EECS 230 Deep Learning
Lecture 5: Training Neural Network

Some slides from Feifei Li

From last lectures:

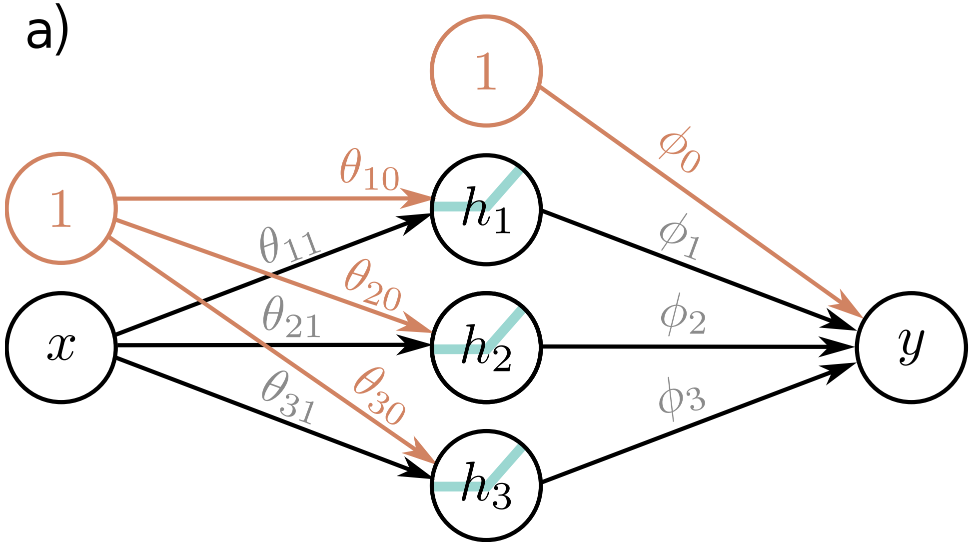
Shallow & Deep Neural network, Losses, Optimization

Depicting shallow neural networks

$$h_1 = \mathrm{a}[\theta_{10} + \theta_{11}x]$$
$$h_2 = \mathrm{a}[\theta_{20} + \theta_{21}x]$$
$$h_3 = \mathrm{a}[\theta_{30} + \theta_{31}x]$$

$$y = \phi_0 + \phi_1 h_1 + \phi_2 h_2 + \phi_3 h_3$$

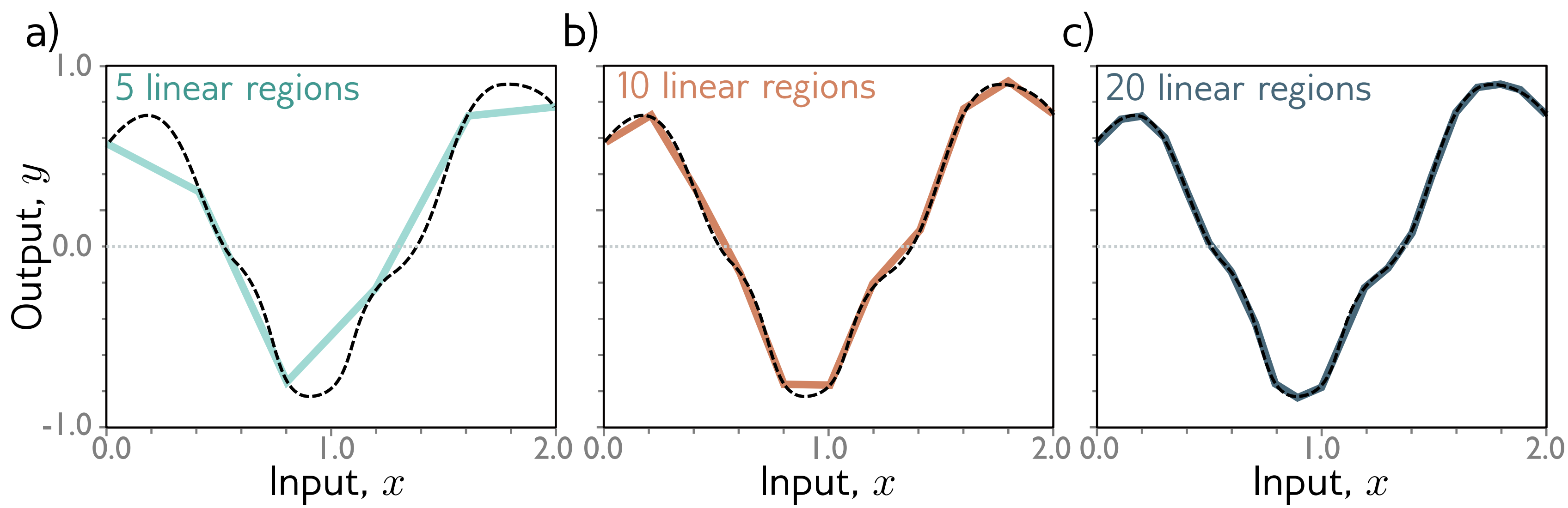
a)



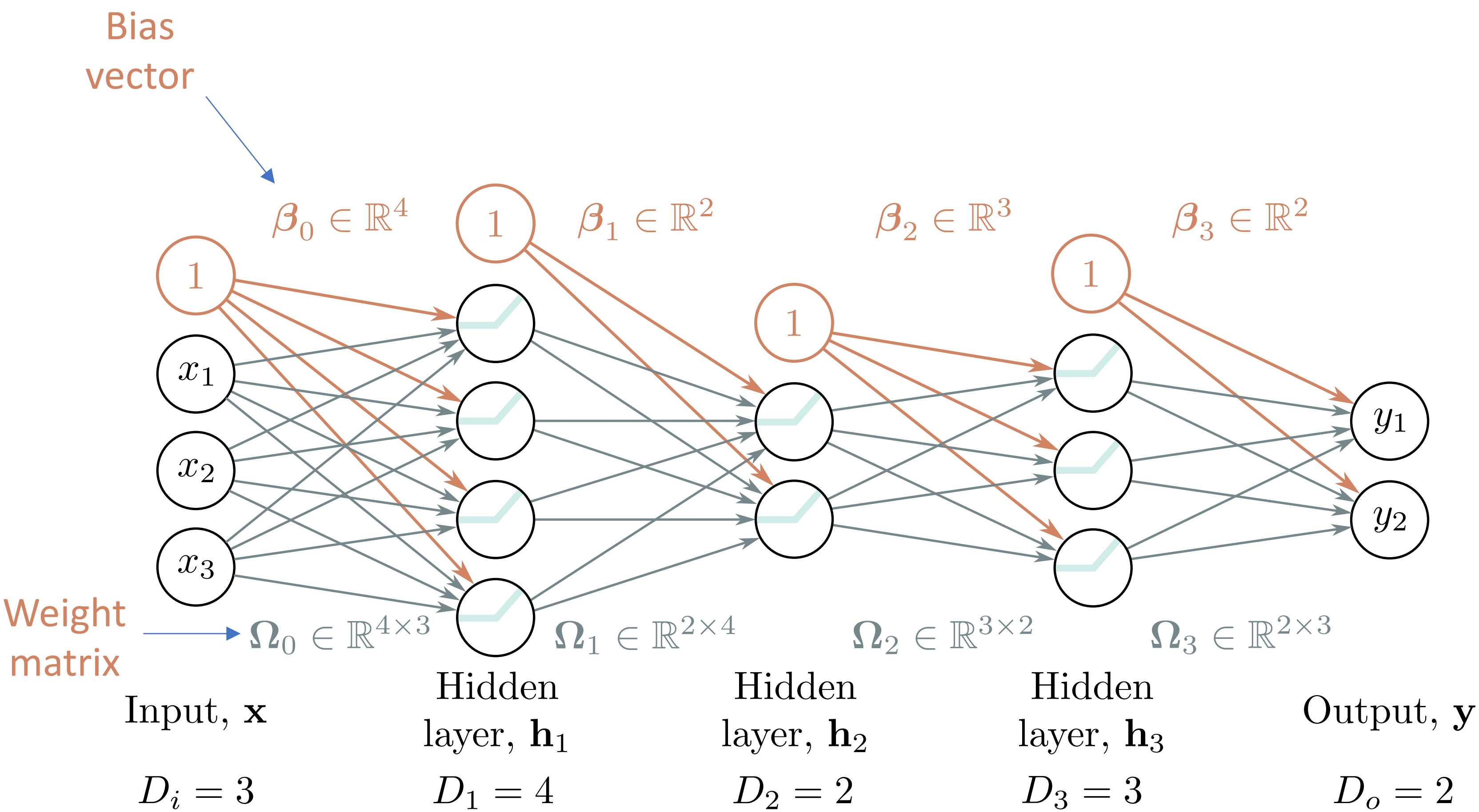
Each parameter multiplies its source and adds to its target

With enough hidden units

- … we can describe any 1D function to arbitrary accuracy



Example of Multi Layer Perceptron (MLP)

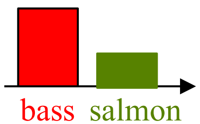


(binary case)

Cross-Entropy Loss (related to *logistic regression* loss)

Perceptron approximation: $\mathbf{f}(\mathbf{w}, \mathbf{x}^i) = u(W^T X^i) \approx \sigma(W^T X^i)$

Consider two probability distributions
over two classes (e.g. bass or salmon) : $(\mathbf{y}, 1-\mathbf{y})$ and $(\sigma, 1-\sigma)$



(binary)
Cross-entropy loss:

$$L(\mathbf{y}, \sigma) = -\mathbf{y} \ln \sigma - (1-\mathbf{y}) \ln(1-\sigma)$$

Distance between two distributions can be evaluated via **cross-entropy**
(equivalent to ***KL divergence*** for fixed target)

$$H(\boldsymbol{p}, \boldsymbol{q}) := -\sum_k p_k \ln q_k$$

(general multi-class case)

Cross-Entropy Loss

K-label perceptron's output: $\bar{\sigma}(\mathbf{W}X^i)$ for example X^i

k-th index

Multi-valued label $\mathbf{y}^i = k$ gives **one-hot** distribution $\bar{\mathbf{y}}^i = (0, 0, 1, 0, \ldots, 0)$

Consider two probability distributions over K classes (e.g. bass, salmon, sturgeon) : $\bar{\mathbf{y}}^i$ and $(\bar{\sigma}_1, \bar{\sigma}_2, \bar{\sigma}_3, \ldots, \bar{\sigma}_K)$

$$\Pr(\mathbf{x}^i \in \text{Class } k \mid W) = \bar{\sigma}_k(WX^i)$$

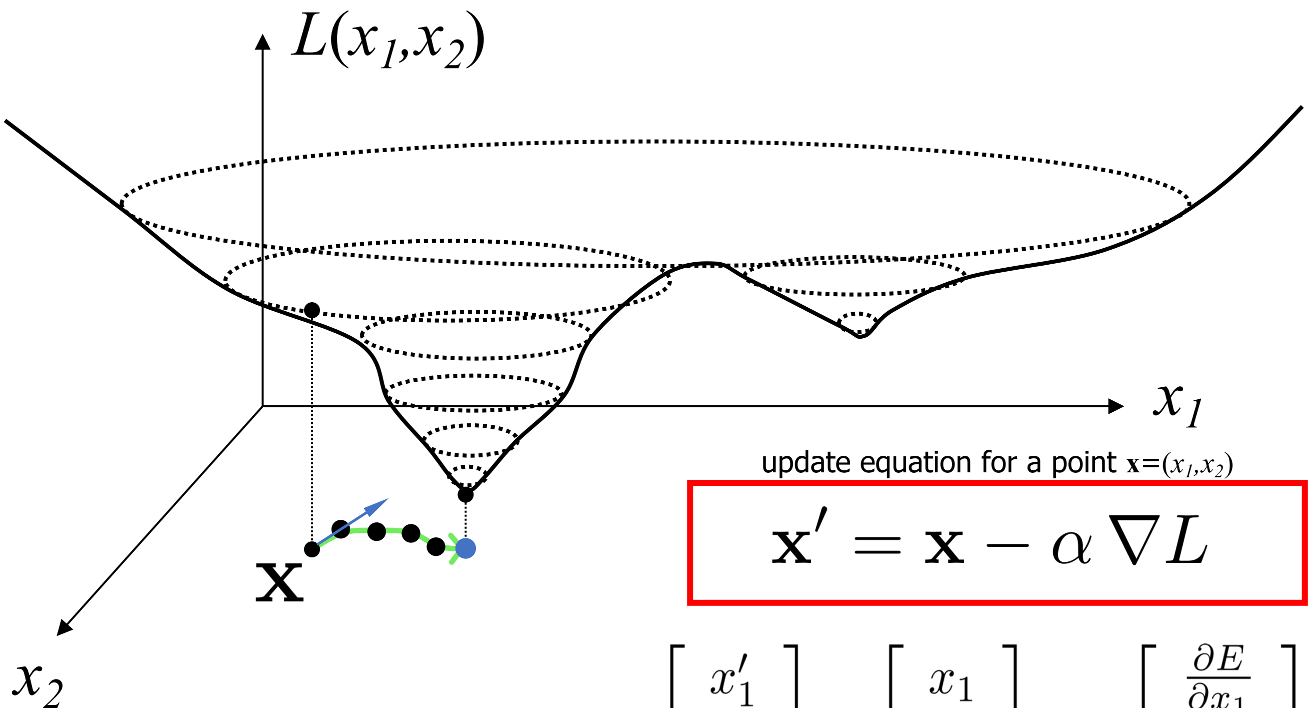
Total loss: $$L(W) = \sum_{i \in \text{train}} \overbrace{\sum_k -\bar{\mathbf{y}}^i_k \ln \bar{\sigma}_k(WX^i)}^{\textbf{cross entropy}}$$

$$\Rightarrow \quad \boxed{L(W) = -\sum_{i \in \text{train}} \ln \bar{\sigma}_{\mathbf{y}^i}(WX^i)}$$

sum of **Negative Log-Likelihoods (NLL)**

From last lecture: Gradient Descent

- Example: for a function of two variables



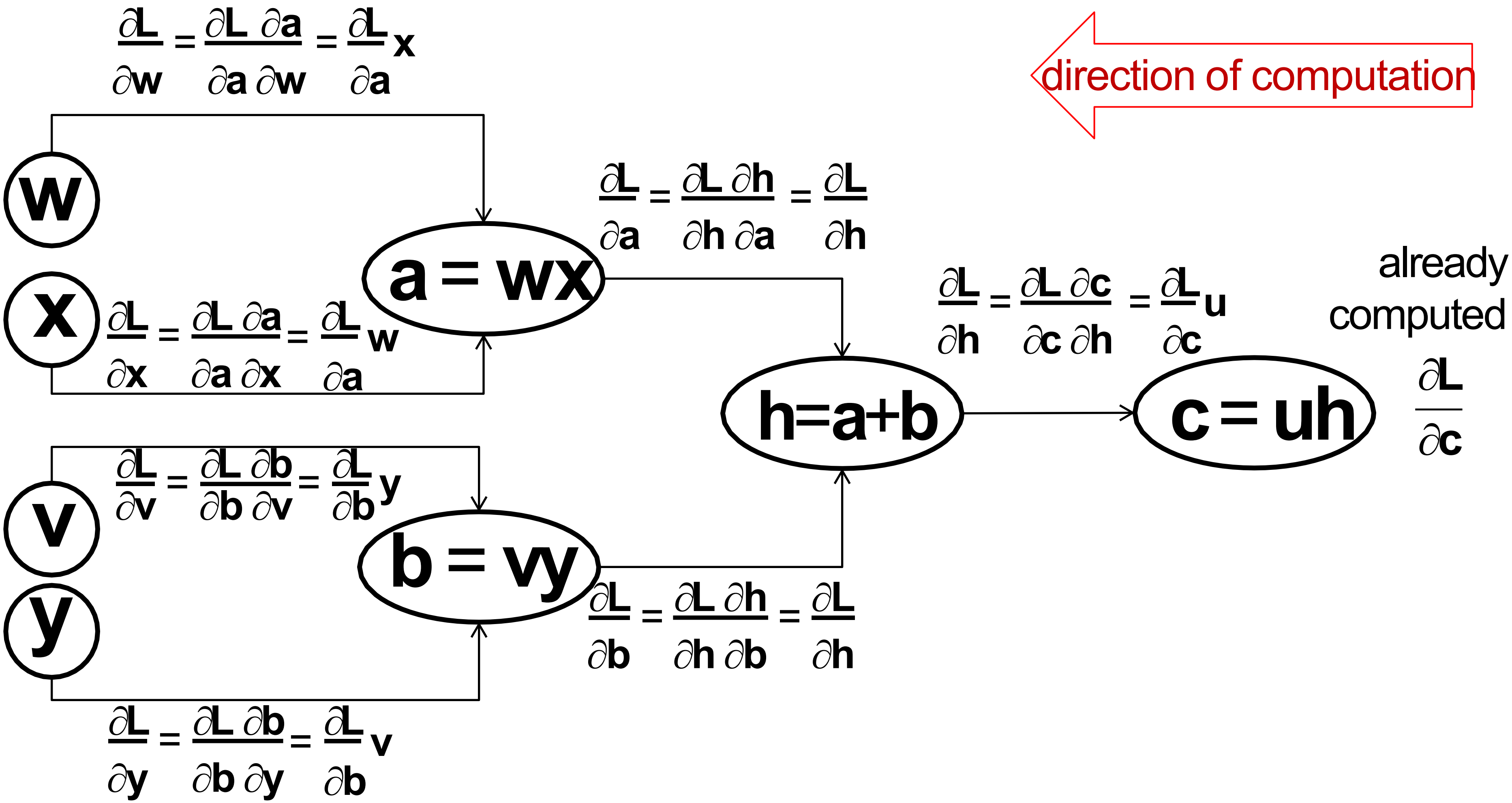
update equation for a point $\mathbf{x}=(x_1,x_2)$

$$\boxed{\mathbf{x}' = \mathbf{x} - \alpha \nabla L}$$

$$\begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \frac{\partial E}{\partial x_2} \end{bmatrix}$$

