Switch
mT5
T0
T5
BART
DeBERTa
ELECTRA
ALBERT
Distill BERT
RoBERTa
ERNIE
BERT
ELMo
ULMFiT
FastText
Word2Vec
GloVe
Encoder-Only
Encoder-Decoder
Decoder-Only
LLaMA-2-Chat
GPT-4
LLaMA
Jurassic-2
Bard PaLM2
Claude-2
Claude
Anthropic LM_v4-s3
ChatGPT
OPT-IML
BLOOMZ
Galactica
Flan PaLM
Sparrow
BLOOM
YaLM
Minerva
OPT
PaLM
Chinchilla
InstructGPT
GPT-NeoX
LaMDA
CodeX
GLaM
Gopher
ERNIE3.0
LM
Cohere
MT-NLG
Jurassic-1
GPT-J
GPT-Neo
GPT-3
XLNet
GPT-2
GPT-1
Open
Closed

Recap: LLMs

Masking



Masked Attention Again!

Similarities: E = (QXT / sqrt(DQ)) * MASK

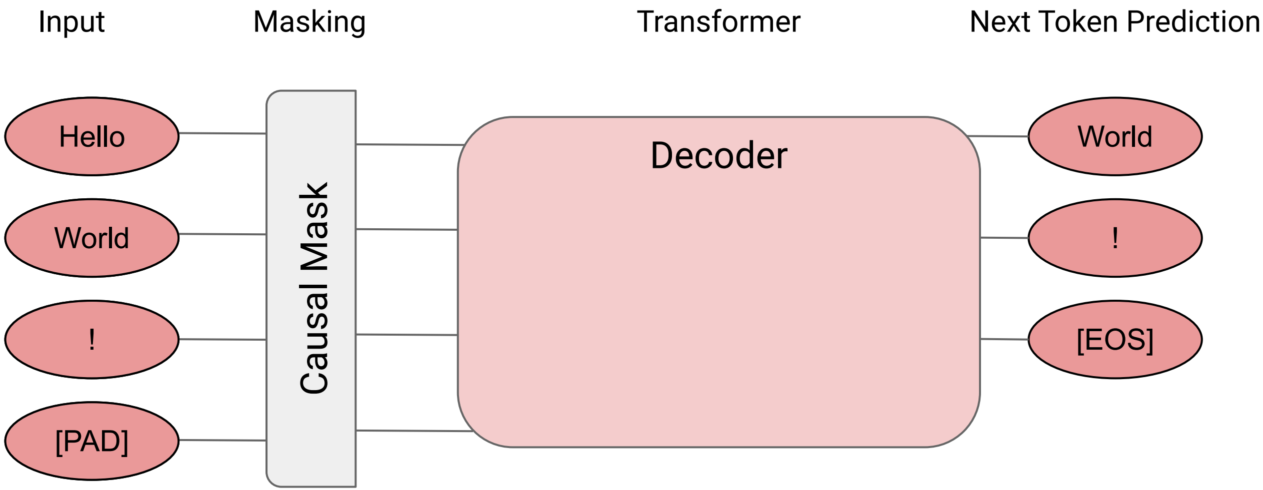
Attention Matrix: A = softmax(E,dim=1)

Output vectors: Y = AX

$Y_i = \sum_j A_{i,j} X$

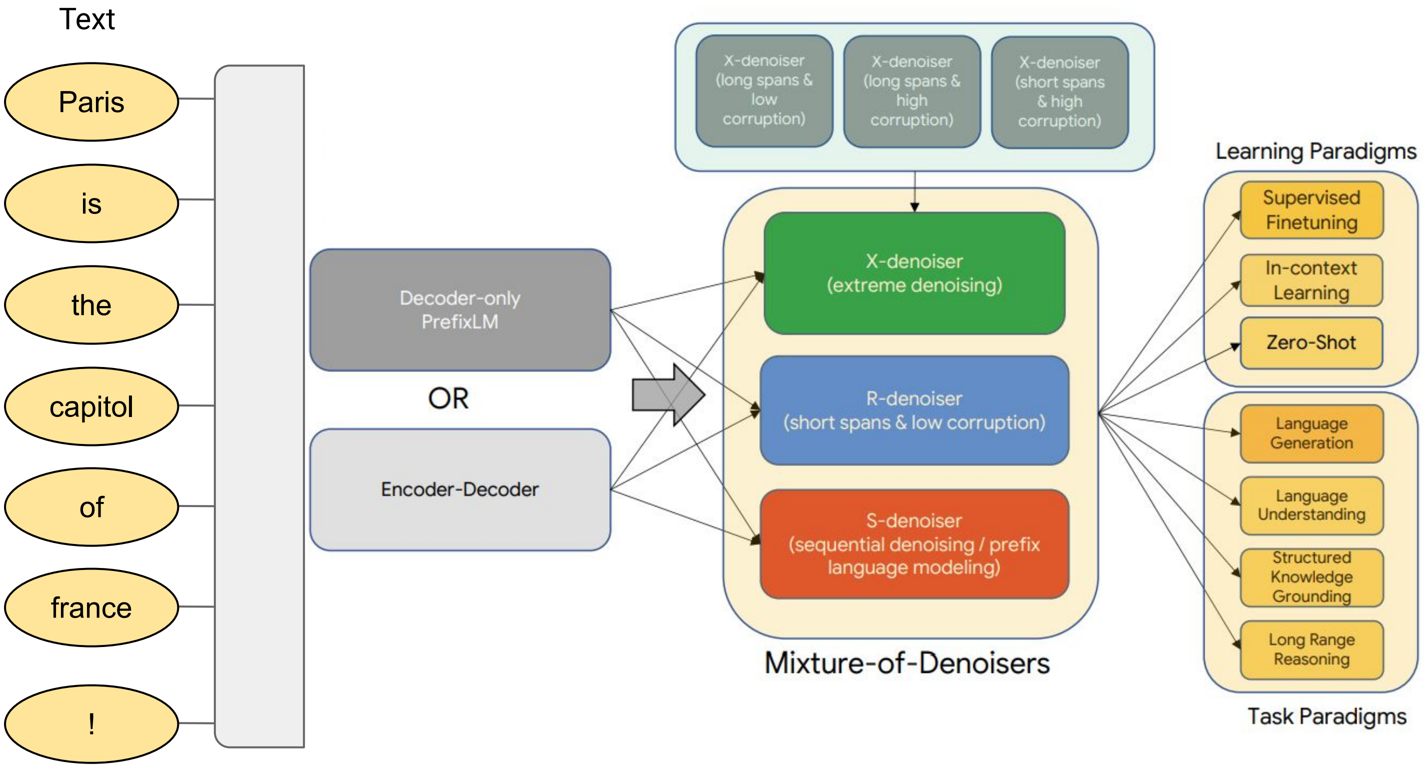
Tokens only affected by preceding tokens

Recap: LLMs



Input
Masking
Transformer
Next Token Prediction
Hello
World
!
[PAD]
Causal Mask
Decoder
World
!
[EOS]

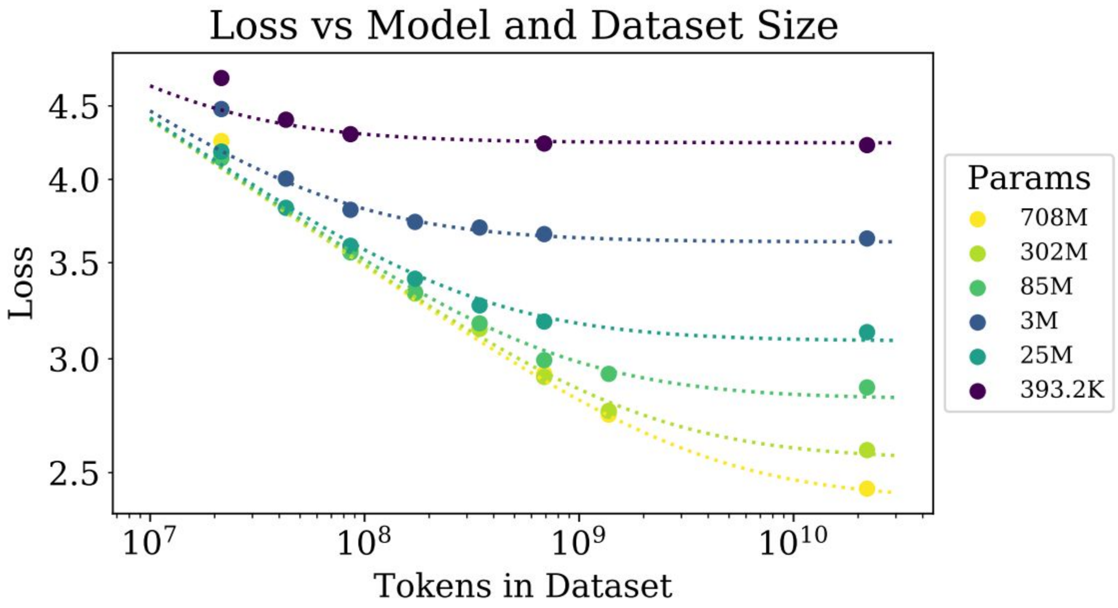
Recap: LLMs



Text
Paris
is
the
capitol
of
france
!
Decoder-only
PrefixLM
OR
Encoder-Decoder
X-denoiser
(long spans &
low
corruption)
X-denoiser
(long spans &
high
corruption)
X-denoiser
(short spans
& high
corruption)
X-denoiser
(extreme denoising)
R-denoiser
(short spans & low corruption)
S-denoiser
(sequential denoising / prefix
language modeling)
Mixture-of-Denoisers
Learning Paradigms
Supervised
Finetuning
In-context
Learning
Zero-Shot
Language
Generation
Language
Understanding
Structured
Knowledge
Grounding
Long Range
Reasoning
Task Paradigms

Recap: LLMs

Today’s LLMs are driven data and model scaling



Recap: LLMs

Llama 2 Corpus

Size
> 2 Trillion Tokens

Quality
Minimal details known

Touvron et al. 2023 (b)

PALM-2 Corpus

Size
> 3.6 Trillion Tokens

Quality
No details known

Anil et al. 202320

GPT-4 Corpus

Size
Unknown (Est. 11T Tokens)

