DeepRob

Lecture 12
Deep Learning Software
University of Michigan | Department of Robotics

DeepRob

Overview

1. **One time setup:**
   - Activation functions, data preprocessing, weight initialization, regularization
2. **Training dynamics:**
   - Learning rate schedules; hyperparameter optimization
3. **After training:**
   - Model ensembles, transfer learning, large-batch training

Model Ensembles

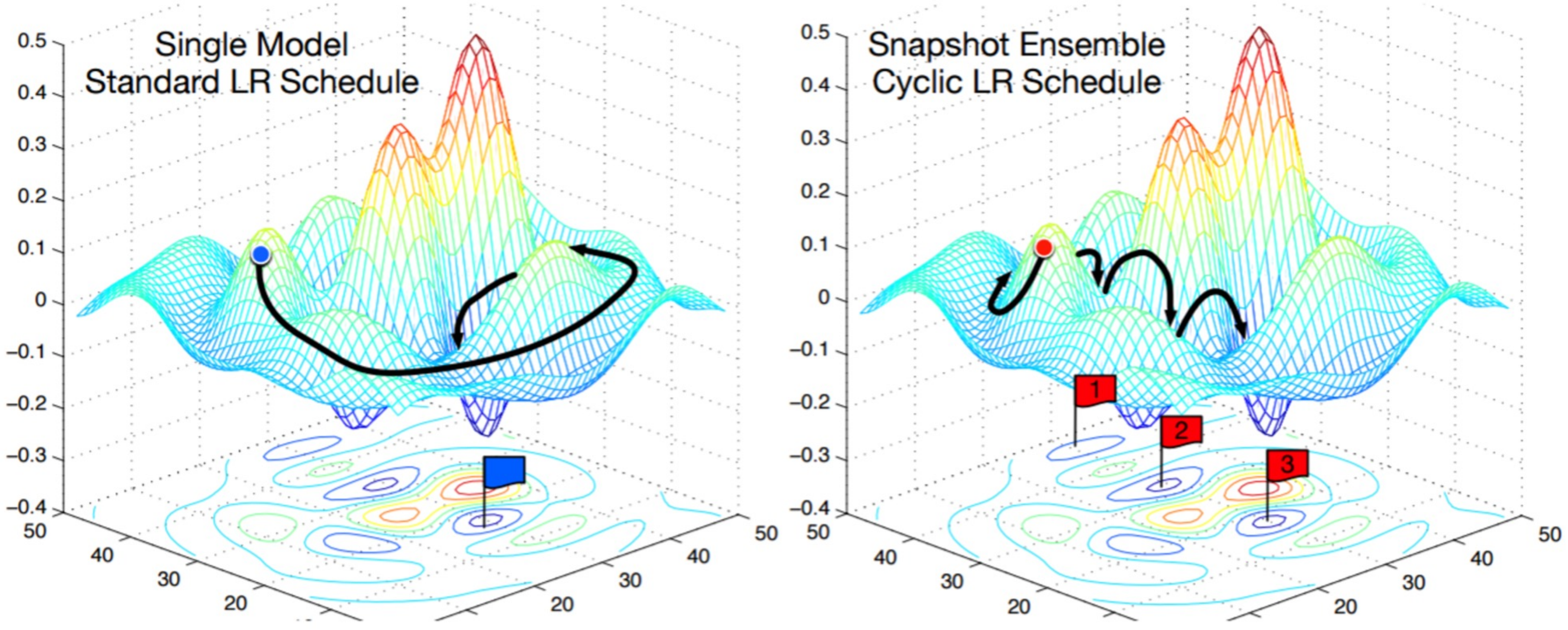
1. **Train multiple independent models**
2. **At test time average their results:**

(Take average of predicted probability distributions, then choose argmax)

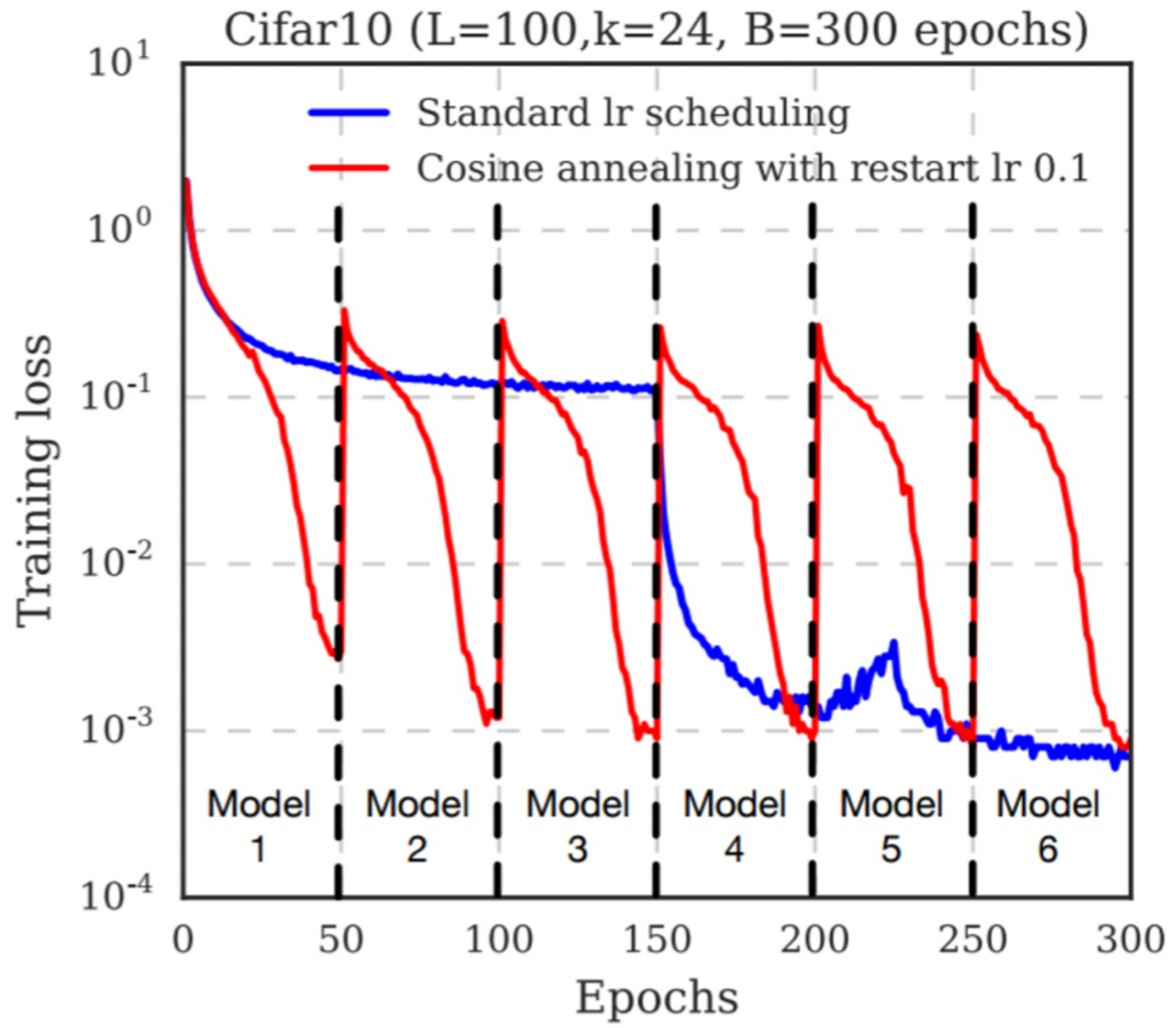
Enjoy 2% extra performance

Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!



Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016



Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017
Figures copyright Yixuan Li and Geoff Pleiss, 2017. Reproduced with permission.

Cyclic learning rate schedules can make this work even better!