Stop at a local minima where $\nabla L = \vec{0}$

From last lecture: Backpropogation



- Some of these partial derivatives are intermediate
  - their values will not be used for gradient descent

Today

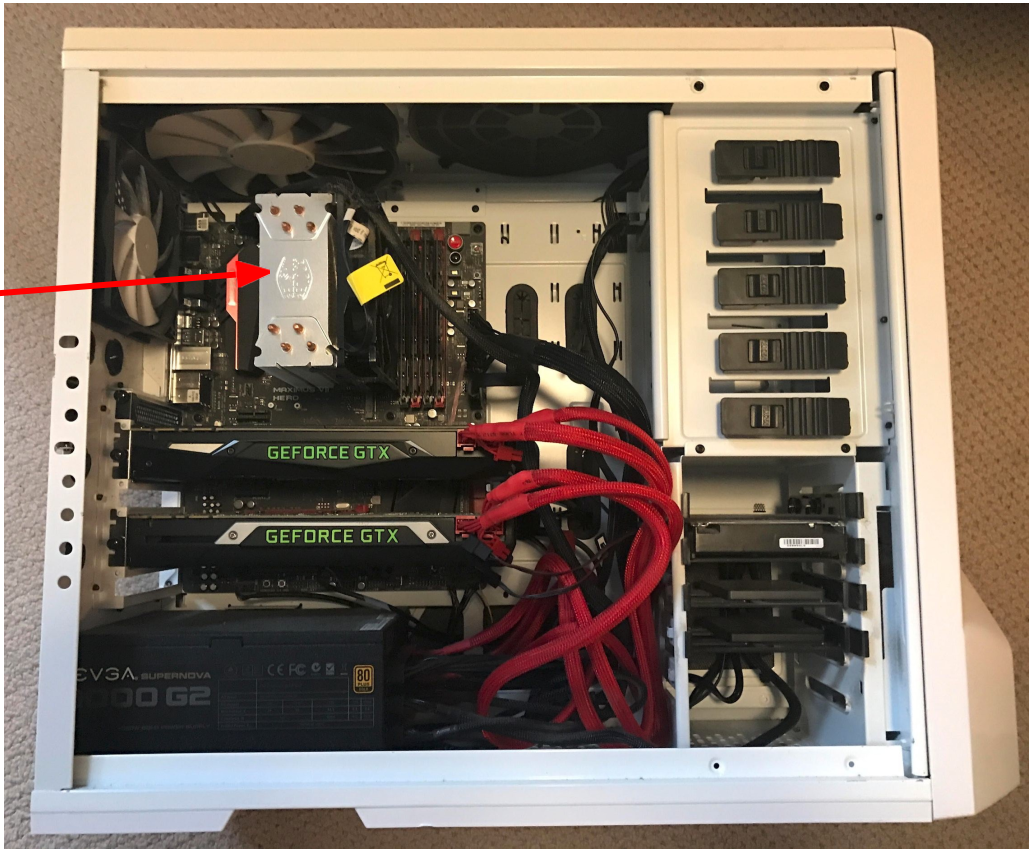
- ❑Deep learning hardware
- ❑Deep learning software
- ❑Tricks for training neural networks
  - ❑Activation function
  - ❑Data Preprocessing
  - ❑Batch normalization
  - ❑Transfer learning

Deep Learning Hardware

Inside a computer

Spot the CPU!

(central processing unit)



Spot the GPUs!

(graphics processing unit)

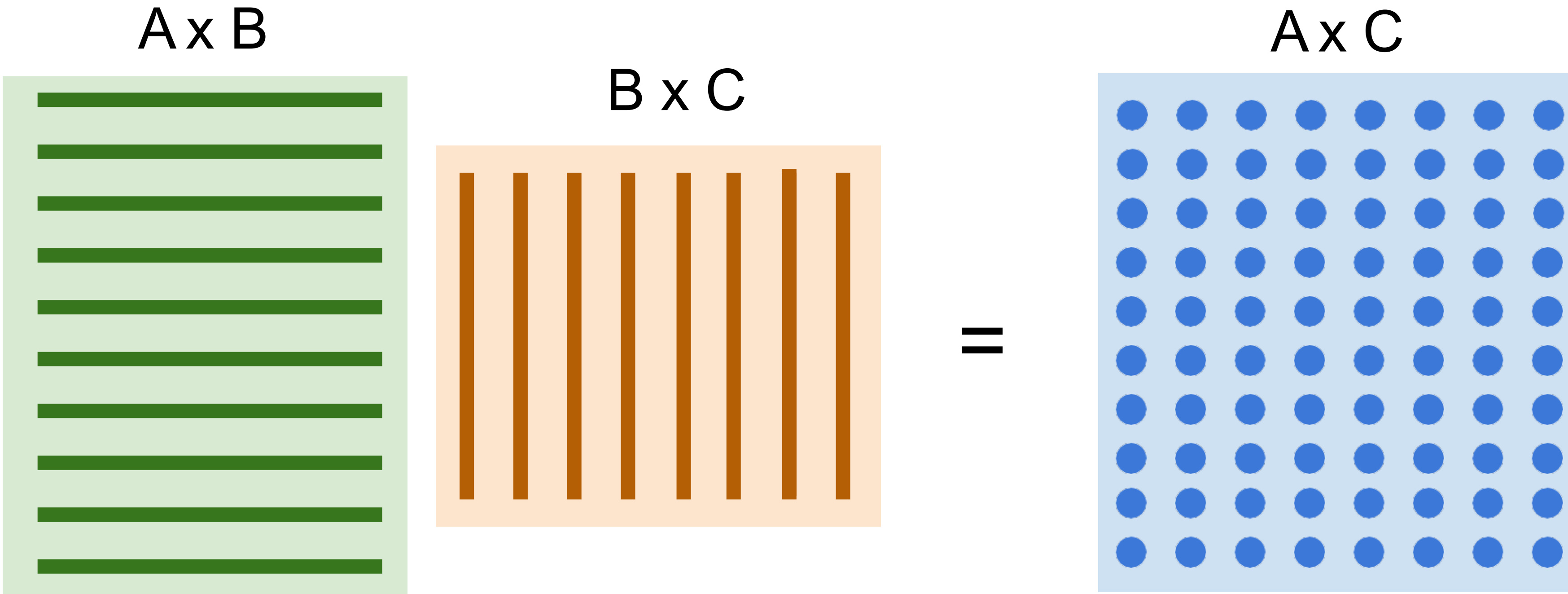
CPU vs GPU

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

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

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

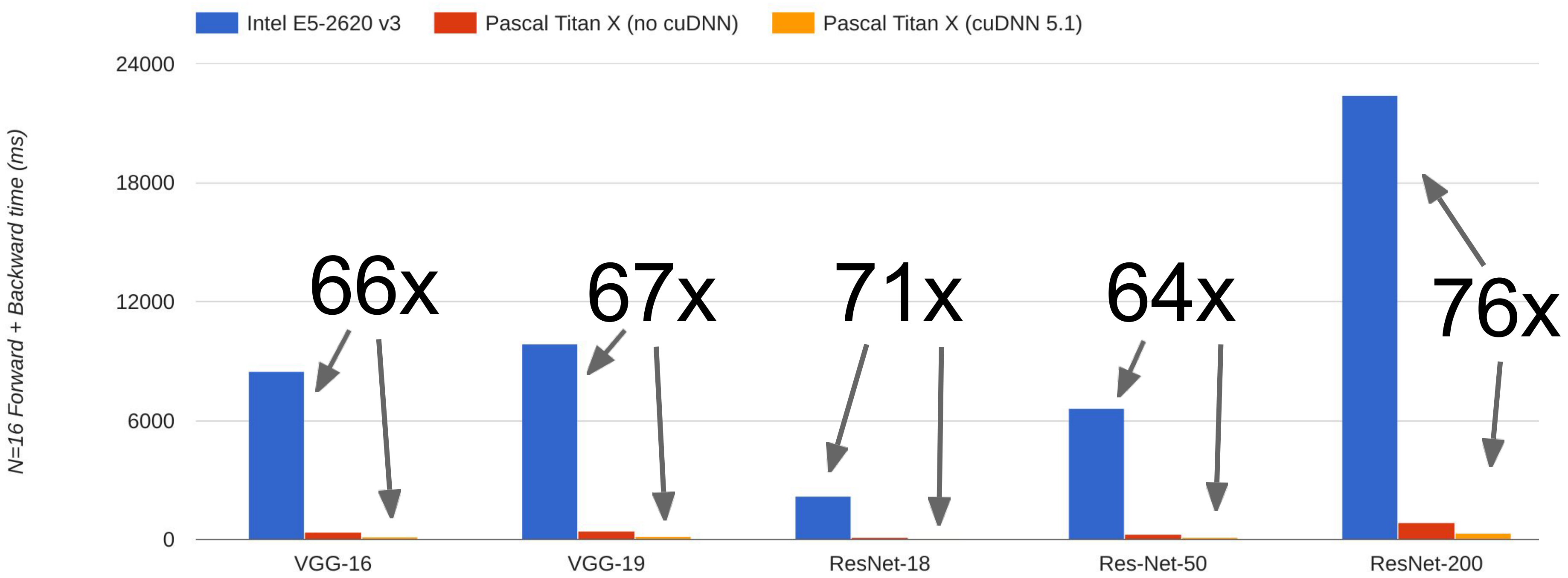
Example: Matrix Multiplication



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

CPU vs GPU in practice

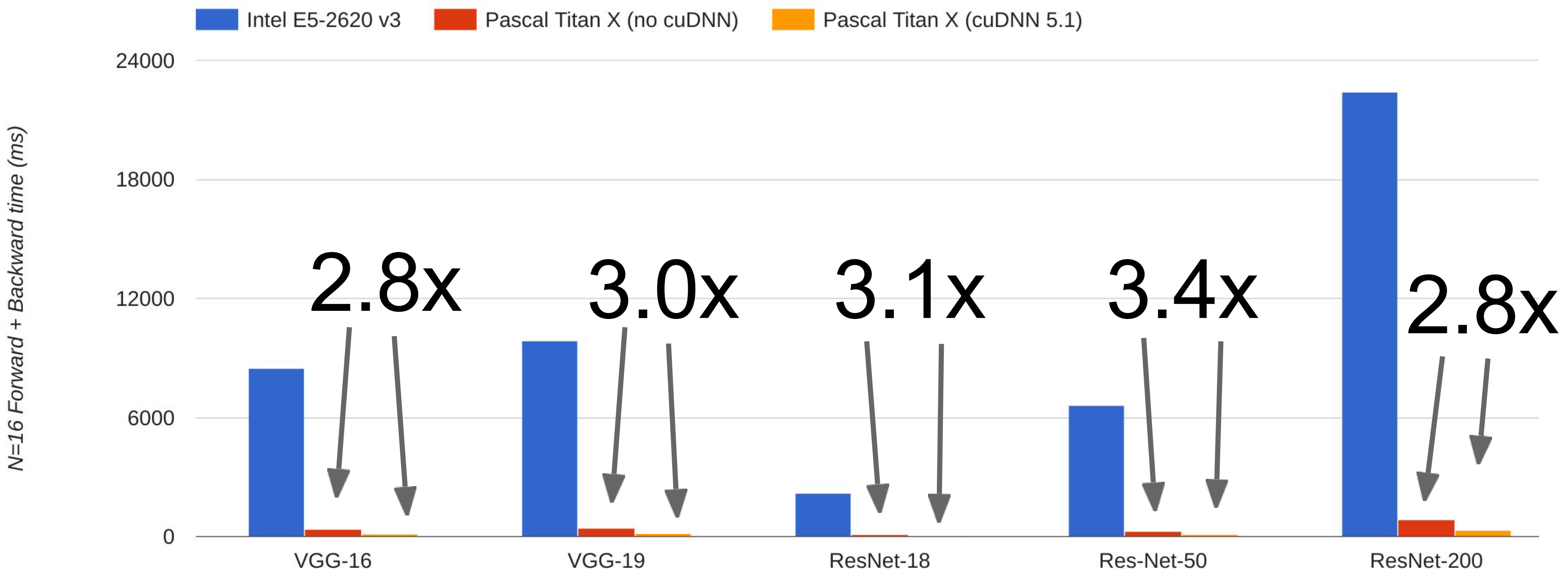
(CPU performance not well-optimized, a little unfair)



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

CPU vs GPU in practice

cuDNN much faster than "unoptimized" CUDA



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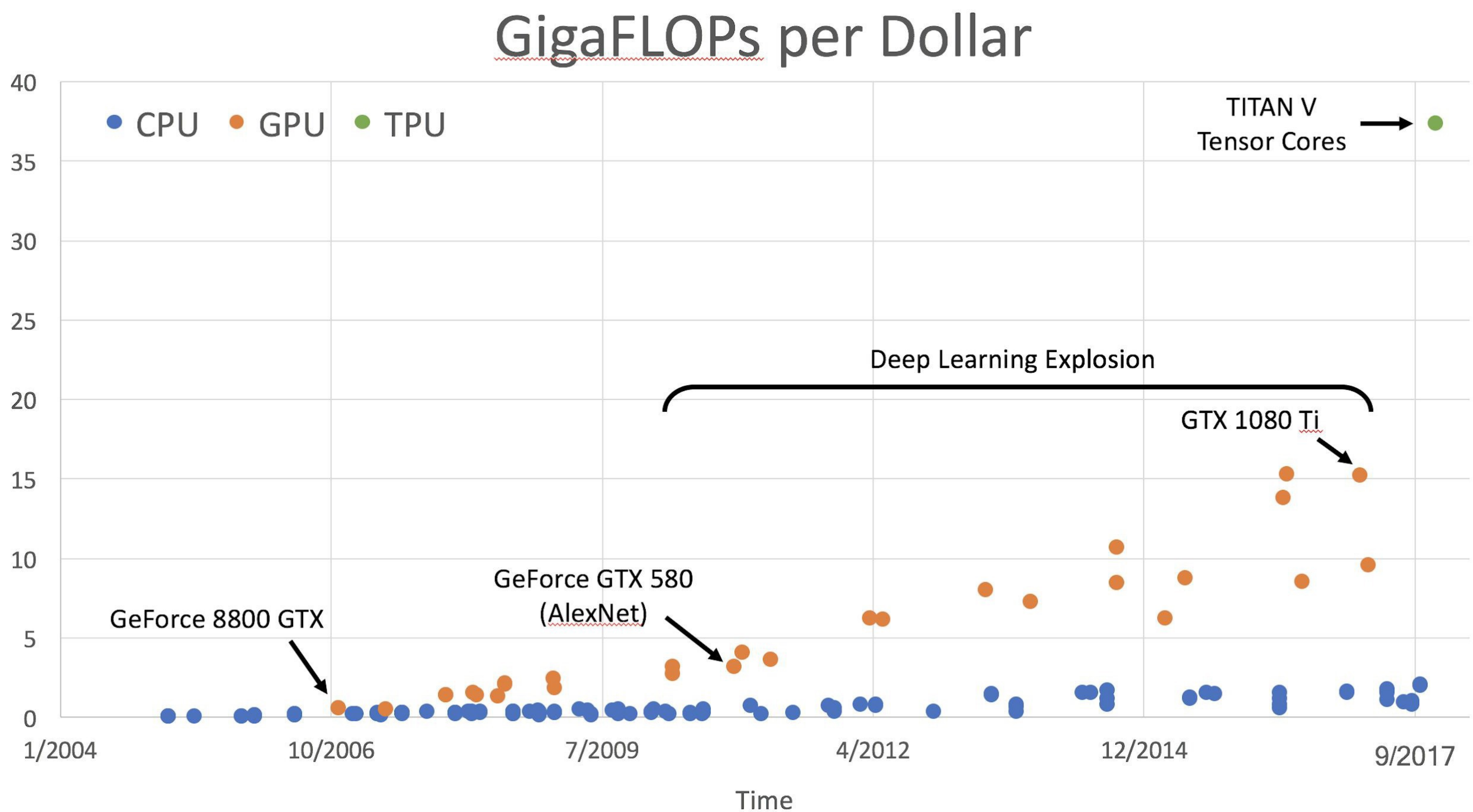
GigaFLOPs per Dollar
CPU
GPU
TPU
TITAN V
Tensor Cores
Deep Learning Explosion
GTX 1080 Ti
GeForce GTX 580
(AlexNet)
GeForce 8800 GTX
40
35
30
25
20
15
10
5
0
1/2004
10/2006
7/2009
4/2012
12/2014
9/2017
Time