Quality
No details known

OpenAI 2023

Today

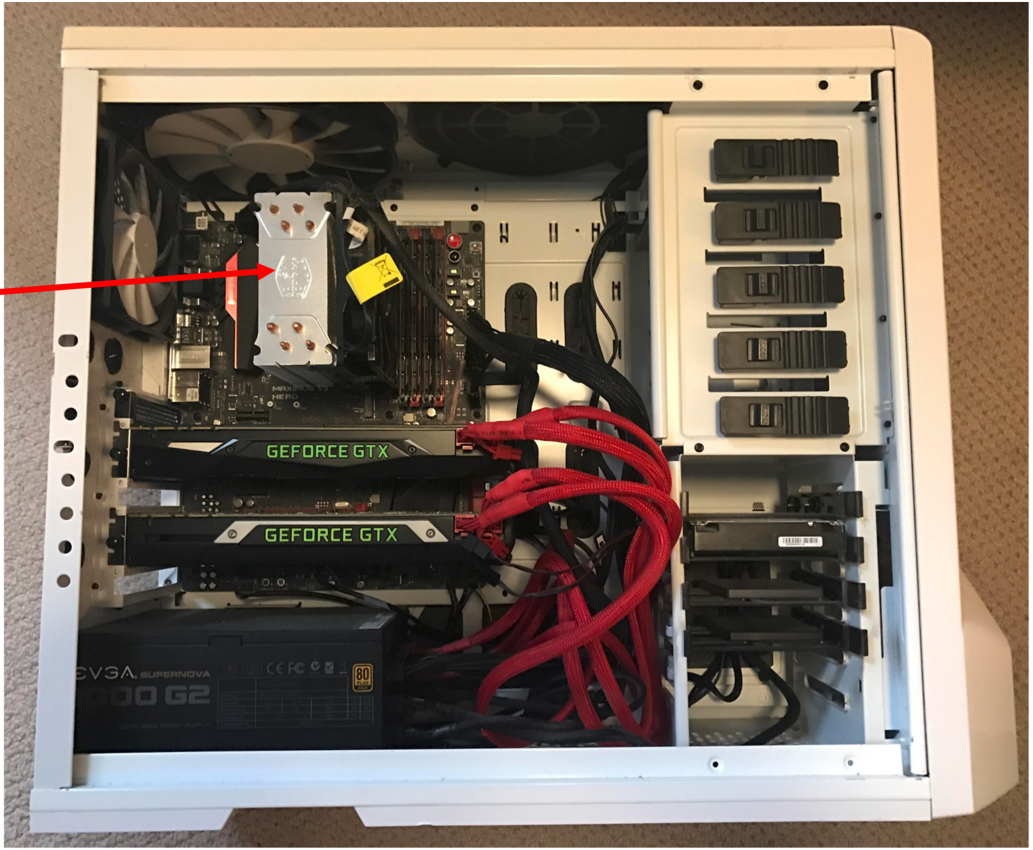
- Deep learning hardware
  - CPU, GPU
- Deep learning software
  - PyTorch and TensorFlow
  - Static and Dynamic computation graphs

Deep Learning Hardware

Inside a computer

Spot the CPU!

(central processing unit)



Spot the GPUs!

(graphics processing unit)

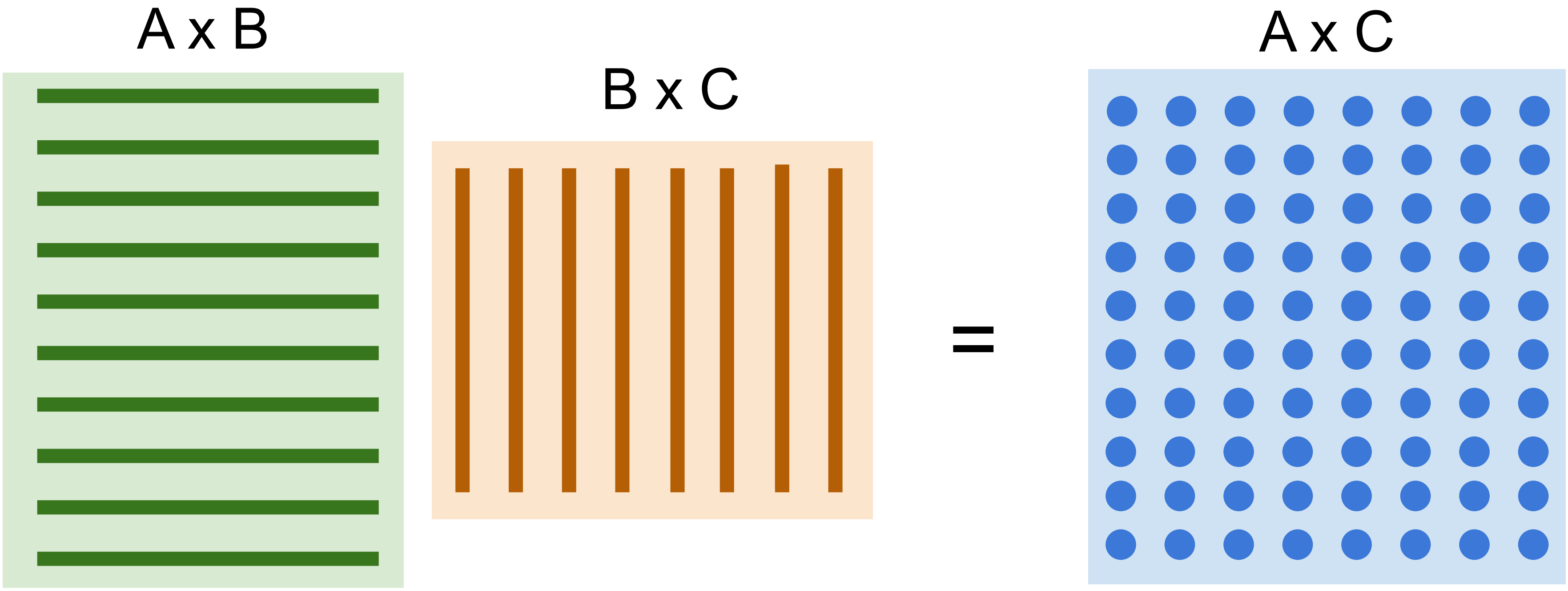
CPU vs GPU

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

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

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

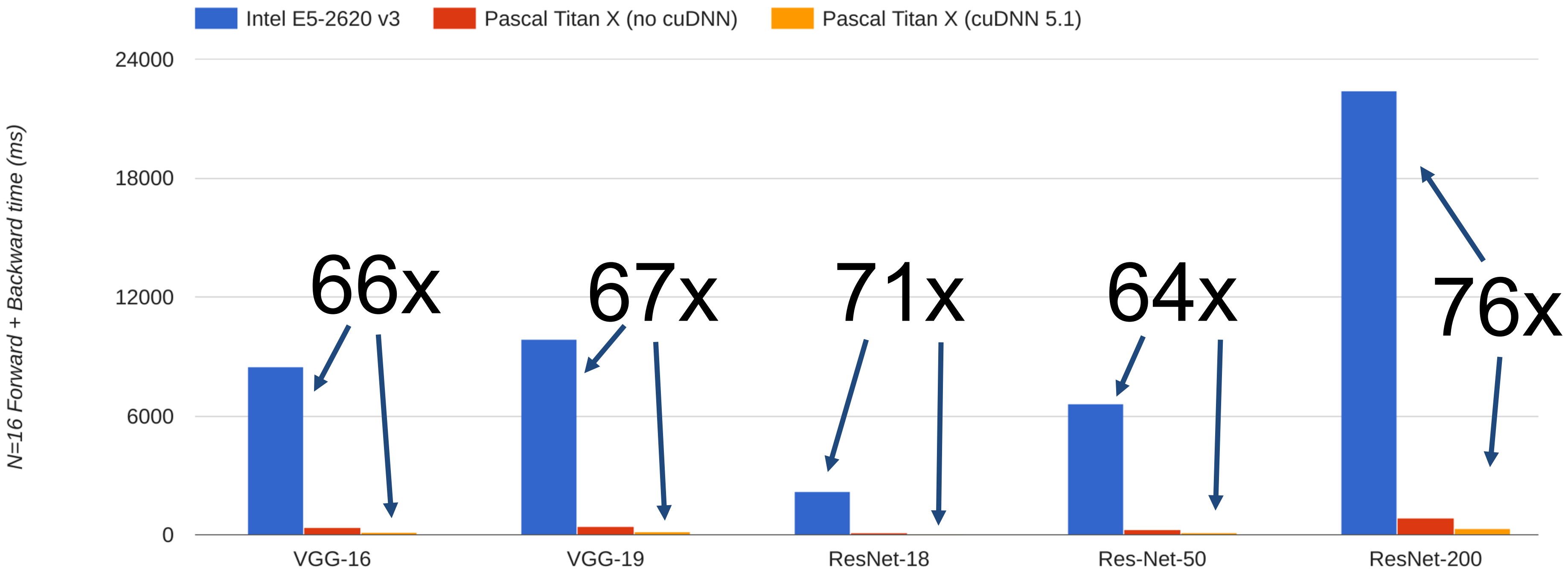
Example: Matrix Multiplication



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

CPU vs GPU in practice

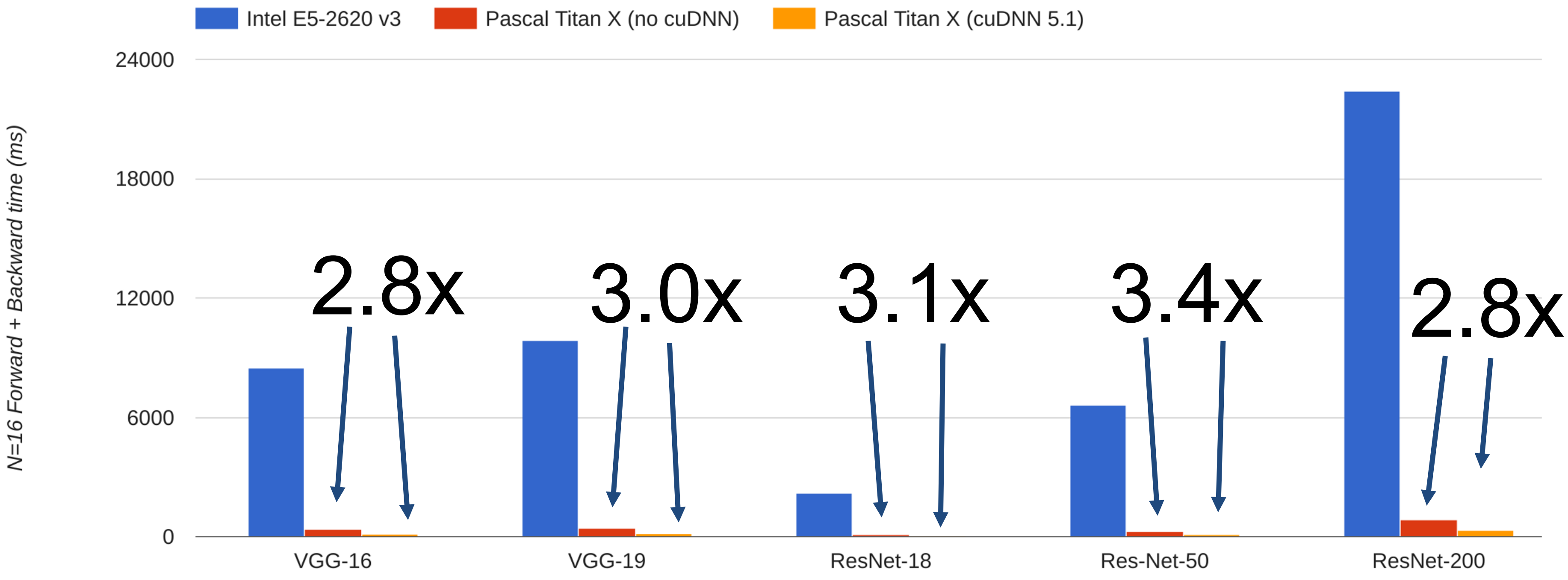
(CPU performance not well-optimized, a little unfair)