Model Ensembles: Tips and Tricks

Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dx = network.backward()
  x += - learning_rate * dx
  x_test = 0.995*x_test + 0.005*x # use for test set
```

Polyak and Juditsky, "Acceleration of stochastic approximation by averaging", SIAM Journal on Control and Optimization, 1992.

Karras et al, "Progressive Growing of GANs for Improved Quality, Stability, and Variation", ICLR 2018

Brock et al, "Large Scale GAN Training for High Fidelity Natural Image Synthesis", ICLR 201

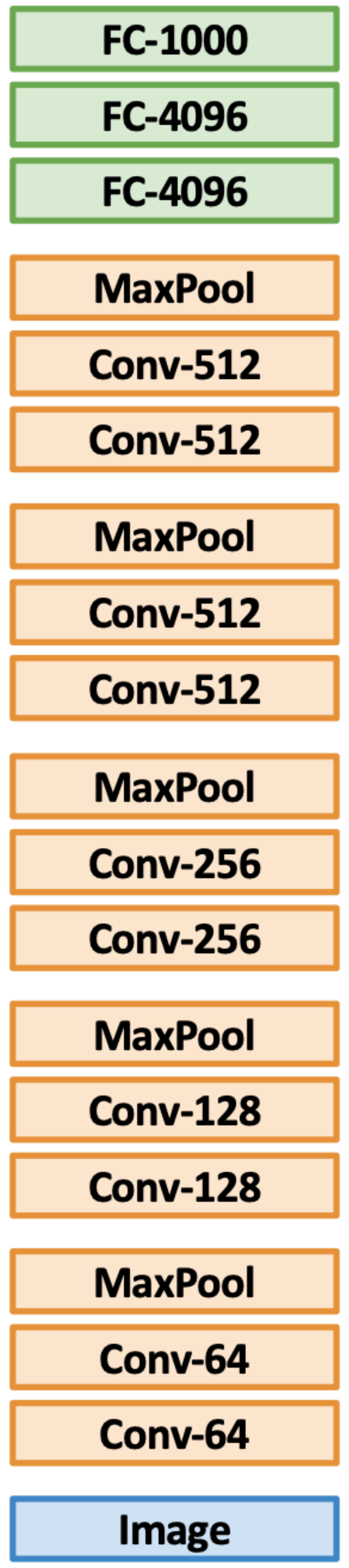
Transfer Learning

"You need a lot of data if you want to train / use CNNs"

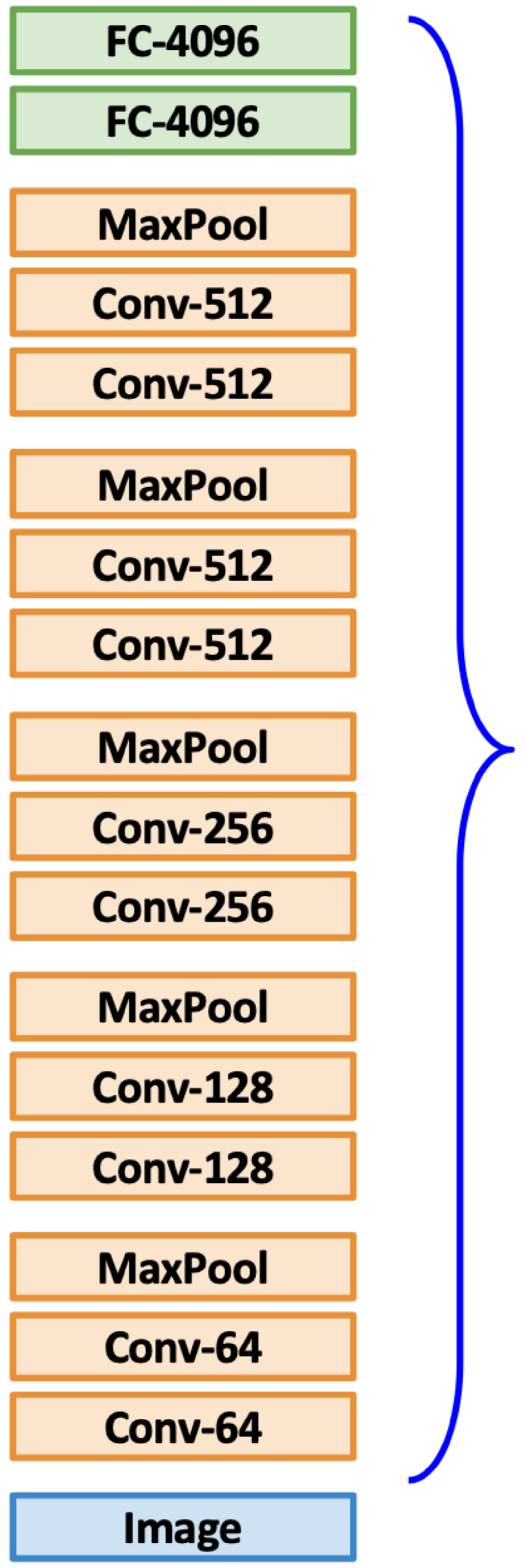
What if data is limited?

Transfer Learning with CNNs

1. Train on ImageNet



2. Use CNN as a feature extractor



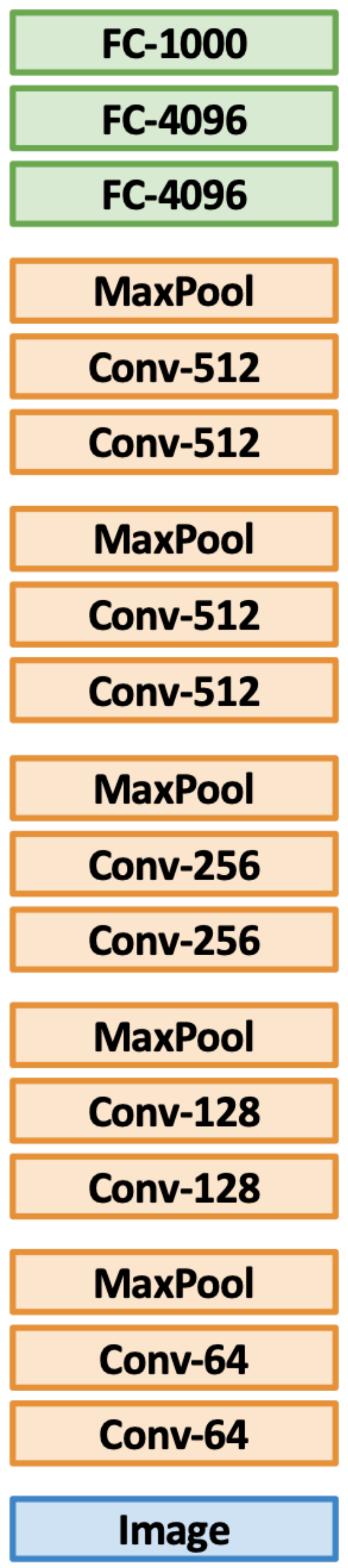
Remove last layer

Freeze these

Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014

Transfer Learning with CNNs

1. Train on ImageNet



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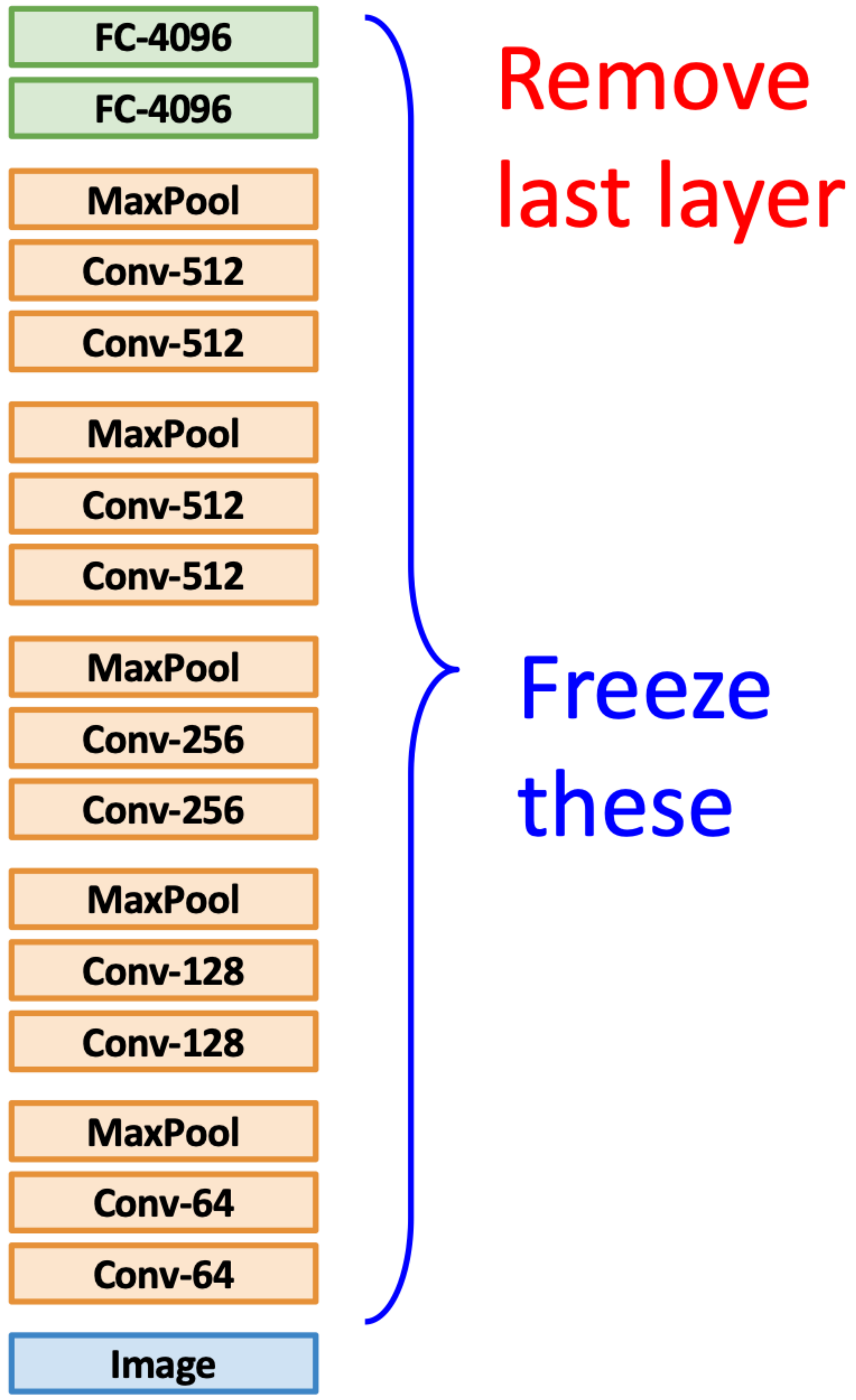
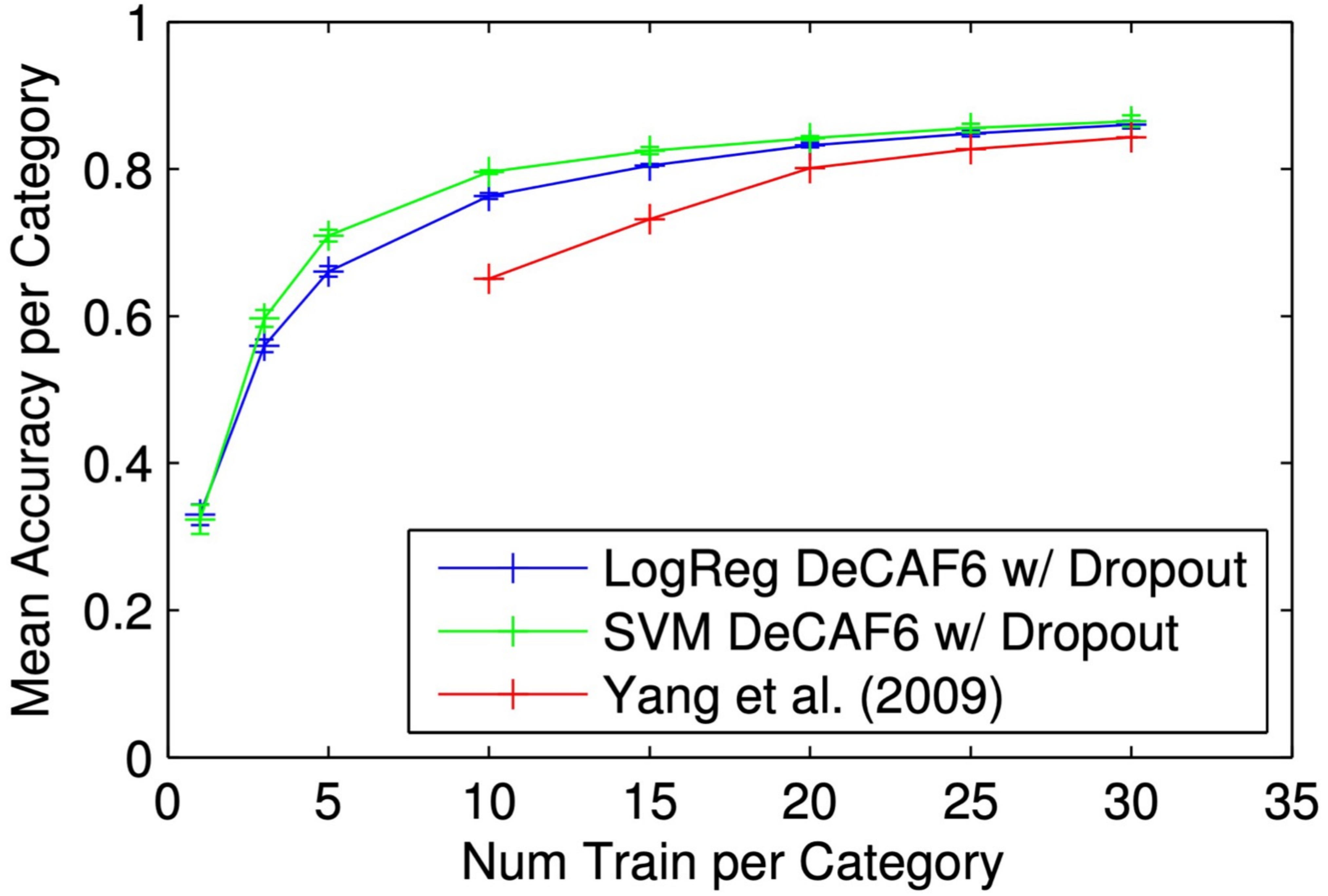


Classification on Caltech-101



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Transfer Learning with CNNs

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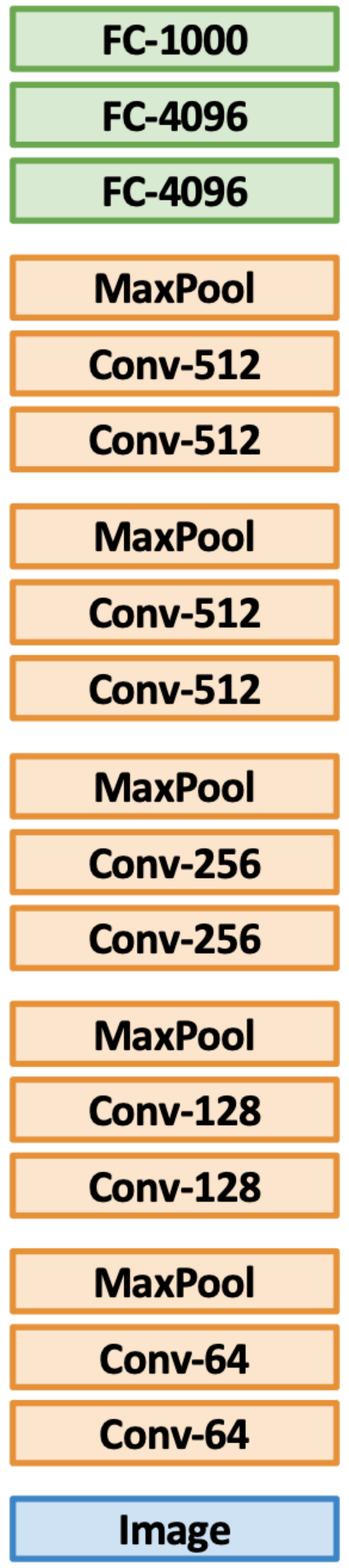

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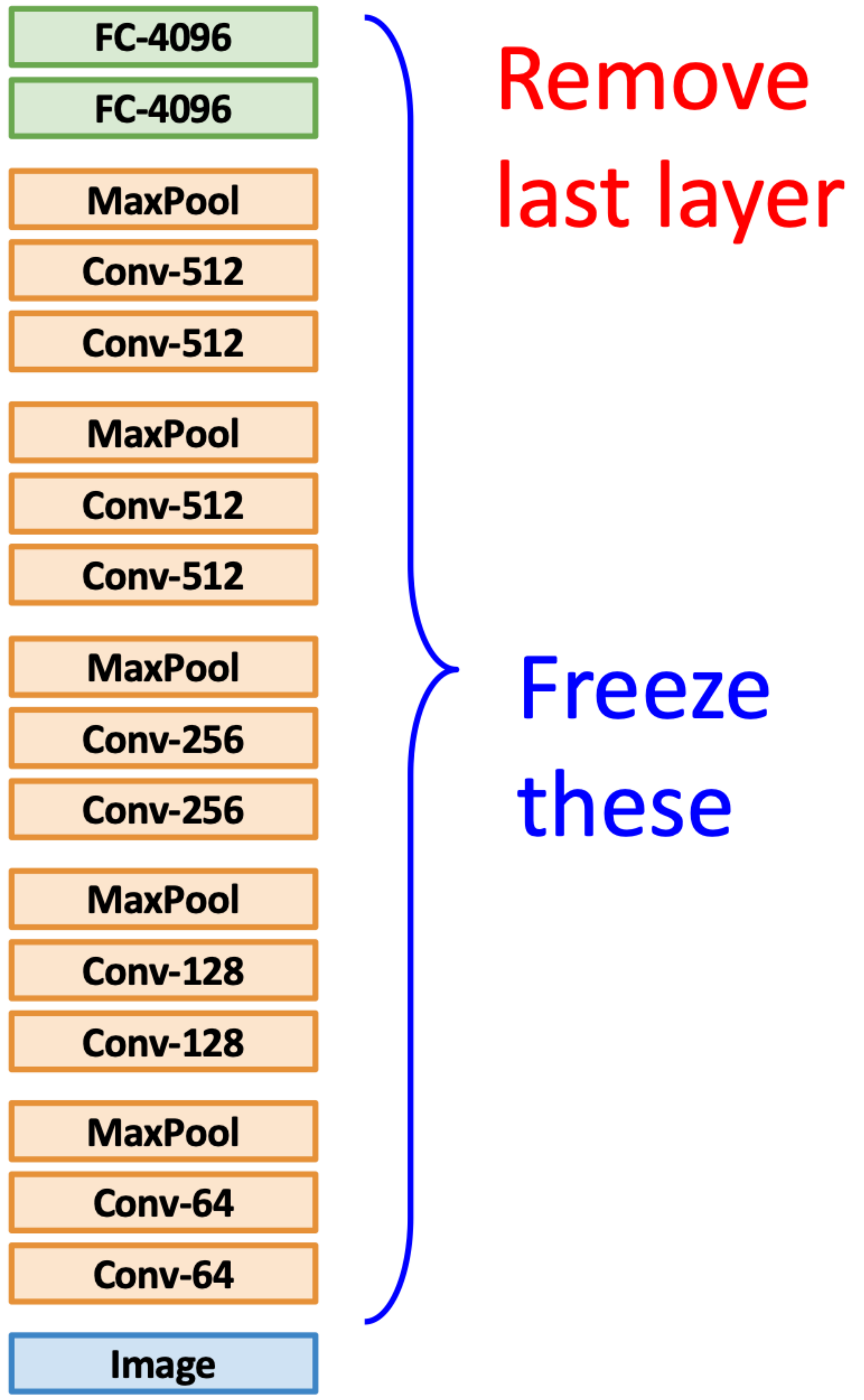
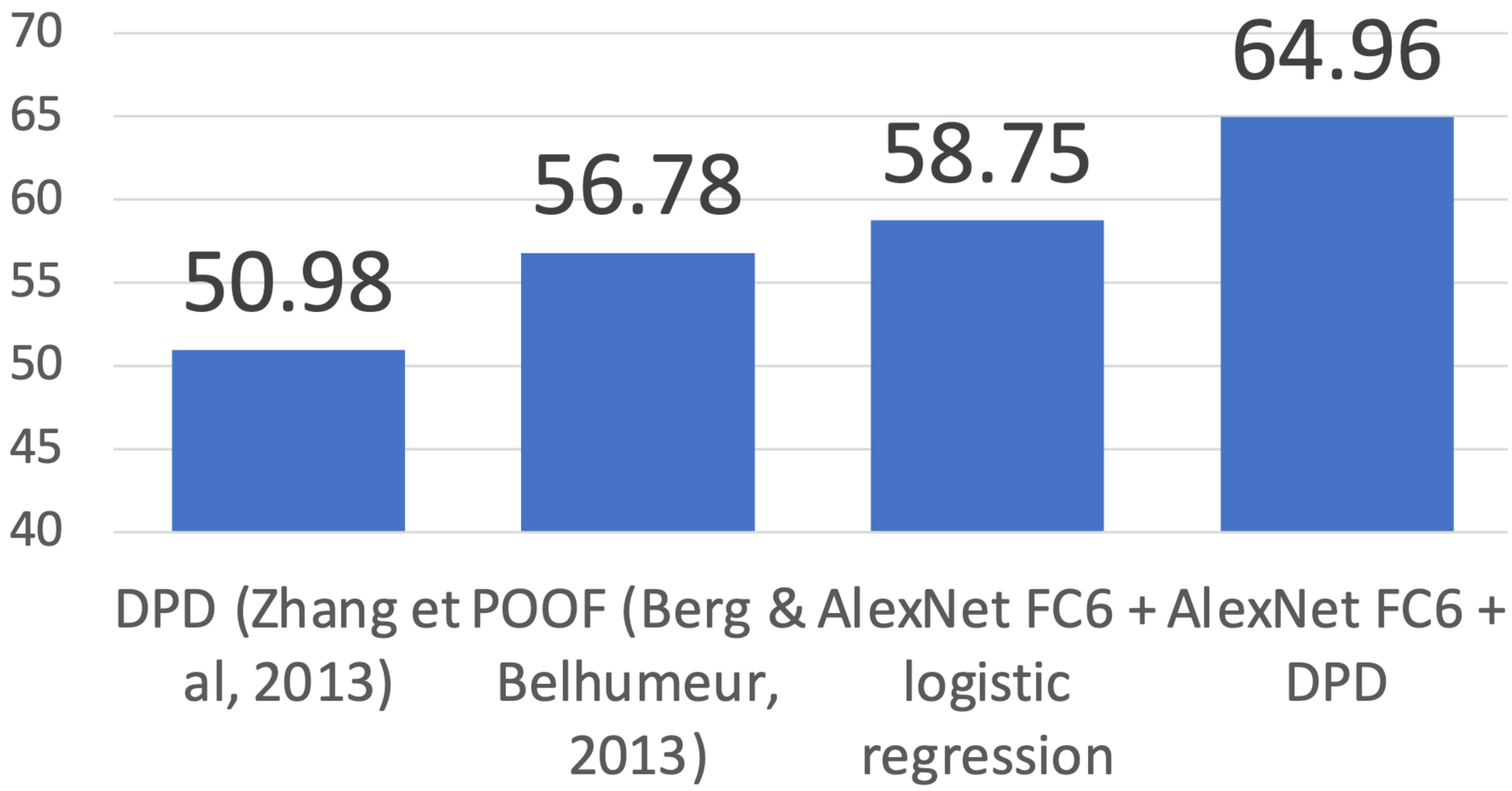


Bird Classification on Caltech-UCSD



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Transfer Learning with CNNs

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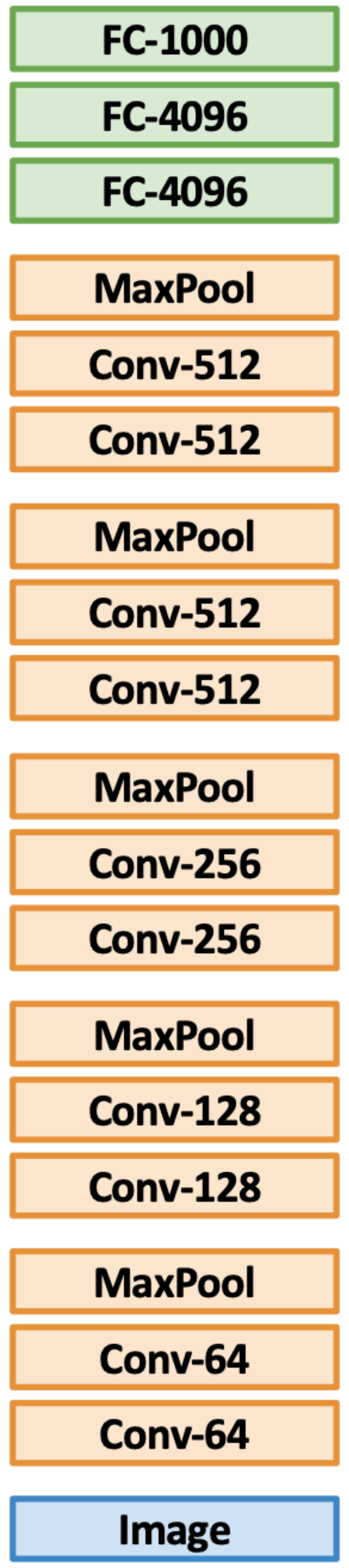

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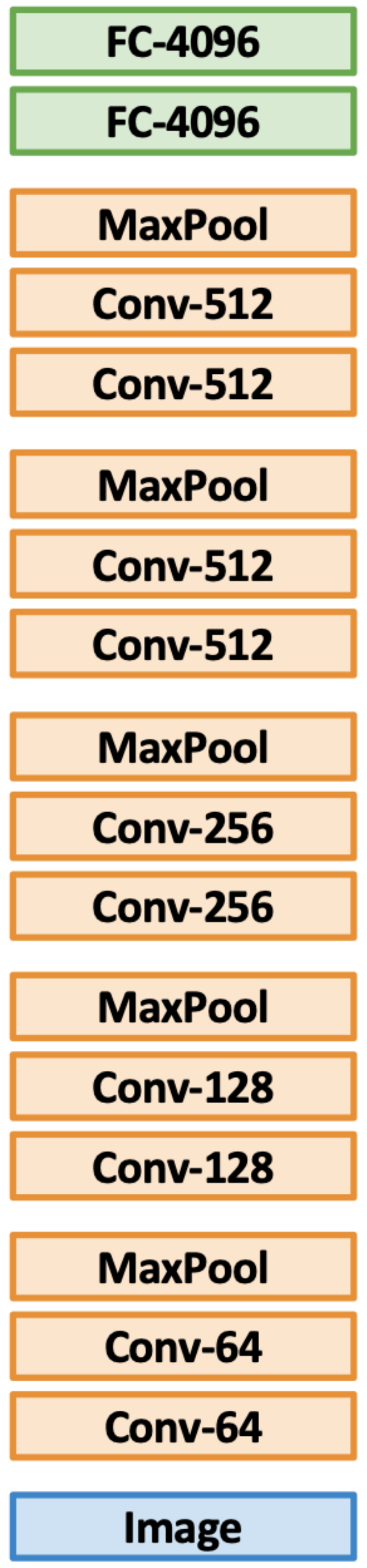

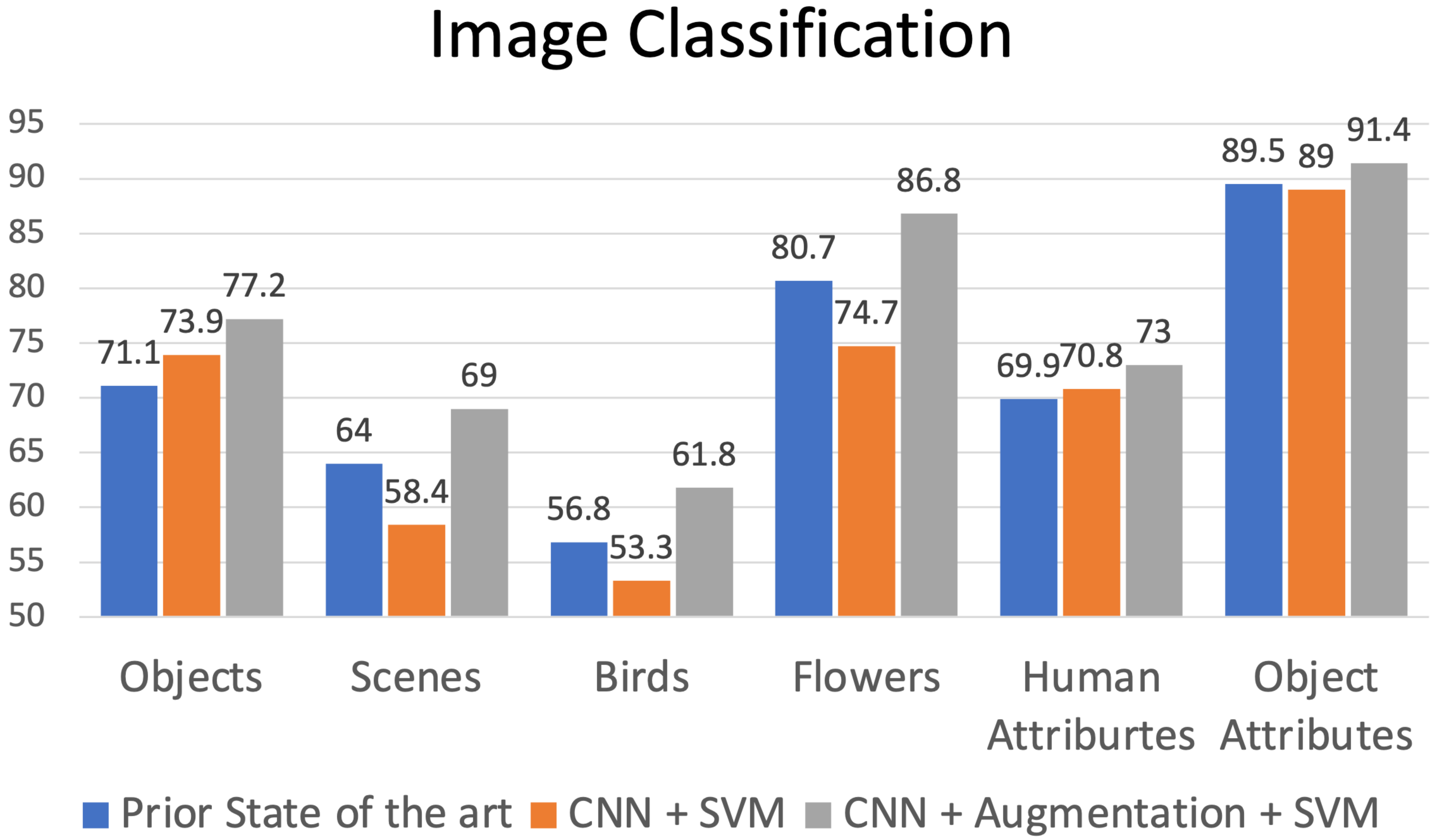

Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

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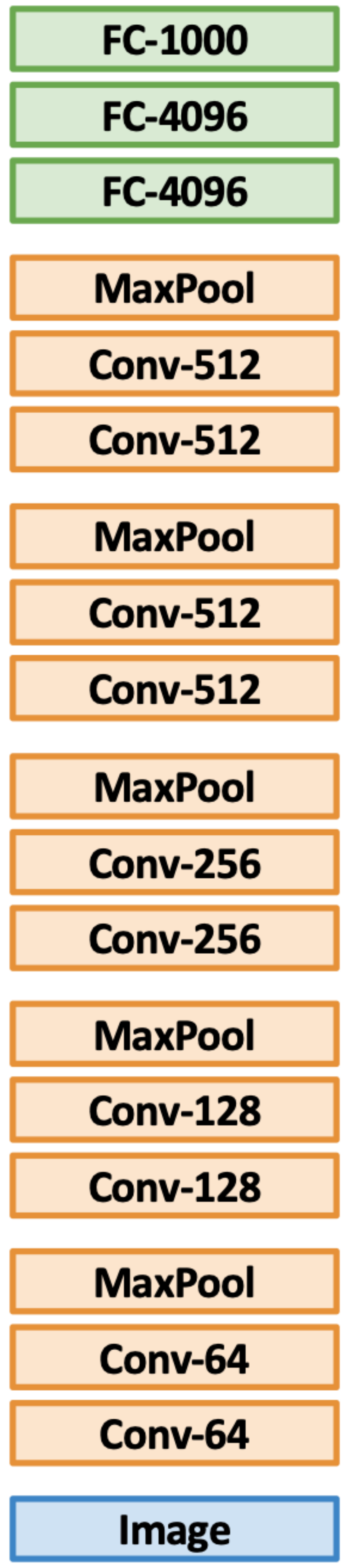

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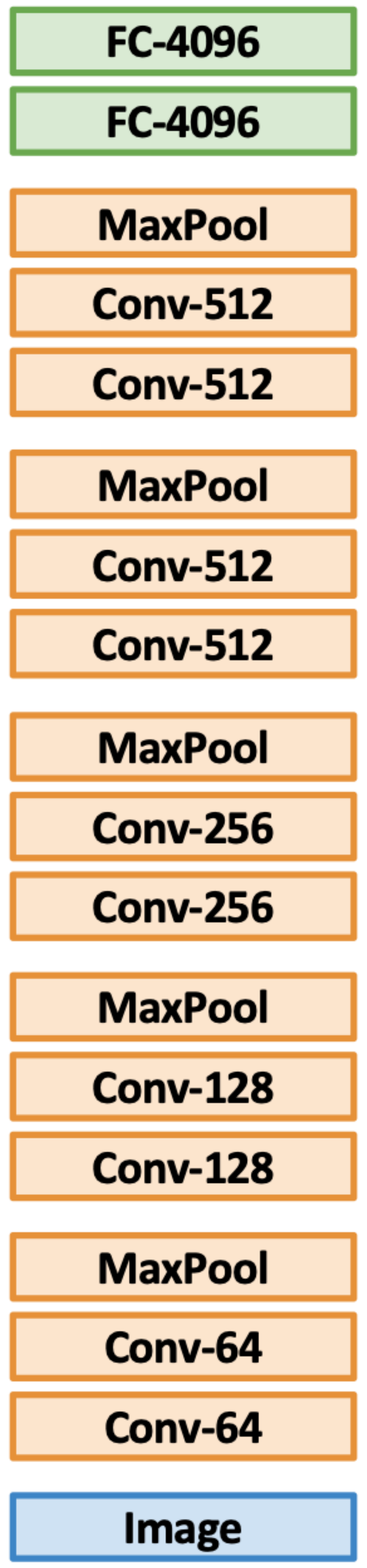
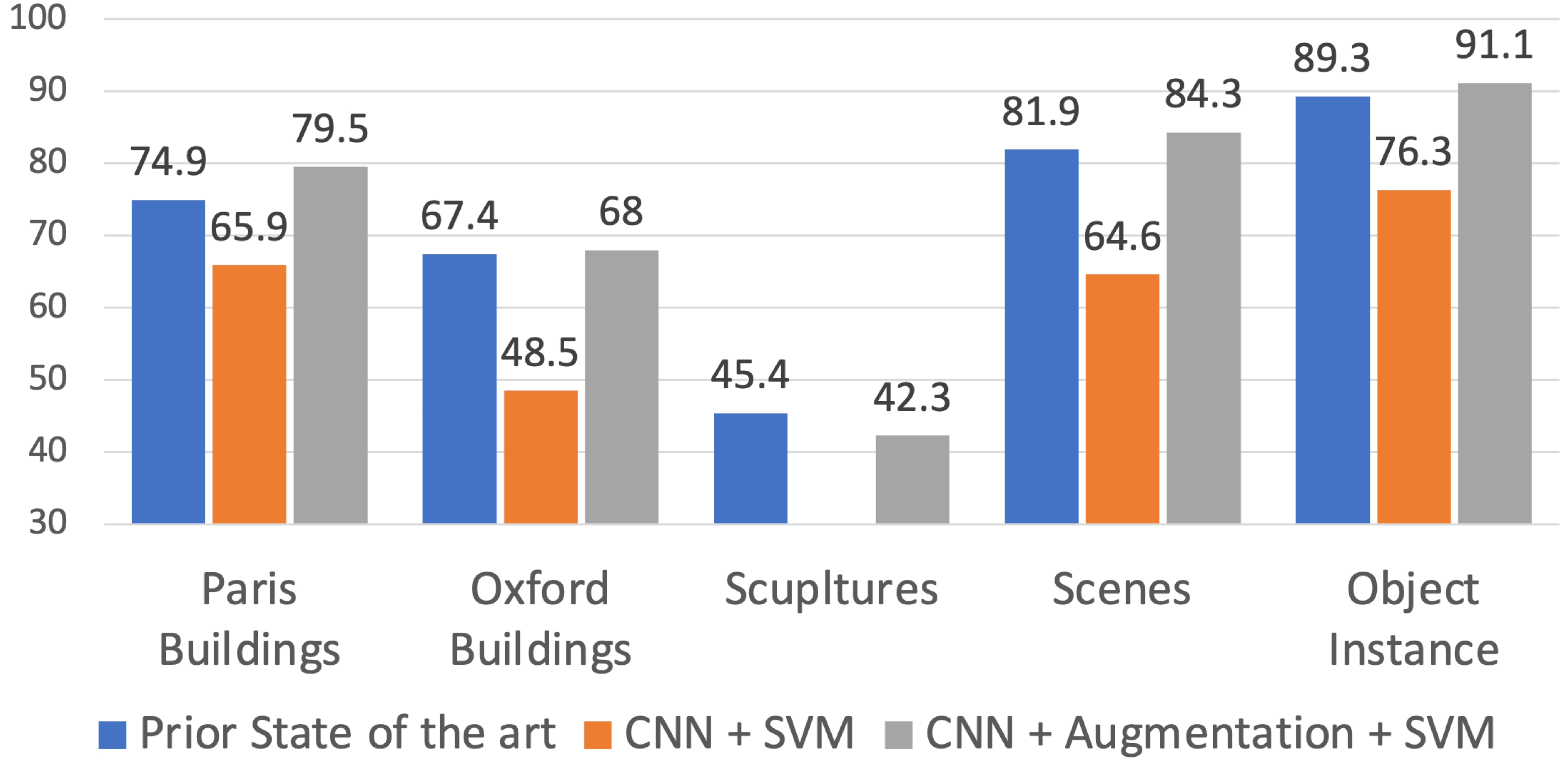


Image Retrieval: Nearest-Neighbor



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Transfer Learning with CNNs

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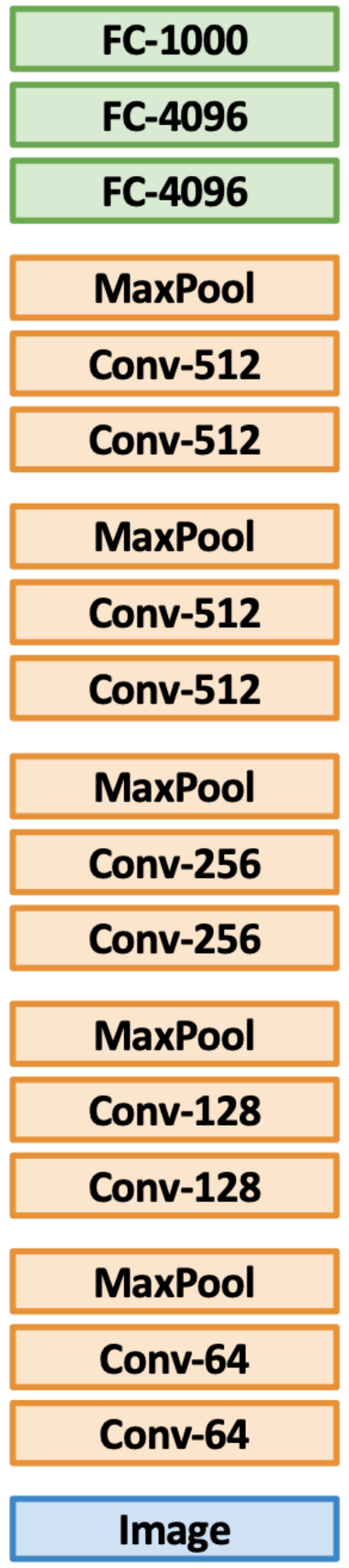

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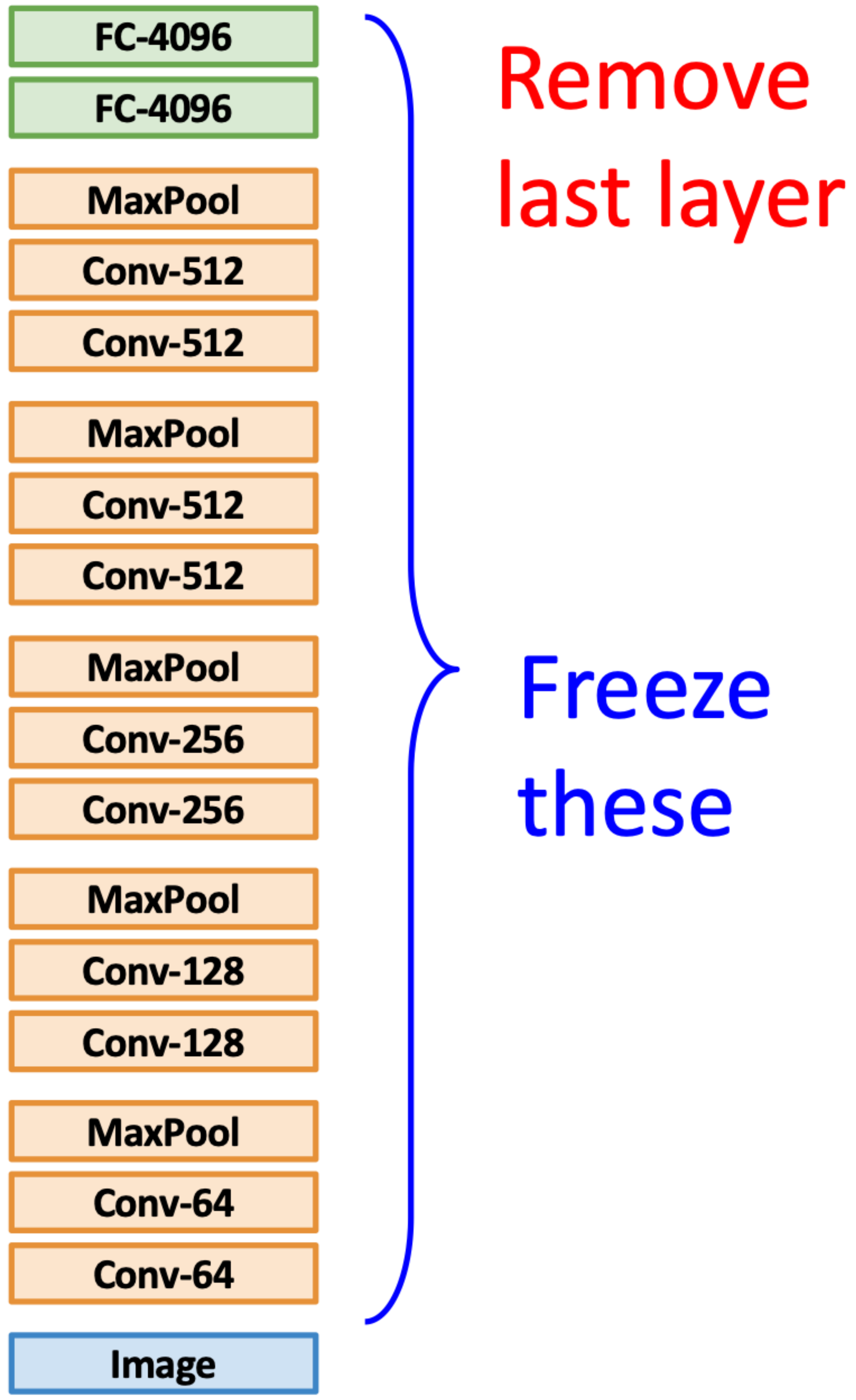
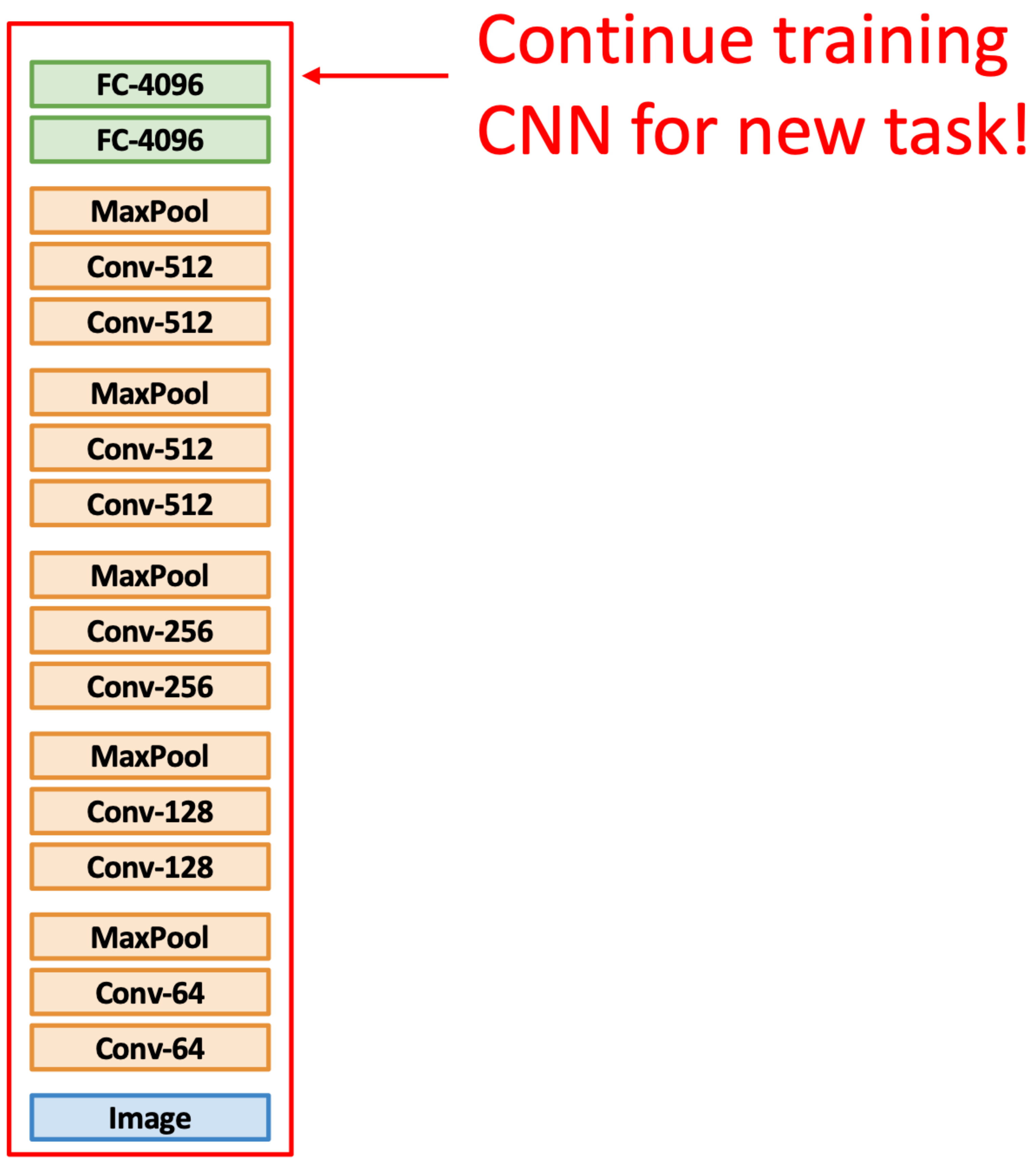


3. Bigger dataset:
Fine-Tuning



Transfer Learning with CNNs

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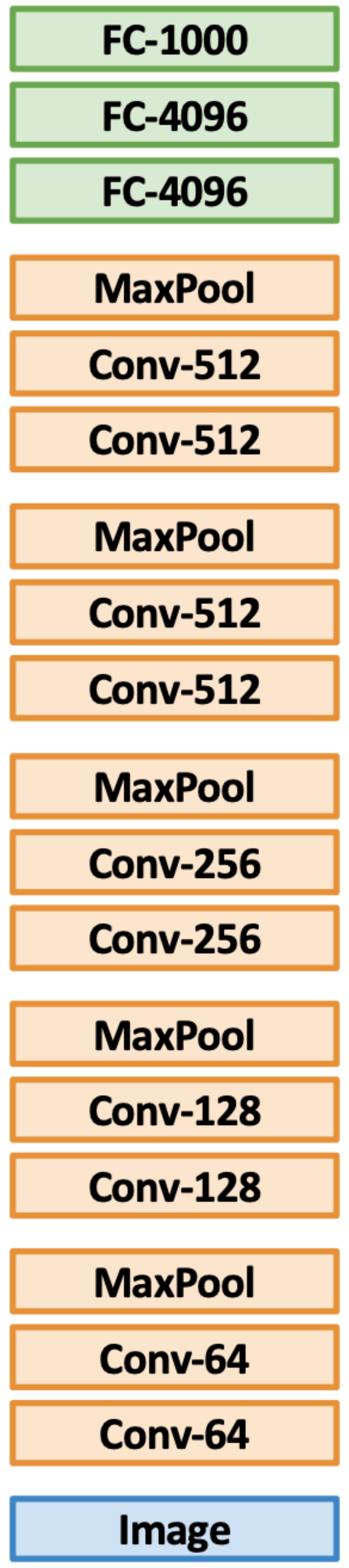

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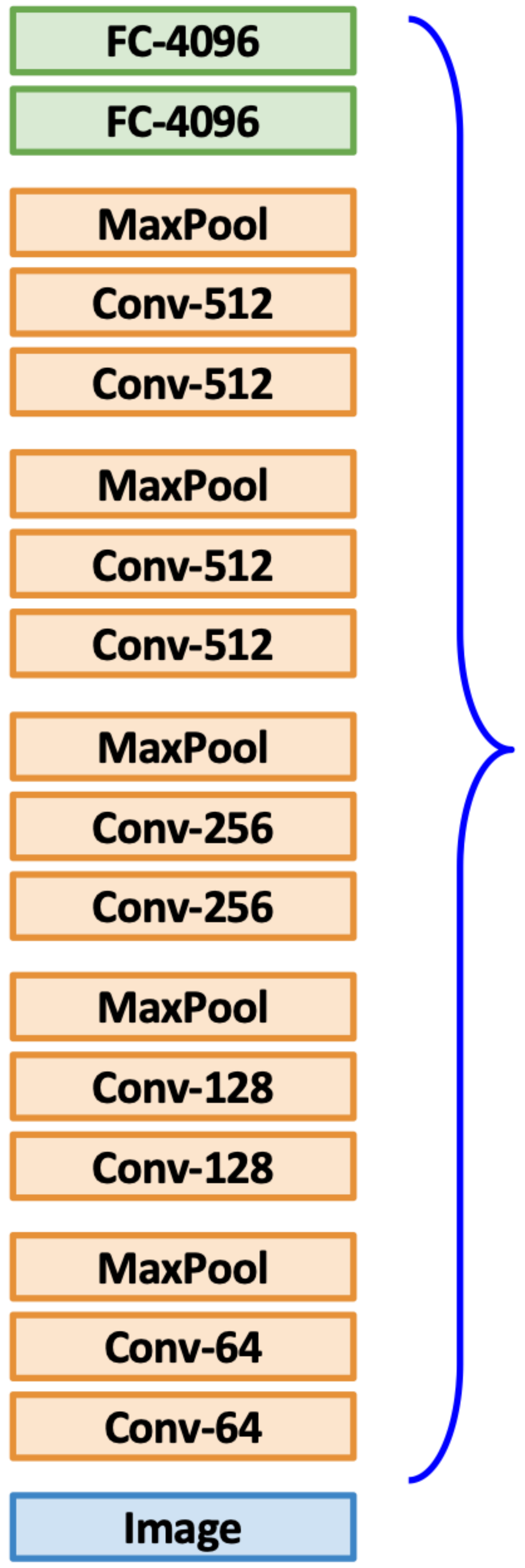