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GPU (Data Center) NVIDIAA100	6912 CUDA, 432 Tensor	1.5 GHz	40/80 GB HBM2	$3/hr (GCP)	~9.7 TFLOPs FP64 ~20 TFLOPs FP32 ~312 TFLOPs FP16
TPU Google Cloud TPUv3	2 Matrix Units (MXUs) per core, 4 cores	?	128 GB HBM	$8/hr (GCP)	~420 TFLOPs (non-standard FP)

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

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

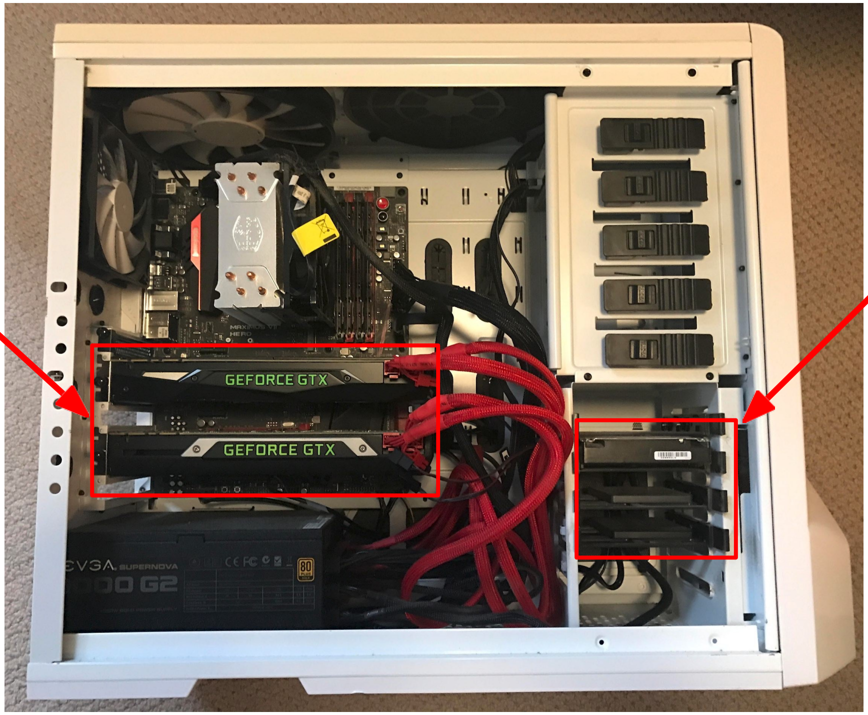
TPU: Specialized hardware for deep learning

Programming GPU

- 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

CPU / GPU Communication

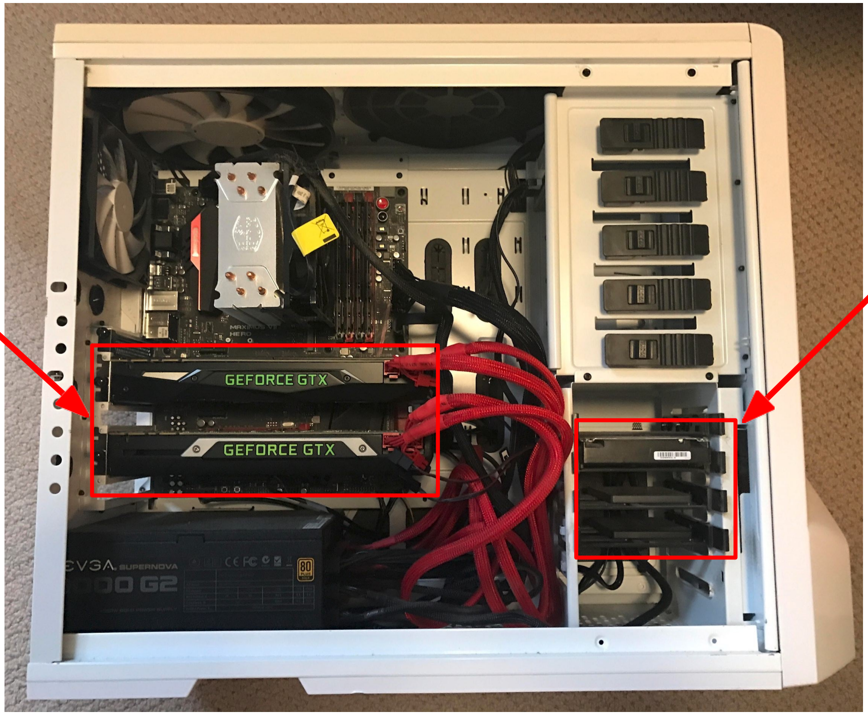
Model
is here



Data is here

CPU / GPU Communication

Model is here



Data is here

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

Solutions:

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

Deep Learning Software

A zoo of frameworks!

Caffe
(UC Berkeley)

Caffe2
(Facebook)
mostly features absorbed by PyTorch

Torch
(NYU / Facebook)

PyTorch
(Facebook)

Theano
(U Montreal)

TensorFlow
(Google)

PaddlePaddle
(Baidu)

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

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

CNTK
(Microsoft)

JAX
(Google)

And others...

A zoo of frameworks!

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We'll focus on this

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And others...

Deep Learning Framework

(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

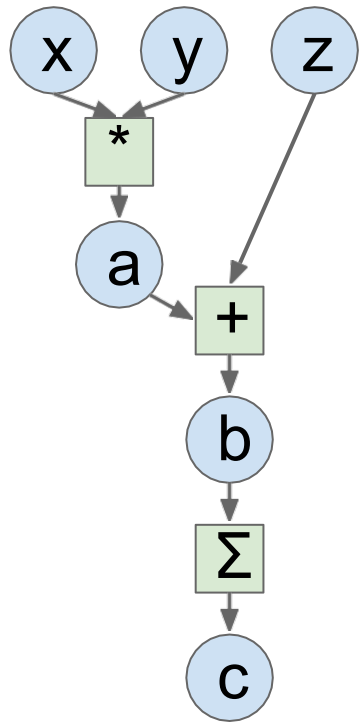
Numpy

```
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)
```



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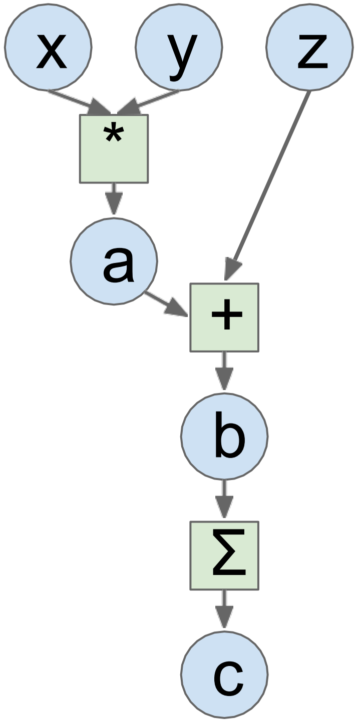
a = x * y
b = a + z
c = np.sum(b)

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
```



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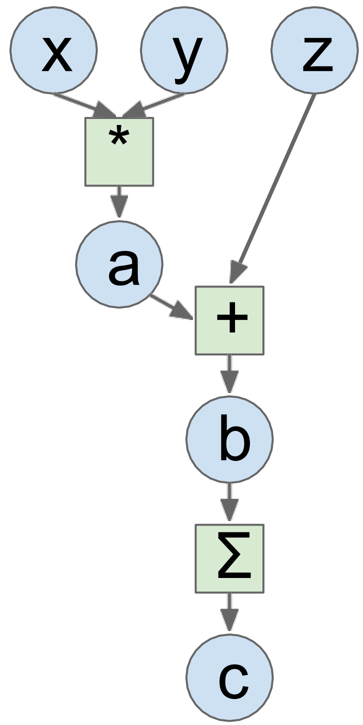

Good:

Clean API, easy to write numeric code

Bad:

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

Computational Graphs

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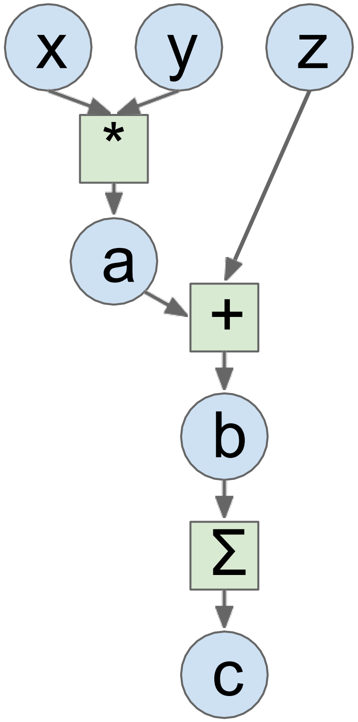

PyTorch

```
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

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

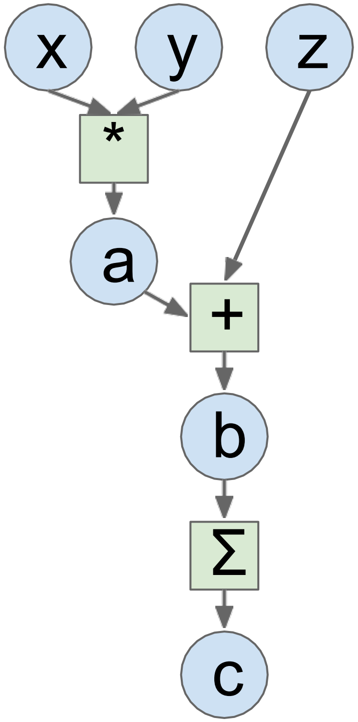

PyTorch

```python
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

```
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grad_x = grad_a * y
grad_y = grad_a * x
```

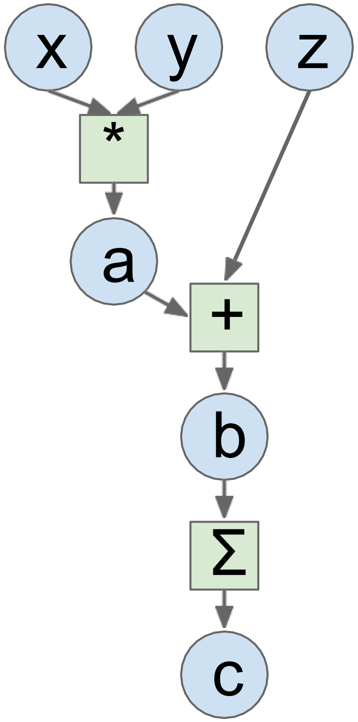

PyTorch

```
import torch

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

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

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

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

PyTorch

(More details)

Pytorch fundamental concepts

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

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

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

Pytorch:Tensor

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
```

UCMERCED

Pytorch:Tensor

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

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

Pytorch:Tensor

Forward pass: compute predictions and loss

```
import torch

device = torch.device('cpu')

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in, device=device)
y = torch.randn(N, D_out, device=device)
w1 = torch.randn(D_in, H, device=device)
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    grad_w1 = x.t().mm(grad_h)

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

Pytorch:Tensor

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
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Pytorch:Tensor

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

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

Gradient descent step on weights

Pytorch:Tensor

To run on GPU, just use a different device!

```
import torch

device = torch.device('cuda:0')

N, D_in, H, D_out = 64, 1000, 100, 10
x = torch.randn(N, D_in, device=device)
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    grad_w1 = x.t().mm(grad_h)

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

Pytorch:Autograd

Creating Tensors with requires_grad=True enables autograd

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

```
import torch

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

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

    loss.backward()

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

Pytorch:Autograd

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

```
import torch

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

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

    loss.backward()

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

Pytorch:Autograd

Compute gradient of loss with respect to w1 and w2

```
import torch

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

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

    loss.backward()

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

Pytorch:Autograd

```
import torch

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

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

    loss.backward()

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

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

Pytorch:Autograd

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

```
import torch

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

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

    loss.backward()

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

PyTorch: New Autograd Functions

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

Use ctx object to “cache” values for the backward pass, just like cache objects from A2

```
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, just like cache objects from A2

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

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

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

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

Can use our new autograd function in the forward pass

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

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

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

    loss.backward()

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

PyTorch: New Autograd Functions

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

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

```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

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

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: nn

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

    loss.backward()

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

After computing gradients, use optimizer to update params and zero gradients

PyTorch: nn
Define new Modules

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

Modules can contain weights or other modules

You can define your own Modules using autograd!

```
import torch

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

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

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

Define our whole model
as a single Module

```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

Initializer sets up two children (Modules can contain modules)

```
import torch

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

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

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn
Define new Modules

Define forward pass using child modules

No need to define backward - autograd will handle it

```
import torch

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

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

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

model = TwoLayerNet(D_in, H, D_out)

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

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

PyTorch: nn Define new Modules

```
import torch

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

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

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

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()
```

Construct and train an instance of our model

PyTorch: nn
Define new Modules

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

```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
Define new 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
Define new Modules

```
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()
```

Stack multiple instances of the component in a sequential

PyTorch: Pretrained Models

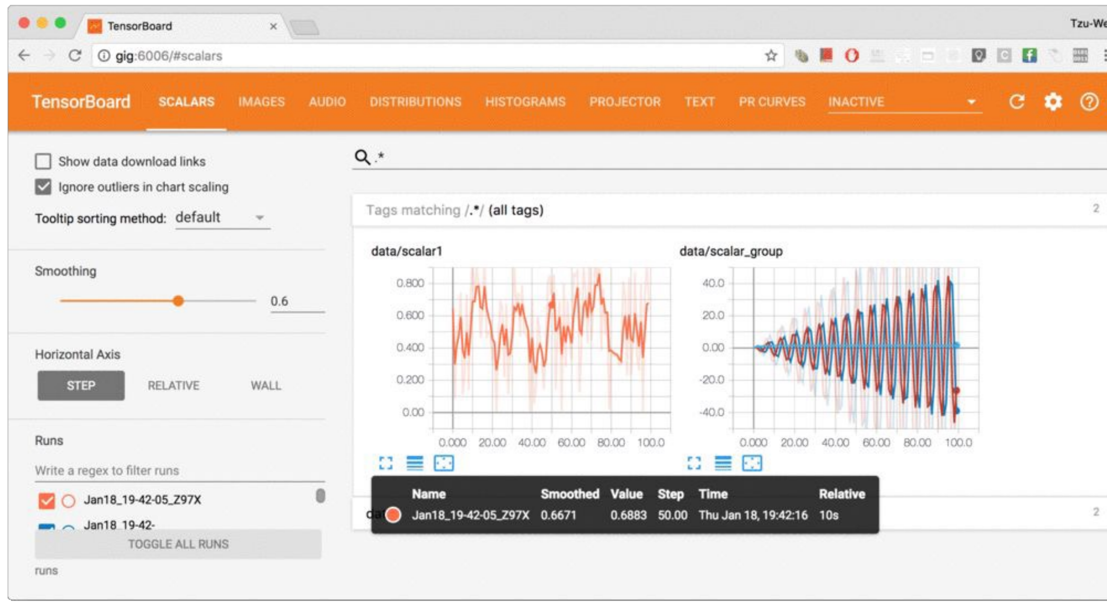
Super easy to use pretrained models with torchvision
https://github.com/pytorch/vision

```
import torch
import torchvision

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

PyTorch: torch.utils.tensorboard

A python wrapper around Tensorflow's web-based visualization tool.