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

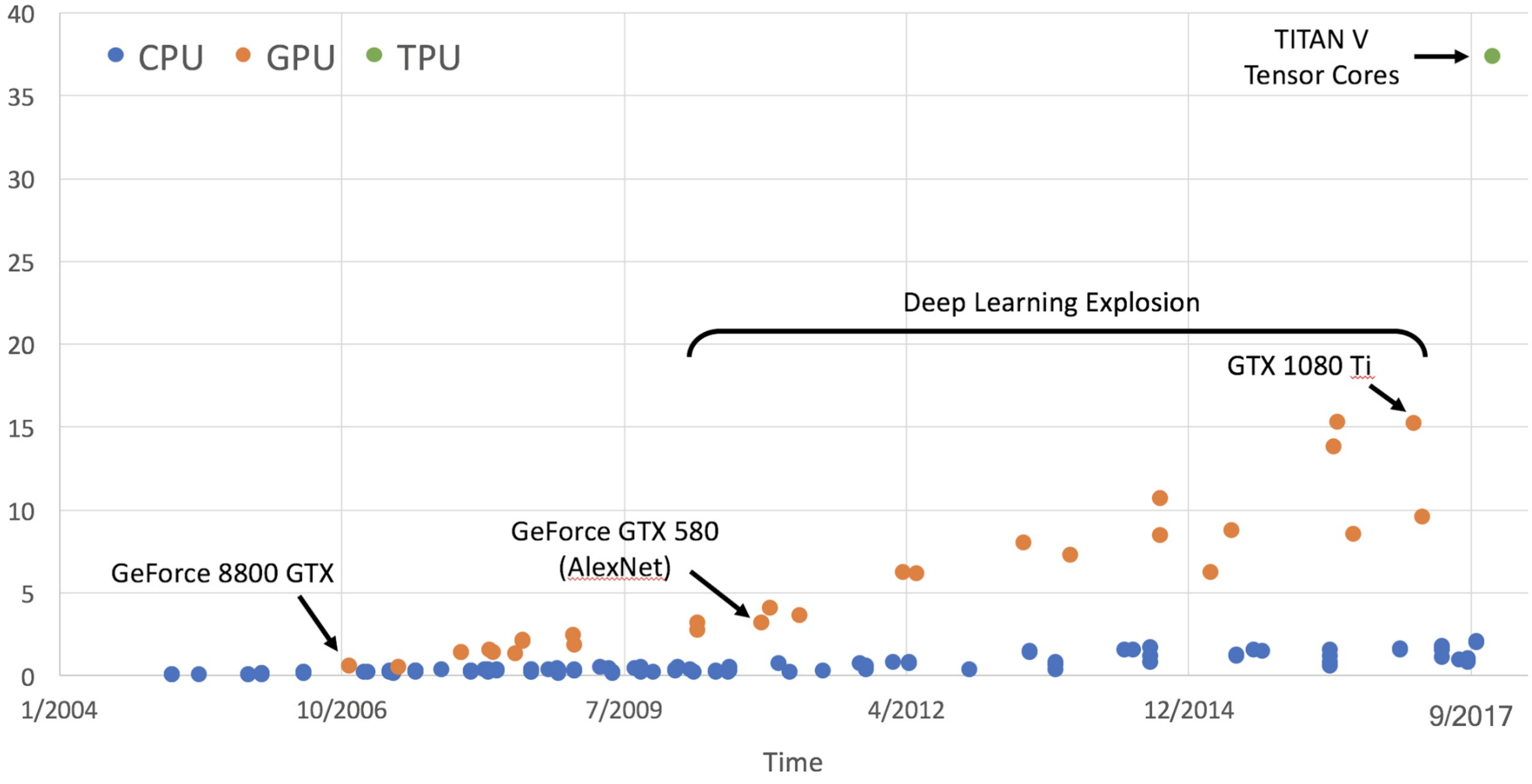
CPU vs GPU in practice

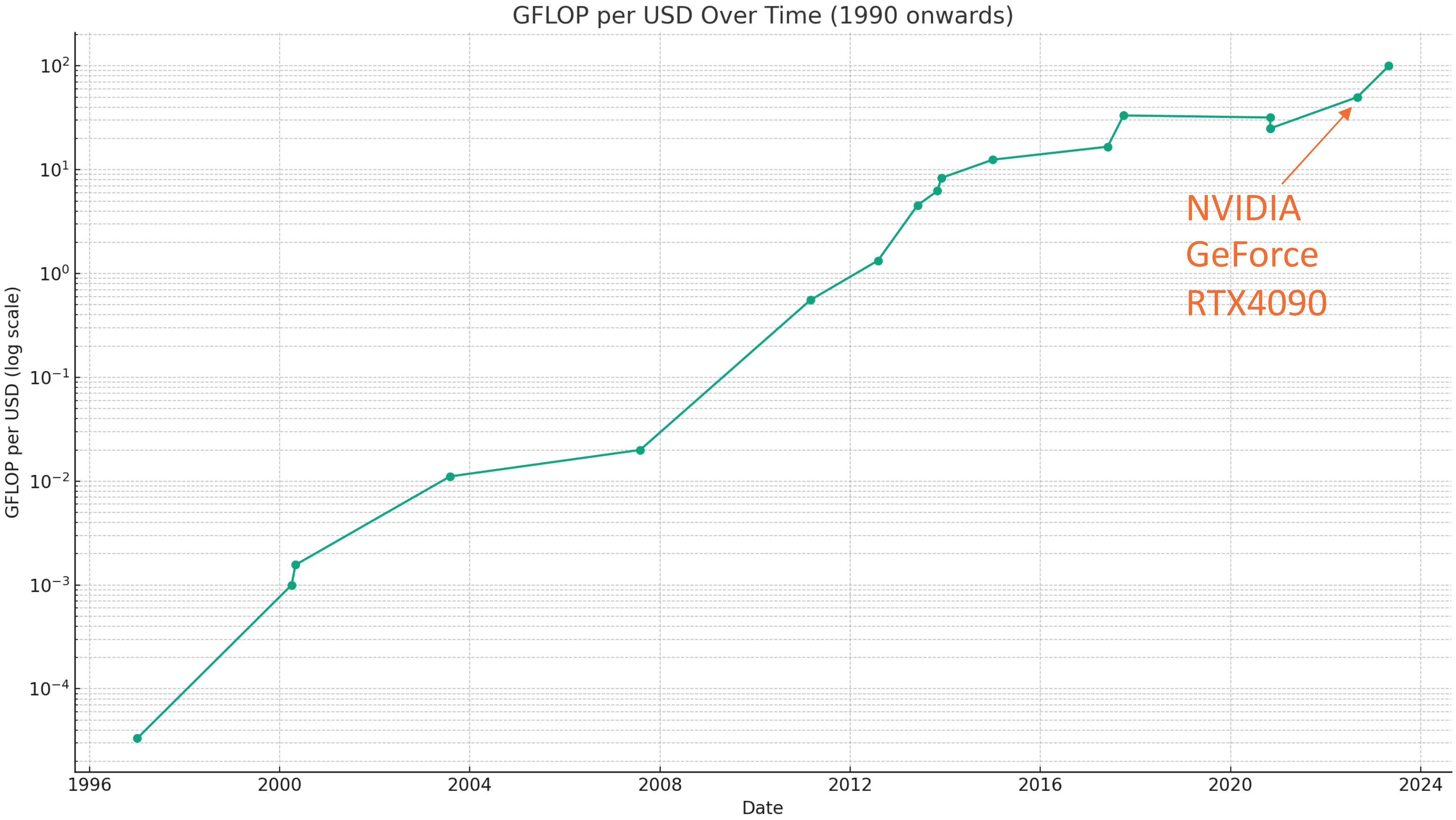
cuDNN much faster than "unoptimized" CUDA



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

GigaFLOPs per Dollar





https://en.wikipedia.org/wiki/FLOPS#Hardware_costs

NVIDIA vs AMD

NVIDIA

vs

AMD

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GPU **(Data Center)** NVIDIA A100	6912 CUDA, 432 Tensor	1.5 GHz	40/80 GB HBM2	$3/hr (GCP)	~9.7 TFLOPs FP64 ~20 TFLOPs FP32 ~312 TFLOPs FP16
TPU Google Cloud TPUv3	2 Matrix Units (MXUs) per core, 4 cores	?	128 GB HBM	$8/hr (GCP)	~420 TFLOPs (non-standard FP)

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

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

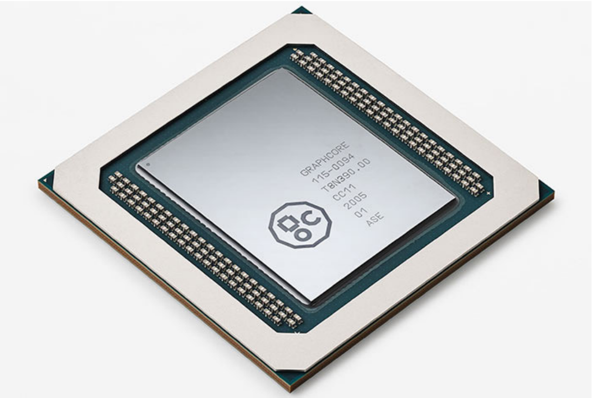
TPU: Specialized hardware for deep learning

Aside: NPUs

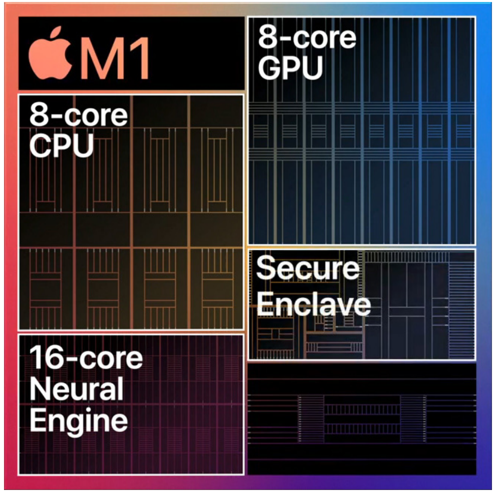
Neural Processing Units (NPUs) are specialized hardware designed for Deep Learning applications. Example: GraphCore IPUs

General pros: larger on-device memory, lower power consumption

General cons: specialized computation units (compared to GPU and CPUs). Smaller instruction sets. Less supported by popular platforms (PyTorch, TensorFlow)