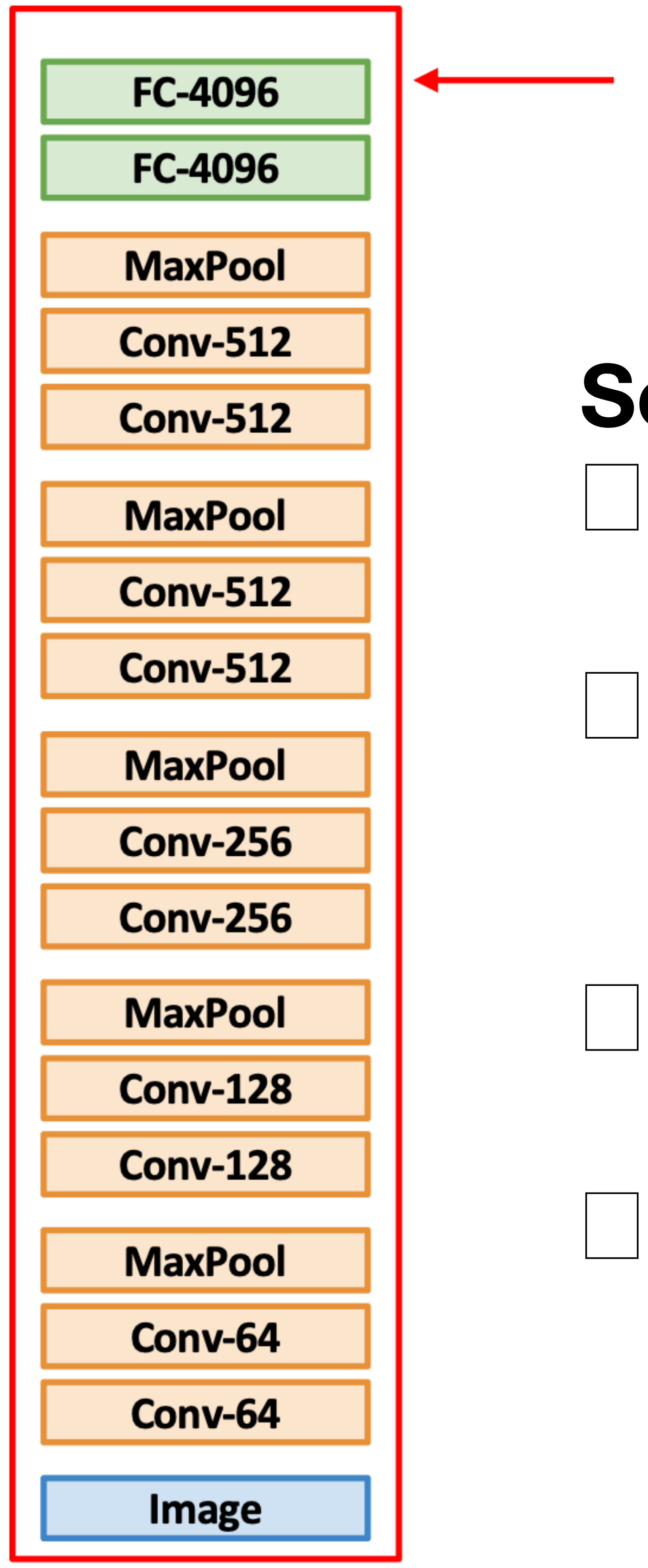


Remove last layer

Freeze these

3. Bigger dataset: **Fine-Tuning**



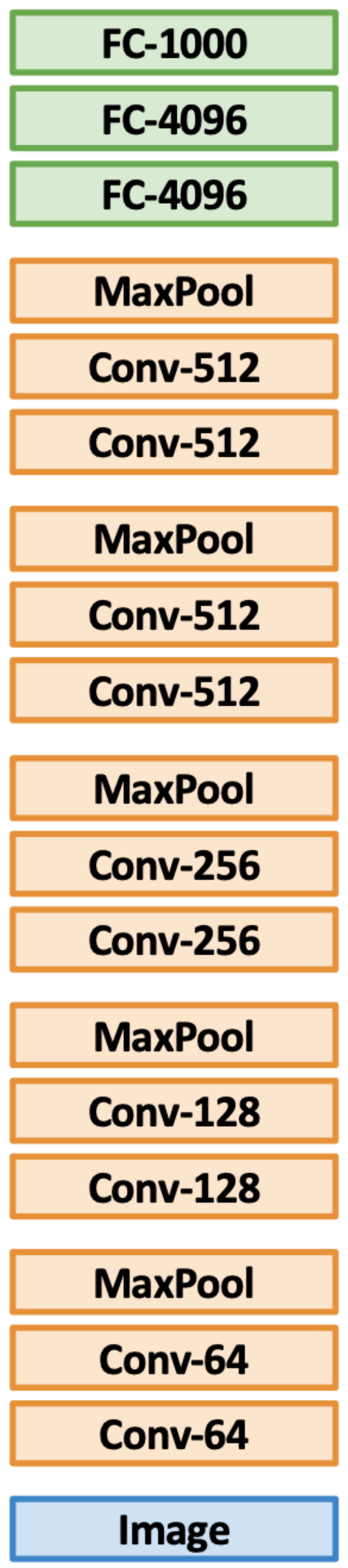
Continue training CNN for new task!

Some tricks:

- Train with feature extraction first before fine-tuning
- Lower the learning rate: use ~1/10 of LR used in original training
- Sometimes freeze lower layers to save computation
- Train with BatchNorm in “test” mode

Transfer Learning with CNNs

1. Train on ImageNet



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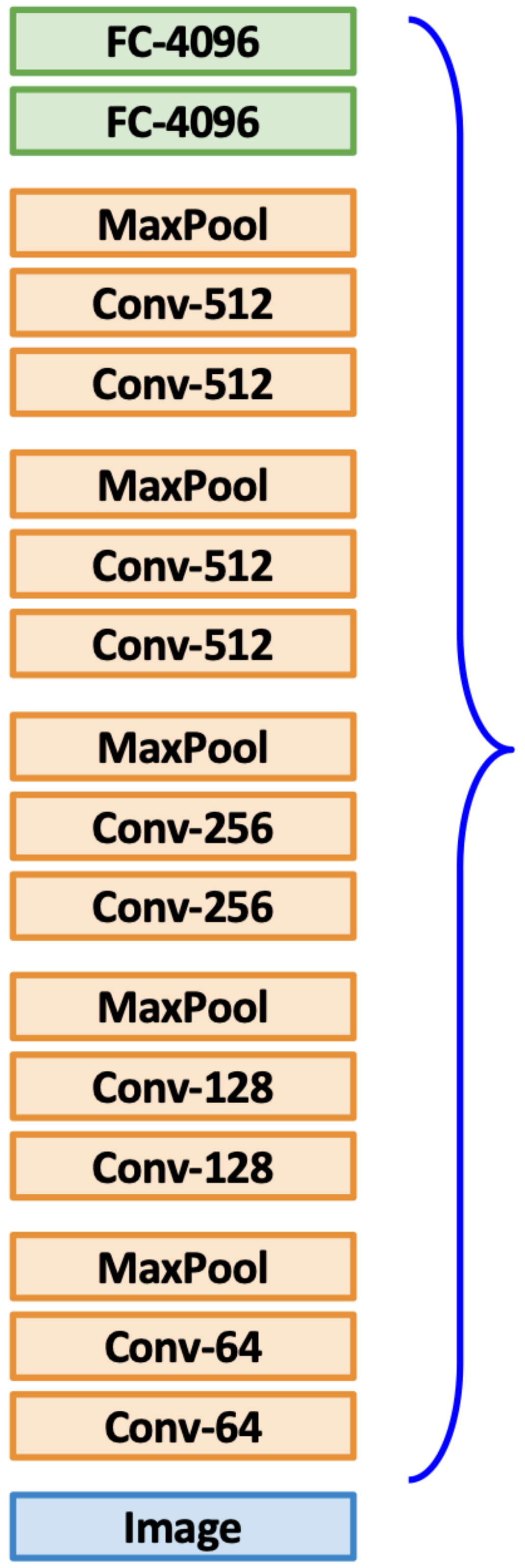

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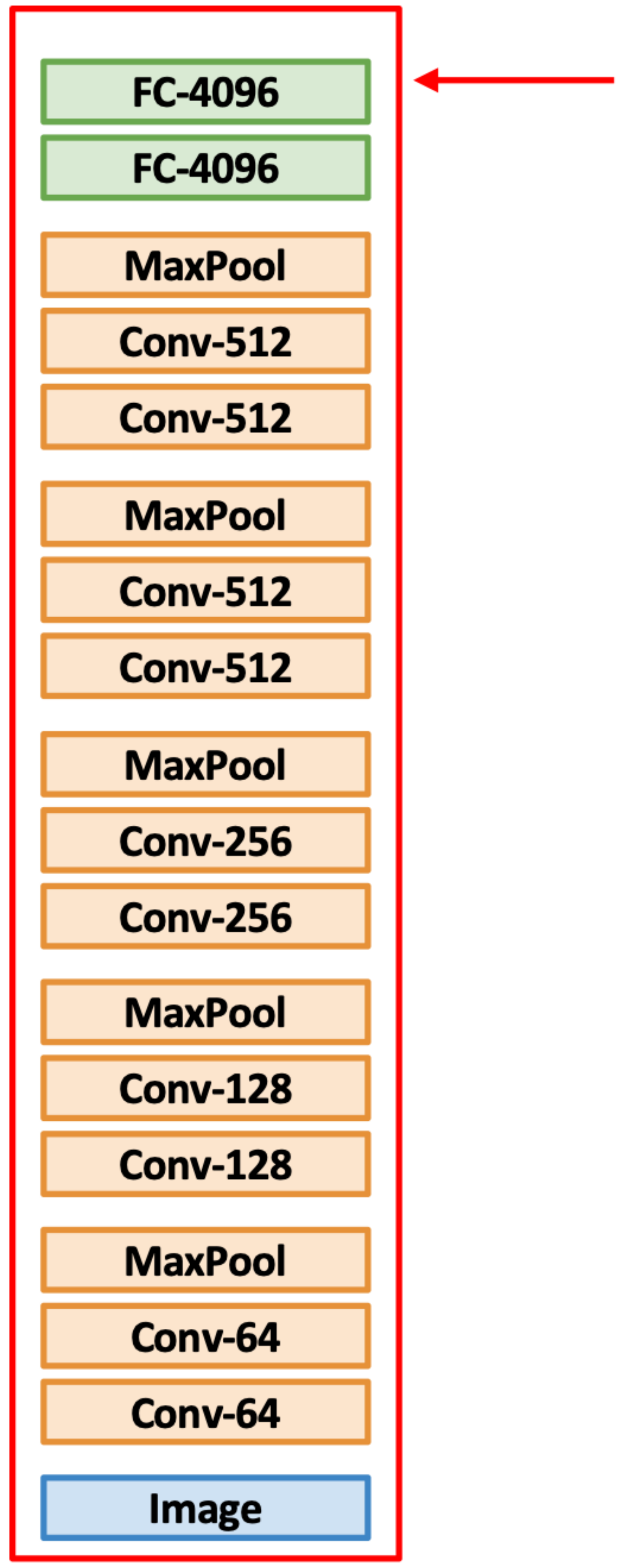
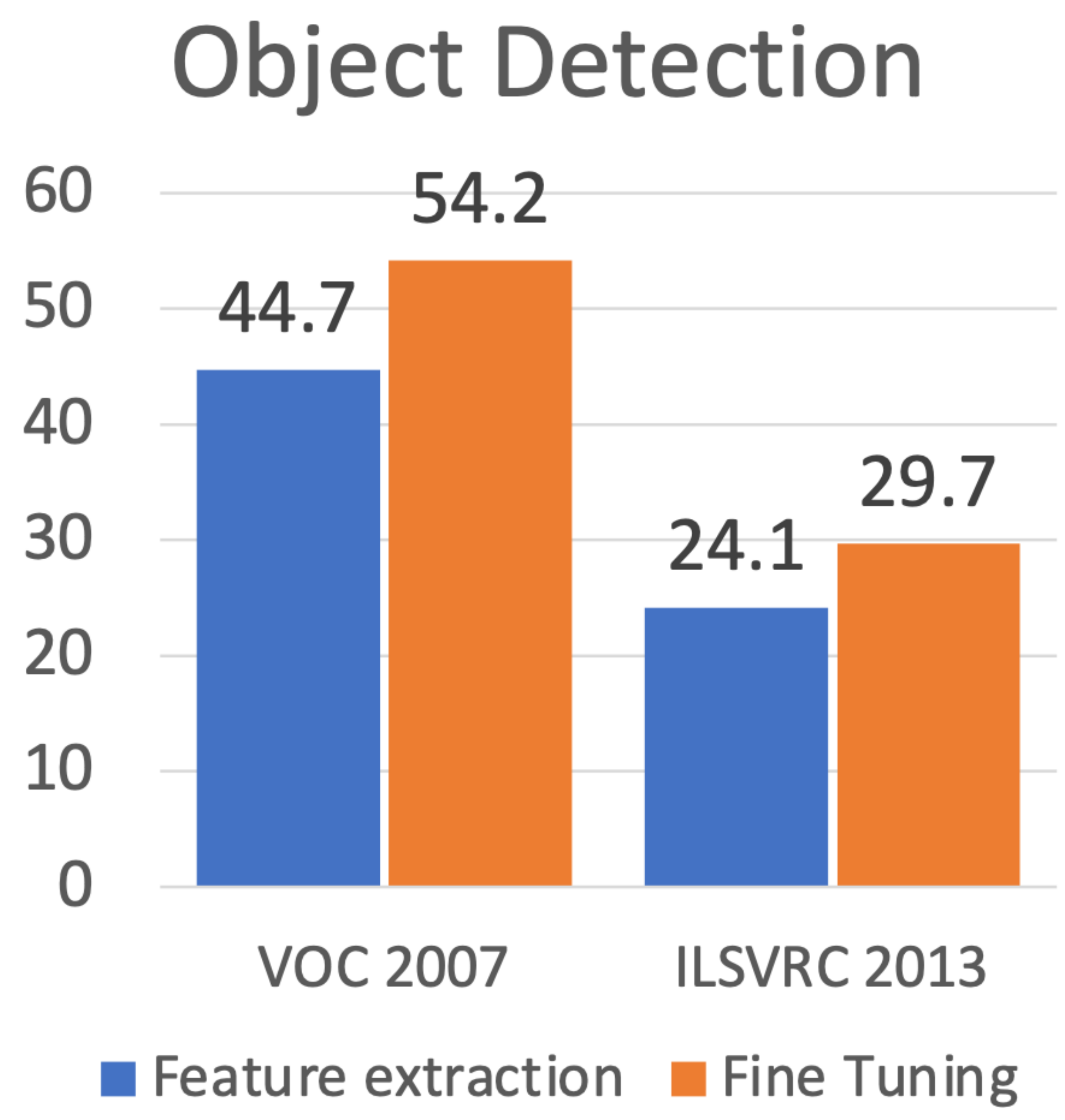
3. Bigger dataset: **Fine-Tuning**

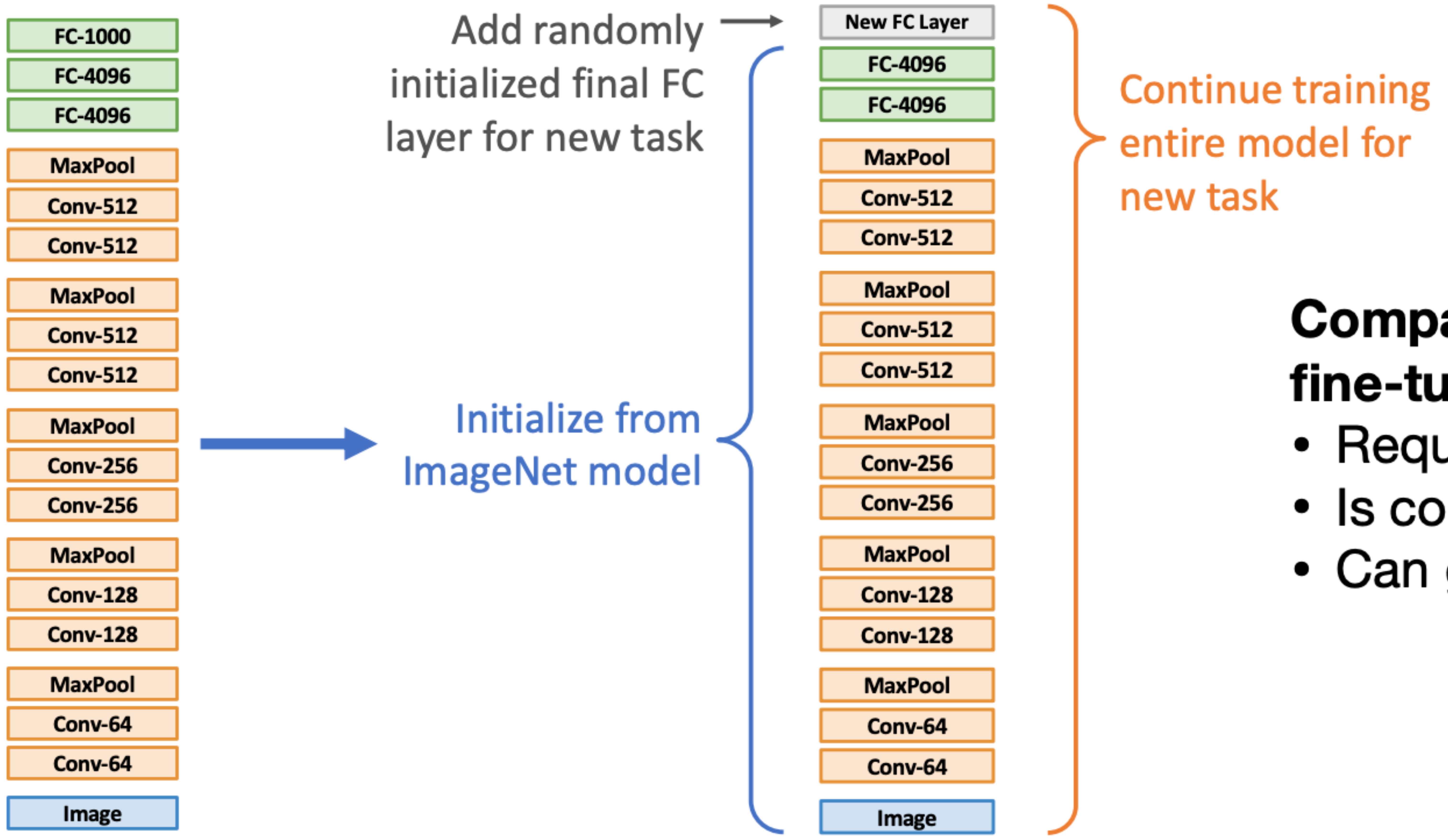


Continue training CNN for new task!



Transfer Learning: Fine Tuning

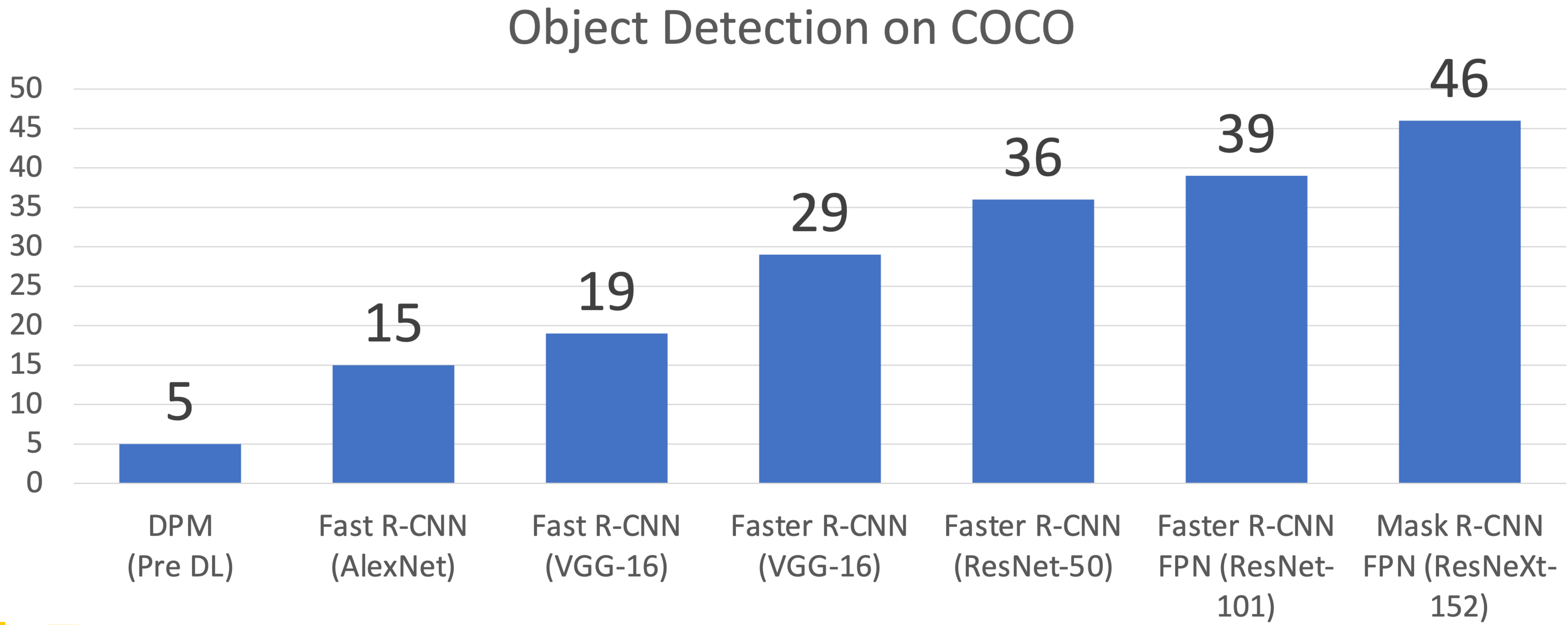
1. Train on ImageNet



Compared with feature extraction, fine-tuning:

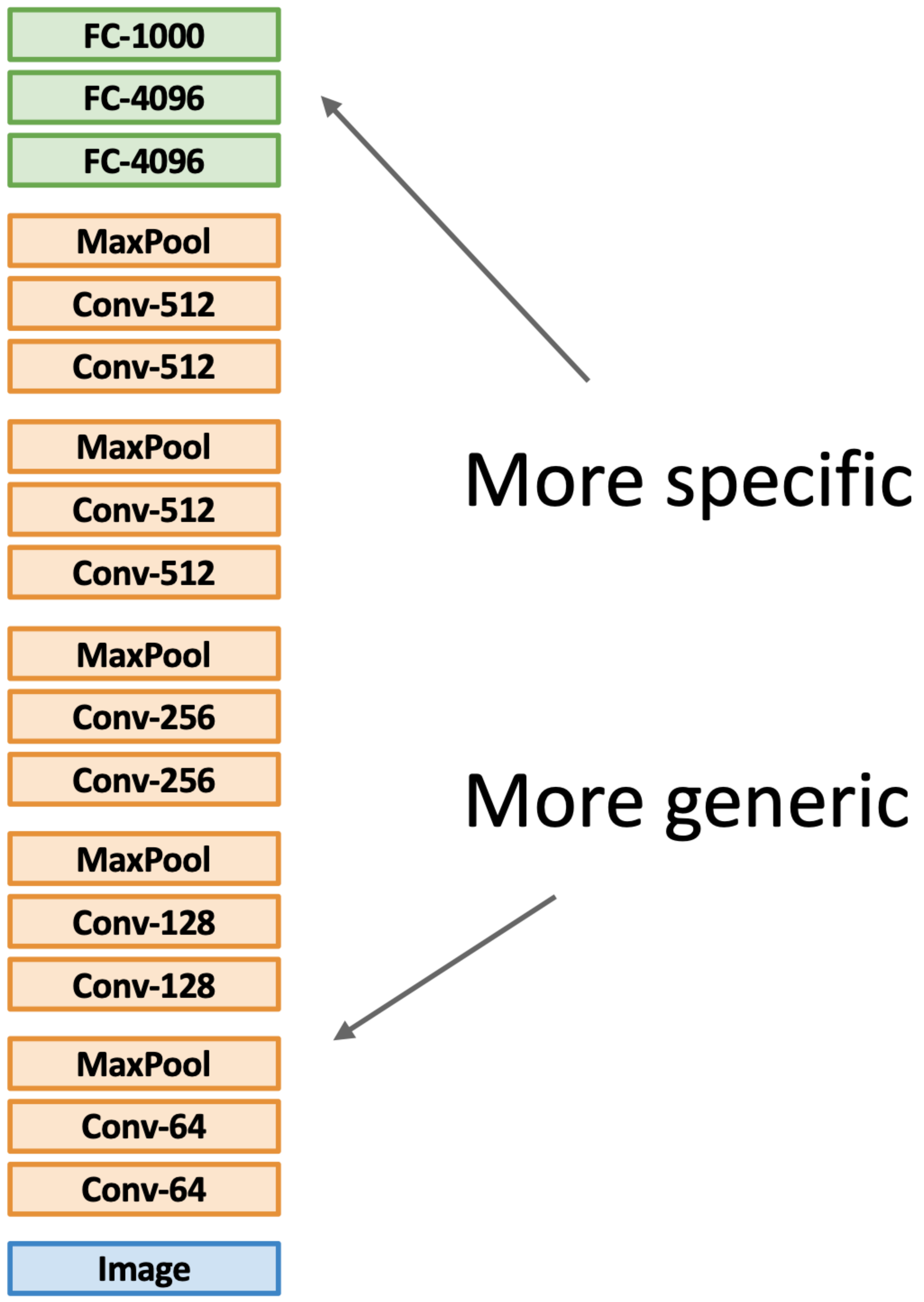
- Requires more data
- Is computationally expensive
- Can give higher accuracies

Transfer Learning with CNNs: Architecture Matters!



Ross Girshick, "The Generalized R-CNN Framework for Object Detection", ICCV 2017 Tutorial on Instance-Level Visual Recognition

Transfer Learning with CNNs

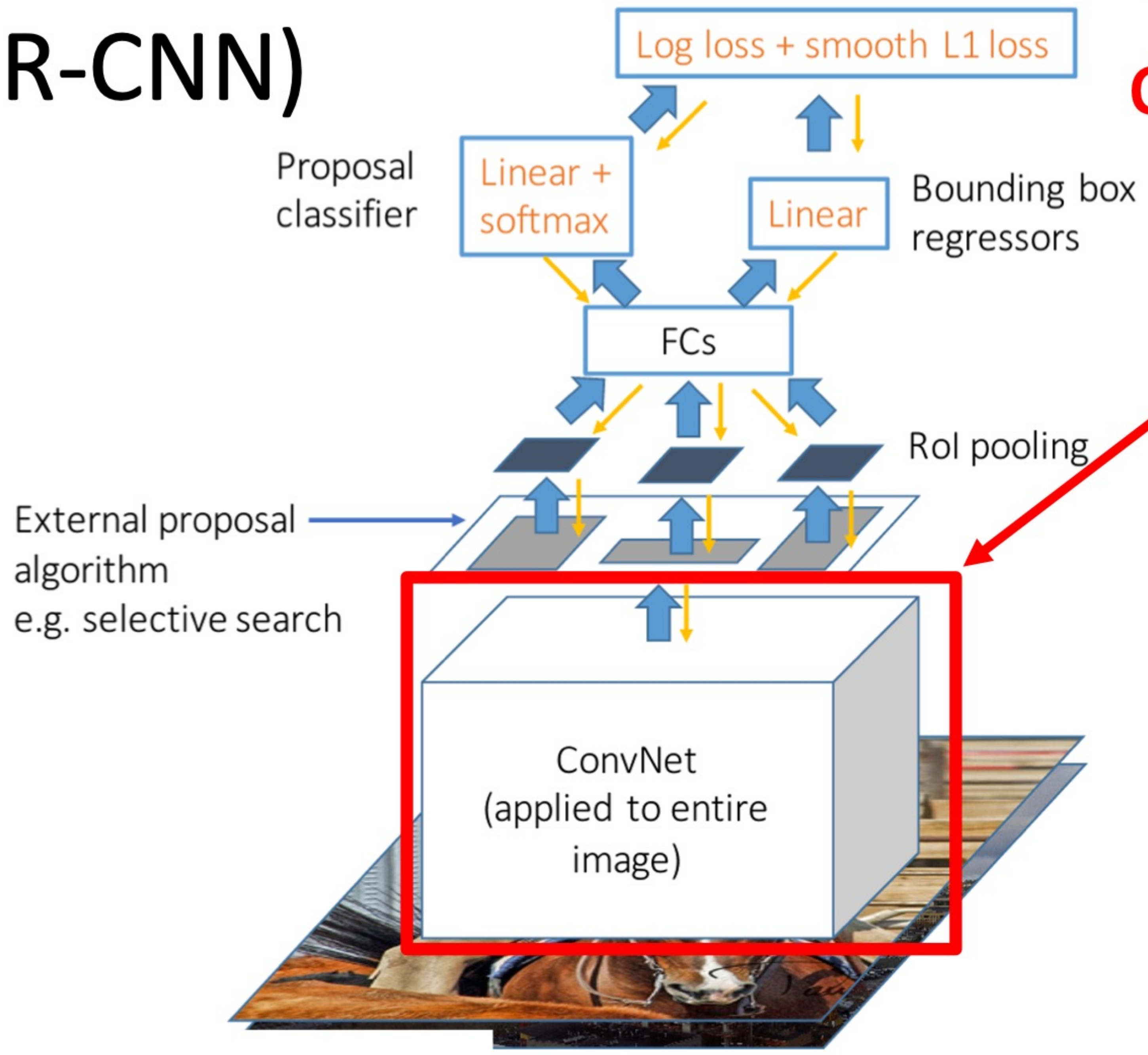


	Dataset similar to ImageNet	Dataset very different from ImageNet
Very little data (10s to 100s)	Use Linear Classifier on top layer	You're in trouble… Try linear classifier from different stages
Quite a lot of data (100s to 1000s)	Finetune a few layers	Finetune a larger number of layers

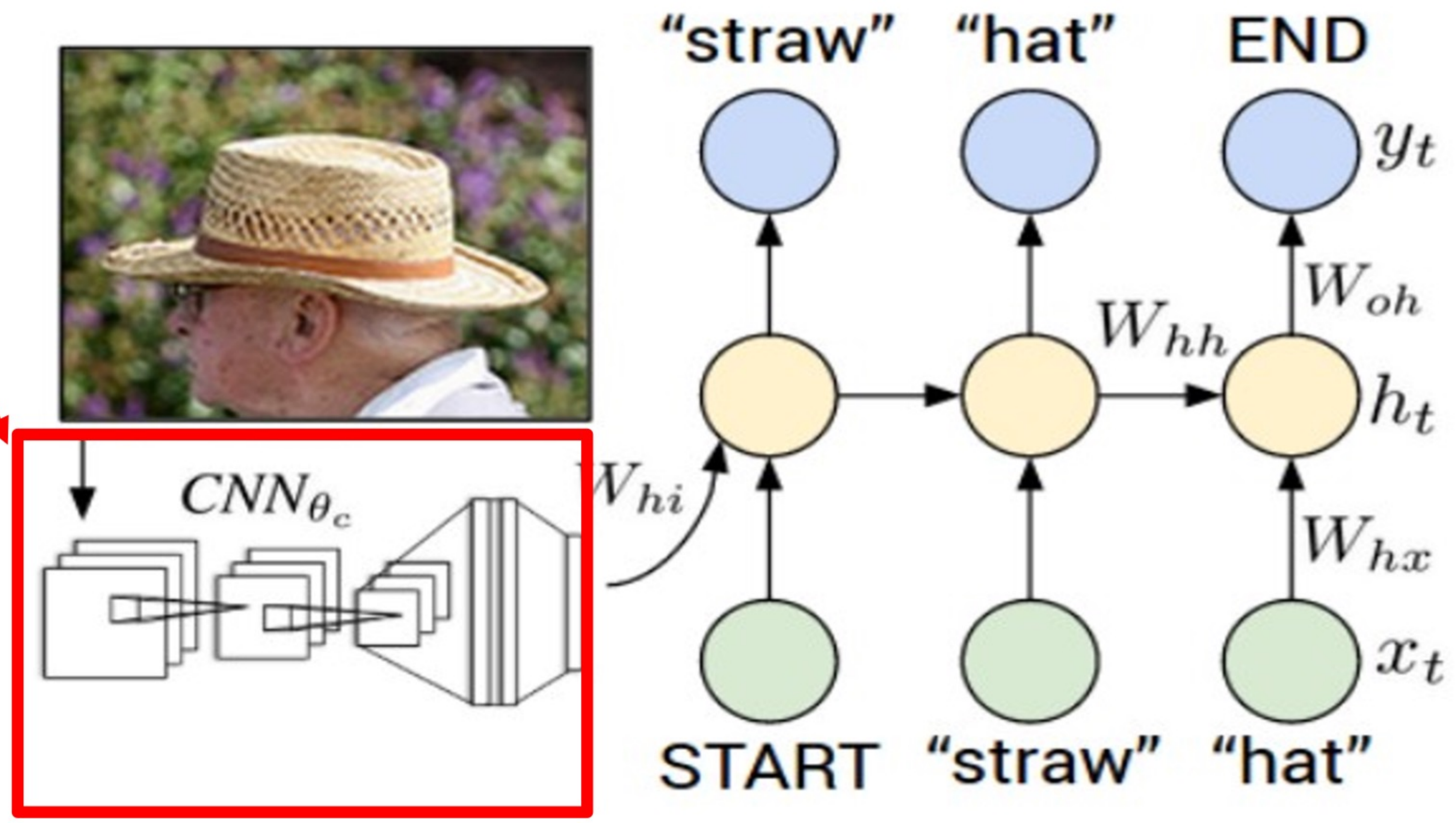
Transfer Learning is pervasive!

Its the norm, not the exception

Object Detection (Fast R-CNN)



CNN pretrained on ImageNet



Girshick, "Fast R-CNN", ICCV 2015
Figure copyright Ross Girshick, 2015. Reproduced with permission.

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

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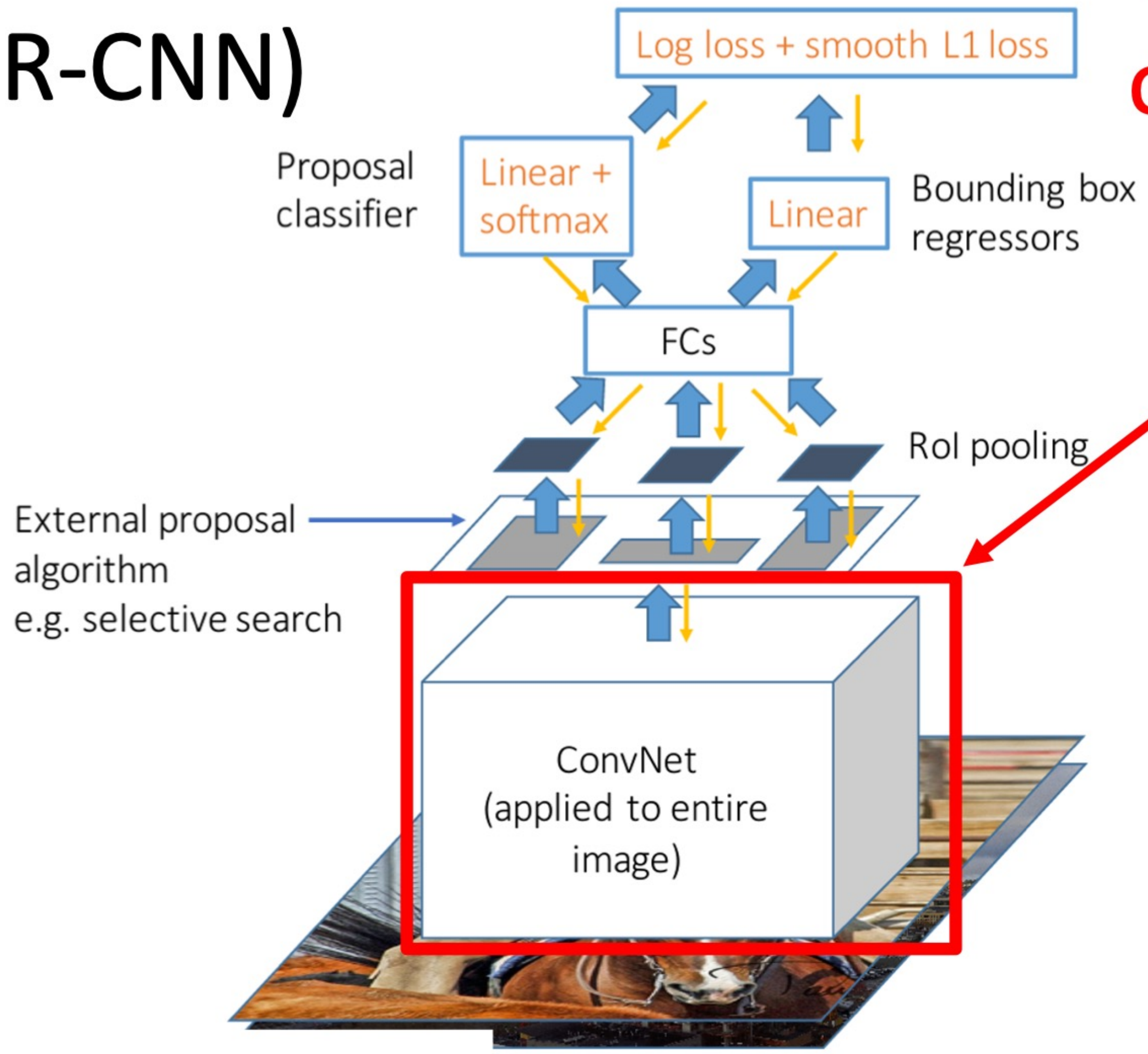

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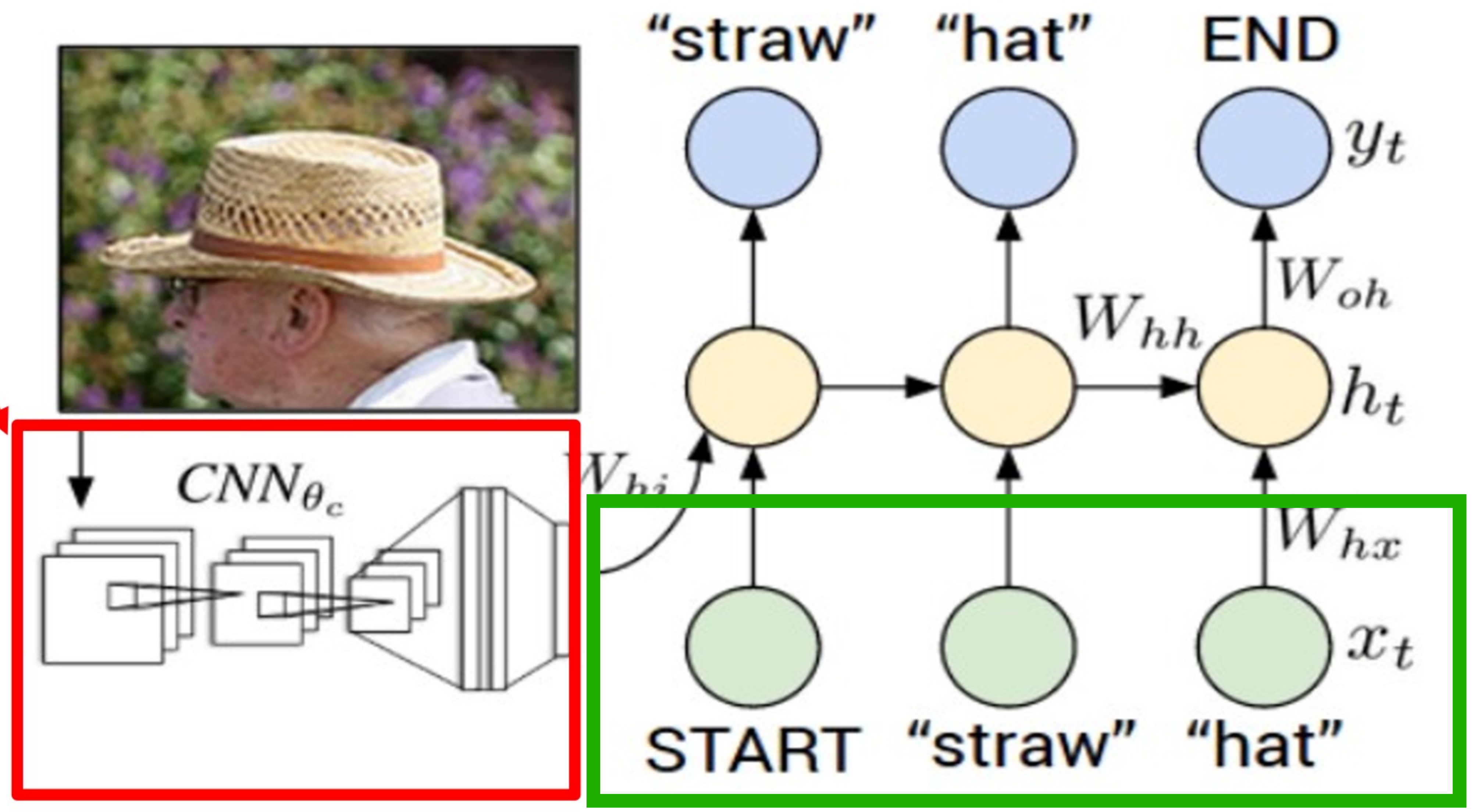

Word vectors pretrained with word2vec

Girshick, "Fast R-CNN", ICCV 2015
Figure copyright Ross Girshick, 2015. Reproduced with permission.

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

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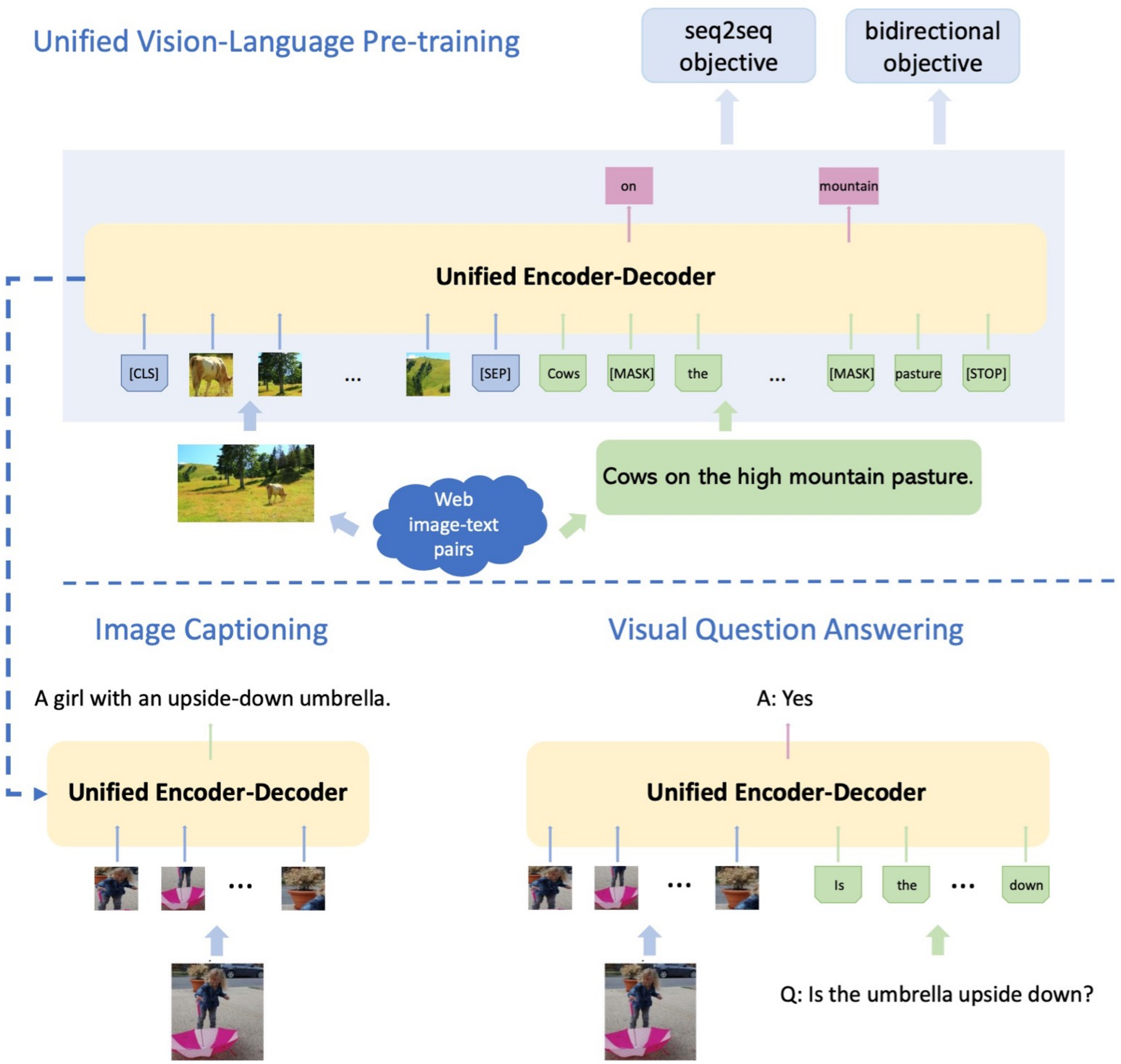


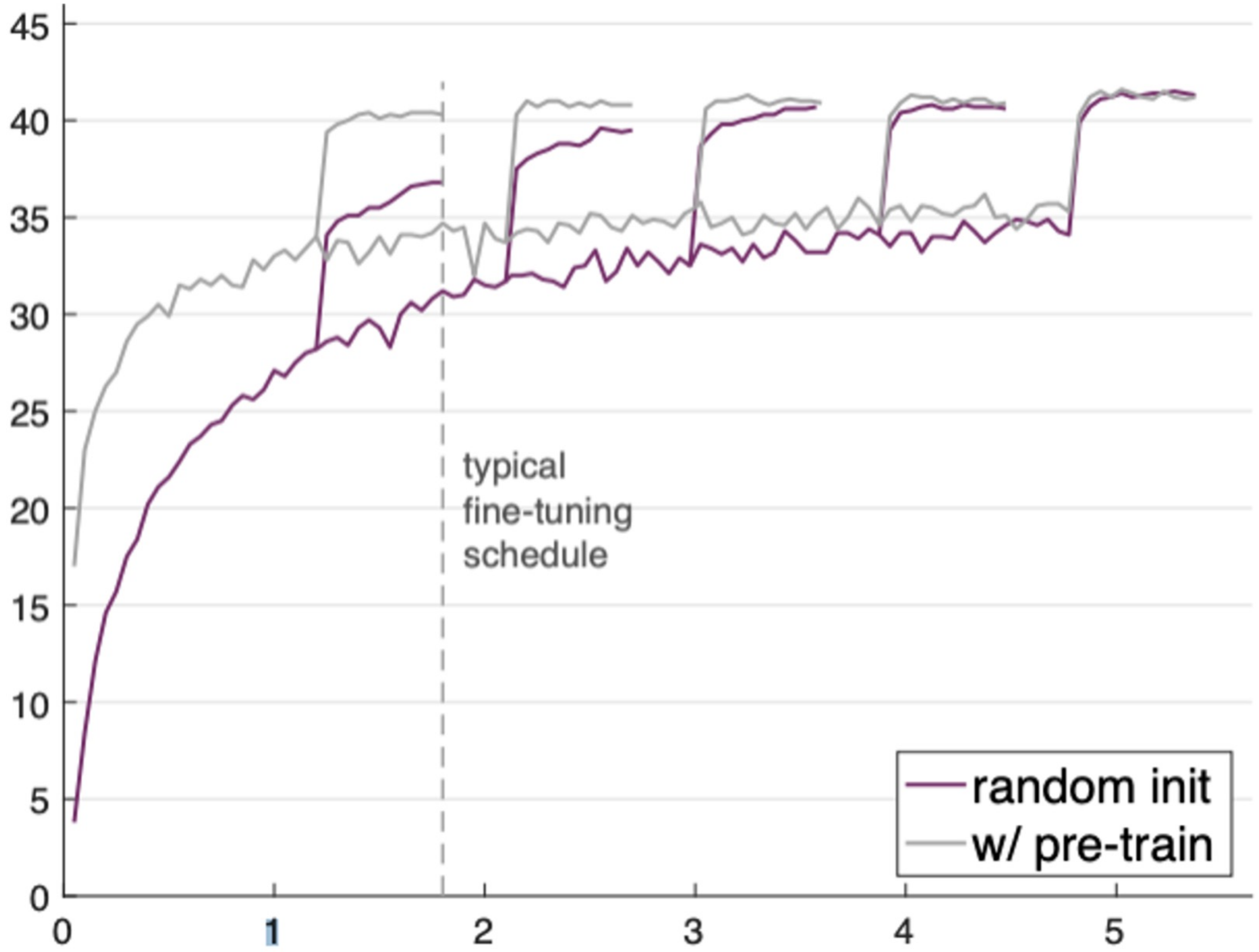
1. Train CNN on ImageNet
2. Fine-Tune (1) for object detection on Visual Genome
3. Train BERT language model on lots of text
4. Combine (2) and (3), train for joint image / language modeling