PyTorch: Computational Graphs

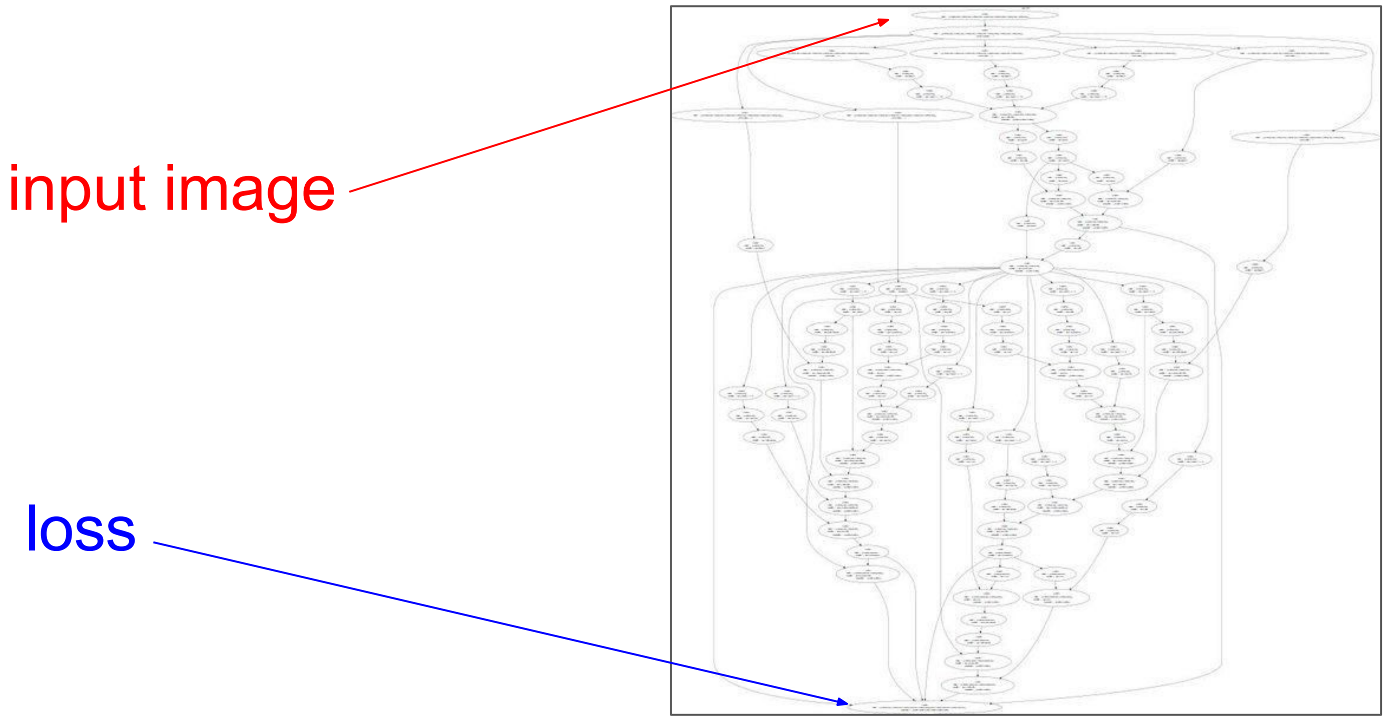
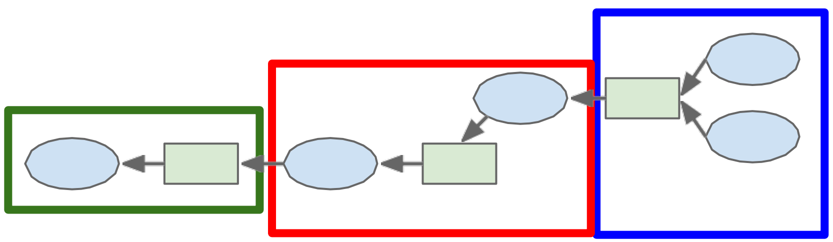


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

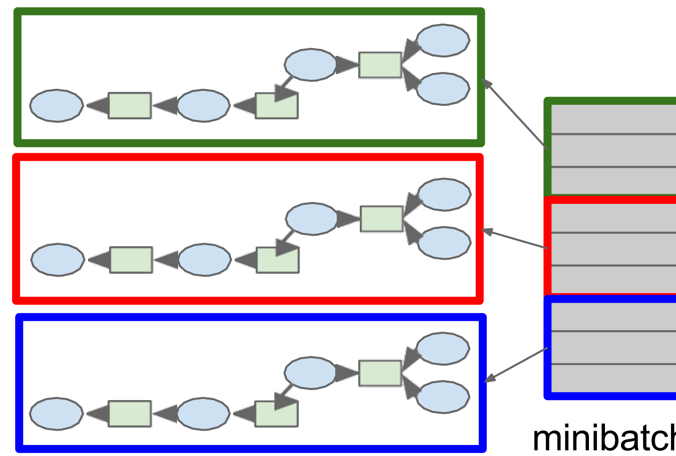
Model Parallel vs. Data Parallel

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

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



Model Parallel

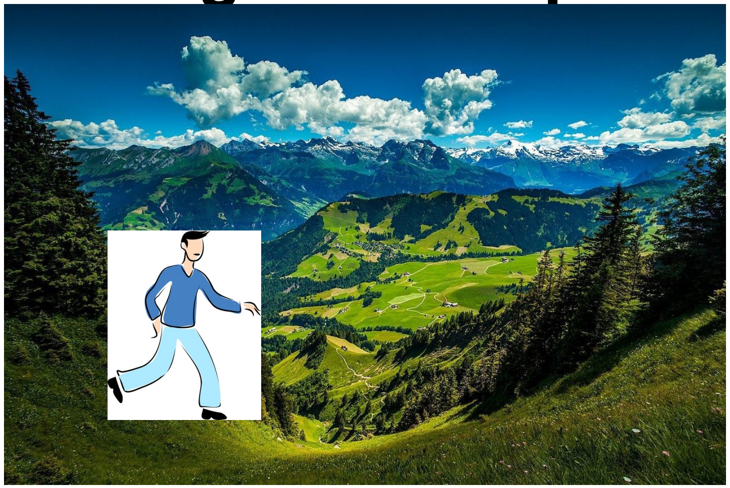


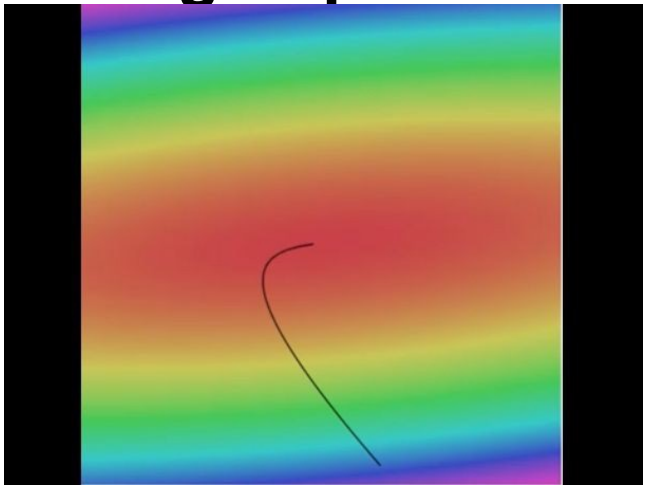
Data Parallel

Tricks for training neural networks

Where we are now...