Graphcore M2000



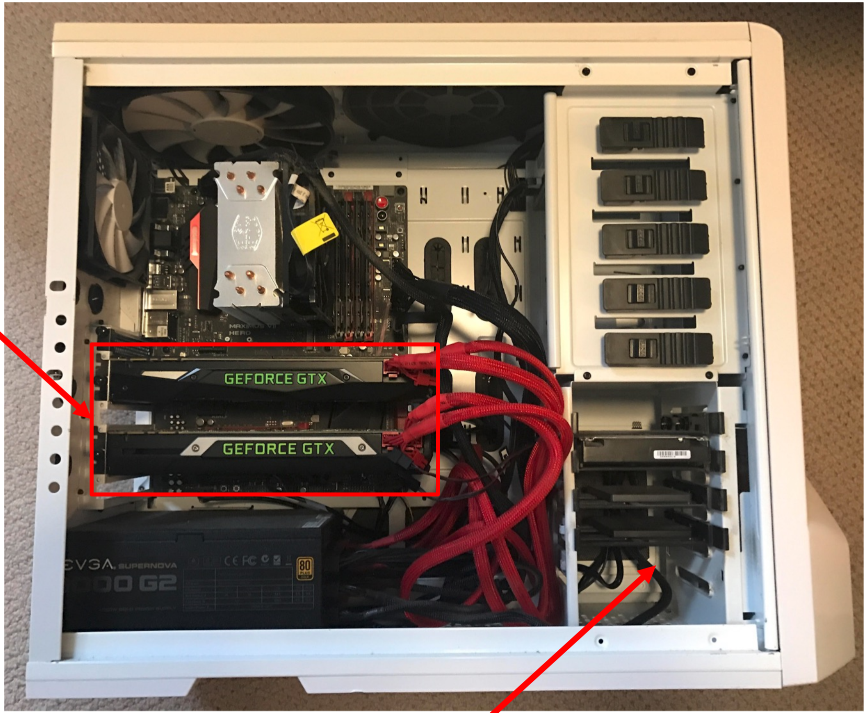
Apple M1

Programming GPUs

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

CPU / GPU Communication

Model is here

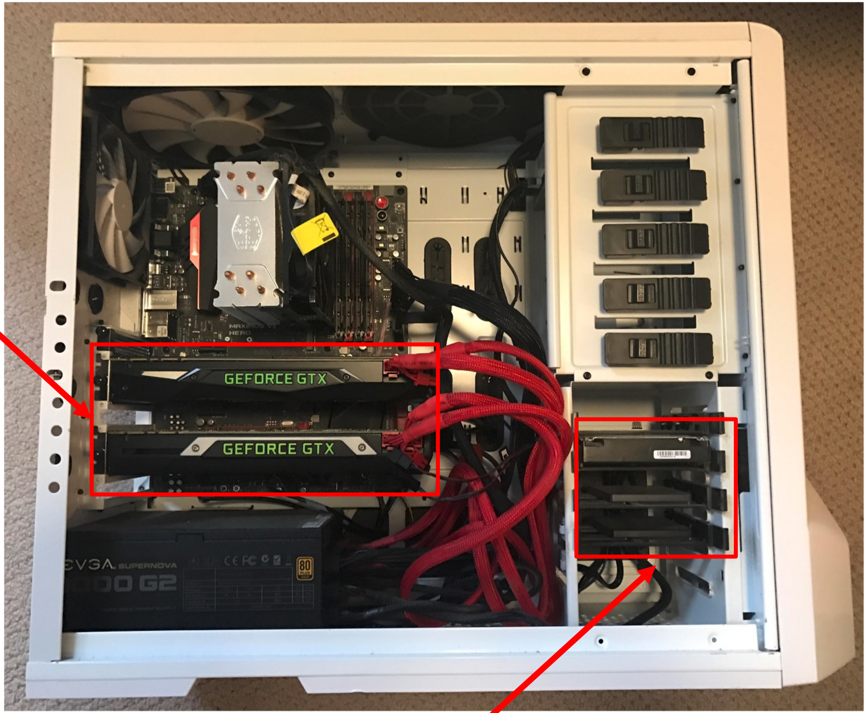


Data is here

Data access rate: RAM and the GPU over PCIe lanes is about **16 GB/s**. GPU's internal memory (like GDDR6) is about **448 GB/s**.

CPU / GPU Communication

Model is here



Data is here

Data access rate: RAM and the GPU over PCIe lanes is about **16 GB/s**. GPU's internal memory (like GDDR6) is about **448 GB/s**.

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

Solutions:

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

Deep Learning Software

A zoo of frameworks!

Caffe
(UC Berkeley)

Caffe2
(Facebook)
mostly features absorbed by PyTorch

Torch
(NYU / Facebook)

PyTorch
(Facebook)

Theano
(U Montreal)

TensorFlow
(Google)

PaddlePaddle
(Baidu)

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

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

CNTK
(Microsoft)

JAX
(Google)

And others...

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TensorFlow
(Google)

We'll focus on these

PaddlePaddle
(Baidu)

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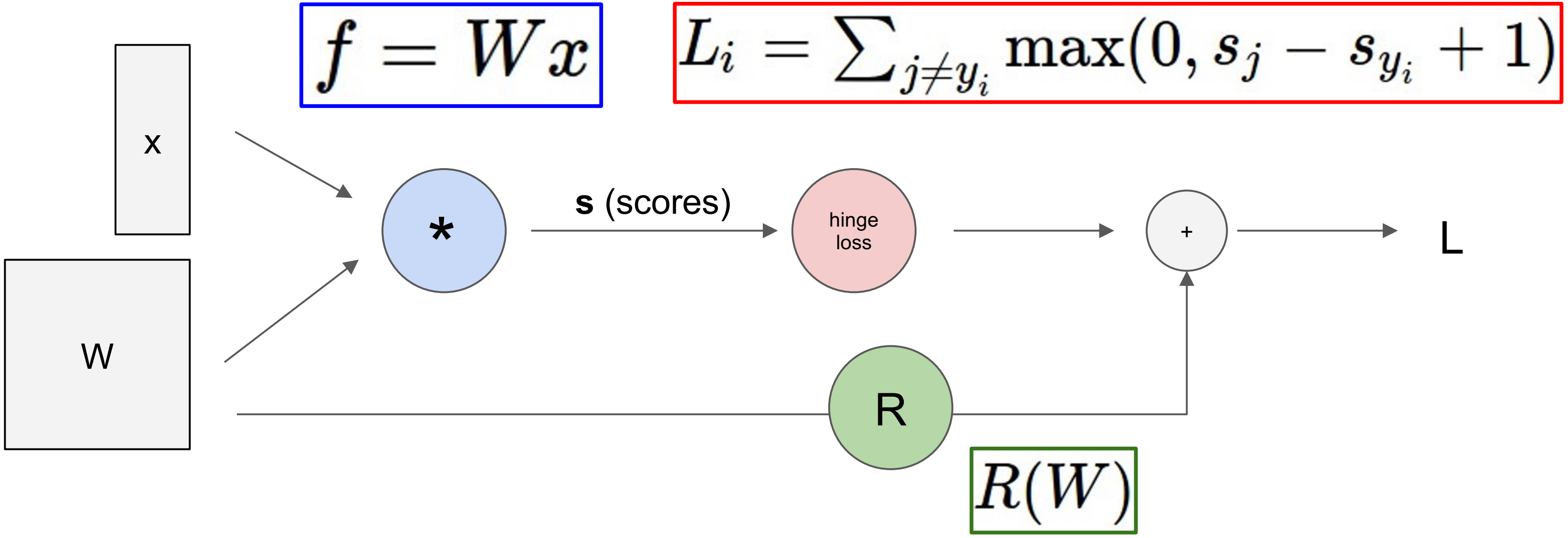
And others...

Recall: Computational Graphs



Recall: Computational Graphs

input image

weights

loss

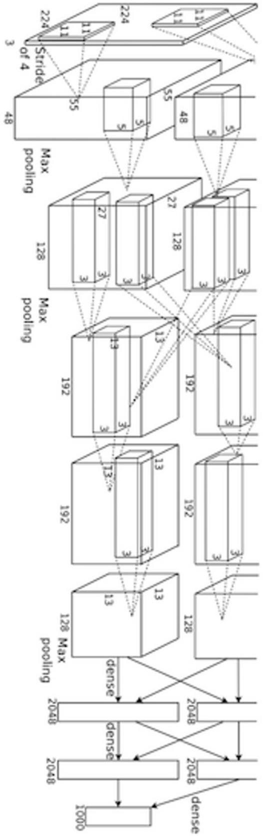


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Recall: Computational Graphs

input image

loss

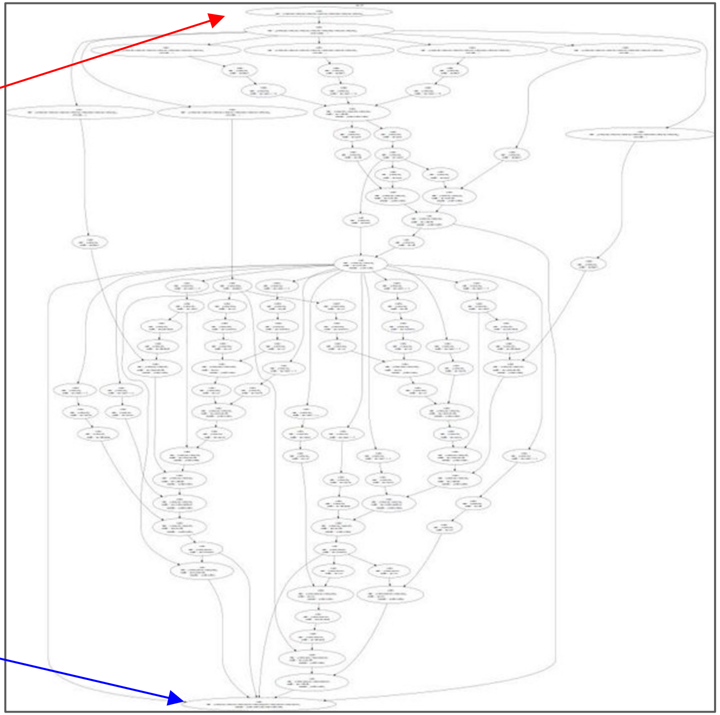


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

The point of deep learning frameworks

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

Computational Graphs

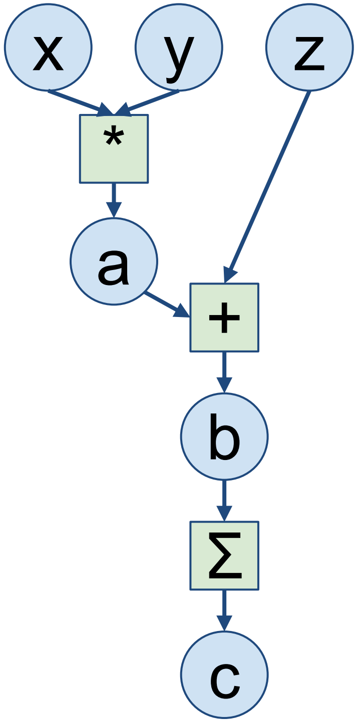
Numpy

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

N, D = 3, 4

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

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



Computational Graphs

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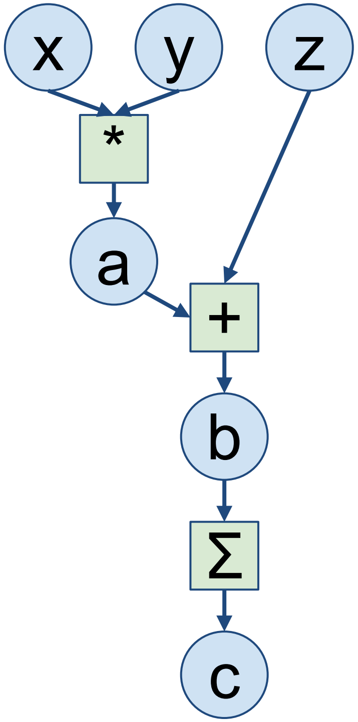
y = np.random.randn(N, D)
z = np.random.randn(N, D)