5. Fine-tune (5) for image captioning, visual question answering, etc.

Zhou et al, "Unified Vision-Language Pre-Training for Image Captioning and VQA", arXiv 2019

Transfer Learning is pervasive!

Some very recent results have questioned it

COCO object detection



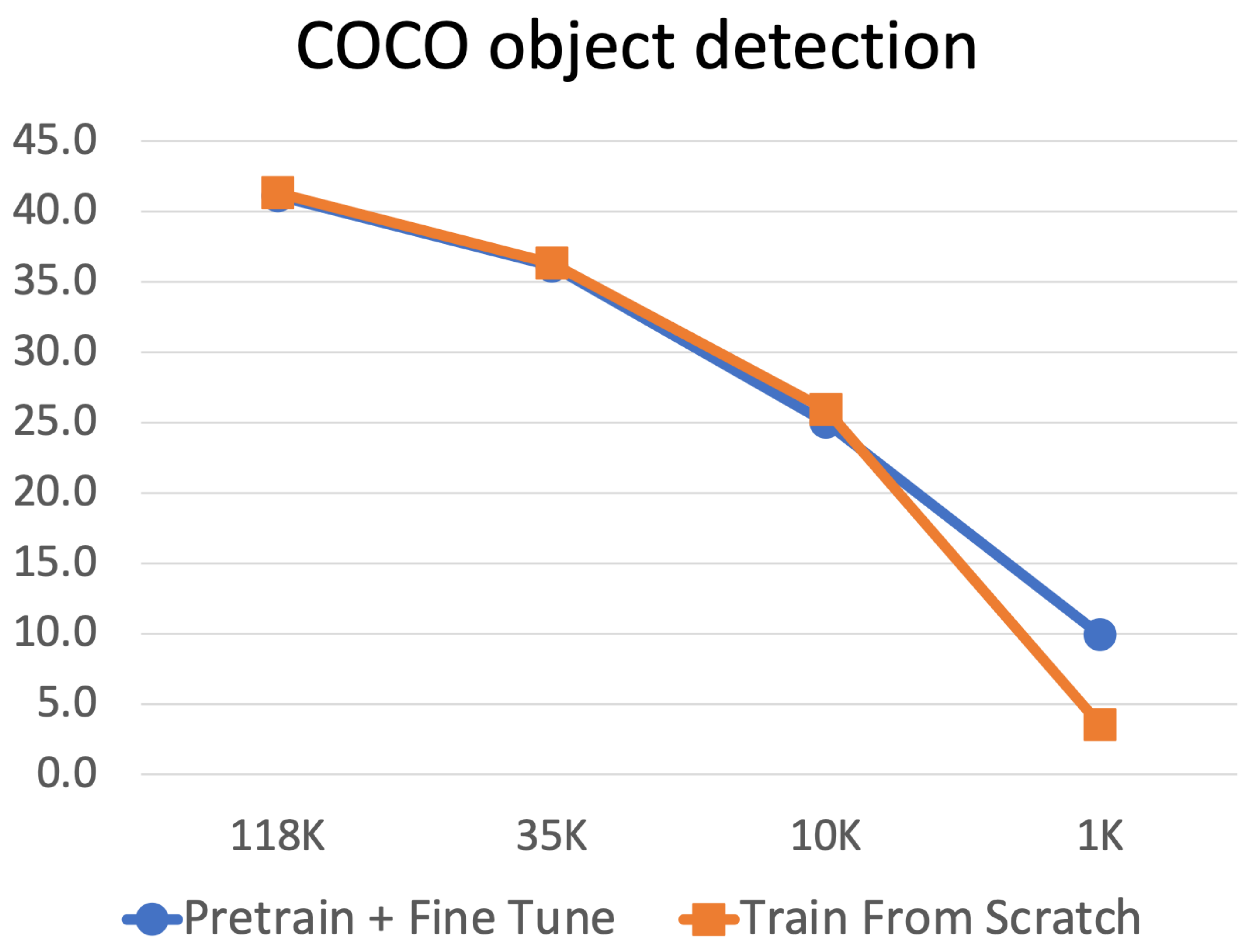
Training from scratch can work as well as pertaining on ImageNet!

… if you train for 3x as long

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

Transfer Learning is pervasive!

Some very recent results have questioned it



Pretraining + Finetuning beats training from scratch when dataset size is very small

Collecting more data is more effective than pretraining

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

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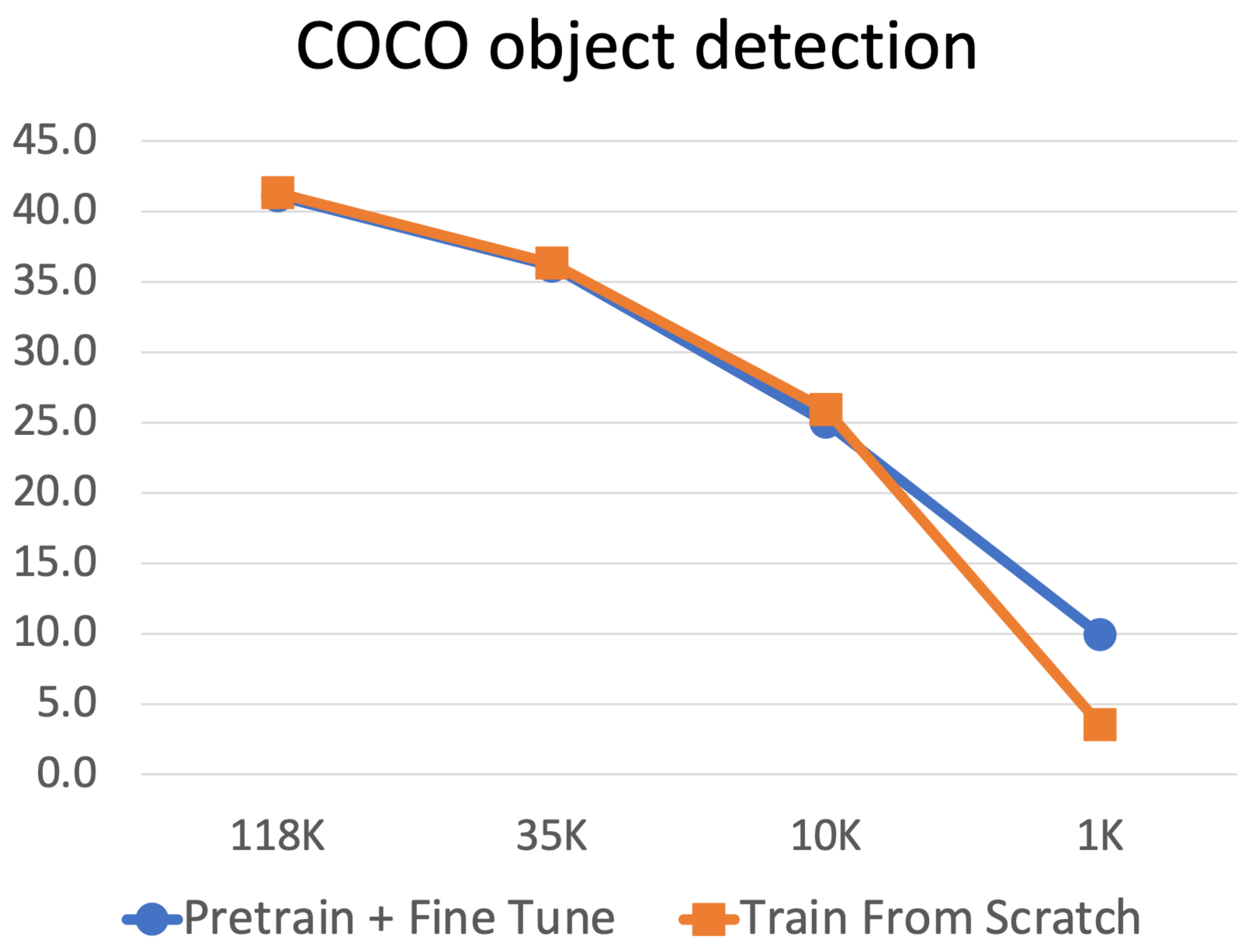
Some very recent results have questioned it



My current view on transfer learning:

- ☐ Pretrain + finetune makes your training faster, so practically very useful
- ☐ Training from scratch works well once you have enough data
- ☐ Lots of work left to be done

He et al, "Rethinking ImageNet Pre-Training", ICCV 2019

Summary

1. **One time setup:**
   - Activation functions, data preprocessing, weight initialization, regularization
2. **Training dynamics:**
   - Learning rate schedules; hyperparameter optimization
3. **After training:**
   - Model ensembles, transfer learning

A zoo of frameworks!

Caffe

(UC Berkeley) → Caffe2

(Facebook)

Torch

(NYU / Facebook) → PyTorch

(Facebook)

Theano

(U Montreal) → TensorFlow

(Google)

Darknet

(Redmon)

Chainer

MXNet

(Amazon)

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

CNTK

(Microsoft)

JAX

(Google)

PaddlePaddle

(Baidu)

A zoo of frameworks!

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We'll focus on these

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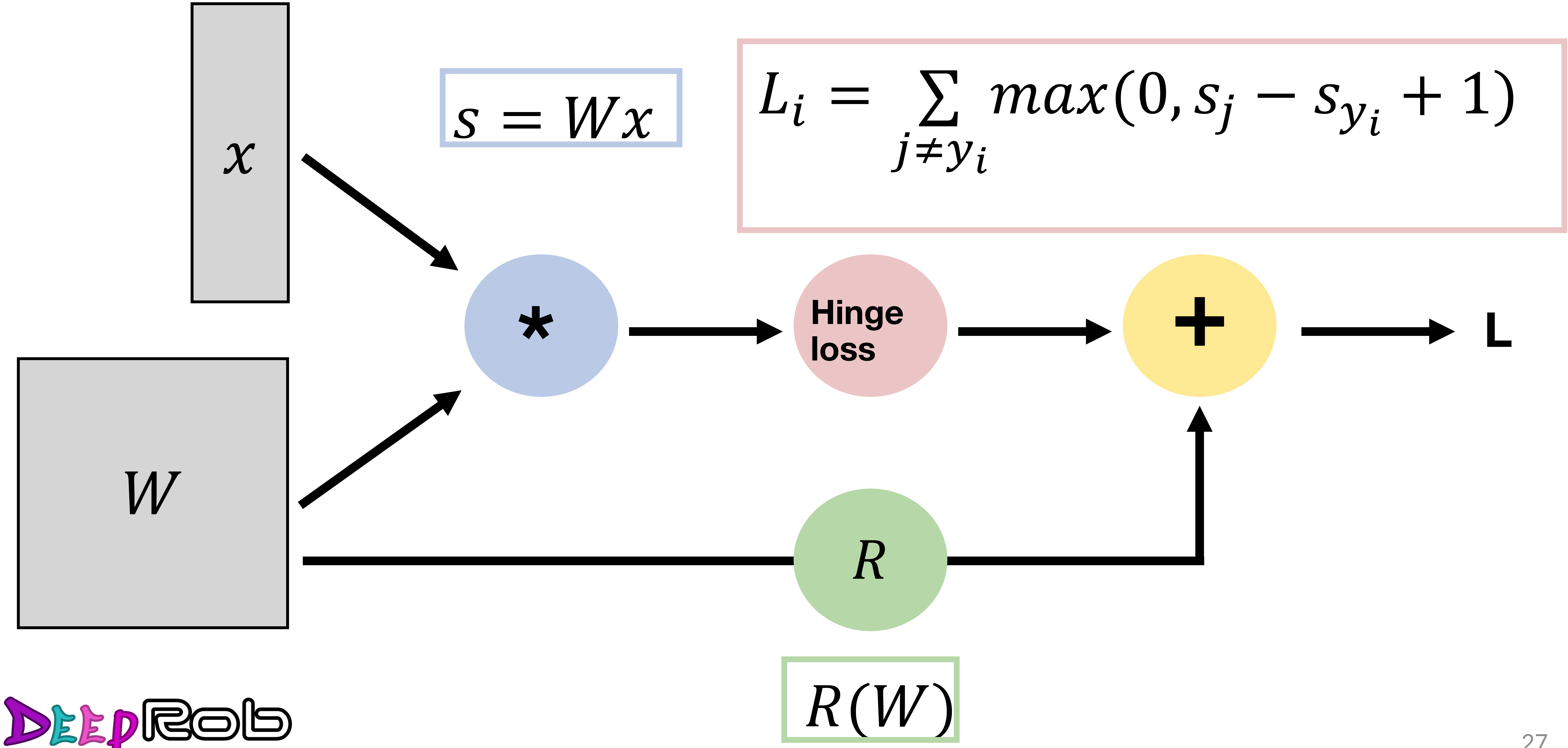
Recall: Computational Graphs



The motivation for 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 hardware

PyTorch: Versions

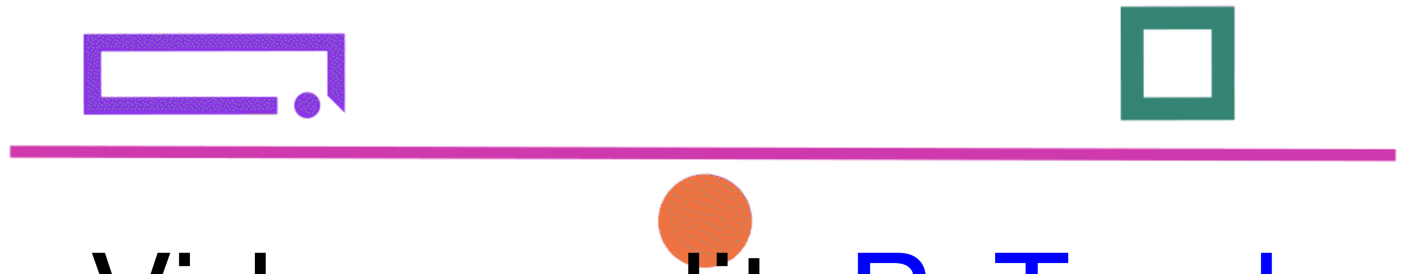
For this class we are using **PyTorch version 1.13** (Released October 2022)

Be careful if you are looking at older PyTorch code—the API changed a lot before 1.0

PyTorch: Version 2.2 (2024)

further optimize models (`torch.compile`, `scaled_dot_product_attention`)

Intended (not committing) to be backwards compatible



Video credit: PyTorch

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: 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
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```

PyTorch: Tensors

Forward pass: compute predictions and loss