Learning network parameters through optimization





```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Where we are now...

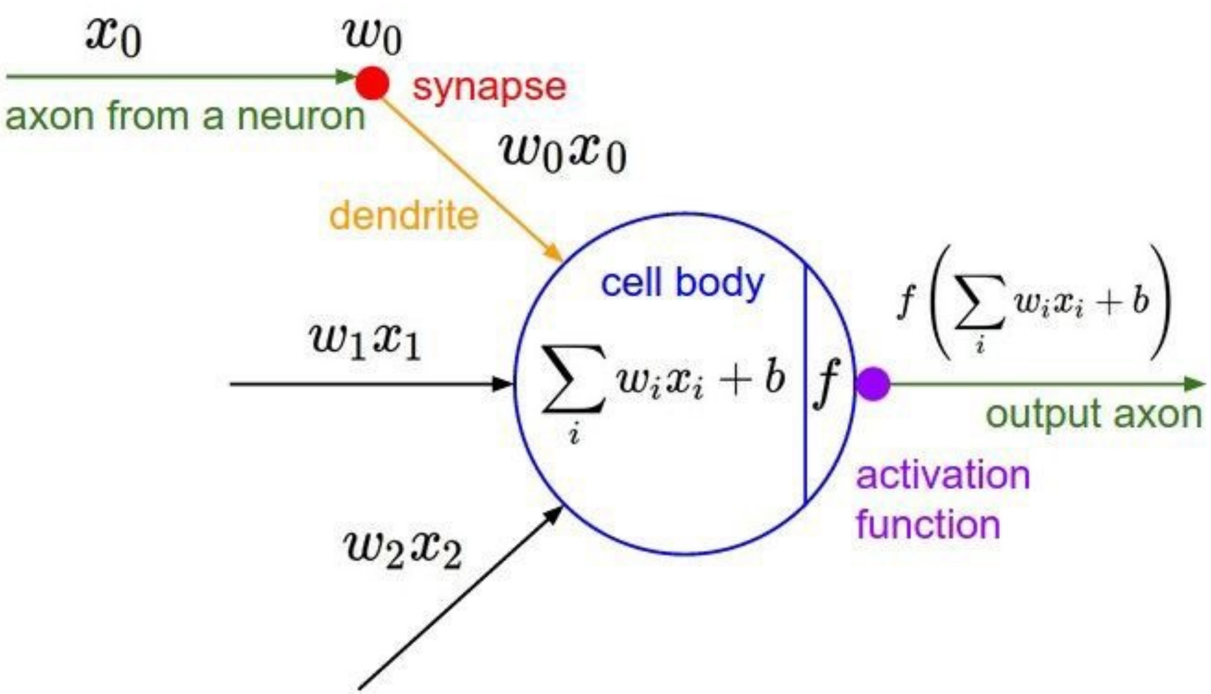
Mini-batch SGD

Loop:

1. **Sample** a batch of data
2. **Forward** prop it through the graph (network), get loss
3. **Backprop** to calculate the gradients
4. **Update** the parameters using the gradient

Activation Functions

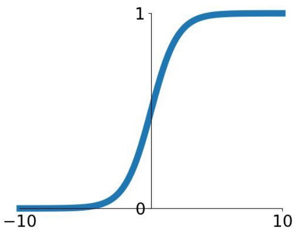
Activation Functions



Activation Functions

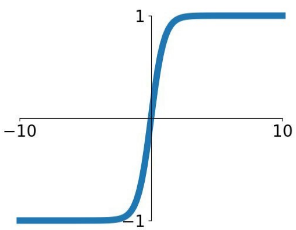
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



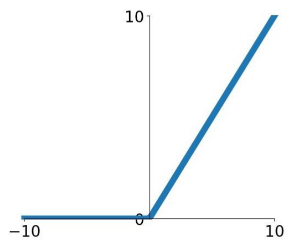
tanh

$$\tanh(x)$$



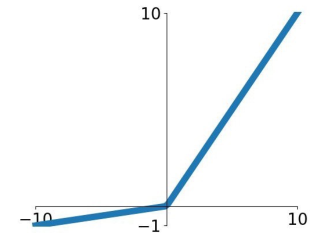
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

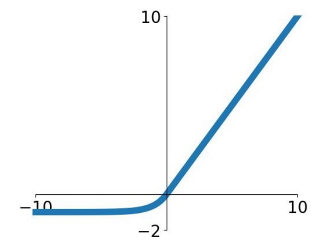


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

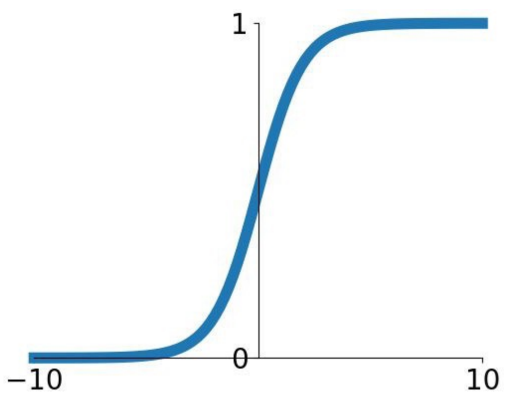
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Activation Functions

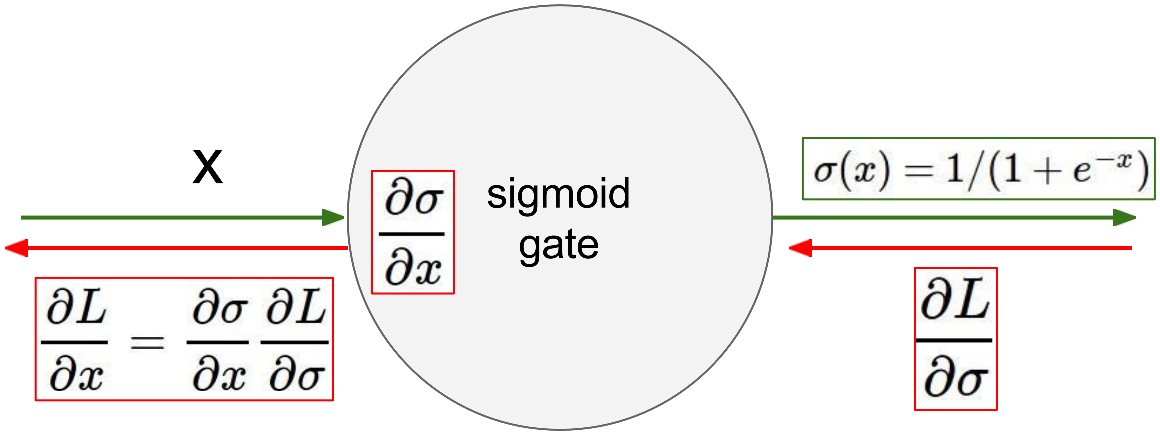
$$\sigma(x) = 1/(1 + e^{-x})$$

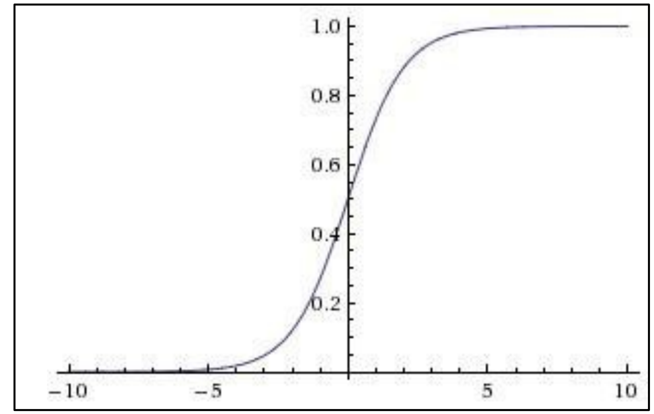
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron



Sigmoid

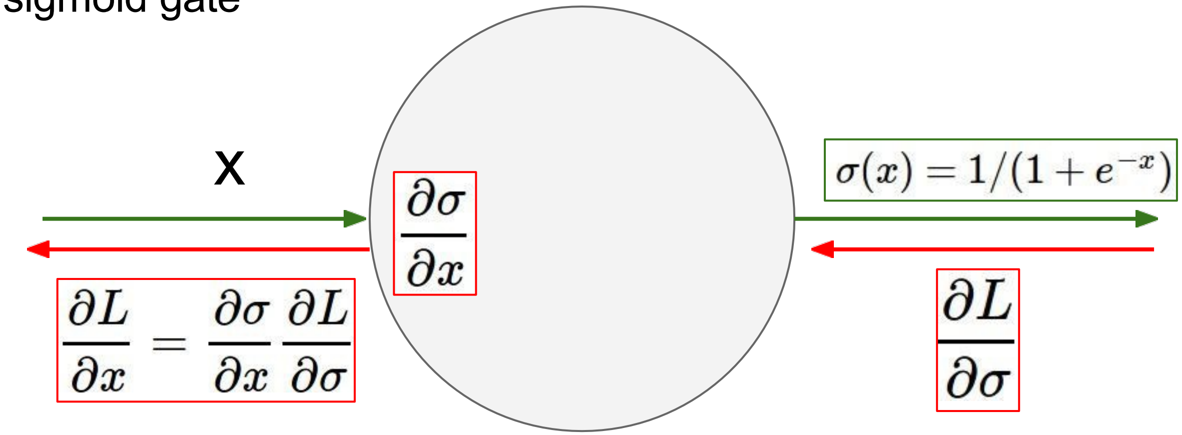
1. Saturated neurons “kill” the gradients

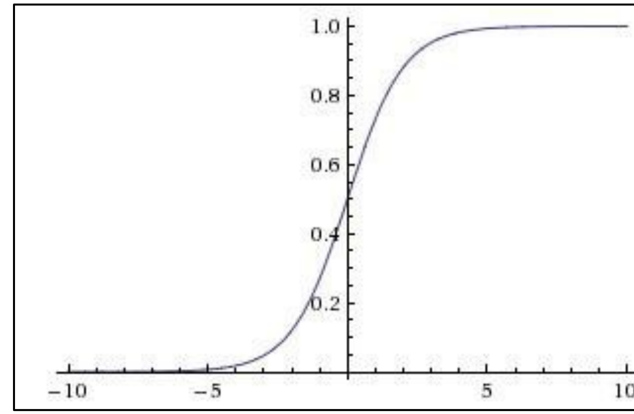




$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

sigmoid gate

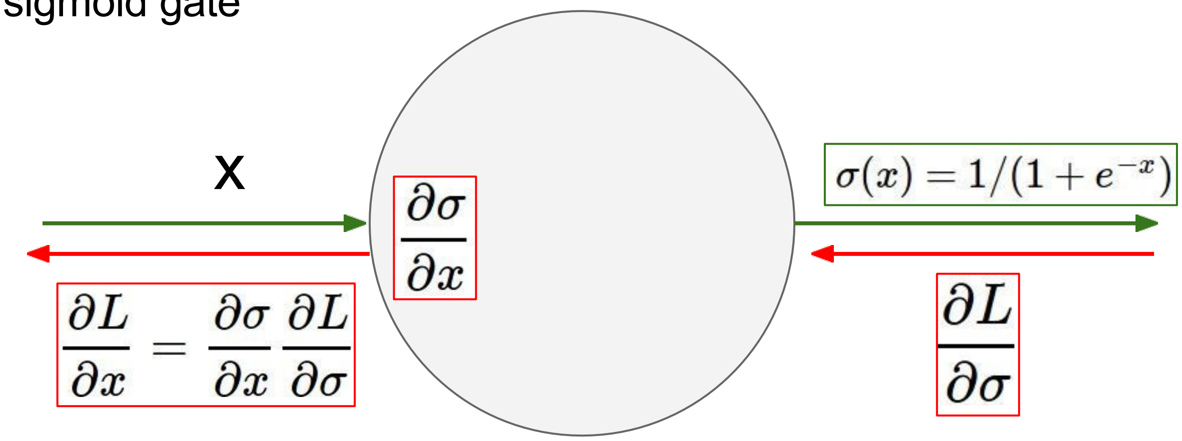


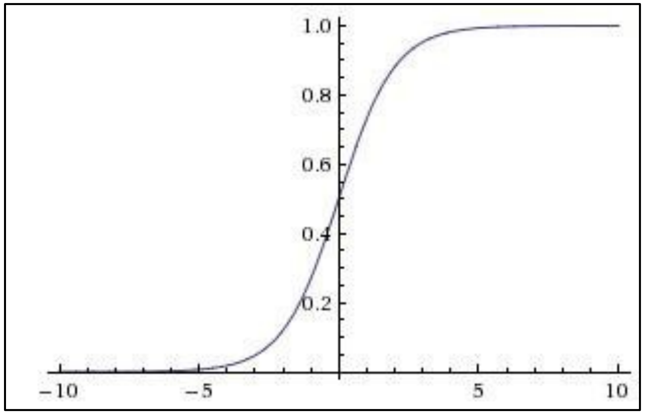


What happens when x = -10?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

sigmoid gate





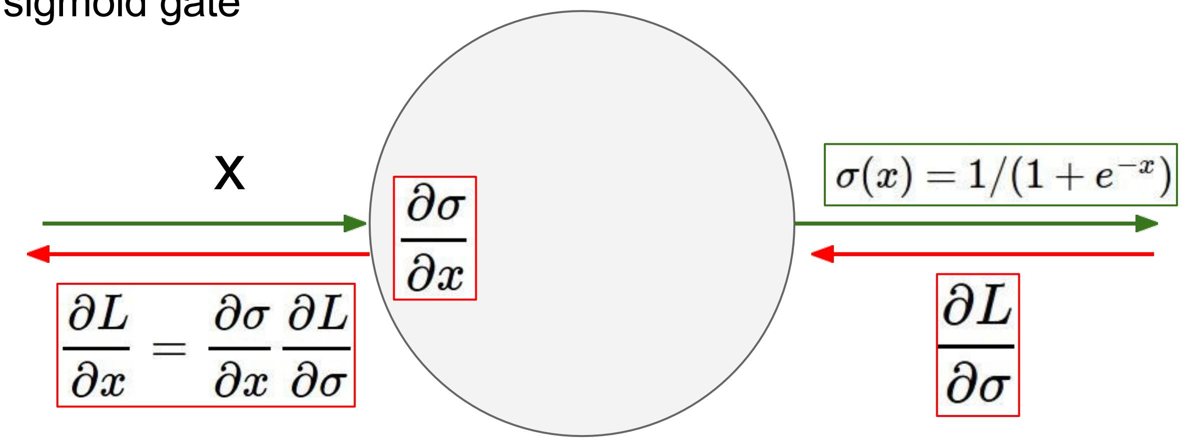
What happens when x = -10?

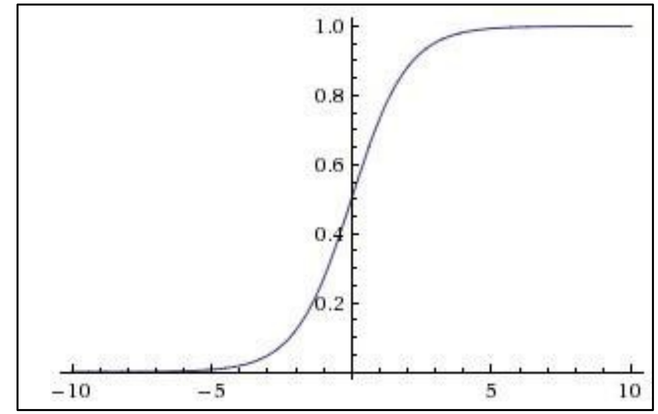
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

$$\sigma(x) \;= \sim 0$$

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,) = 0(1-0) \;=\; 0$$

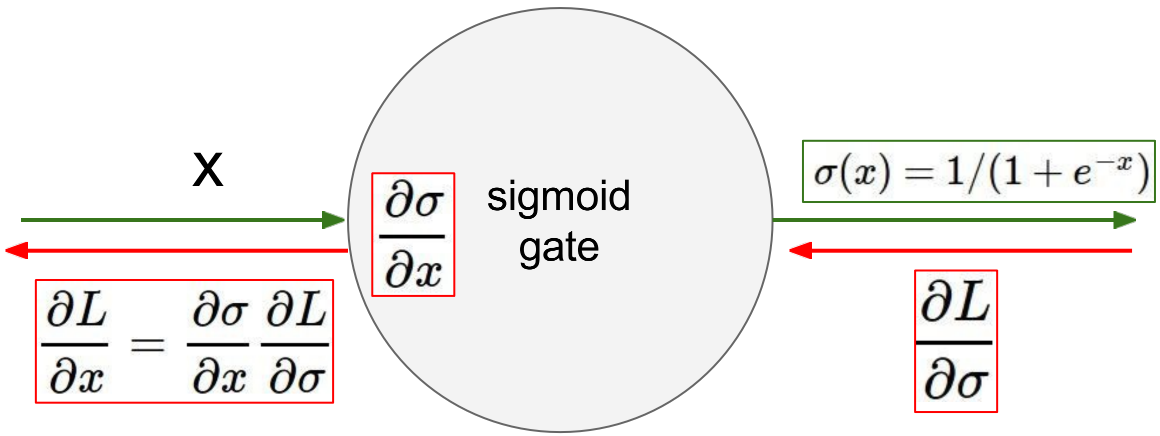
sigmoid gate

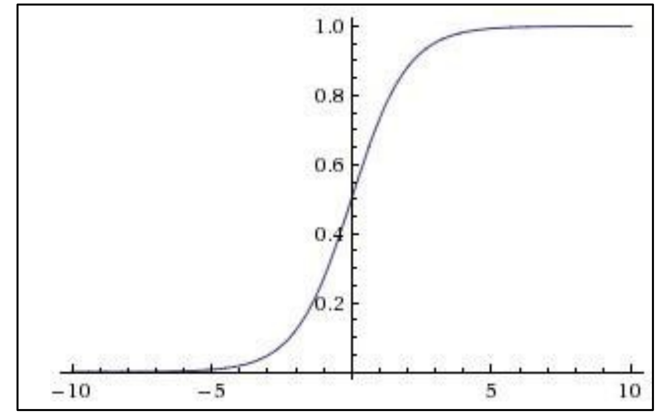




$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

- What happens when x = -10? What happens when x = 0?

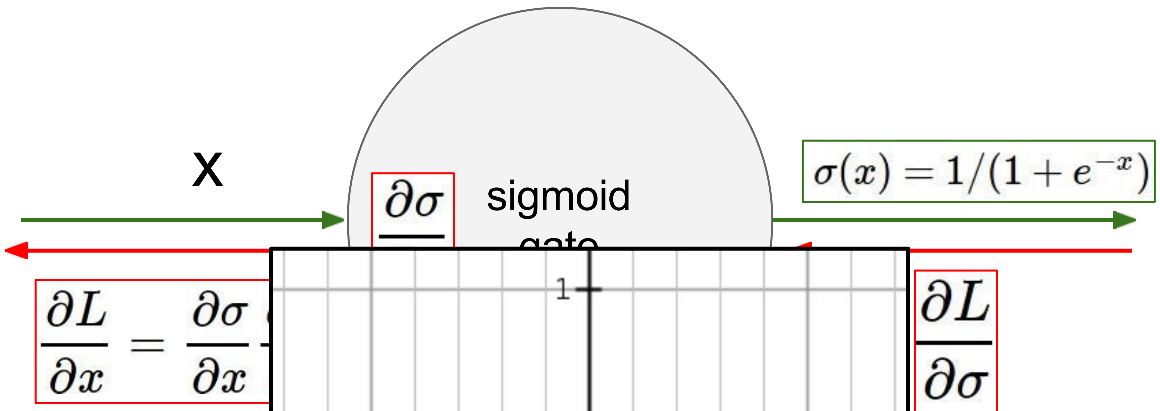


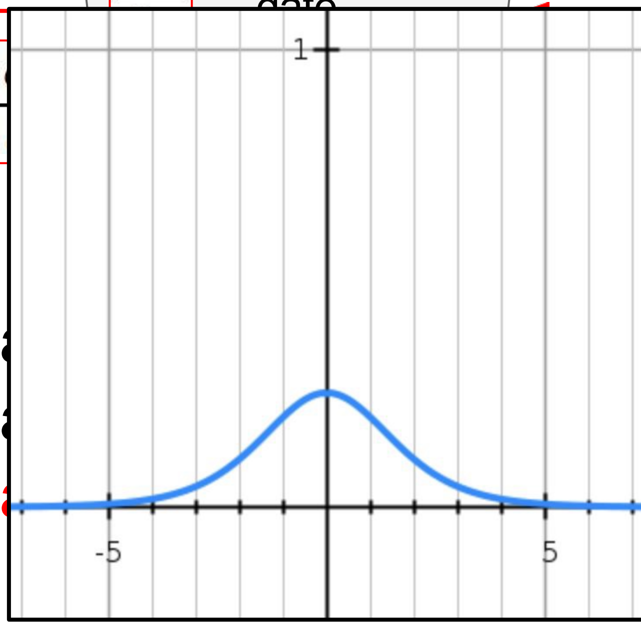


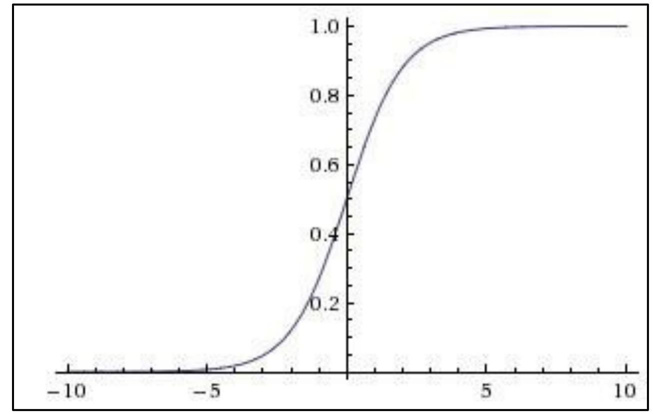