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

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



Computational Graphs

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grad_a = grad_b.copy()
grad_z = grad_b.copy()
grad_x = grad_a * y
grad_y = grad_a * x
```
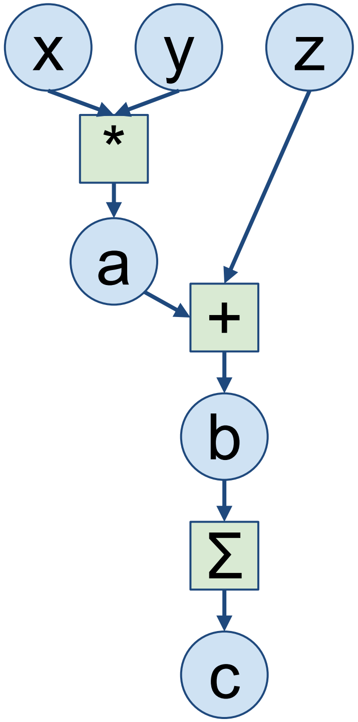



Good:

Clean API, easy to write numeric code

Bad:

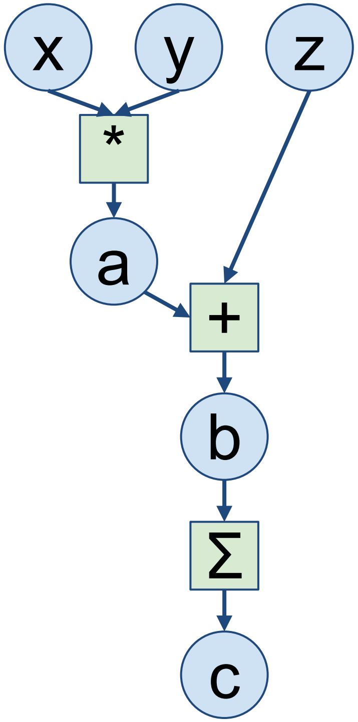
- Have to compute our own gradients
- Can't run on GPU

Computational Graphs

Numpy

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

N, D = 3, 4

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

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

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



PyTorch

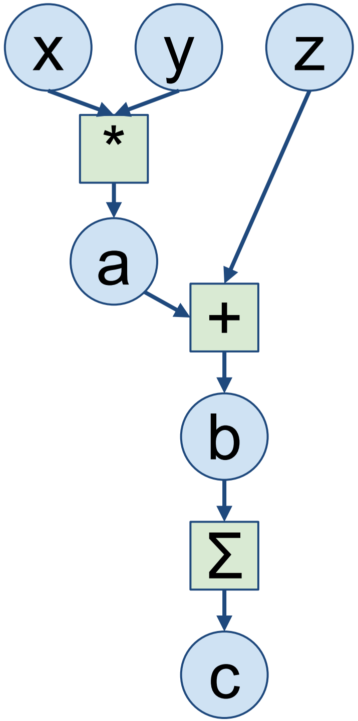
```
import torch

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

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

Looks exactly like numpy!

Computational Graphs

Numpy

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

N, D = 3, 4

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

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

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



PyTorch

```
import torch

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

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

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

PyTorch handles gradients for us!

Computational Graphs

Numpy

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

N, D = 3, 4

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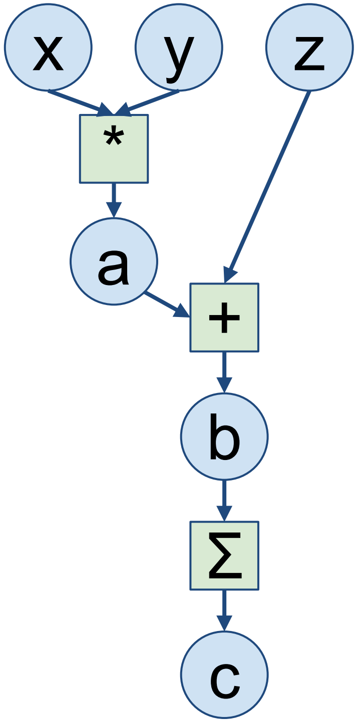



PyTorch

```python
import torch

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

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

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

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

PyTorch

(More details)

PyTorch: Fundamental Concepts

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

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

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

PyTorch: Versions

For this class we are using **PyTorch version >= 2.0.0 (newest is v2.1.0)**

Major API change in release 1.0

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

PyTorch: Tensors

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

```
import torch

device = torch.device('cpu')

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

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

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

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

PyTorch: Tensors

Create random tensors for data and weights

```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

Forward pass: compute predictions and 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

Backward pass: manually compute gradients

```
import torch

device = torch.device('cpu')

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

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

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

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

PyTorch: Tensors

```
import torch

device = torch.device('cpu')

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

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

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

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

Gradient descent
step on weights

PyTorch: Tensors

To run on GPU, just use a different device!

```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)
w2 = torch.randn(H, D_out, device=device)

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

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

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

PyTorch: Autograd

Creating Tensors with requires_grad=True enables autograd

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

```
import torch

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

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

    loss.backward()

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

PyTorch: Autograd

Forward pass looks exactly the same as before, but we don’t need to track intermediate values - PyTorch keeps track of them for us in the graph

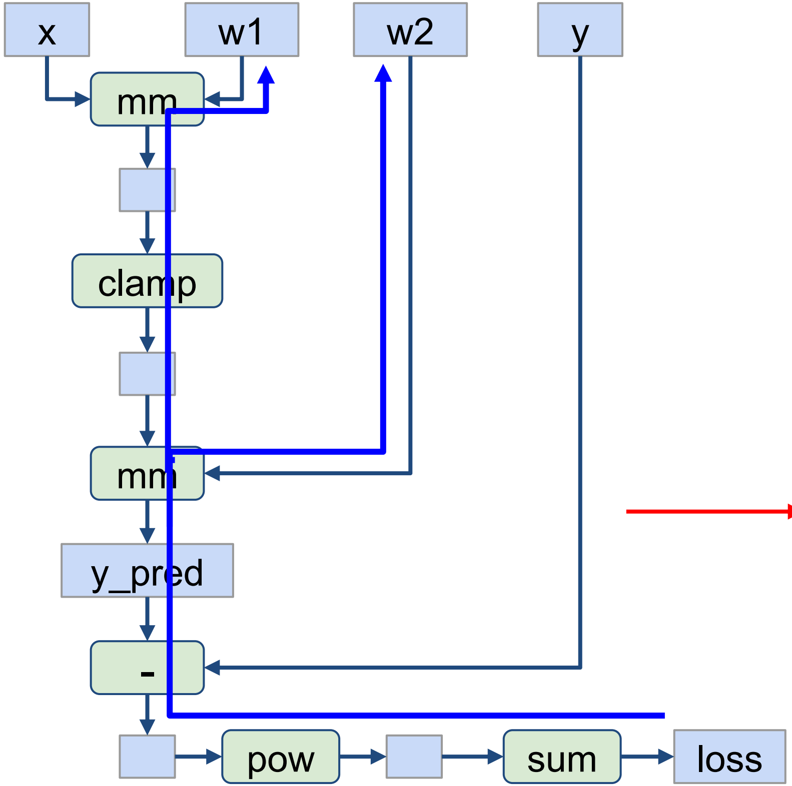
```
import torch

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

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

    loss.backward()

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

PyTorch: Autograd

Compute gradient of loss with respect to w1 and w2

```
import torch

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

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

    loss.backward()

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

PyTorch: Autograd




```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

```
import torch

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

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

    loss.backward()

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

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

PyTorch: Autograd

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

PyTorch: New Autograd Functions

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

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

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

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

PyTorch: New Autograd Functions

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

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

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

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

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

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

PyTorch: New Autograd Functions

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

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

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

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

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

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

    loss.backward()

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

Can use our new autograd function in the forward pass

PyTorch: New Autograd Functions

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

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

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

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

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

    loss.backward()

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

PyTorch: nn

Higher-level wrapper for working with neural nets

Use this! It will make your life easier

```
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

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

```
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

Forward pass: feed data to model, and compute loss

```
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

Forward pass: feed data to model, and compute loss

torch.nn.functional has useful helpers like loss functions

```
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

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

```
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

```
import torch

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

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

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

    loss.backward()

    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 params and zero gradients

PyTorch: nn
Define new Modules

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

Modules can contain weights or other modules

You can define your own Modules using autograd!

```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
Define new Modules

Define our whole model
as a single Module

```
import torch

class TwoLayerNet(torch.nn.Module):
    def __init__(self, D_in, H, D_out):
        super(TwoLayerNet, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, H)
        self.linear2 = torch.nn.Linear(H, D_out)

    def forward(self, x):
        h_relu = self.linear1(x).clamp(min=0)
        y_pred = self.linear2(h_relu)
        return y_pred

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

Initializer sets up two children (Modules can contain modules)

```
import torch

class TwoLayerNet(torch.nn.Module):
    def __init__(self, D_in, H, D_out):
        super(TwoLayerNet, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, H)
        self.linear2 = torch.nn.Linear(H, D_out)

    def forward(self, x):
        h_relu = self.linear1(x).clamp(min=0)
        y_pred = self.linear2(h_relu)
        return y_pred

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

Define forward pass using child modules

No need to define backward - autograd will handle it

```
import torch

class TwoLayerNet(torch.nn.Module):
    def __init__(self, D_in, H, D_out):
        super(TwoLayerNet, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, H)
        self.linear2 = torch.nn.Linear(H, D_out)

    def forward(self, x):
        h_relu = self.linear1(x).clamp(min=0)
        y_pred = self.linear2(h_relu)
        return y_pred

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

Construct and train an instance of our model

```
import torch

class TwoLayerNet(torch.nn.Module):
    def __init__(self, D_in, H, D_out):
        super(TwoLayerNet, self).__init__()
        self.linear1 = torch.nn.Linear(D_in, H)
        self.linear2 = torch.nn.Linear(H, D_out)

    def forward(self, x):
        h_relu = self.linear1(x).clamp(min=0)
        y_pred = self.linear2(h_relu)
        return y_pred

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

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

```
import torch

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

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

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

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

PyTorch: nn
Define new Modules

Define network component as a Module subclass

```
import torch

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

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

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

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

PyTorch: nn
Define new Modules

Stack multiple instances of the component in a sequential