```
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```

PyTorch: Tensors

Backward pass: manually compute gradients

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```

PyTorch: Tensors

Gradient descent step on weights

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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: Tensors

To run on GPU, just use a different device!

```
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: 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

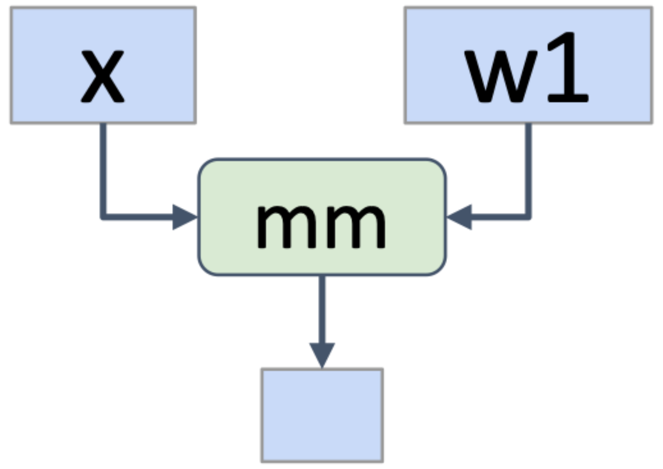
```
import torch

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

Compute gradients with respect to all inputs that 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_()
```

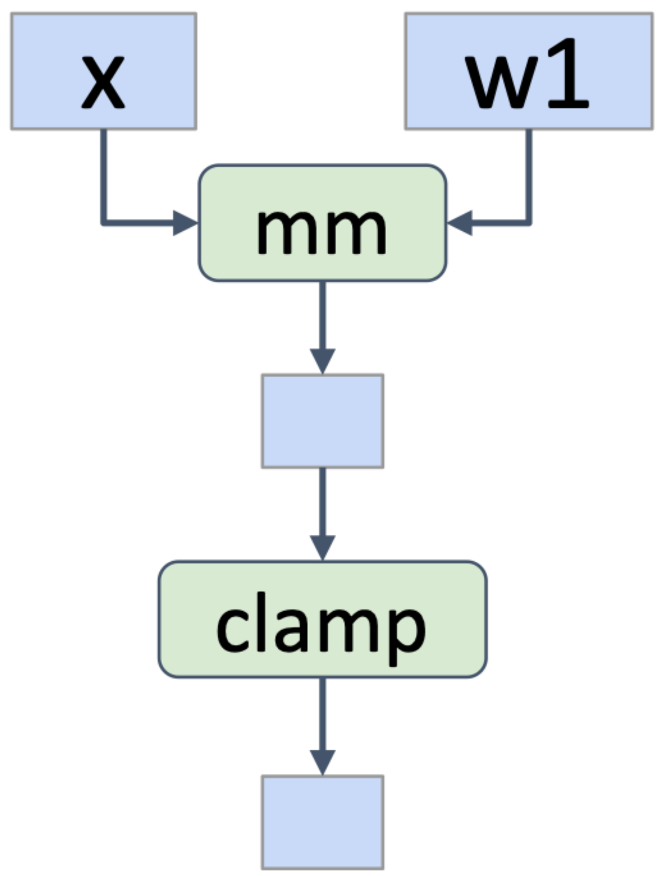
PyTorch: Autograd



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_()
```

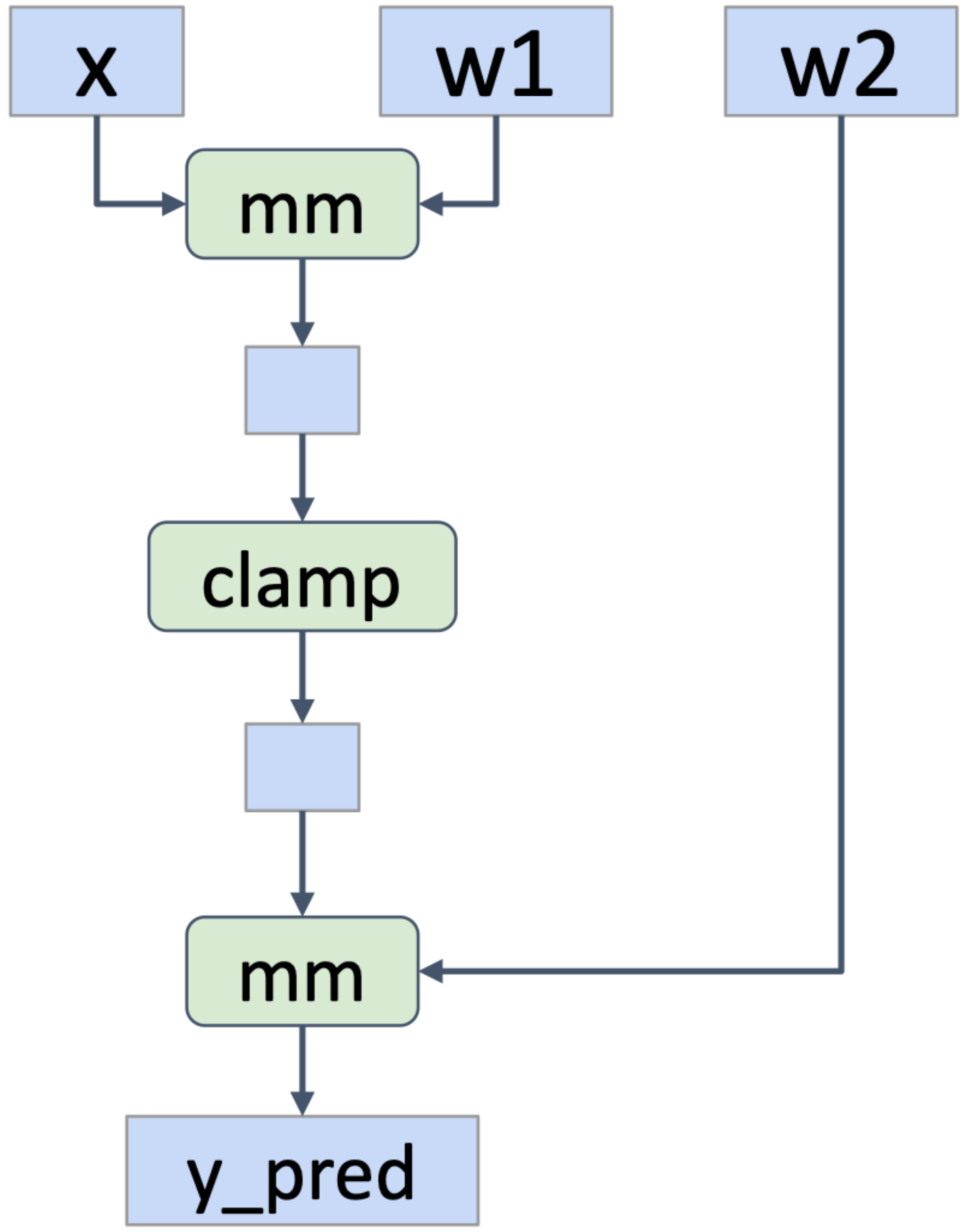
PyTorch: Autograd



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

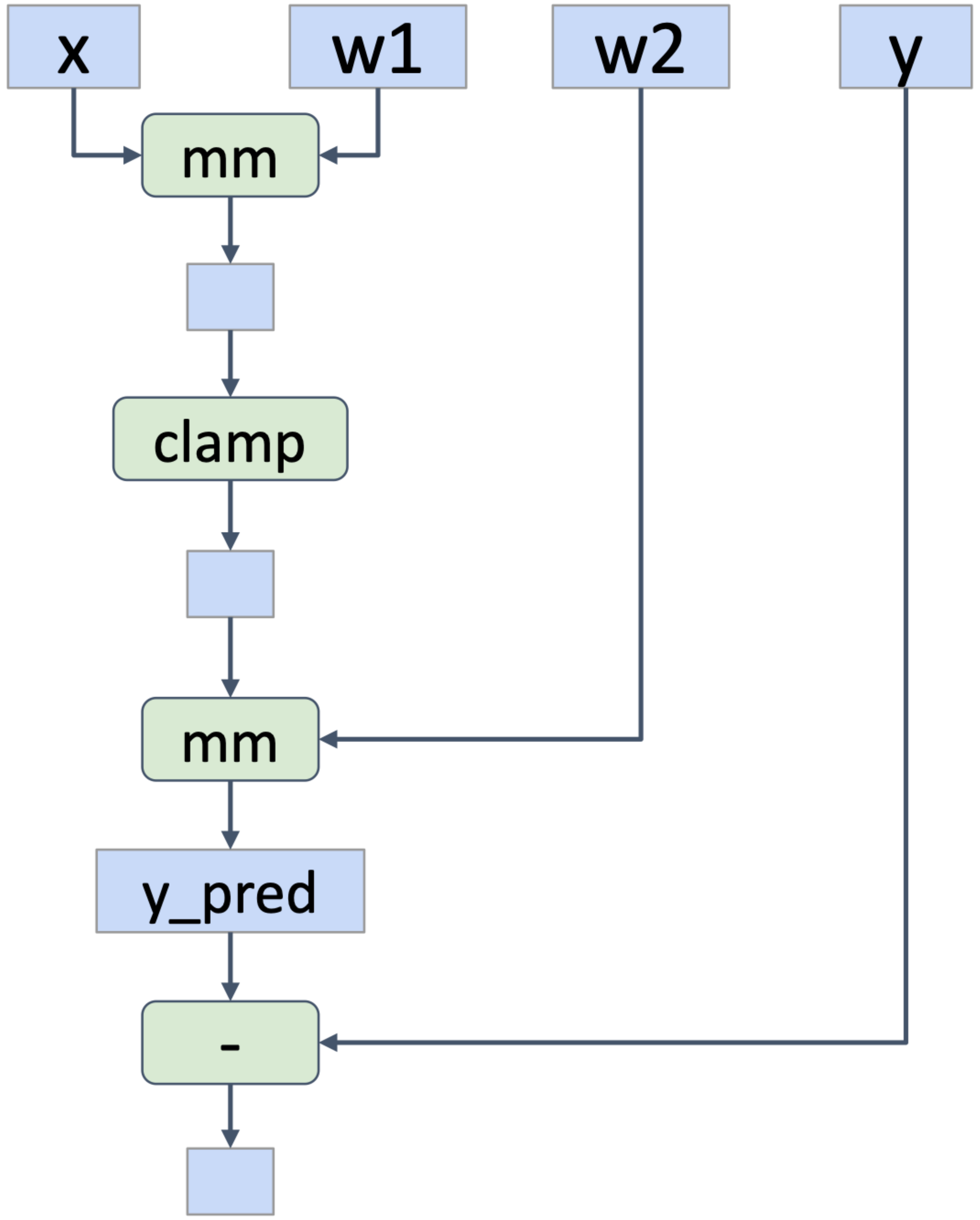
```python
import torch

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



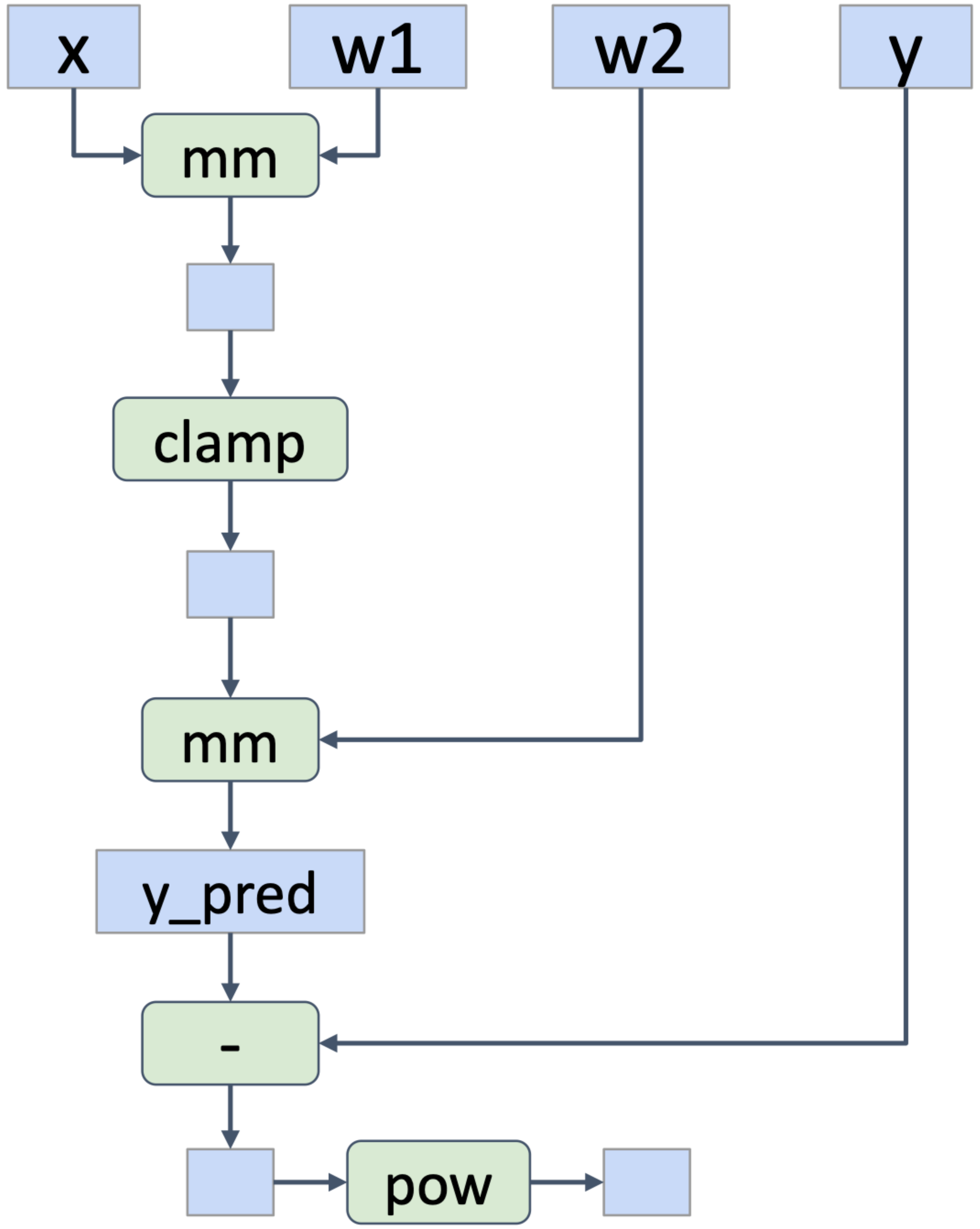