What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

$$\sigma(x) \;= \sim 1 \qquad \frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,) = 1(1-1) \;=\; 0$$





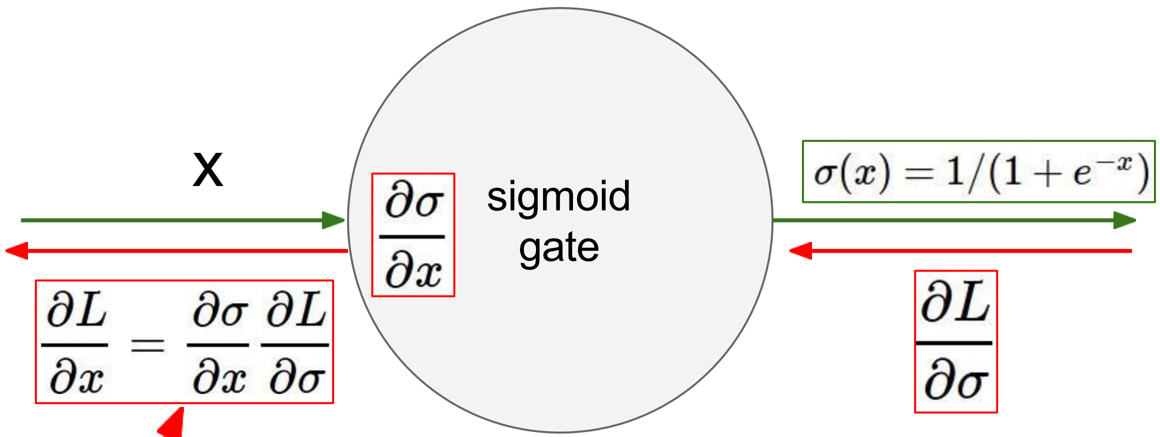


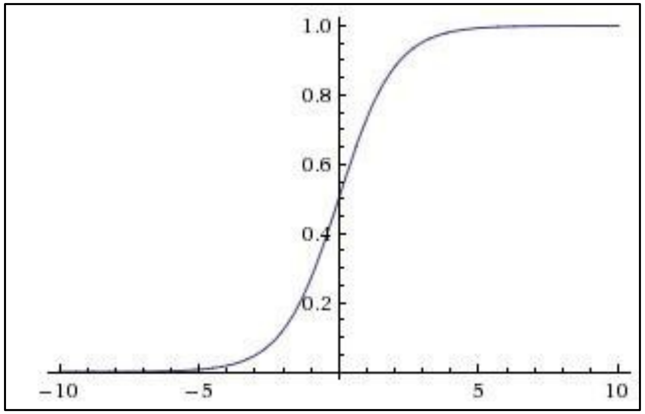
What ha

What ha

What ha

$$\frac{\partial\sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$





$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

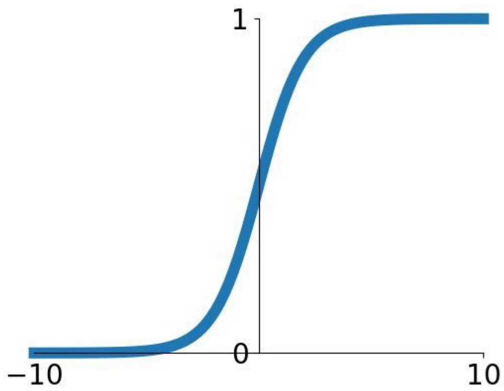
Why is this a problem?

If all the gradients flowing back will be zero and weights will never change

Activation Functions

$$\sigma(x) = 1/(1+e^{-x})$$

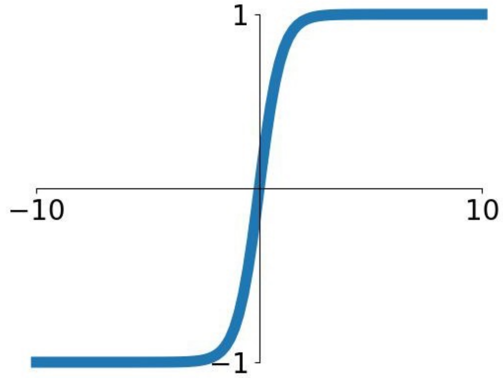
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron



Sigmoid

1. Saturated neurons “kill” the gradients
2. exp() is a bit expensive

Activation Functions

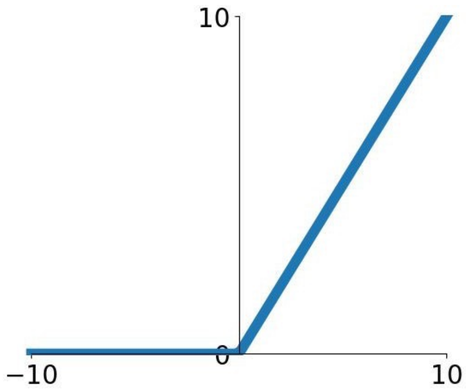


tanh(x)

- Squashes numbers to range [-1,1]
- still kills gradients when saturated :(

[LeCun et al., 1991]

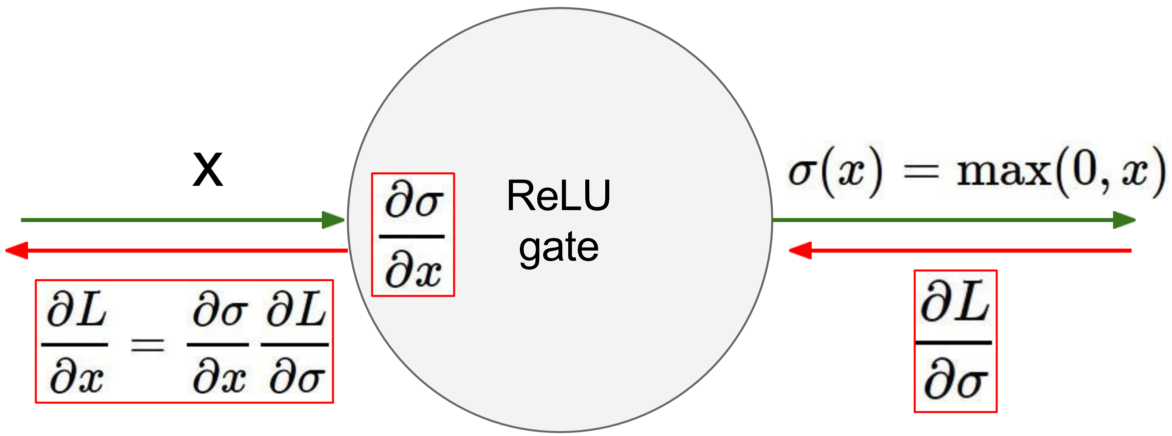
Activation Functions

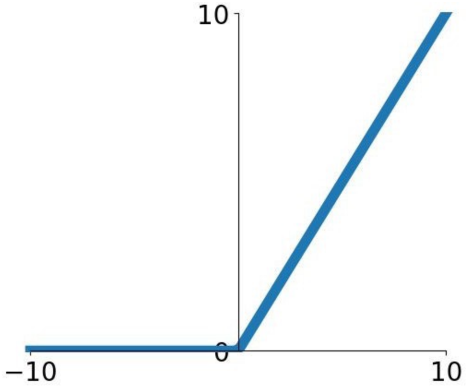


ReLU
(Rectified Linear Unit)

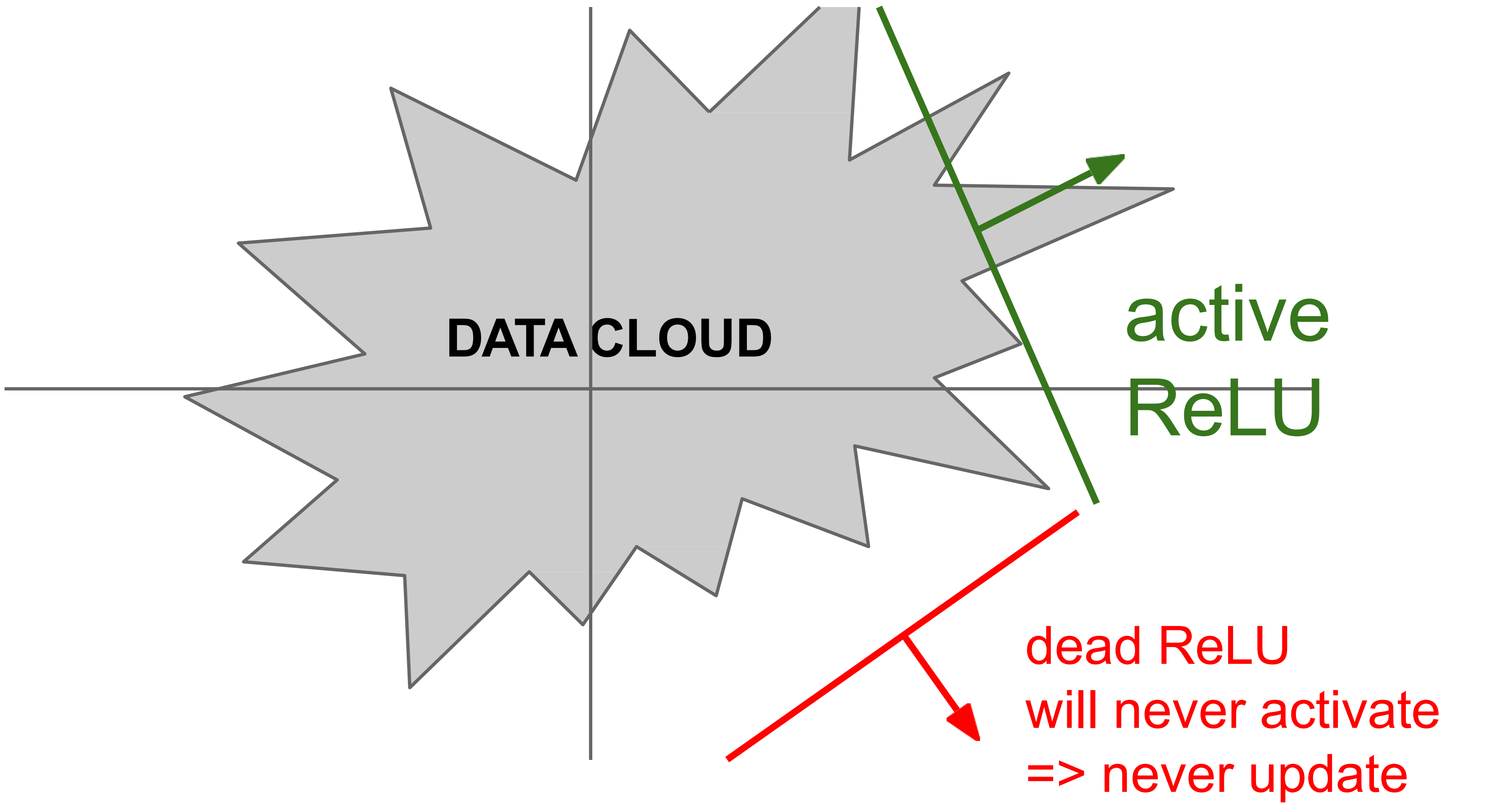
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

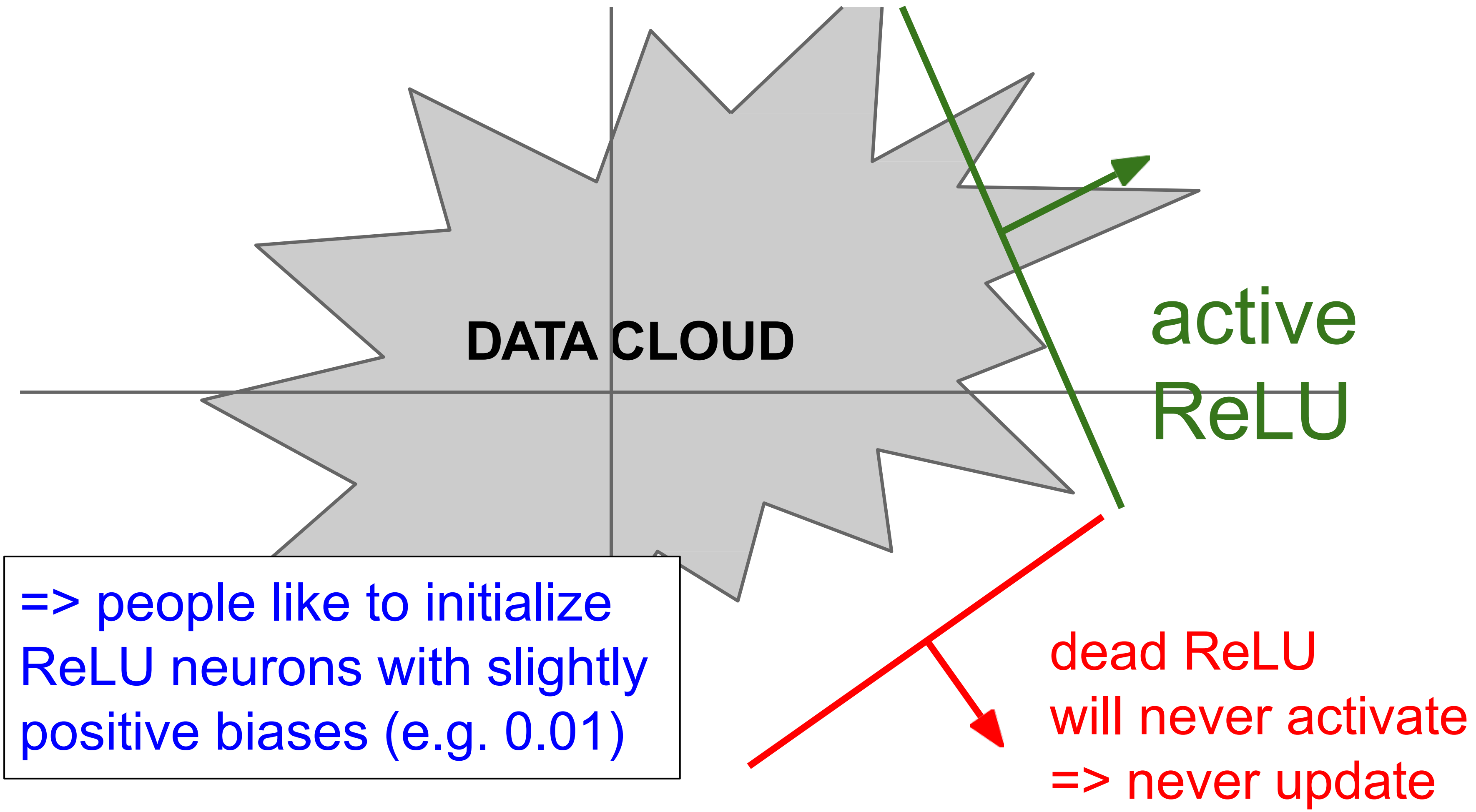
[Krizhevsky et al., 2012]





What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

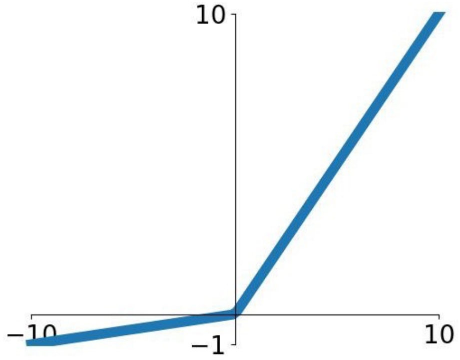

DATA CLOUD
active
ReLU
dead ReLU
will never activate
=> never update



=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

Activation Functions

[Mass et al., 2013]
[He et al., 2015]



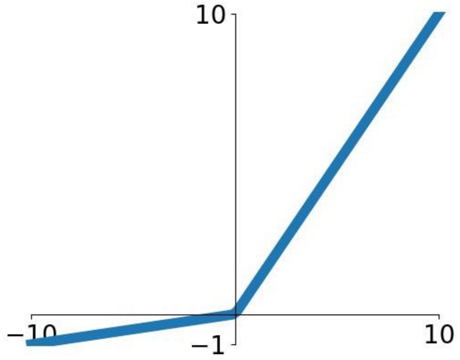
Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Activation Functions

[Mass et al., 2013]
[He et al., 2015]



Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Parametric Rectifier (PReLU)

$$f(x) = \max(\alpha x, x)$$

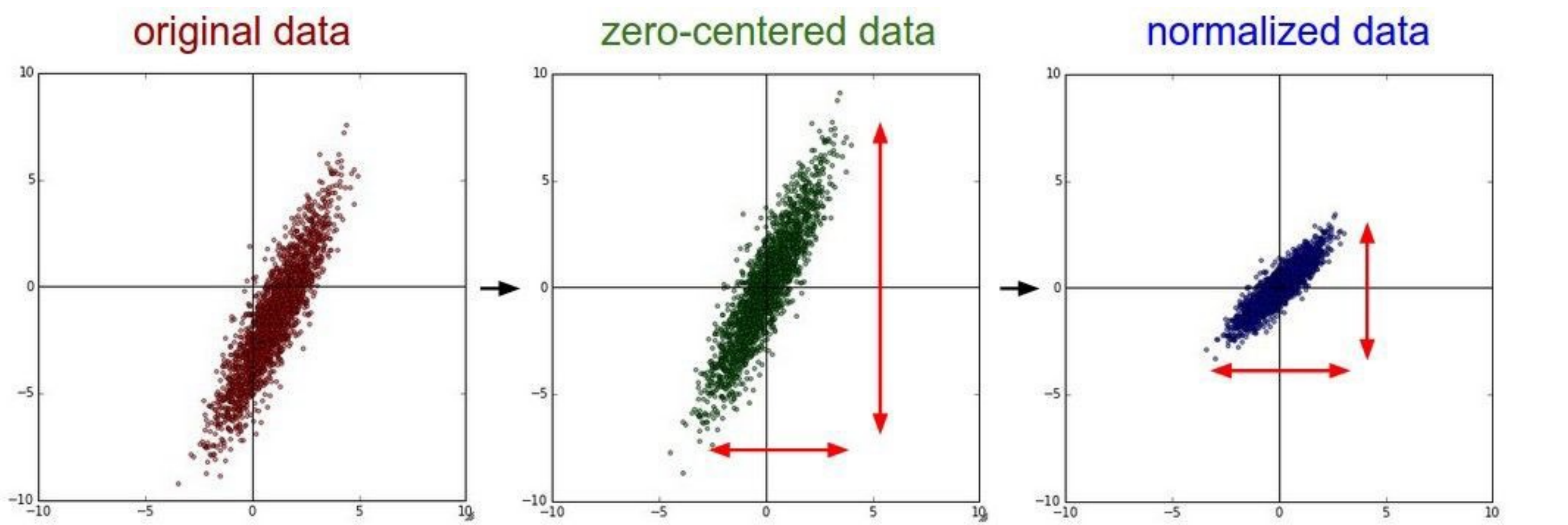
backprop into \alpha
(parameter)

TLDR: In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU
  - To squeeze out some marginal gains
- Don't use sigmoid or tanh

Data Preprocessing

Data Preprocessing



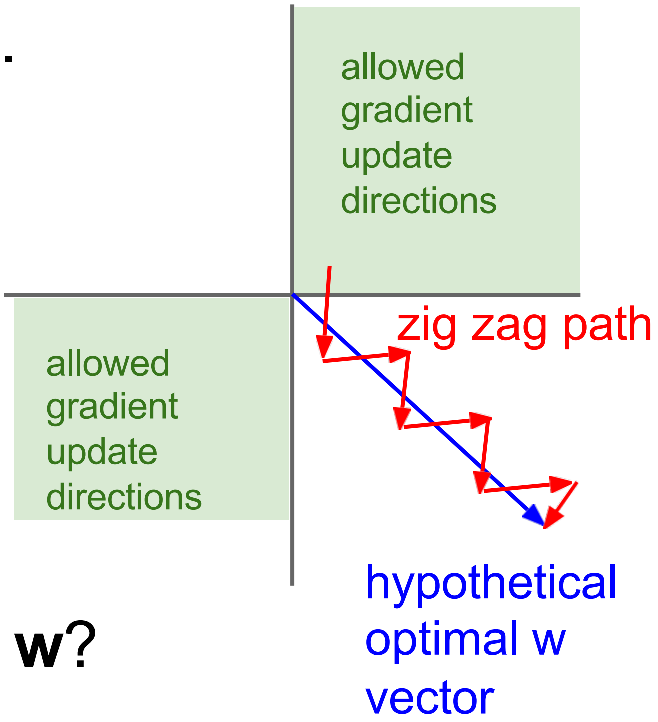