```
import torch

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

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

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

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

PyTorch: Pretrained Models

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

```
import torch
import torchvision

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

PyTorch: Computational Graphs

input image

loss

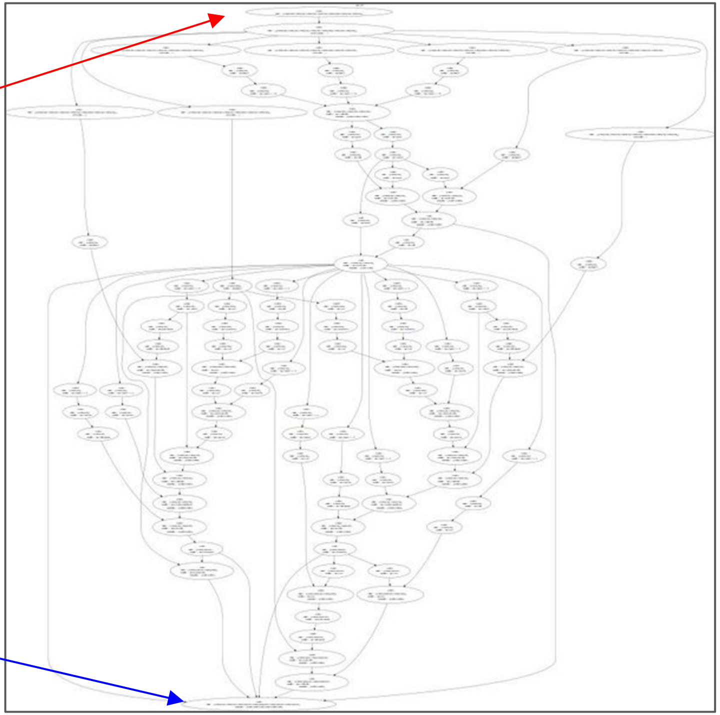


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

PyTorch: **Dynamic** Computation Graphs

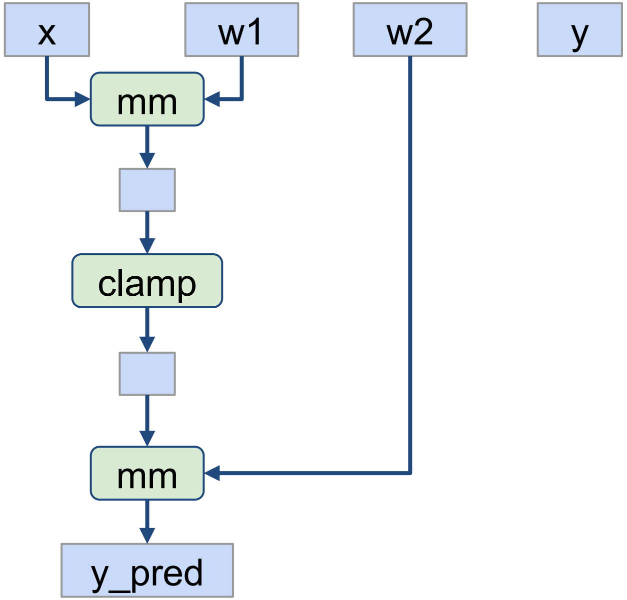
```
import torch

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

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

    loss.backward()
```

PyTorch: **Dynamic** Computation Graphs


```
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

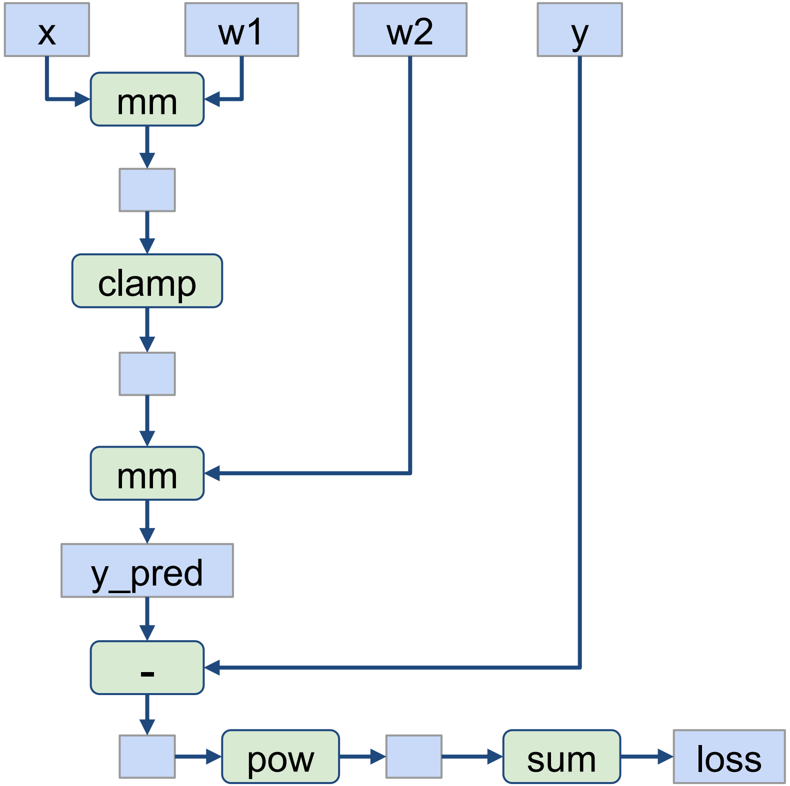
PyTorch: **Dynamic** Computation Graphs




```
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

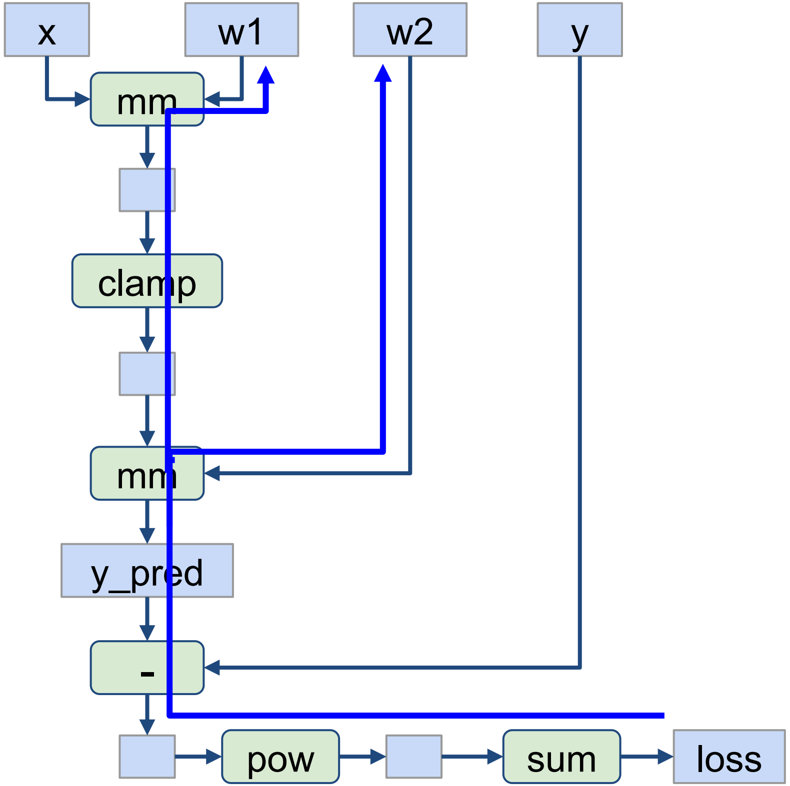
PyTorch: **Dynamic** Computation Graphs




```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()
```

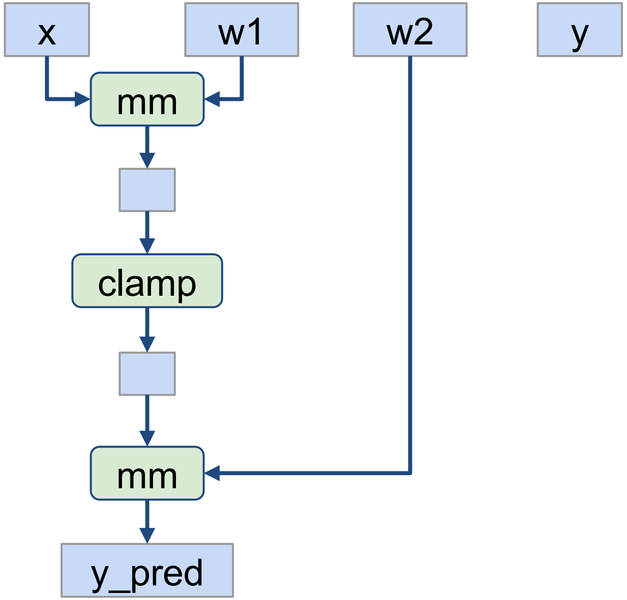
Search for path between loss and w1, w2 (for backprop) AND perform computation

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()
```

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

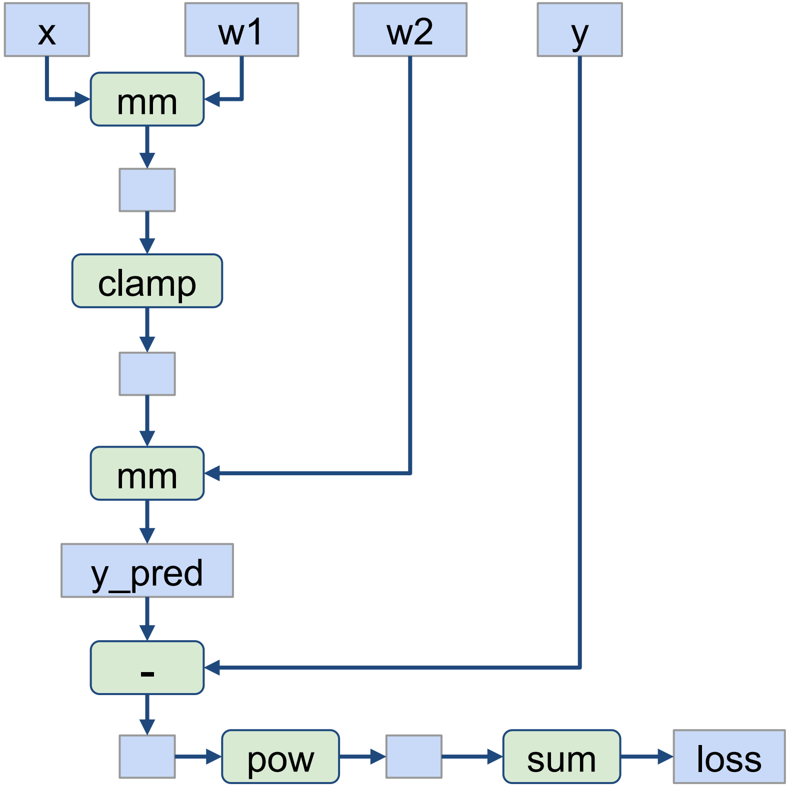
PyTorch: **Dynamic** Computation Graphs




```
import torch

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

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

    loss.backward()
```