```
import torch

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



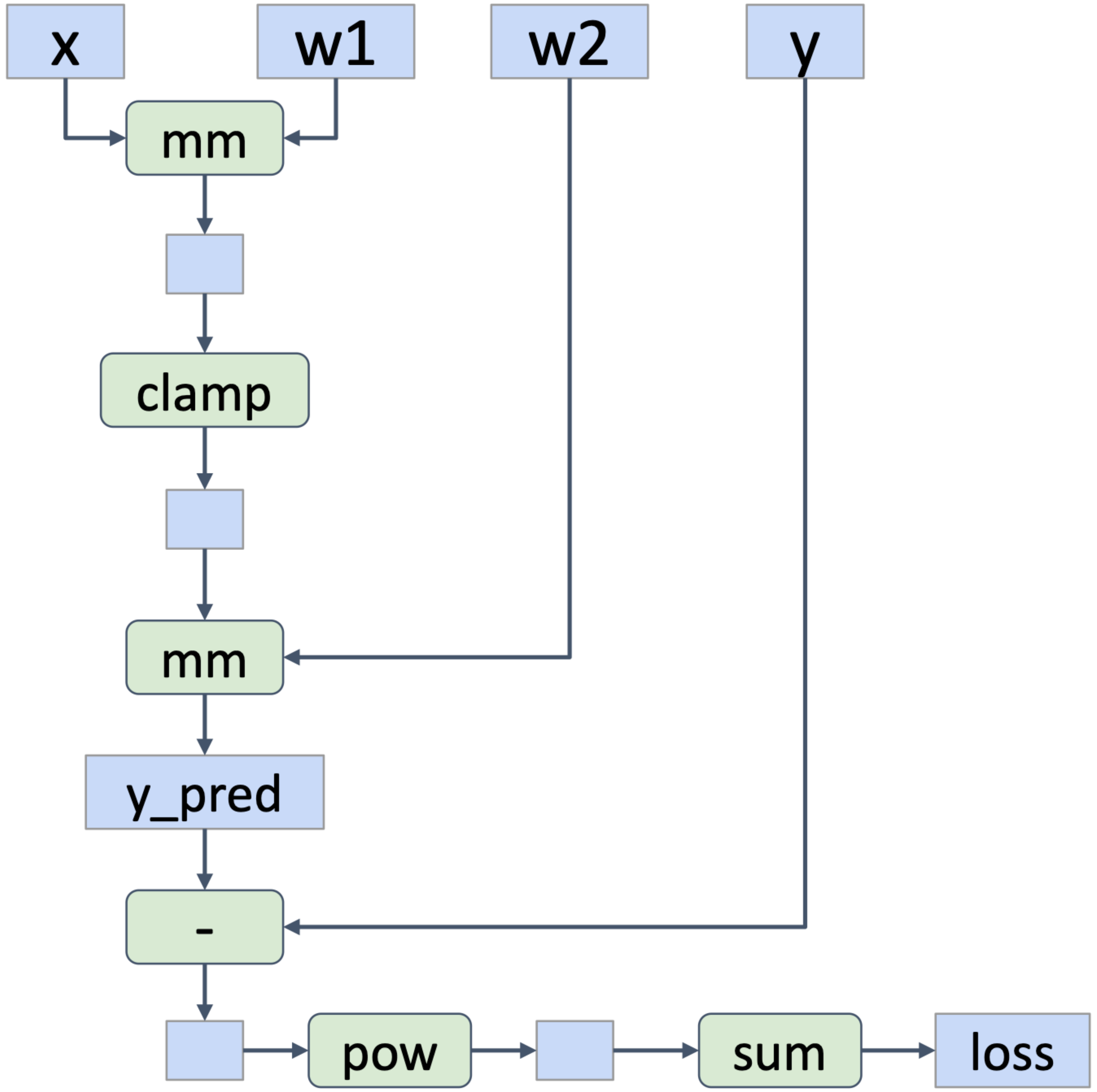

```python
import torch

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



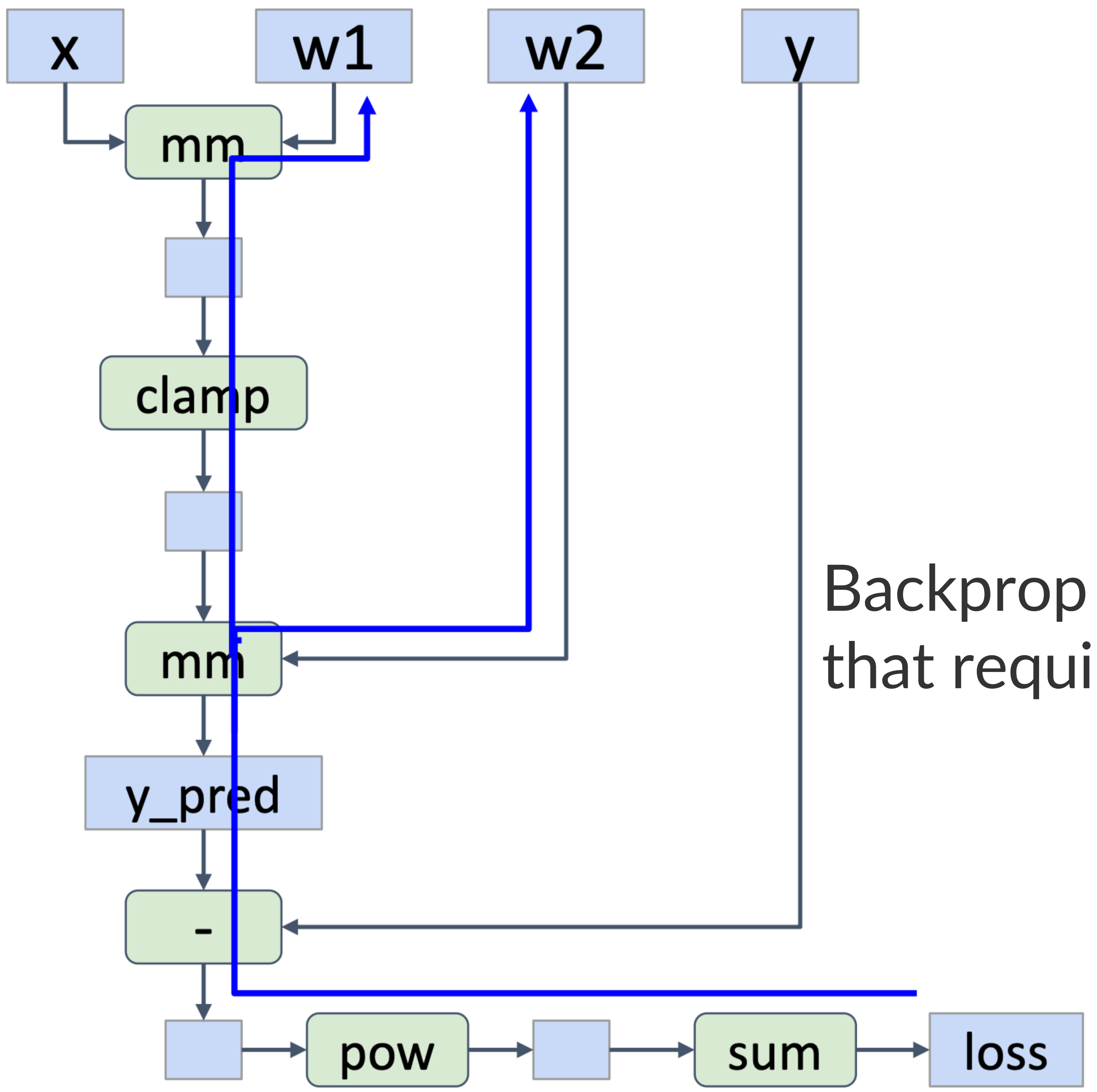

```python
import torch

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

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

Make gradient step on 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

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

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

```
import torch

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

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

    loss.backward()

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

PyTorch: New Functions

Can define new operations using Python functions

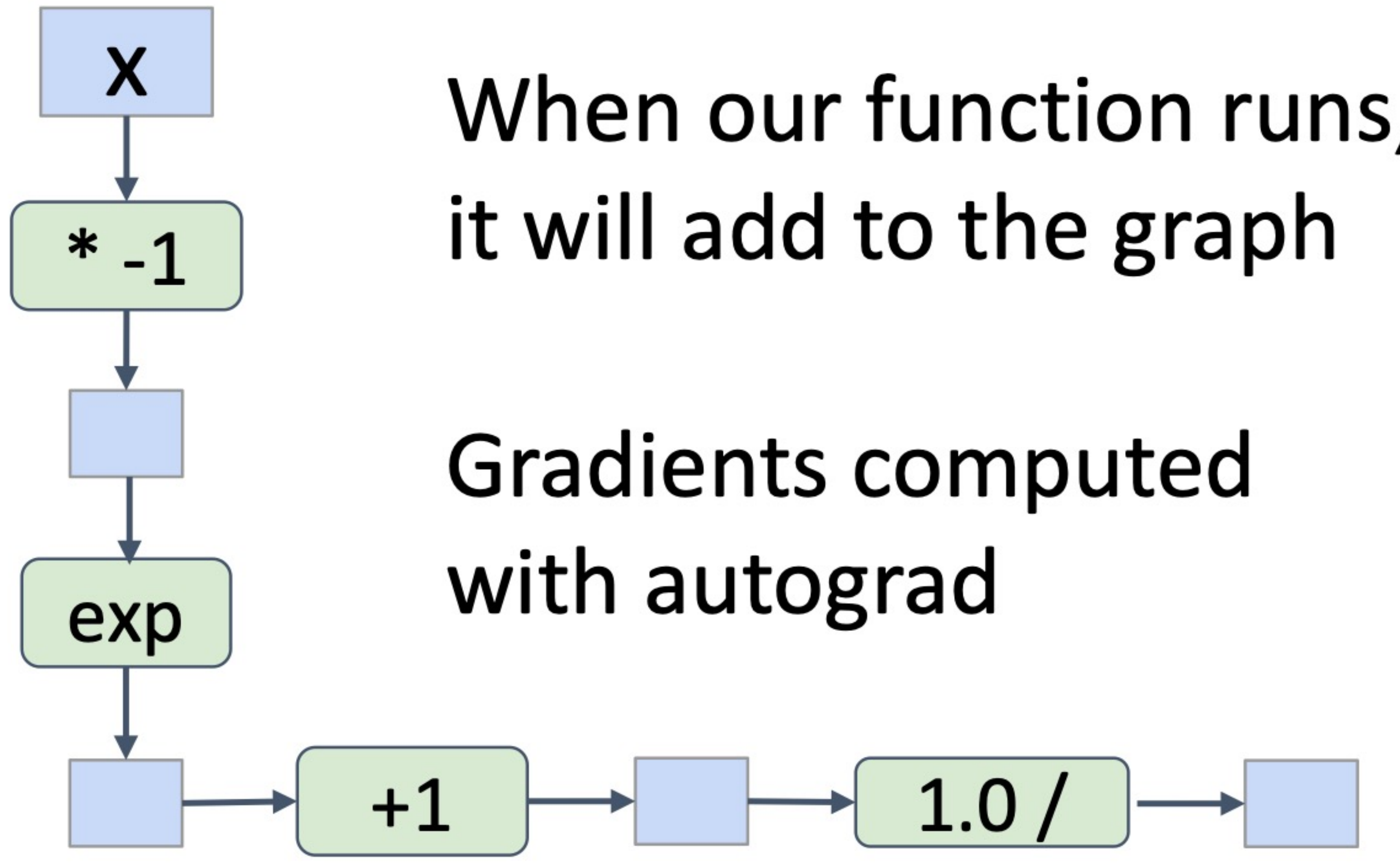
```python
def sigmoid(x):
  return 1.0 / (1.0 + (-x).exp())
```

```python
import torch

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

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

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

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

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

PyTorch: New Functions

Can define new operations using Python functions

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



When our function runs, it will add to the graph

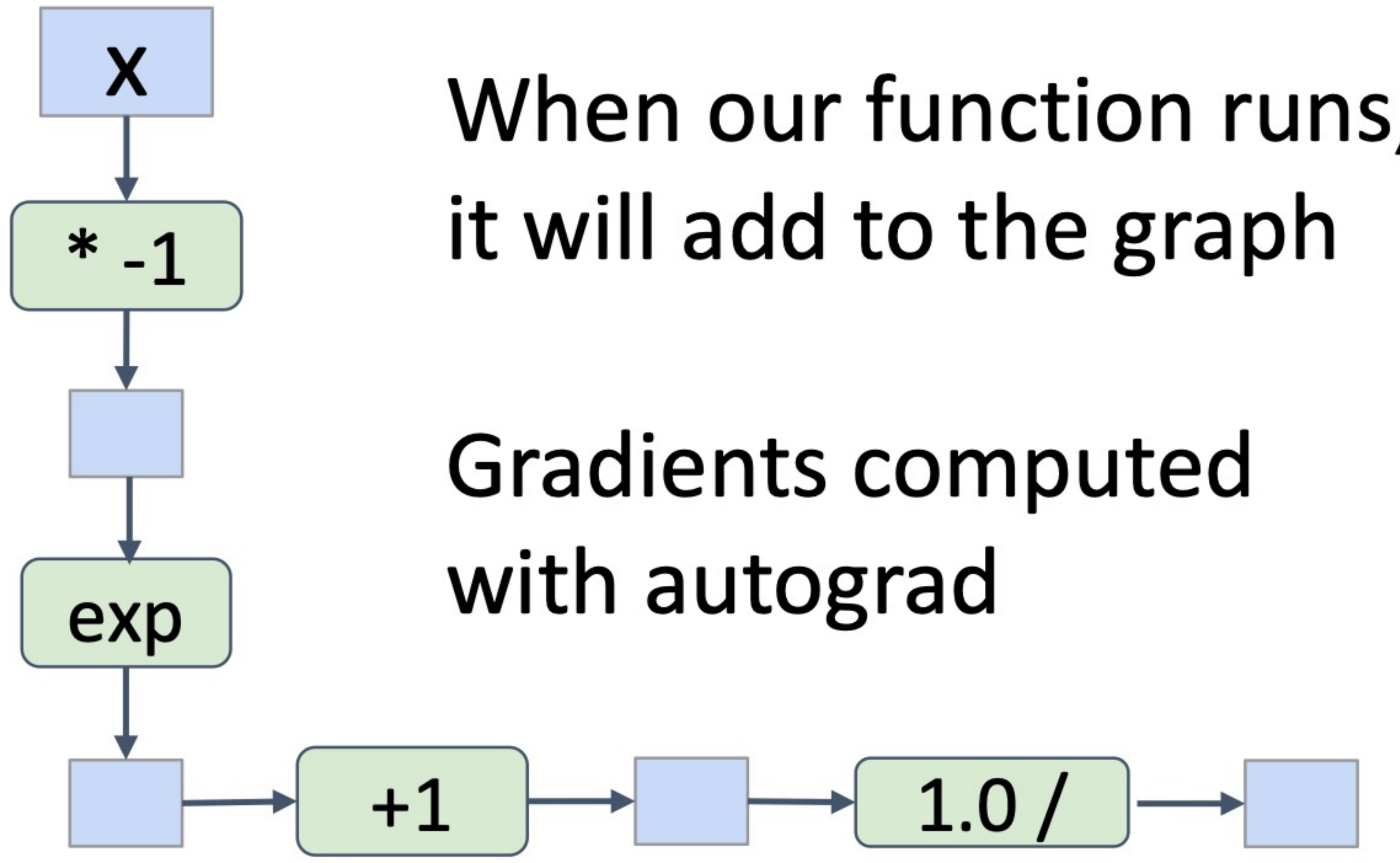
Gradients computed with autograd

```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

```
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

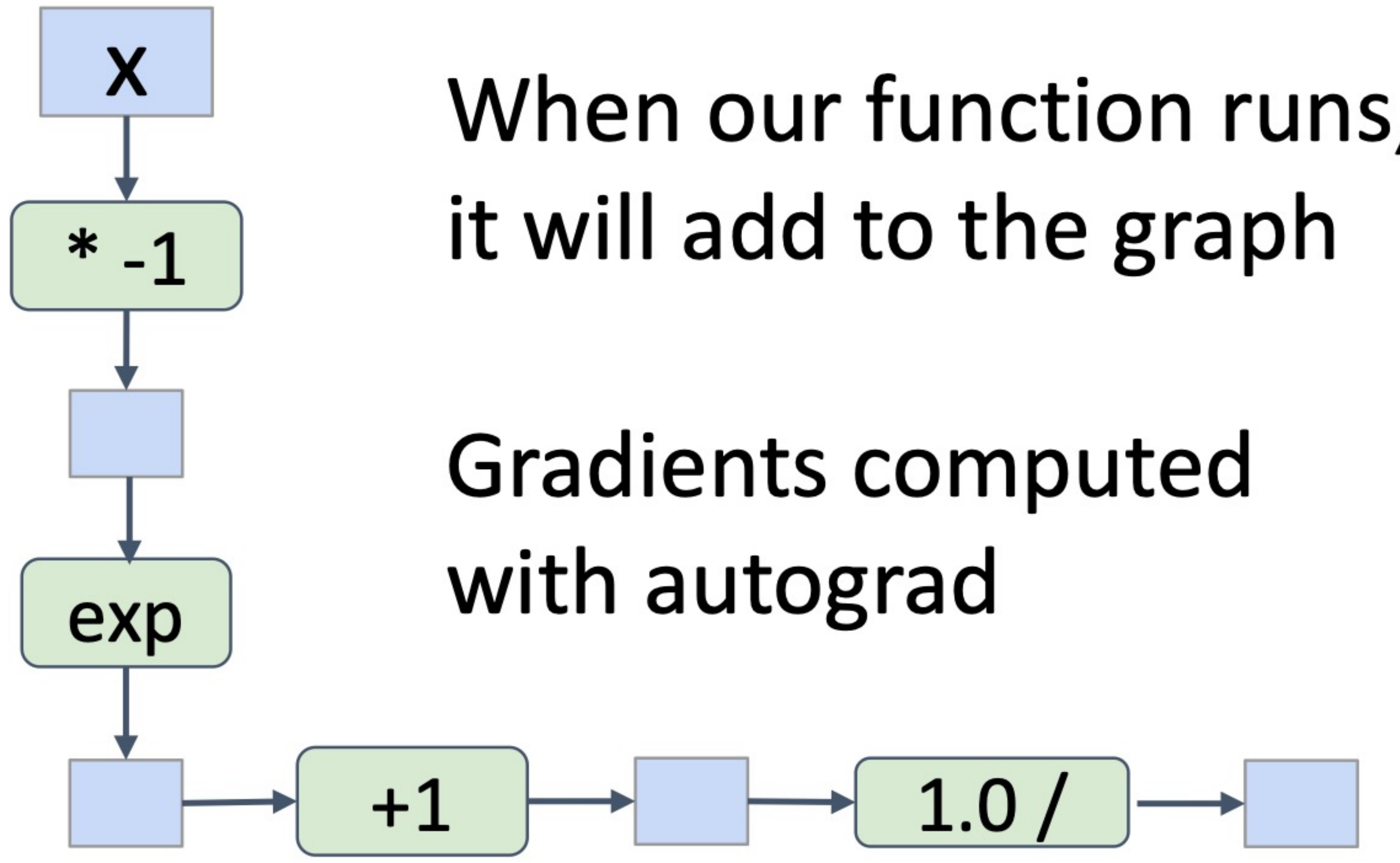
```
class Sigmoid(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x):
    y = 1.0 / (1.0 + (-x).exp())
    ctx.save_for_backward(y)
    return y

  @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)
```

Recall: $$\frac{\partial}{\partial x}\Big[\sigma(x)\Big] = (1-\sigma(x))\sigma(x)$$

PyTorch: New Functions

Can define new operations using Python functions

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



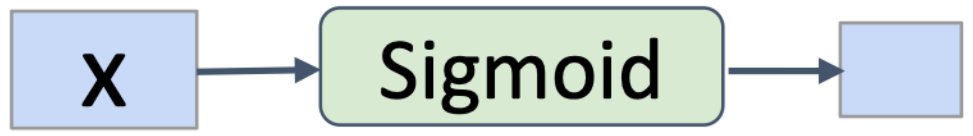
When our function runs, it will add to the graph

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)
```

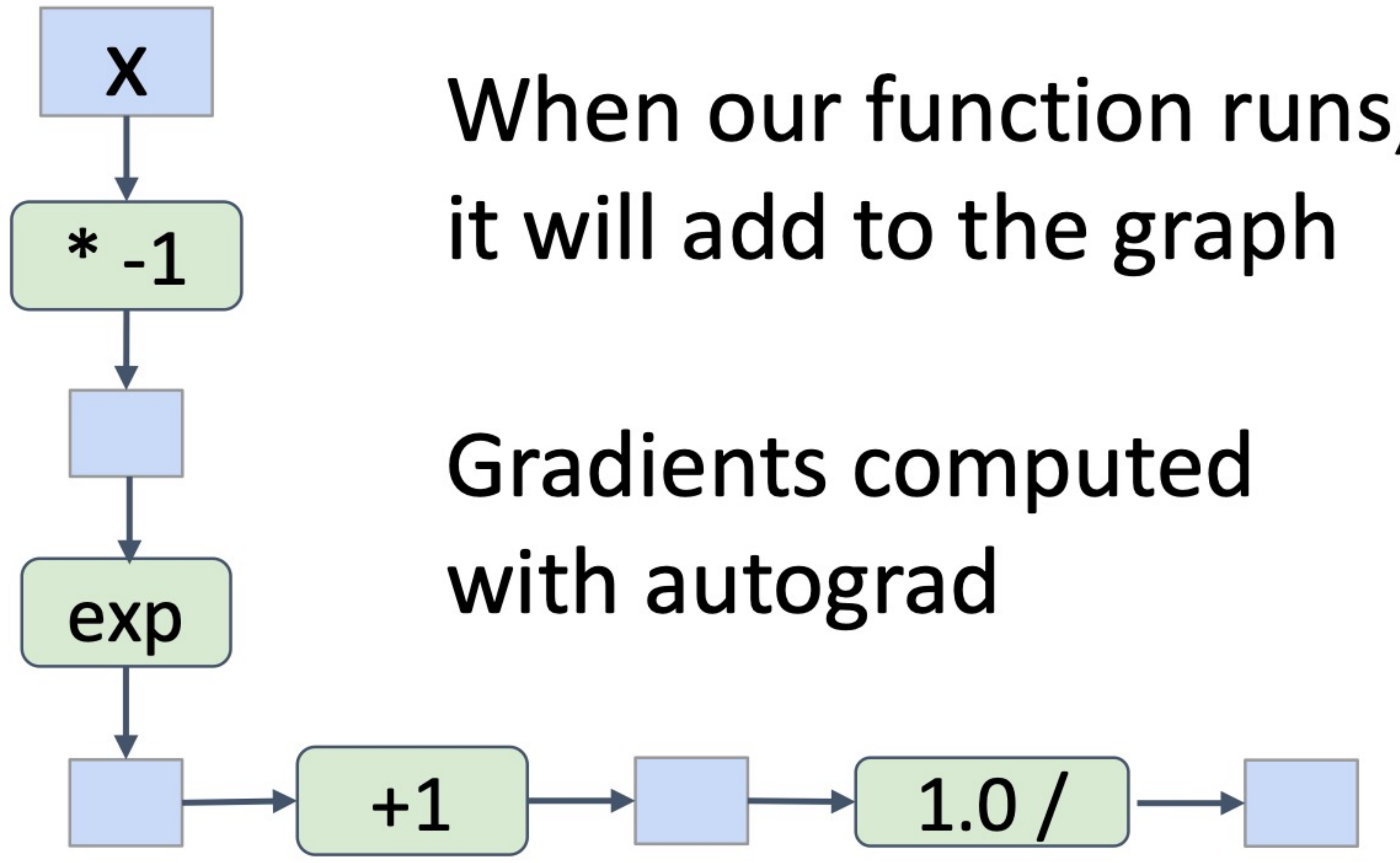
Now when our function runs, it adds one node to the graph!



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

```python
import torch

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

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

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

    loss.backward()

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

PyTorch: nn

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

```
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

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

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

```
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: 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

After computing gradients, use optimizer to update and zero gradients

```
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: 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

```
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

```
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()
```