```
X -= np.mean(X, axis = 0)
```

```
X /= np.std(X, axis = 0)
```

(Assume X [NxD] is data matrix,
each example in a row)

Remember: Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b\right)$$

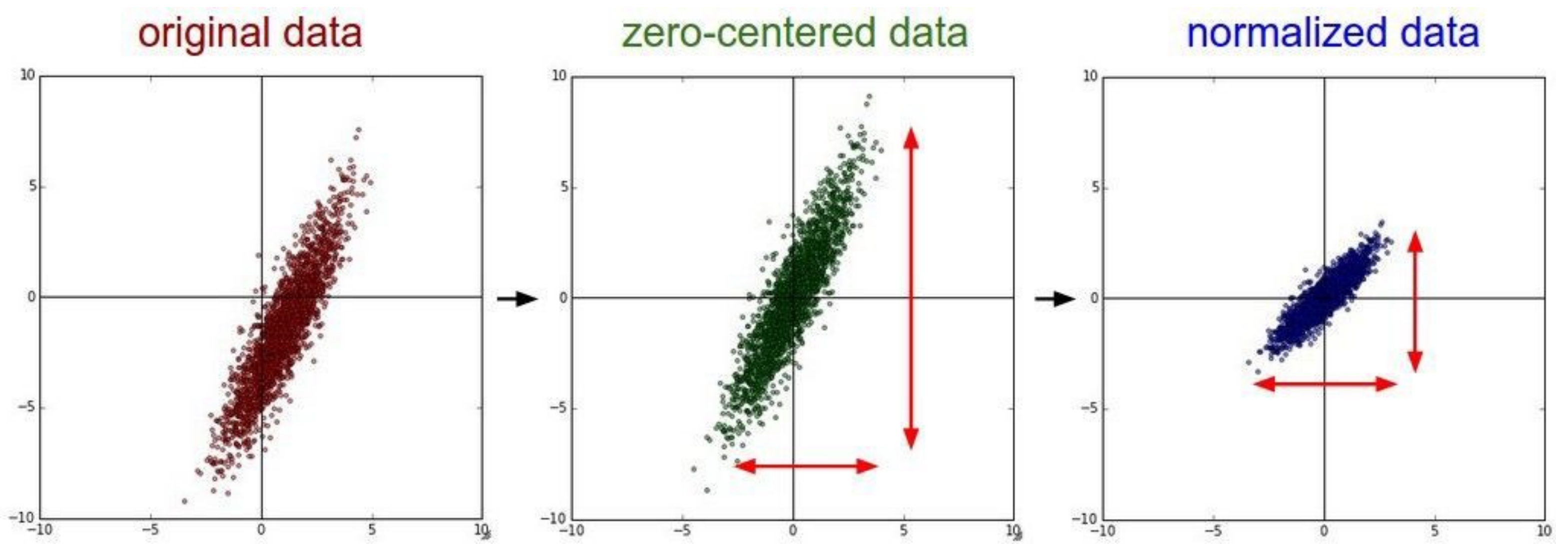


What can we say about the gradients on **w**?

Always all positive or all negative :(

(this is also why you want zero-mean data!)

Data Preprocessing



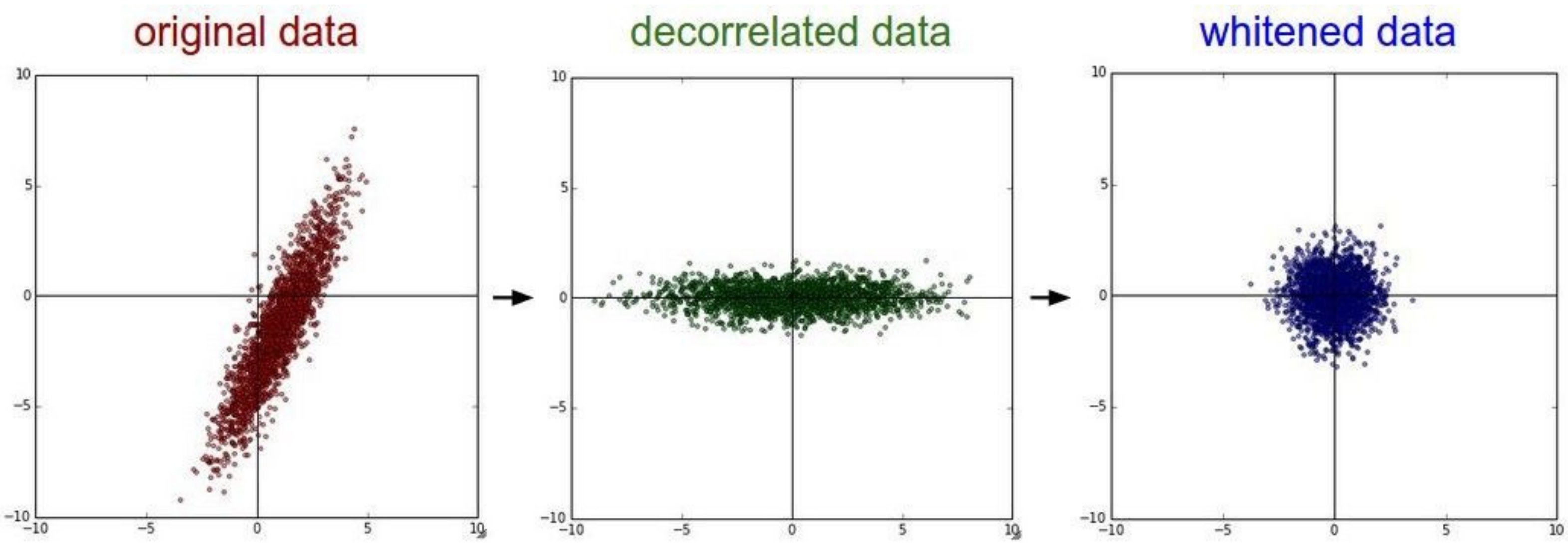