Build graph data structure AND
perform computation

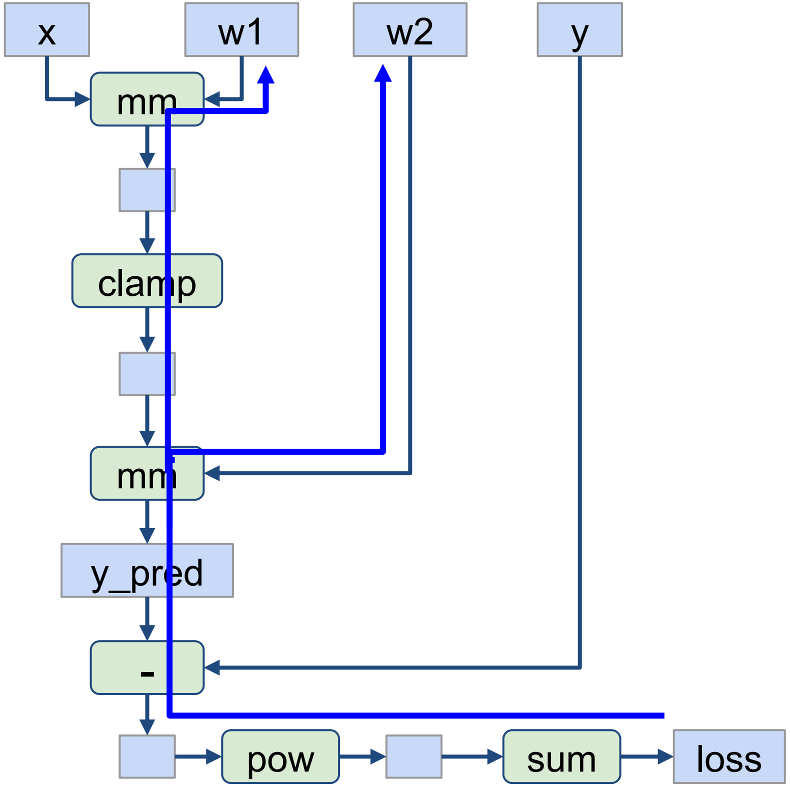
PyTorch: **Dynamic** Computation Graphs




```
import torch

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

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

    loss.backward()
```

Build graph data structure AND perform computation

PyTorch: **Dynamic** Computation Graphs




```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()
```

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

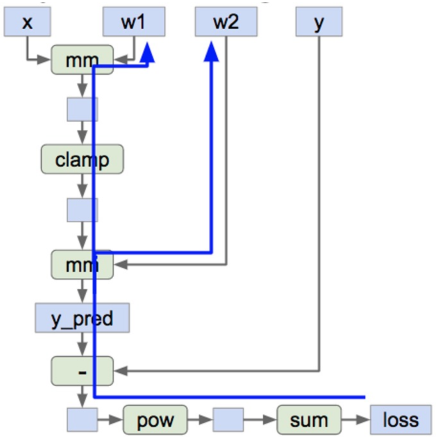
PyTorch: **Dynamic** Computation Graphs

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

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

```
import torch

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

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

    loss.backward()
```

Static Computation Graphs



Alternative: **Static** graphs

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

Step 2: Reuse the same graph on every iteration

```
graph = build_graph()

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

TensorFlow

TensorFlow Versions

Pre-2.0 (1.14 latest)

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

2.0+

Default dynamic graph, optionally static graph.

TensorFlow: Neural Net (Pre-2.0)

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

(Assume imports at the top of each snippet)

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

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

grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])

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

TensorFlow: Neural Net (Pre-2.0)

First **define** computational graph

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

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

grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])
```

Then **run** the graph many times

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

TensorFlow: 2.0+ vs. pre-2.0

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:
"Eager" Mode by default

`assert(tf.executing_eagerly())`

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

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

grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])

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

Tensorflow 1.13

TensorFlow: 2.0+ vs. pre-2.0

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:
"Eager" Mode by default

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

```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 1.13

TensorFlow: 2.0+ vs. pre-2.0

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

Tensorflow 2.0+:
"Eager" Mode by default

`assert(tf.executing_eagerly())`

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

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

grad_w1, grad_w2 = tf.gradients(loss, [w1, w2])

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

Tensorflow 1.13

TensorFlow: Neural Net

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

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net

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

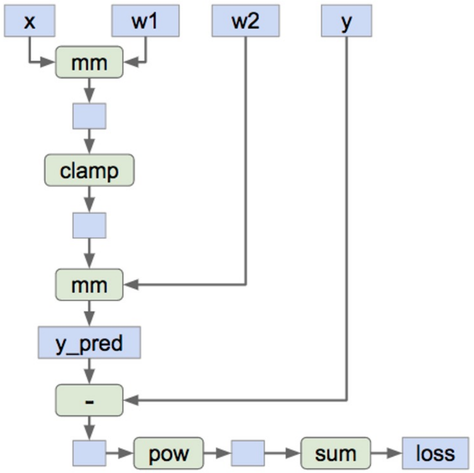
```
N, D, H = 64, 1000, 100

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net

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

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net



Forward pass

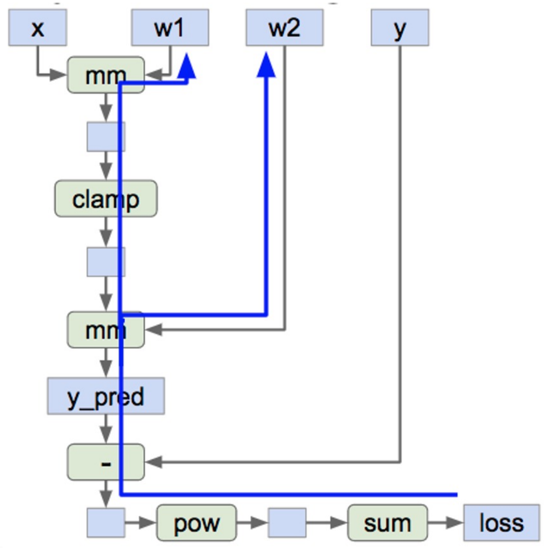
```
N, D, H = 64, 1000, 100

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net

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

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

TensorFlow: Neural Net



Backward pass

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

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

with tf.GradientTape() as tape:
  h = tf.maximum(tf.matmul(x, w1), 0)
  y_pred = tf.matmul(h, w2)
  diff = y_pred - y
  loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
gradients = tape.gradient(loss, [w1, w2])
```

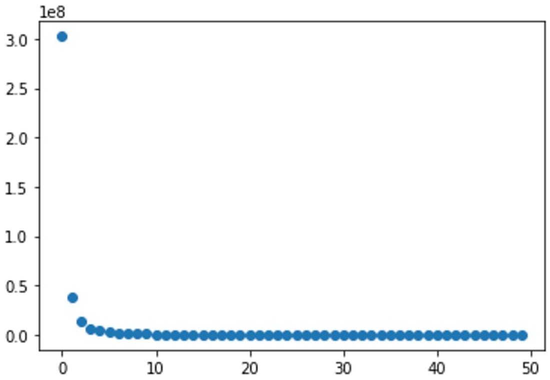
TensorFlow: Neural Net

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

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

```
learning_rate = 1e-6
for t in range(50):
  with tf.GradientTape() as tape:
    h = tf.maximum(tf.matmul(x, w1), 0)
    y_pred = tf.matmul(h, w2)
    diff = y_pred - y
    loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
  gradients = tape.gradient(loss, [w1, w2])
  w1.assign(w1 - learning_rate * gradients[0])
  w2.assign(w2 - learning_rate * gradients[1])
```

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

TensorFlow: Neural Net



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

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

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

```
learning_rate = 1e-6
for t in range(50):
  with tf.GradientTape() as tape:
    h = tf.maximum(tf.matmul(x, w1), 0)
    y_pred = tf.matmul(h, w2)
    diff = y_pred - y
    loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
  gradients = tape.gradient(loss, [w1, w2])
  w1.assign(w1 - learning_rate * gradients[0])
  w2.assign(w2 - learning_rate * gradients[1])
```

TensorFlow: Optimizer

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

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

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

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

learning_rate = 1e-6
for t in range(50):
  with tf.GradientTape() as tape:
    h = tf.maximum(tf.matmul(x, w1), 0)
    y_pred = tf.matmul(h, w2)
    diff = y_pred - y
    loss = tf.reduce_mean(tf.reduce_sum(diff ** 2, axis=1))
  gradients = tape.gradient(loss, [w1, w2])
  optimizer.apply_gradients(zip(gradients, [w1, w2]))
```

TensorFlow: Loss

Use predefined loss functions

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

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

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

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

TensorFlow: High-Level Wrappers

Keras (https://keras.io/)

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

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

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

TFLearn (http://tflearn.org/)

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

@tf.function: compile static graph

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

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

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

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

@tf.function: compile static graph

Ran on Google Colab, April 2020

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

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

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


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

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

dynamic graph:  0.02520249200000535
static graph:  0.03932226699998864
```

@tf.function: compile static graph

Ran on Google Colab, April 2020

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

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


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

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

dynamic graph:  0.02520249200000535
static graph:  0.03932226699998864
```

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

@tf.function: compile static graph

Ran on Google Colab, April 2020

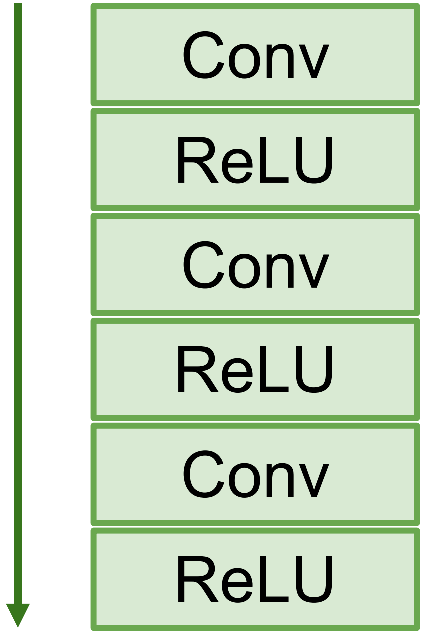
```
N, D, H = 64, 1000, 100
x = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
y = tf.convert_to_tensor(np.random.randn(N, D), np.float32)
model = tf.keras.Sequential()
model.add(tf.keras.layers.Dense(H, input_shape=(D,), activation=tf.nn.relu))
model.add(tf.keras.layers.Dense(D))
optimizer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

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

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

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

dynamic graph: 2.3648411540000325
static graph: 1.1723986679999143
```

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

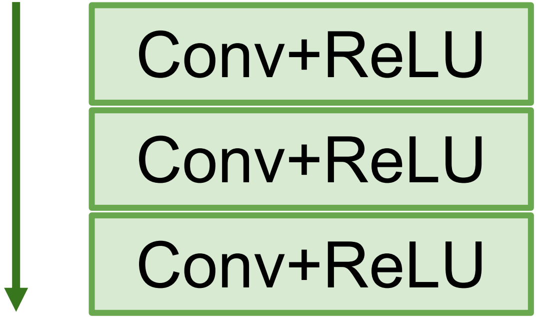
<u>Static</u> vs Dynamic: Optimization

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

The graph you wrote



Equivalent graph with **fused operations**



Static PyTorch: TorchScript