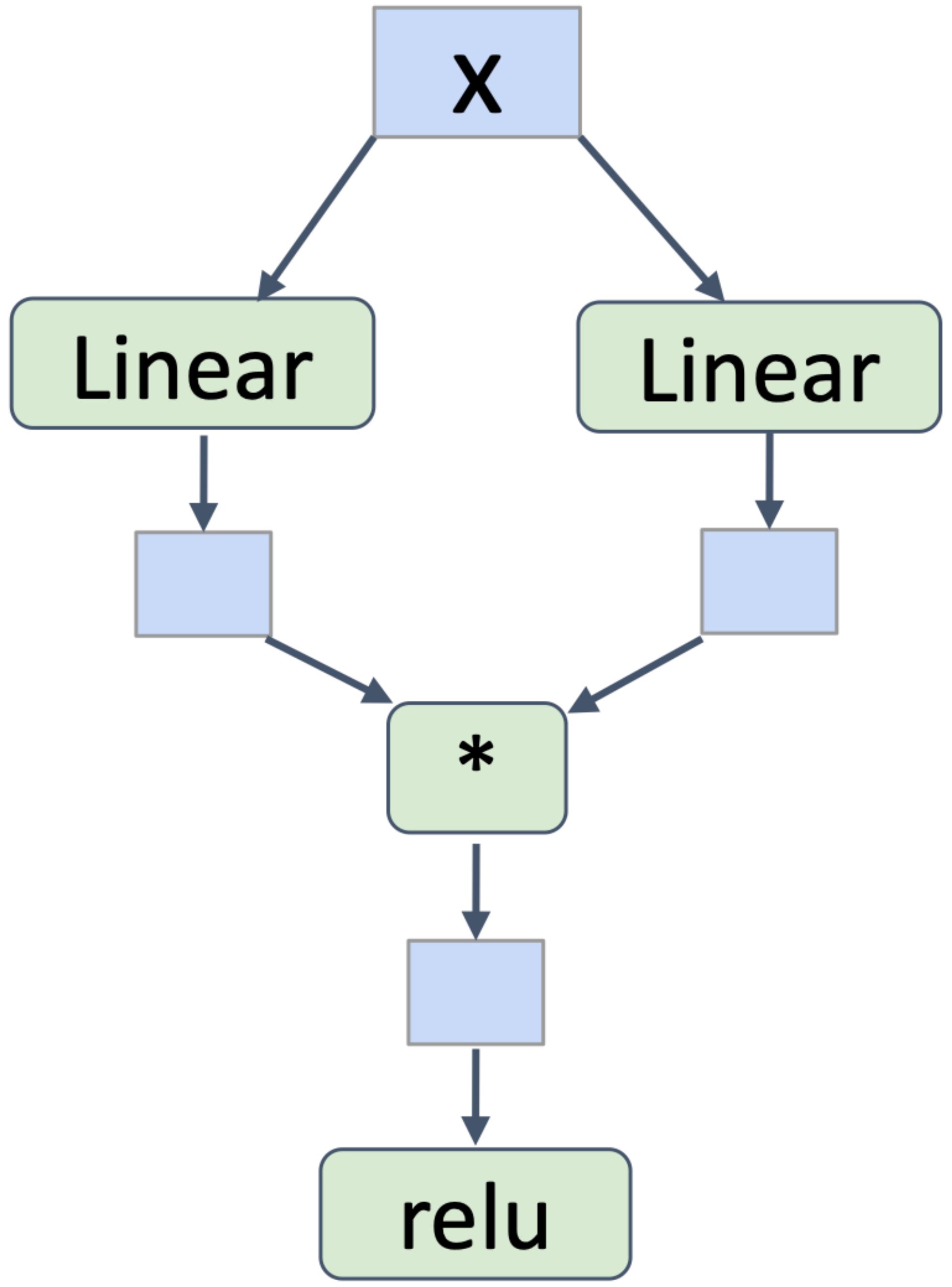
PyTorch: nn
Defining Modules

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

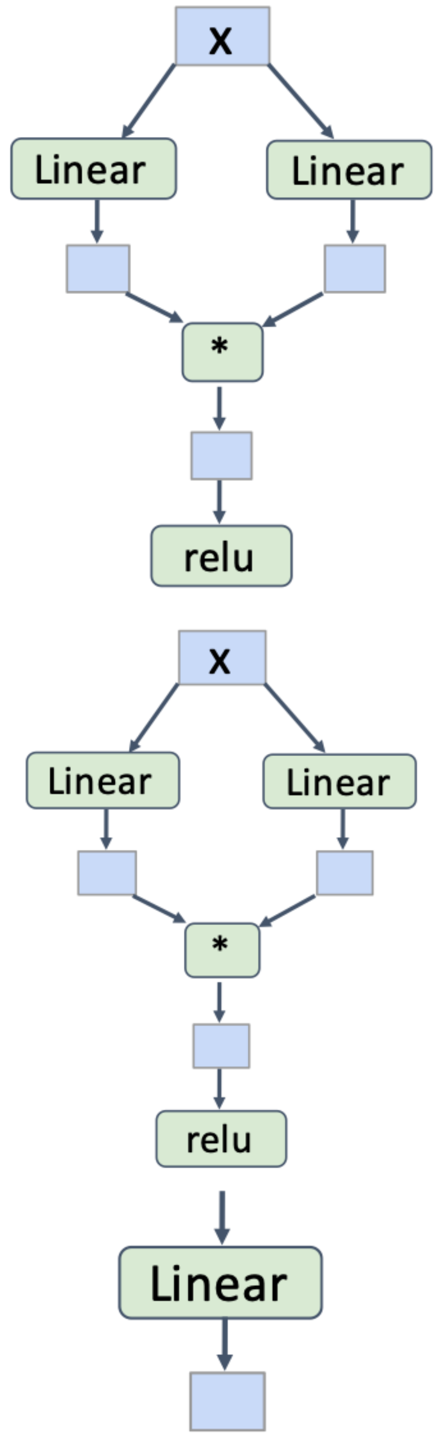



```python
import torch

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: Pretrained Models

Super easy to use pertained models with torch vision

https://pytorch.org/vision/stable/

```
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()
```

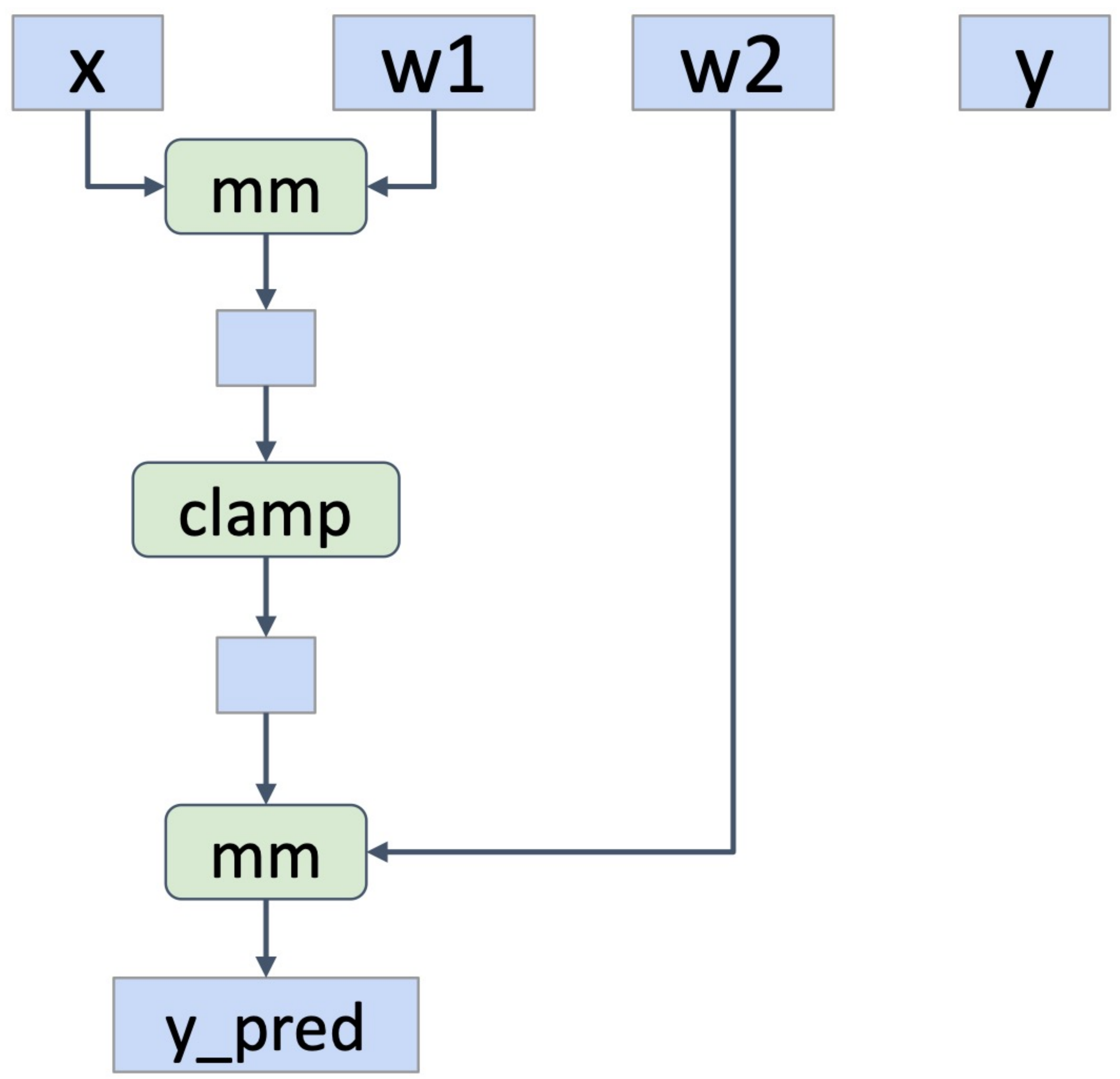
PyTorch: Dynamic Computation Graphs

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

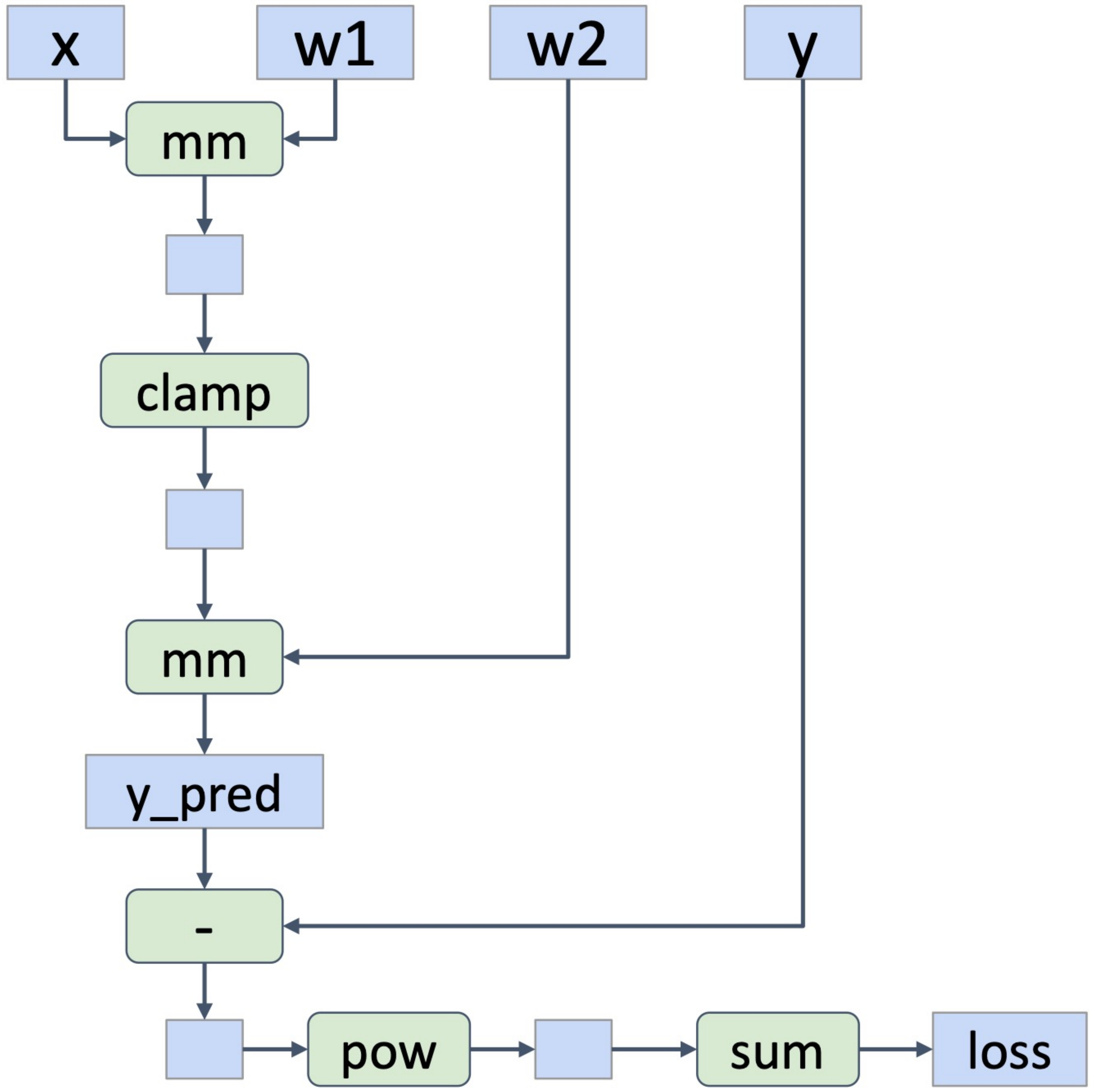
PyTorch: Dynamic Computation Graphs




```
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

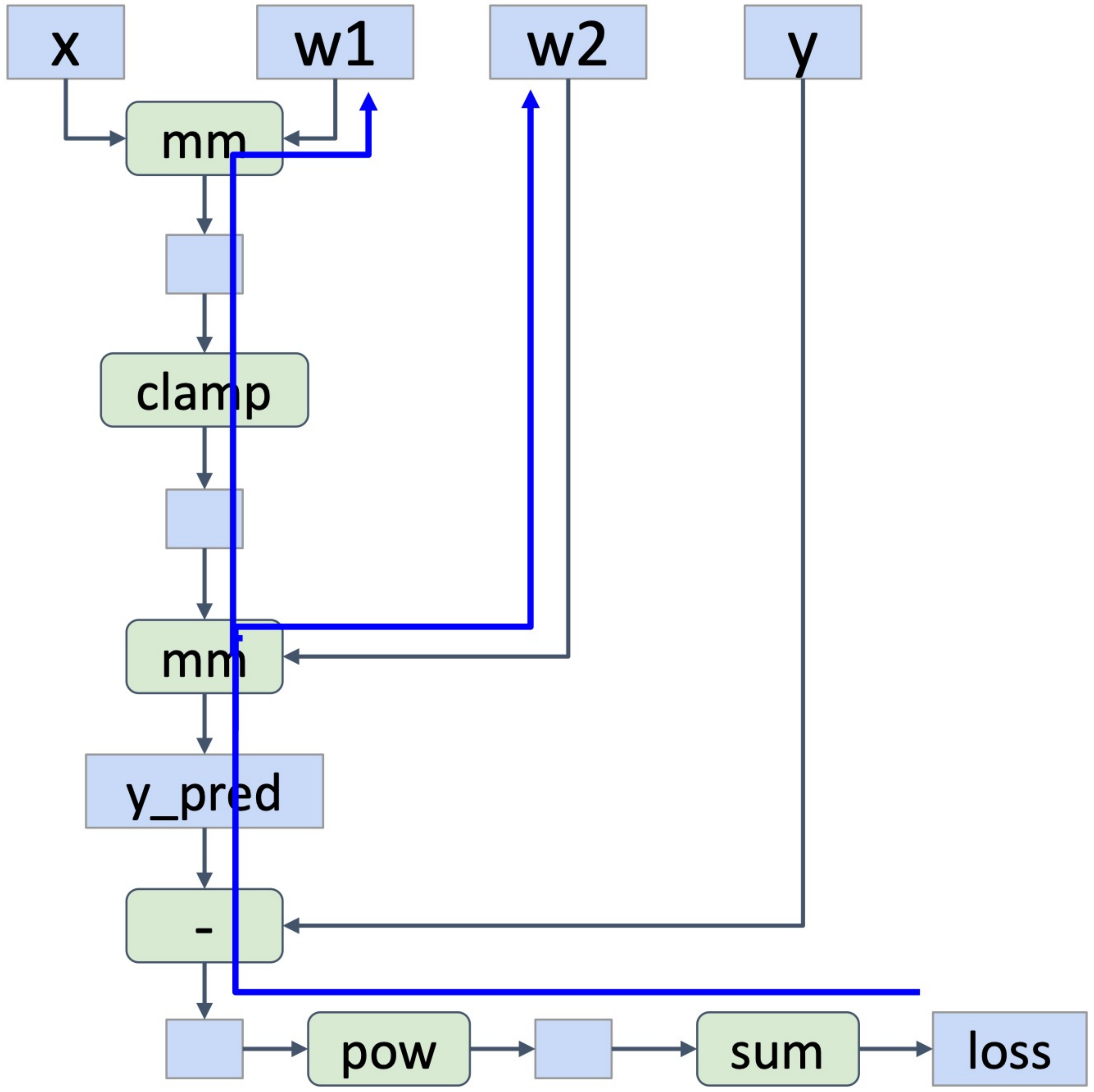
PyTorch: Dynamic Computation Graphs




```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()
```

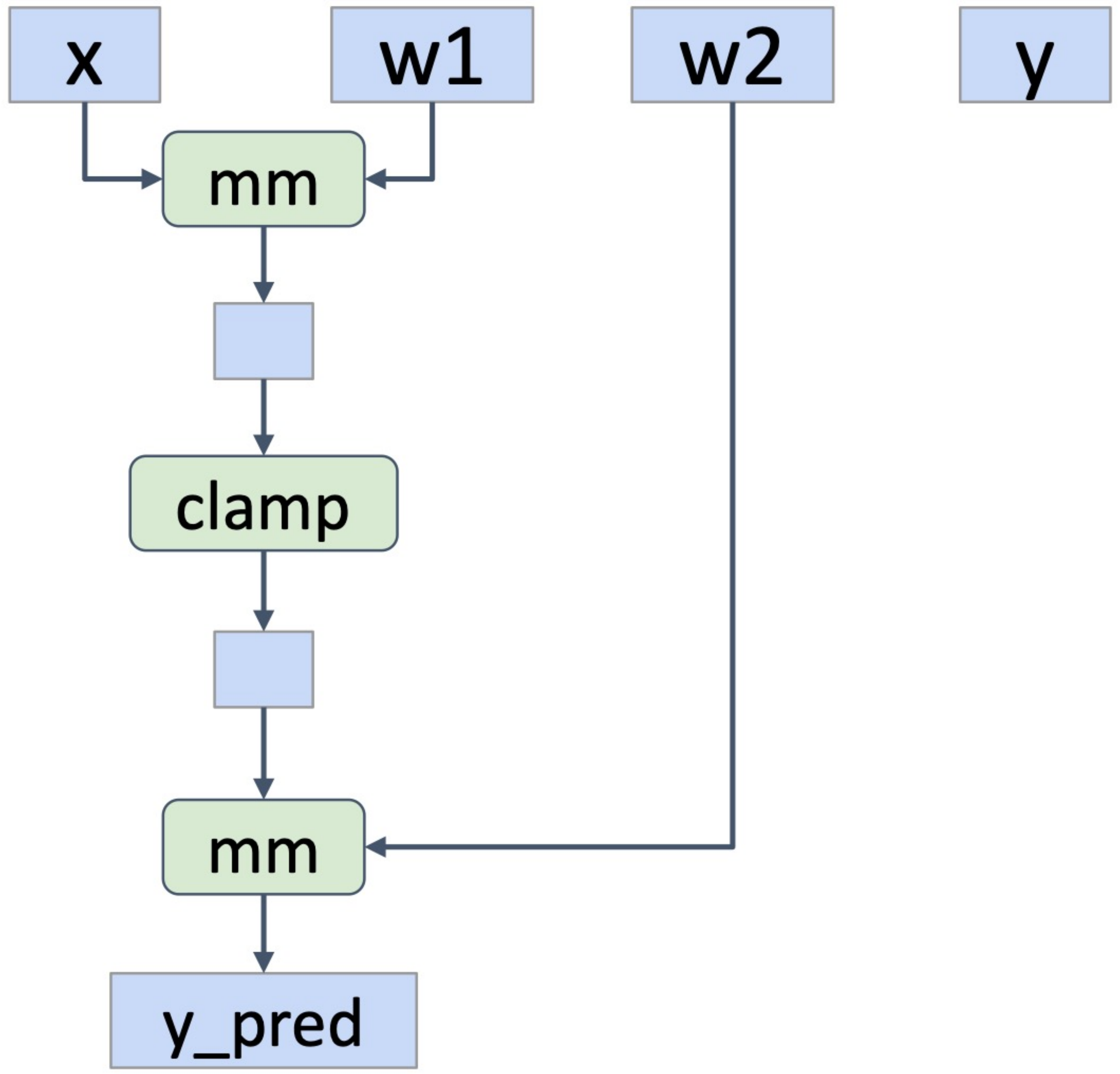
Perform backprop, throw away graph

PyTorch: Dynamic Computation Graphs


```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

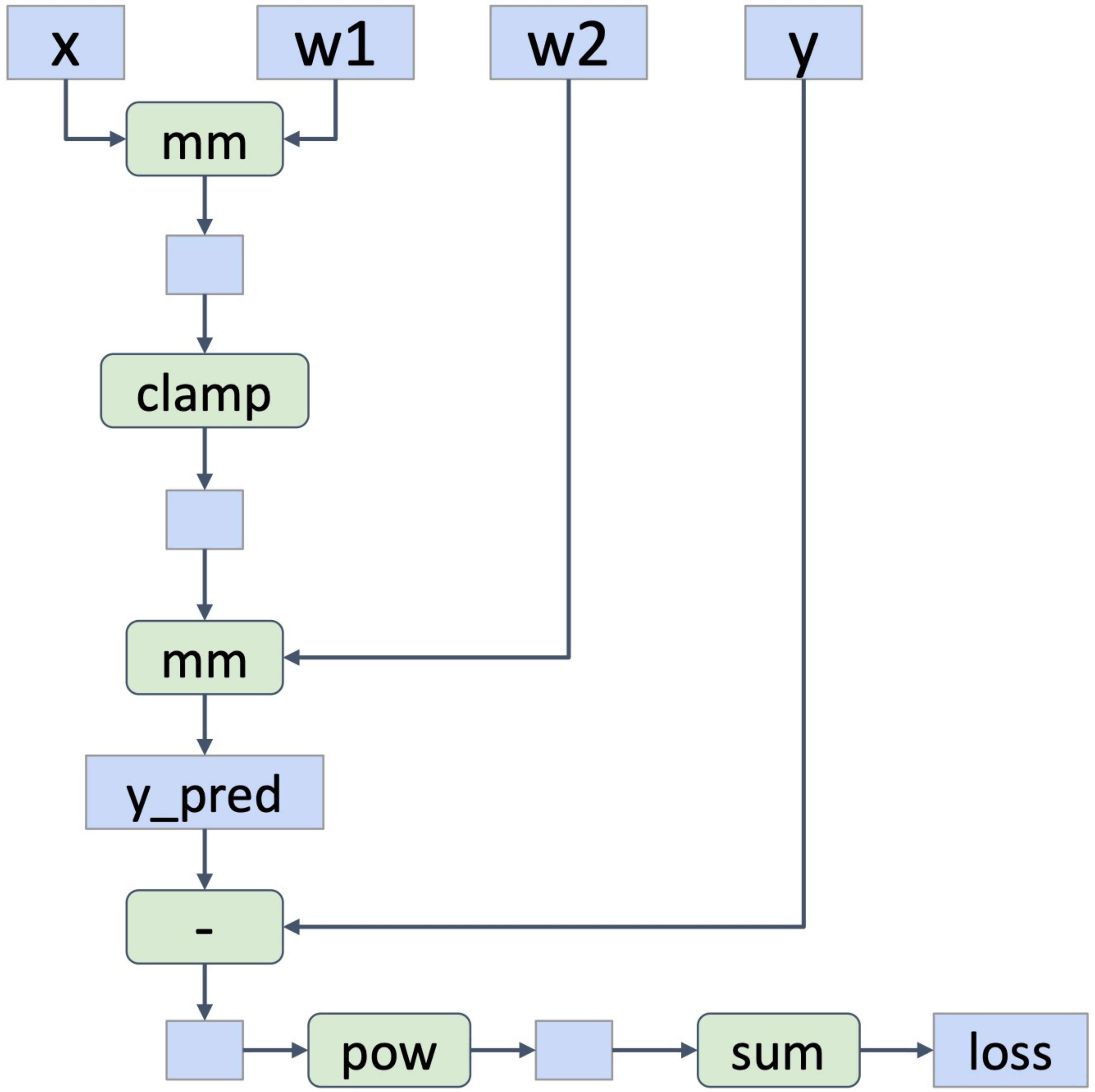
PyTorch: Dynamic Computation Graphs