```
X -= np.mean(X, axis = 0)
```

```
X /= np.std(X, axis = 0)
```

(Assume X [NxD] is data matrix, each example in a row)

Data Preprocessing

In practice, you may also see **PCA** and **Whitening** of the data

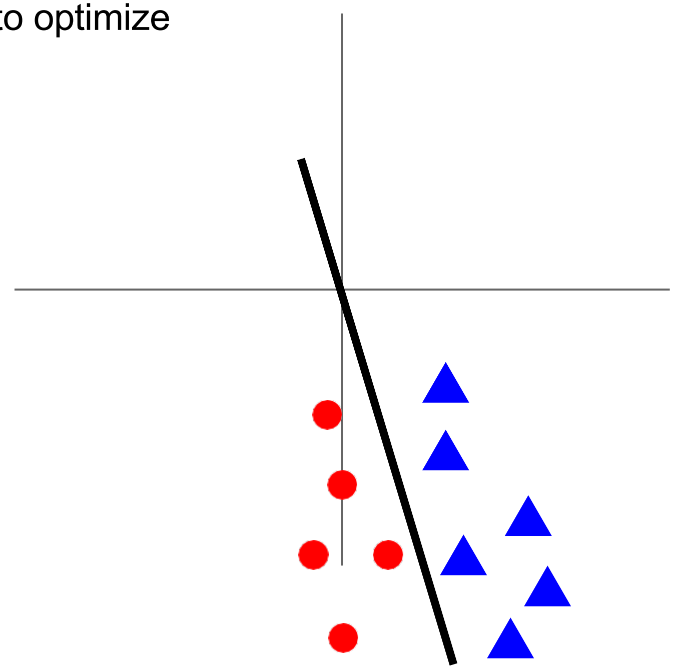


(data has diagonal covariance matrix)

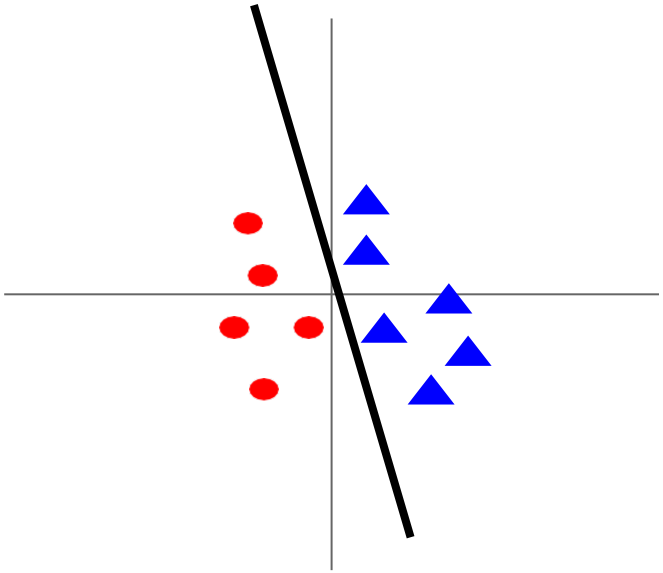
(covariance matrix is the identity matrix)

Data Preprocessing

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize



After normalization: less sensitive to small changes in weights; easier to optimize



TLDR: In practice for Images: center only

e.g. consider CIFAR-10 example with [32,32,3] images

- Subtract the mean image (e.g. AlexNet)
  (mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet)
  (mean along each channel = 3 numbers)
- Subtract per-channel mean and
  Divide by per-channel std (e.g. ResNet)
  (mean along each channel = 3 numbers)

Not common to do PCA or whitening

Batch Normalization

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want zero-mean unit-variance activations? just make them so."

consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

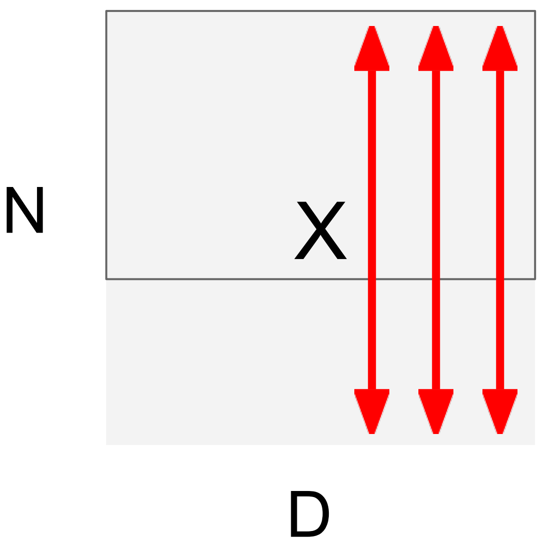
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



$$\mu_j = \frac{1}{N} \sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

$$\mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization: Test-Time

Estimates depend on minibatch; can't do this at test-time!

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

$$\mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization: Test-Time

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

During testing batchnorm becomes a linear operator! Can be fused with the previous fully-connected or conv layer

$\mu_j =$ (Running) average of values seen during training — Per-channel mean, shape is D

$\sigma_j^2 =$ (Running) average of values seen during training — Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

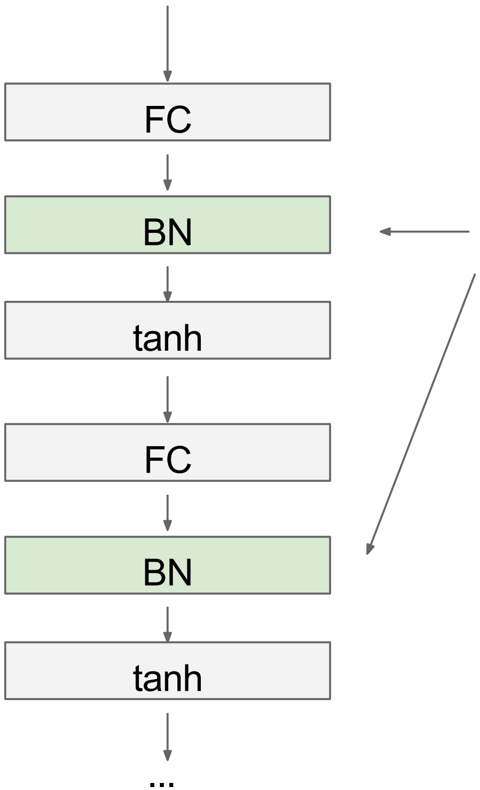
Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization

[Ioffe and Szegedy, 2015]

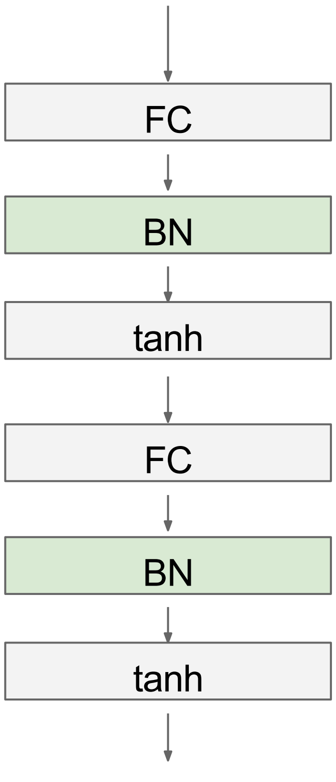


Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Batch Normalization

[Ioffe and Szegedy, 2015]



- Makes deep networks **much** easier to train!
- Improves gradient flow
- Allows higher learning rates, faster convergence
- Networks become more robust to initialization
- Acts as regularization during training
- Zero overhead at test-time: can be fused with conv!
- Behaves differently during training and testing: this is a very common source of bugs!

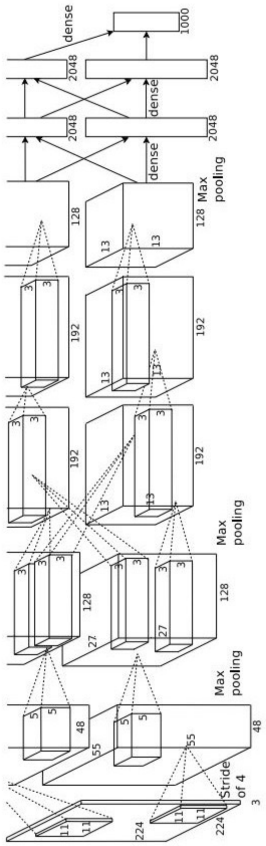
Transfer learning

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

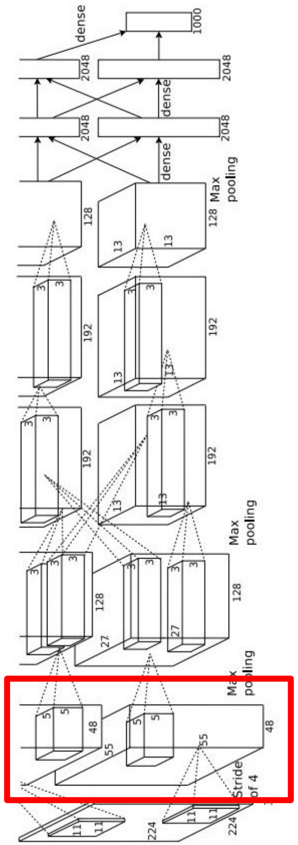
“You need a lot of a data if you want to train/use CNNs”

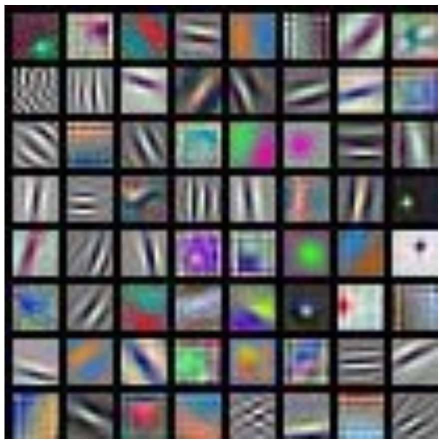
BUSTED

Transfer Learning with CNNs



Transfer Learning with CNNs

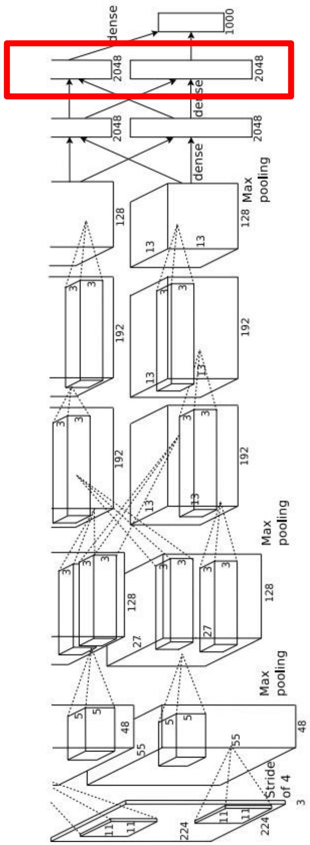




AlexNet:
64 x 3 x 11 x 11

(More on this in Lecture 13)

Transfer Learning with CNNs



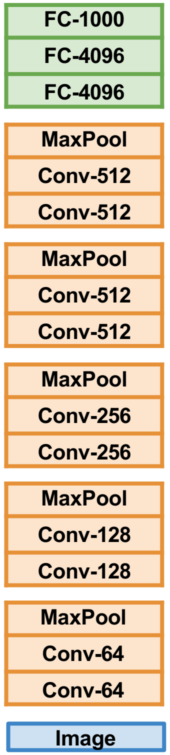
Test image L2 Nearest neighbors in <u>feature</u> space

(More on this in Lecture 13)

Transfer Learning with CNNs

Donahue et al, “DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition”, ICML 2014
Razavian et al, “CNN Features Off-the-Shelf: An Astounding Baseline for Recognition”, CVPR Workshops 2014

1. Train on Imagenet



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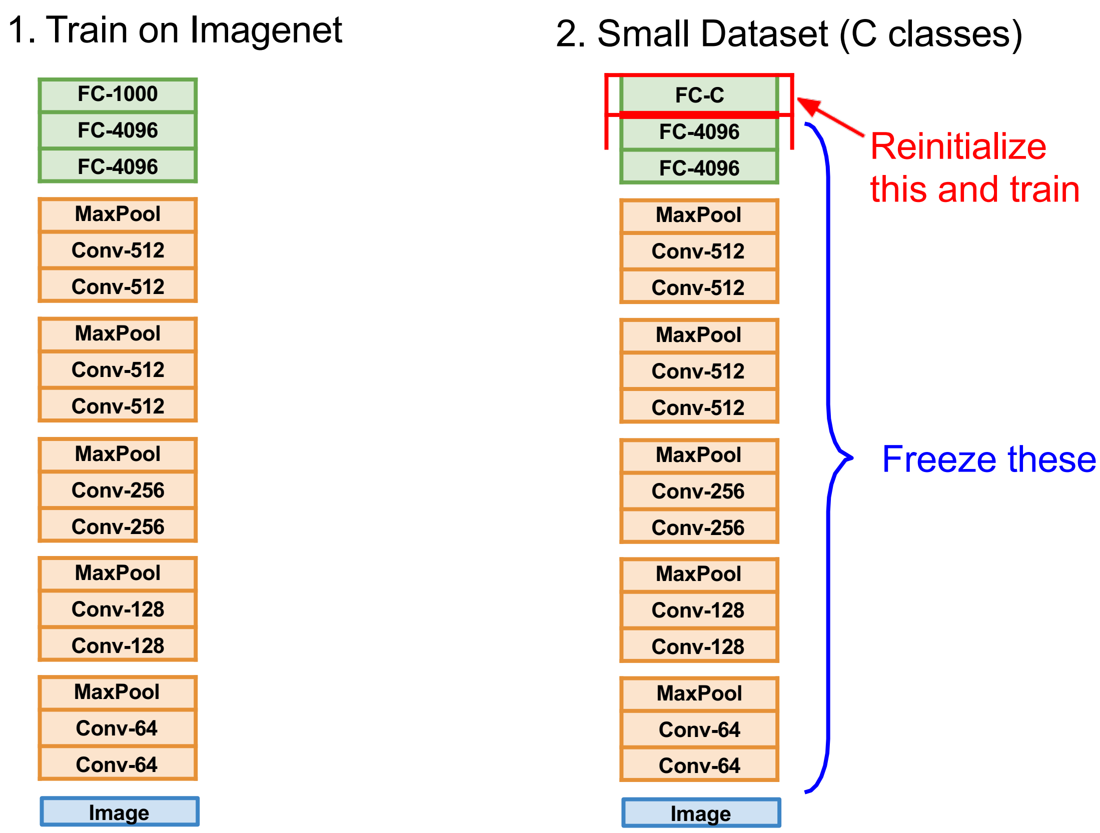
Transfer Learning with CNNs



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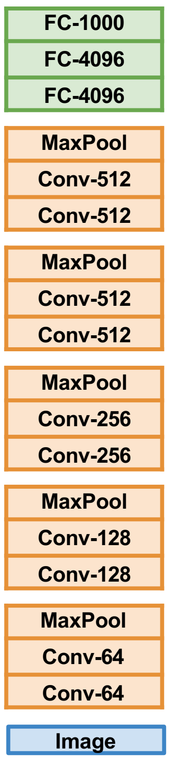
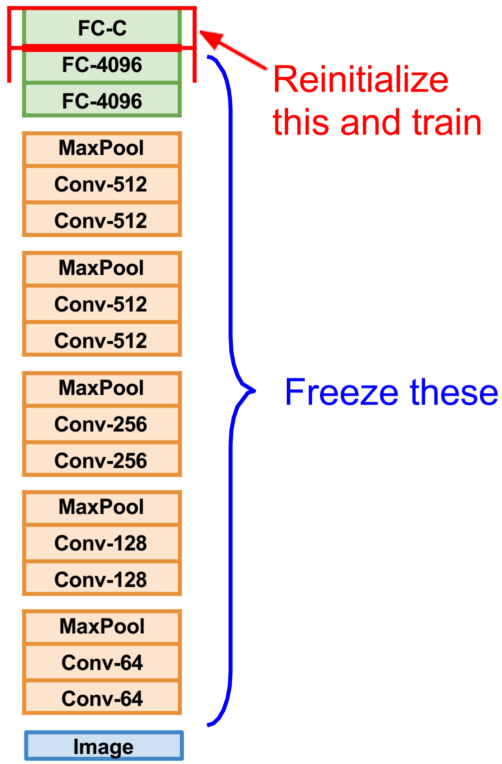
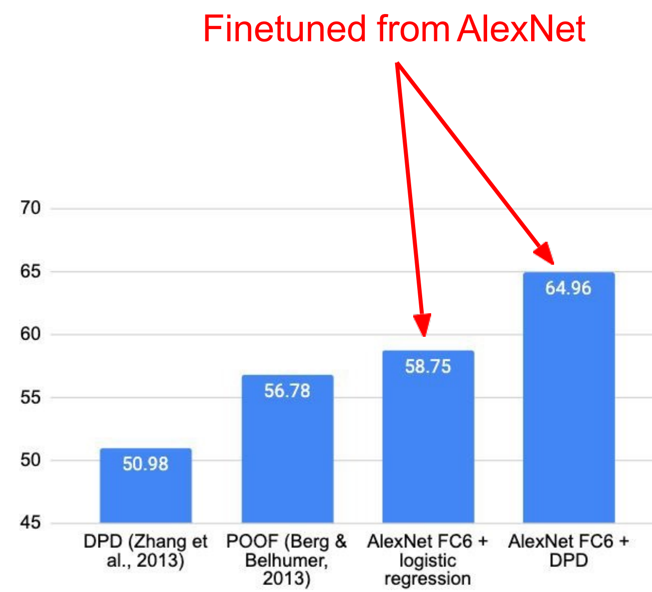
Transfer Learning with CNNs

1. Train on Imagenet



2. Small Dataset (C classes)



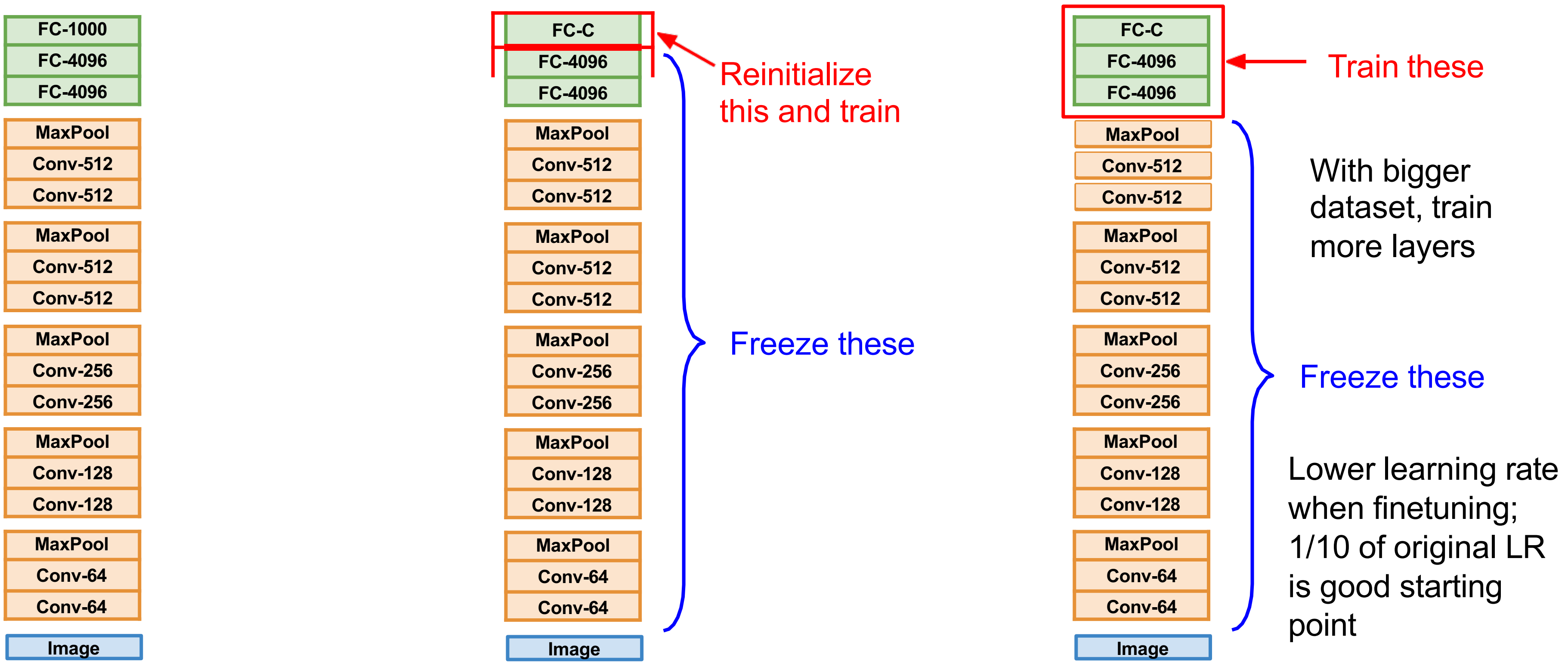


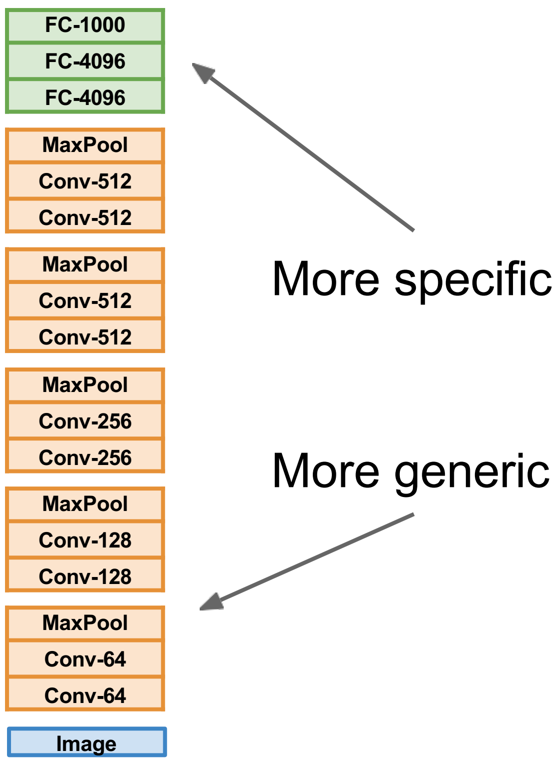
Donahue et al, “DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition”, ICML 2014

Transfer Learning with CNNs

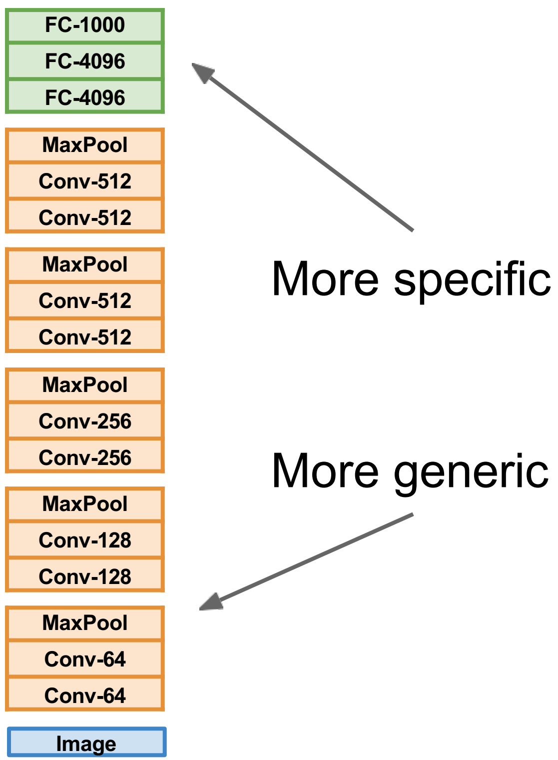
Donahue et al, “DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition”, ICML 2014
Razavian et al, “CNN Features Off-the-Shelf: An Astounding Baseline for Recognition”, CVPR Workshops 2014

1. Train on Imagenet
2. Small Dataset (C classes)
3. Bigger dataset

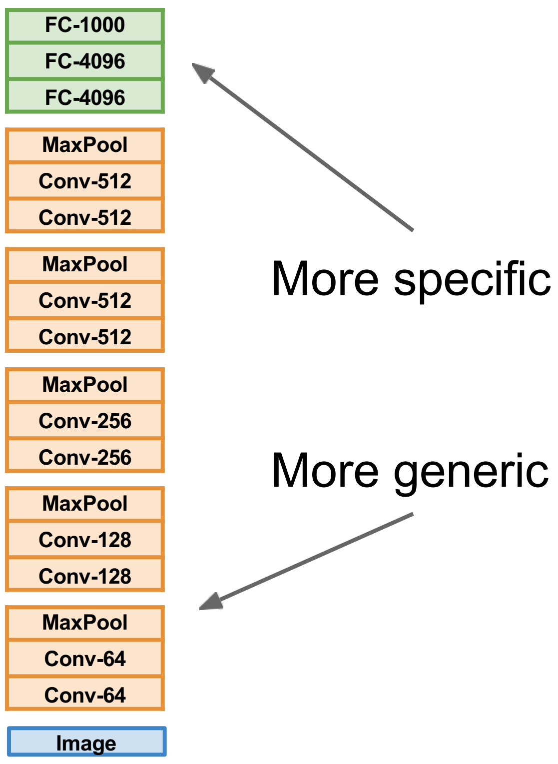




	very similar dataset	**very different dataset**
very little data	?	?
quite a lot of data	?	?



	very similar dataset	**very different dataset**
very little data	Use Linear Classifier on top layer	?
quite a lot of data	Finetune a few layers	?



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

Summary
We looked in detail at:

TLDRs

- Activation Functions (use ReLU)
- Data Preprocessing (images: subtract mean)
- Batch Normalization (use this!)
- Transfer learning (use this if you can!)