```
graph(%self.1 :
__torch__.torch.nn.modules.module.___torch_mangl
e_4.Module,
      %input : Float(3, 4),
      %h : Float(3, 4)):
  %19 :
__torch__.torch.nn.modules.module.___torch_mangl
e_3.Module =
prim::GetAttr[name="linear"](%self.1)
  %21 : Tensor =
prim::CallMethod[name="forward"](%19, %input)
  %12 : int = prim::Constant[value=1]() #
<ipython-input-40-26946221023e>:7:0
  %13 : Float(3, 4) = aten::add(%21, %h, %12) #
<ipython-input-40-26946221023e>:7:0
  %14 : Float(3, 4) = aten::tanh(%13) #
<ipython-input-40-26946221023e>:7:0
  %15 : (Float(3, 4), Float(3, 4)) =
prim::TupleConstruct(%14, %14)
  return (%15)
```

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

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

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

Build static graph with torch.jit.trace

PyTorch vs TensorFlow, Static vs Dynamic

PyTorch
Dynamic Graphs
Static: TorchScript

TensorFlow
Dynamic: Eager
Static: @tf.function

Static vs Dynamic: Serialization

Static

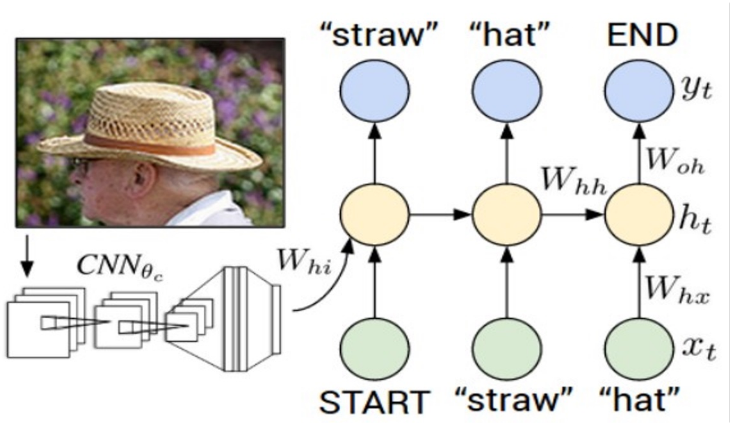
Once graph is built, can **serialize** it and run it without the code that built the graph!

Dynamic

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

Dynamic Graph Applications

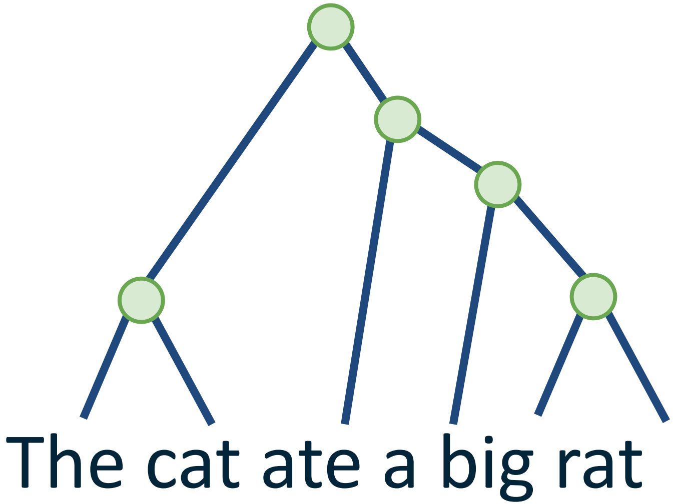
- Recurrent networks



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

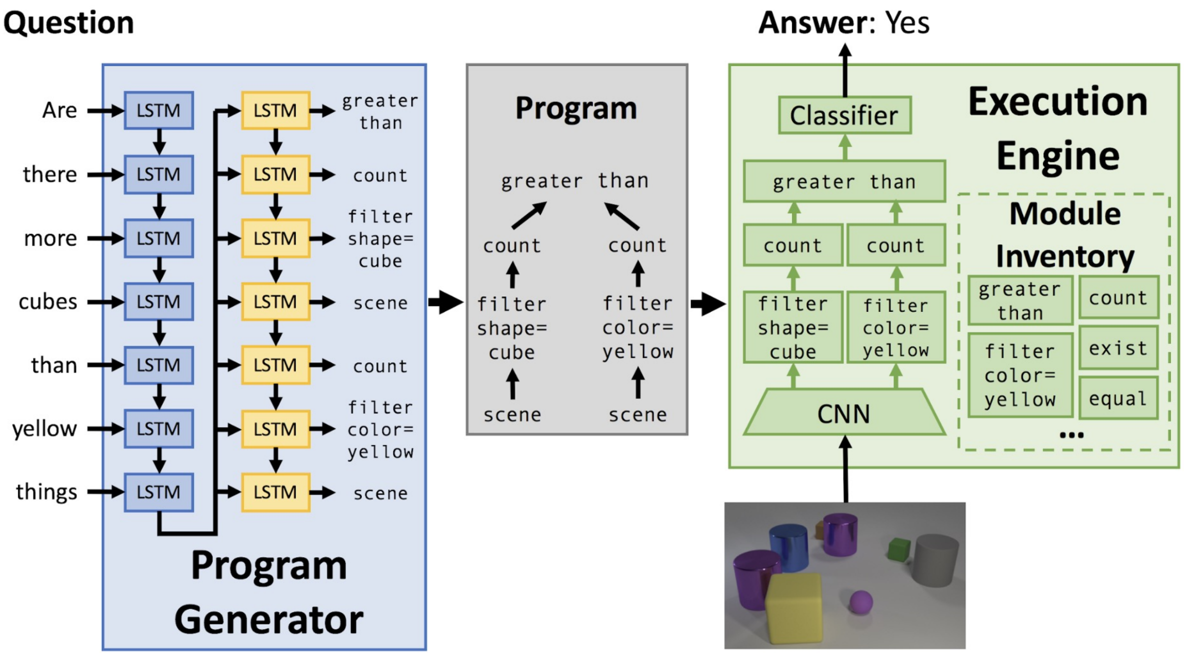
Dynamic Graph Applications

- Recurrent networks
- Recursive networks



Dynamic Graph Applications

- 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

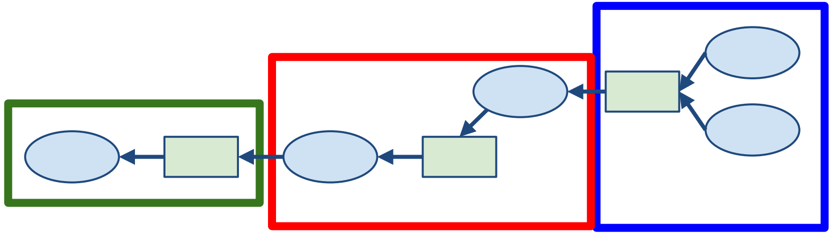
Dynamic Graph Applications

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

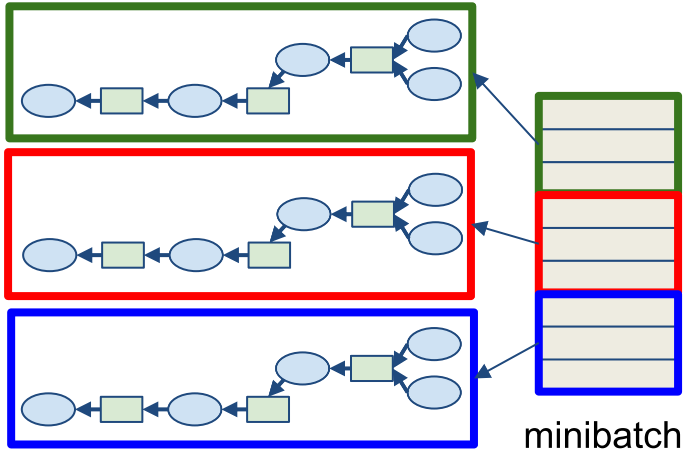
Model Parallel vs. Data Parallel

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

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



Model Parallel



Data Parallel

PyTorch: Data Parallel

`nn.DataParallel`

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

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

`nn.DistributedDataParallel`

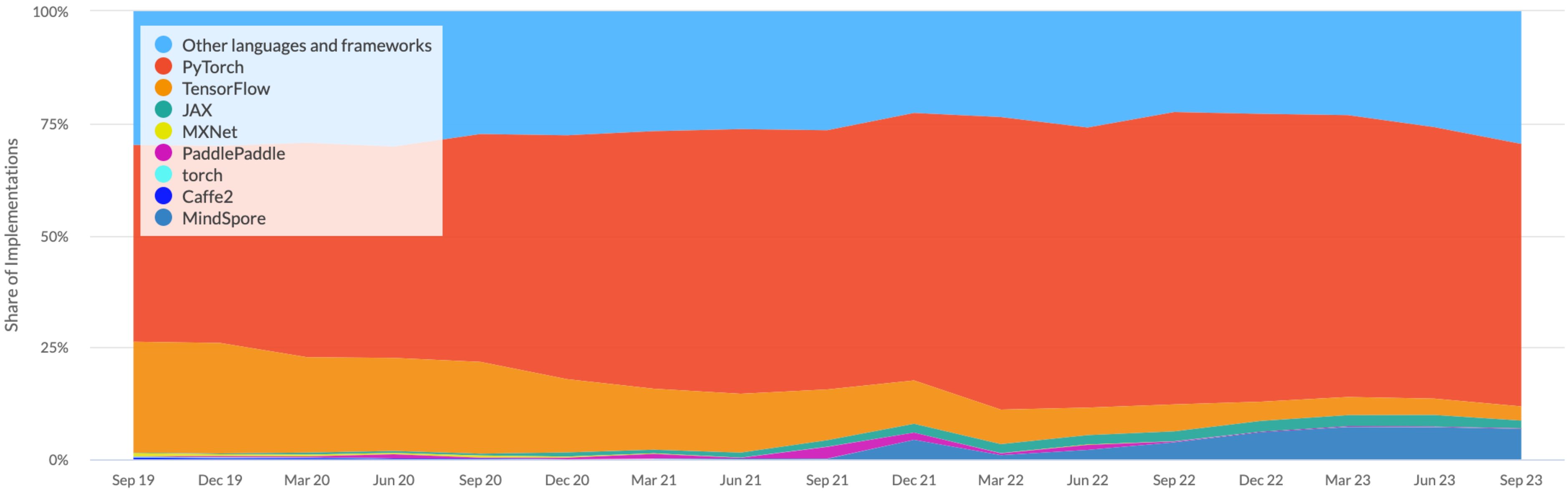
Pro: Multi-nodes & multi-process training

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

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

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

PyTorch vs. TensorFlow



My Advice:

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

TensorFlow's syntax became a lot more intuitive after 2.0. Not perfect but still has a wide industry usage. Can use same framework for research and production.