```
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

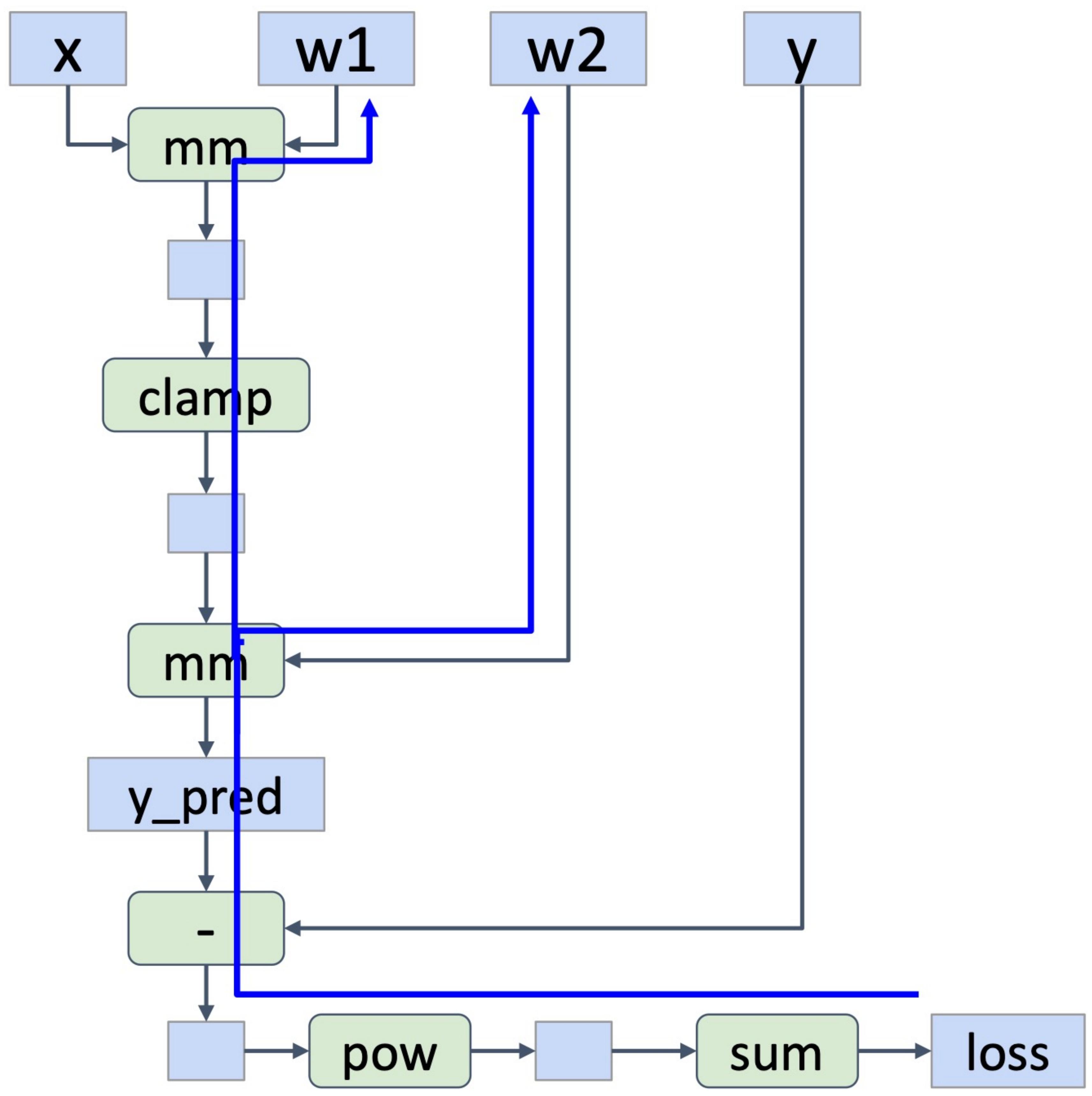
PyTorch: Dynamic Computation Graphs




```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)

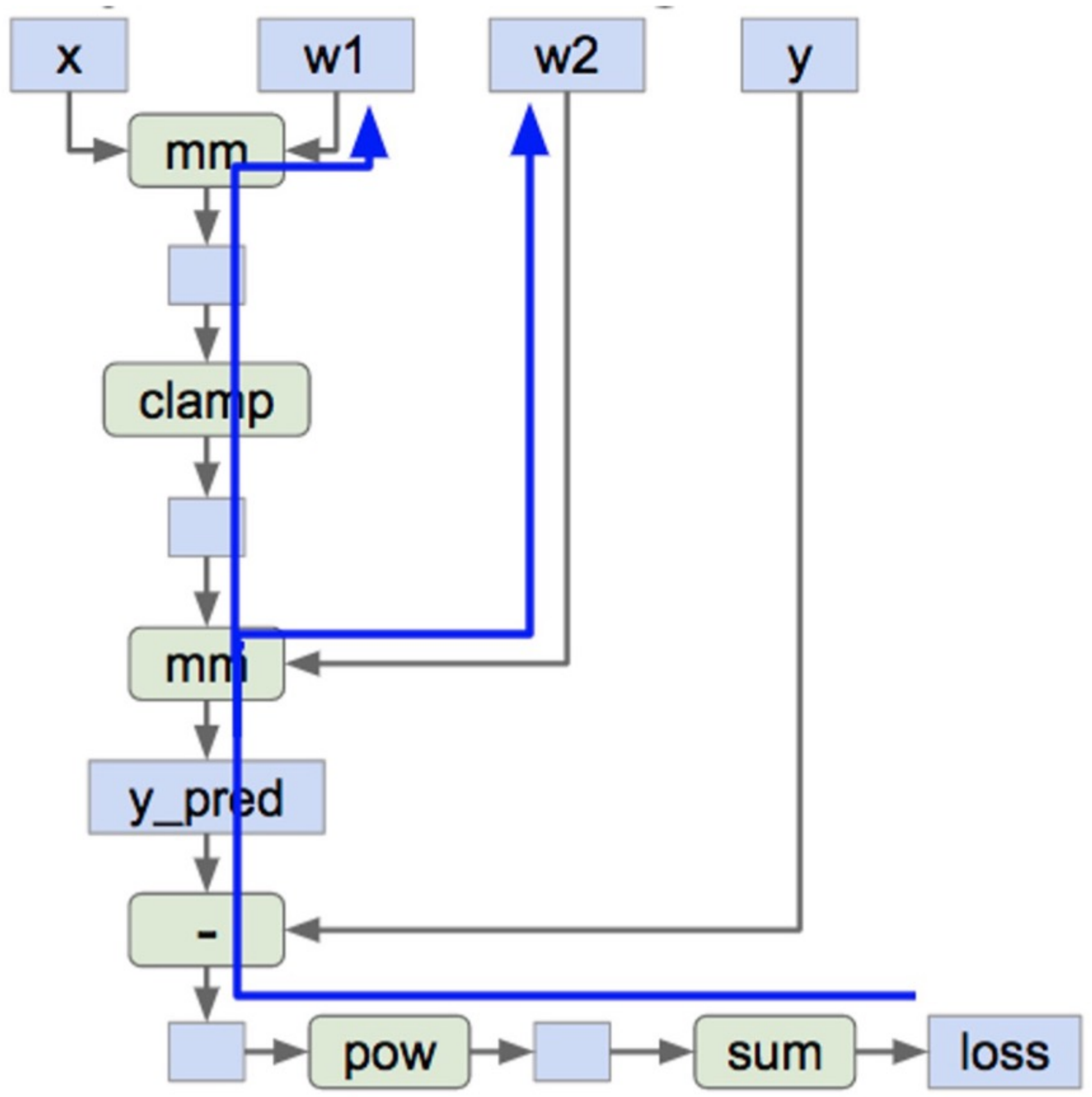
```
import torch

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)
```

Alternative: 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()
```

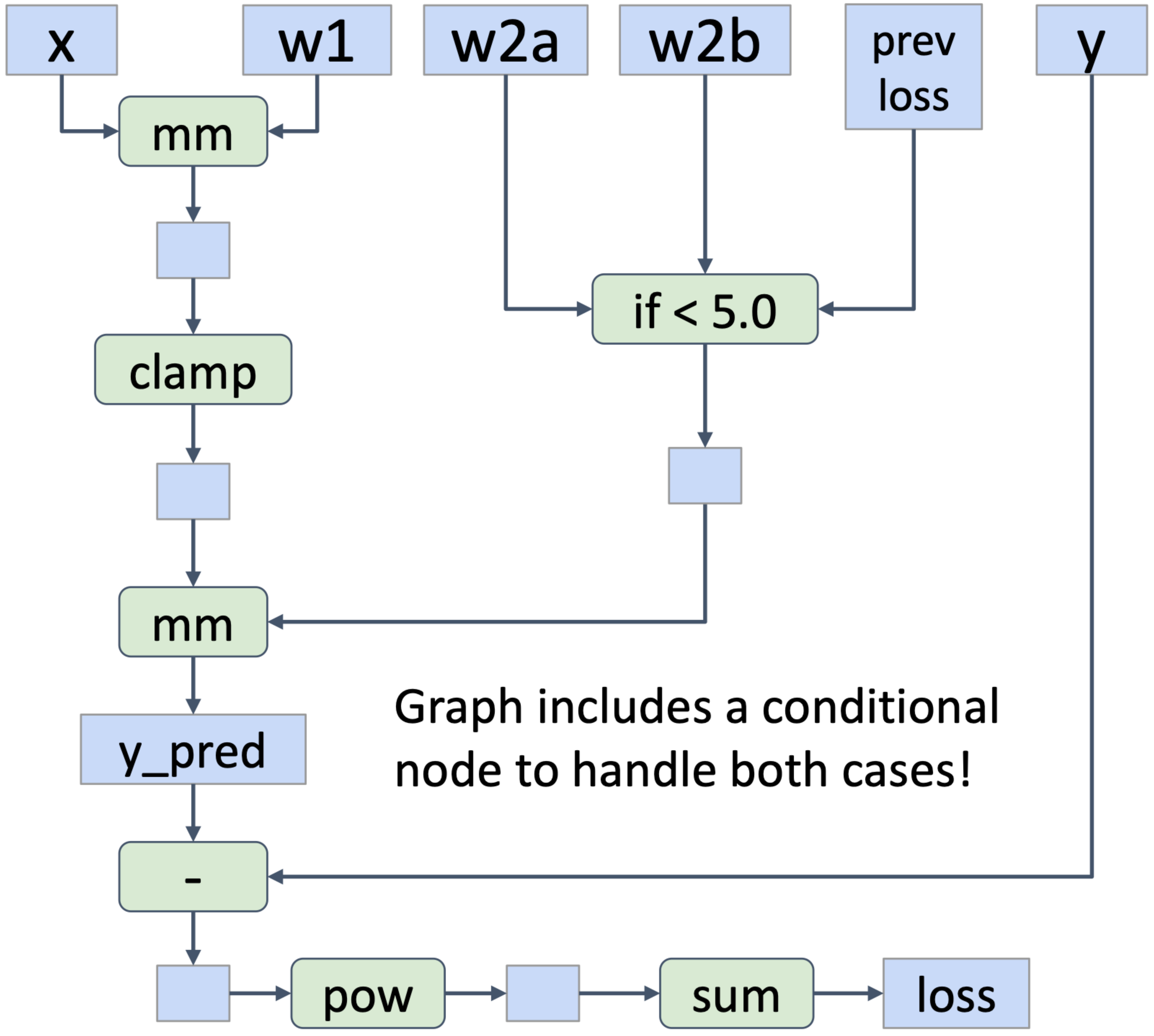
Alternative: Static Graphs with JIT

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()
```

Alternative: Static Graphs with JIT



Graph includes a conditional node to handle both cases!

```
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()
```

Alternative: Static Graphs with JIT

Use our compiled graph object at each forward pass

```
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()
```

Alternative: 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: Optimization

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: Optimization

Static

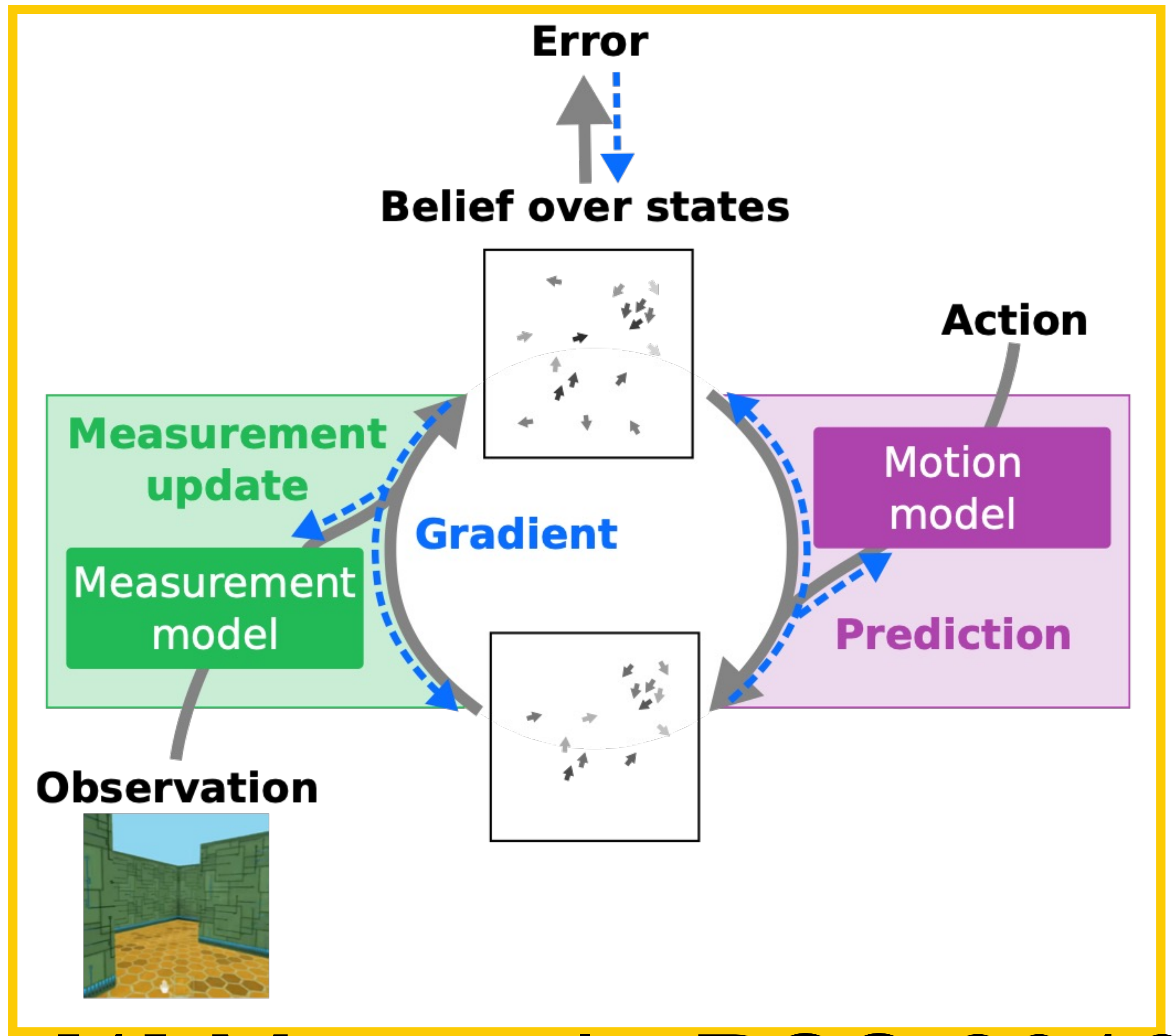
Lots of indirection between the code you write and the code that runs – can be hard to debug, benchmark, etc

Dynamic

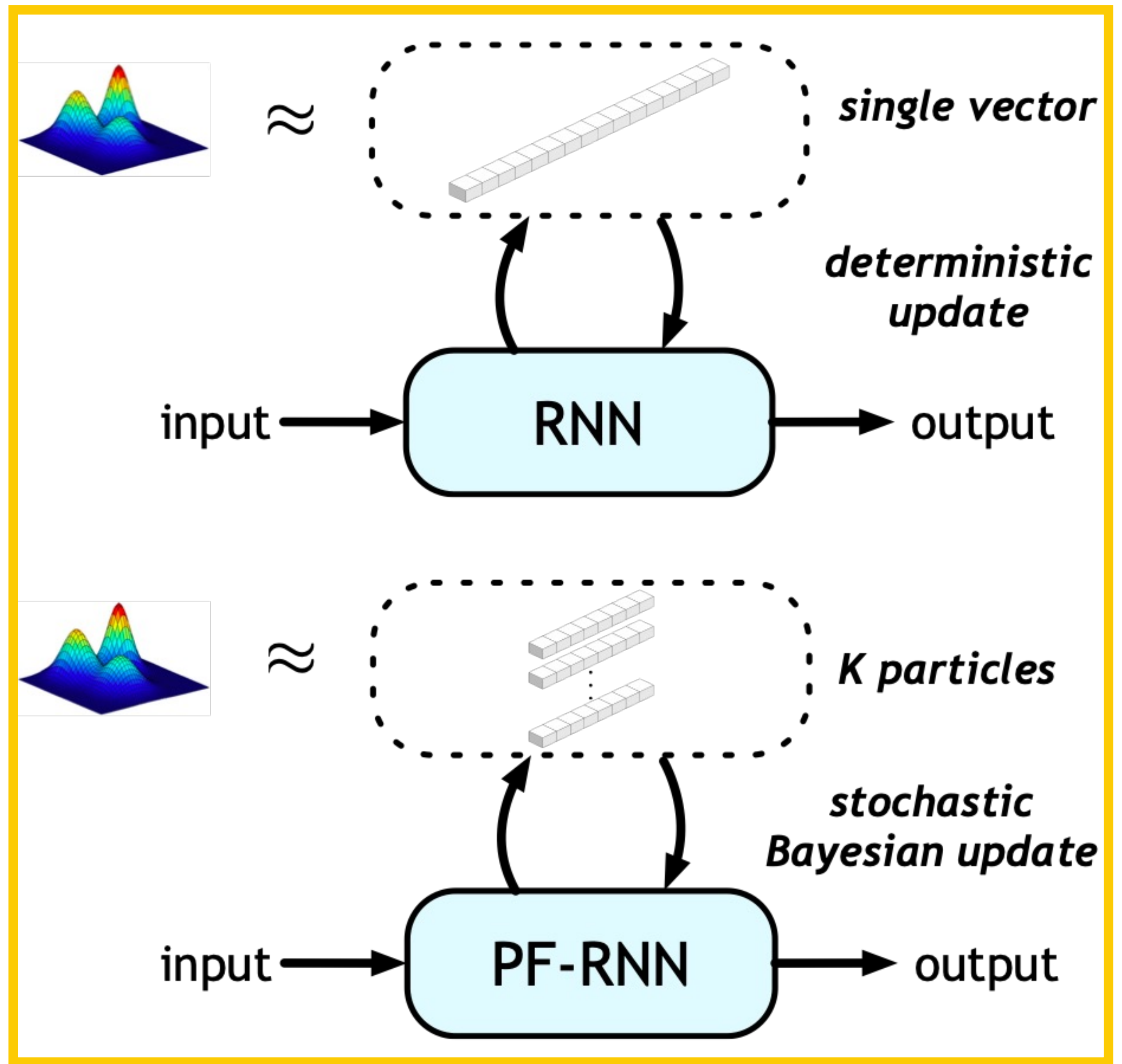
The code you write is the code that runs! Easy to reason about, debug, profile, etc

Dynamic Graph Applications

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



[1] Ma et al., RSS 2018

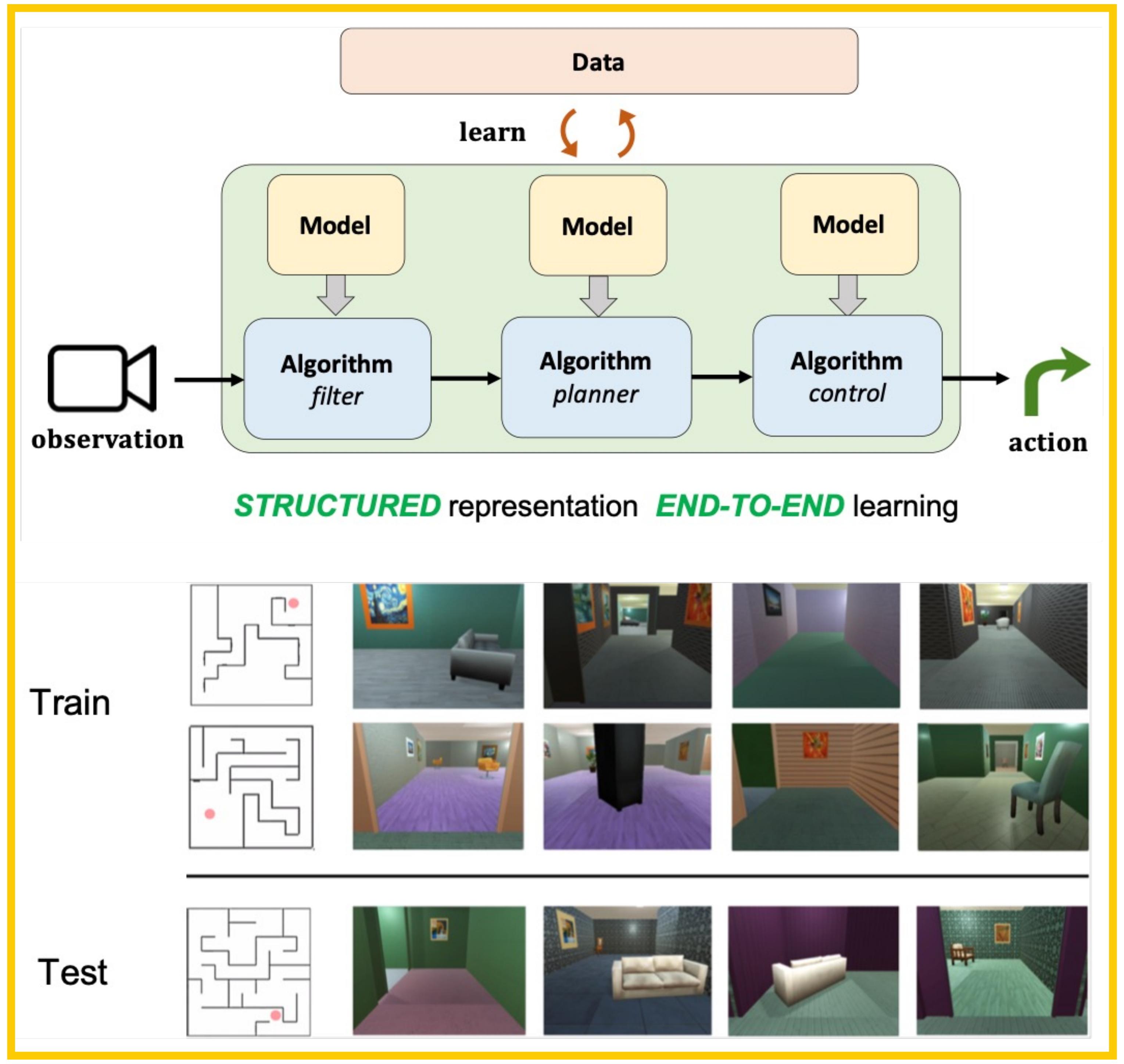


[2] Ma et al., AAAI 2020

[1] Rico Jonschkowski, Divyam Rastogi, Oliver Brock. "Differentiable Particle Filters: End-to-End Learning with Algorithmic Priors" RSS, 2018
[2] Xiao Ma, Peter Karkus, David Hsu, Wee Sun Lee. "Particle Filter Recurrent Neural Networks" AAAI, 2020.

Dynamic Graph Applications

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



[1] Karkus et al., RSS 2019

[1] Peter Karkus, Xiao Ma, David Hsu, Leslie Pack Kaelbling, Wee Sun Lee, Tomas Lozano-Perez. "Differentiable Algorithm Networks for Composable Robot Learning" RSS, 2019

Dynamic Graph Applications

Model structure depends on the input:

- Recurrent Networks
- Recursive Networks
- Modular Networks
- (Your idea here!)

Final Project

TensorFlow: Versions

TensorFlow 1.0

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

TensorFlow 2.0

- Current release: 2.8.0
  - Released 2/2/2022
- Default**: dynamic graphs**
- Optional: static graphs

TensorFlow 1.0: Static Graphs

```
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 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

```
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

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)
```

In PyTorch, all ops build graph by default; **opt out** via torch.no_grad
In Tensorflow, ops do not build graph by default; **opt in** via GradientTape

TensorFlow 2.0: Dynamic Graphs

Ask the tape to compute gradients

```
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)
```

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

Call the compiled step function in the training loop

```
@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)
```

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
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

Keras gives you common loss functions and optimization algorithms

```
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

Forward pass:
Compute loss,
build graph

Backward pass:
compute gradients

```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

Optimizer object updates parameters

```
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

Define a function that returns the loss

```
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))

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

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

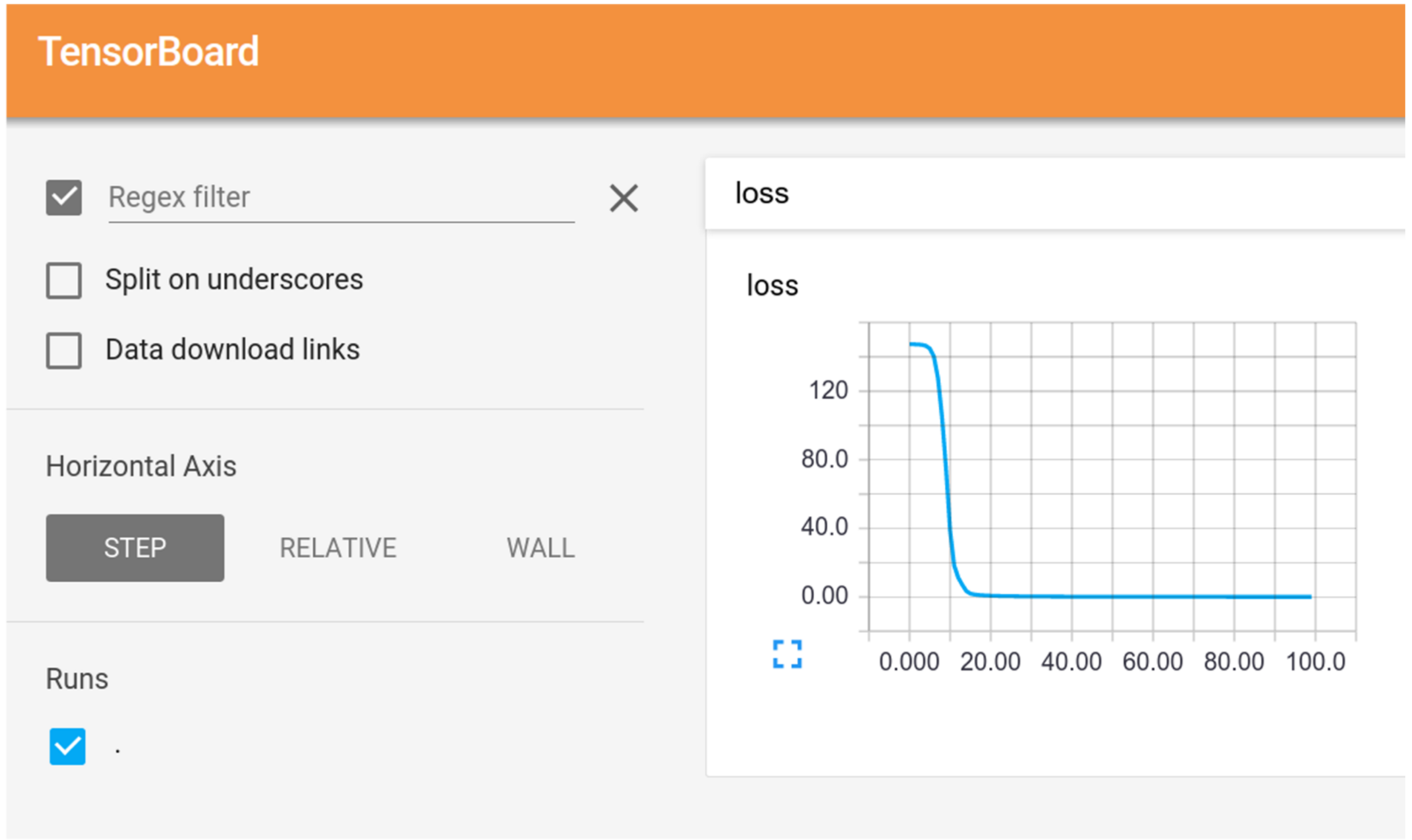
Keras: High-level API

```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))

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!



Summary: PyTorch vs TensorFlow

- **Pytorch**
  - Clean, imperative API
  - Dynamic graphs for easy debugging
  - JIT allows static graphs for production
  - Hard/inefficient to use on TPUs
  - Not easy to deploy on mobile
- **Tensorflow 1.0**: static graphs by default; can be confusing to debug; API could be messy
- **Tensorflow 2.0**: dynamic by default; standardized on Keras API

DeepRob

Lecture 12
Deep Learning Software
University of Michigan | Department of Robotics