

# Lecture 7: Training Neural Networks

# Administrative: assignments

A2 is out, due Monday May 8th, 11:59pm

[Important] Q6 is moved from A2 to A3, please re-download the assignment if you have the version before the change

We are working on grading A1 by the end of the week

Where we are now...

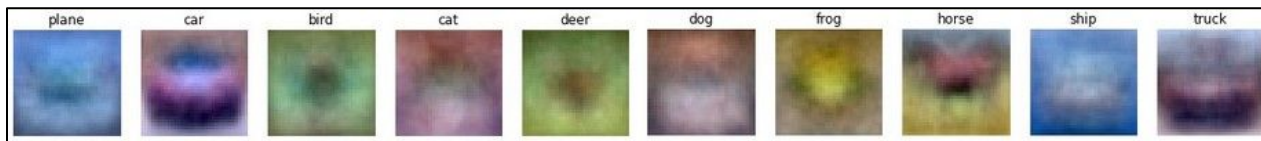
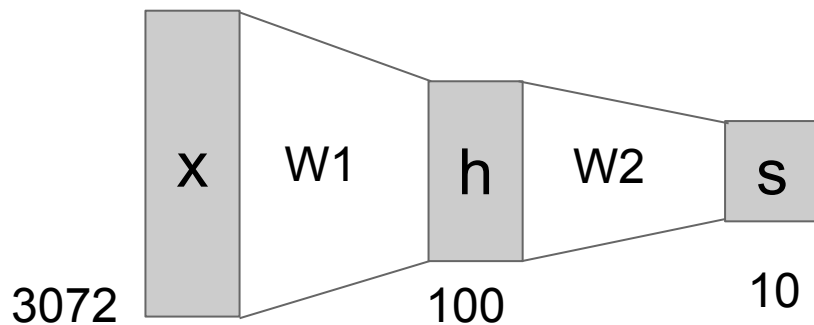
## Neural Networks

Linear score function:

$$f = Wx$$

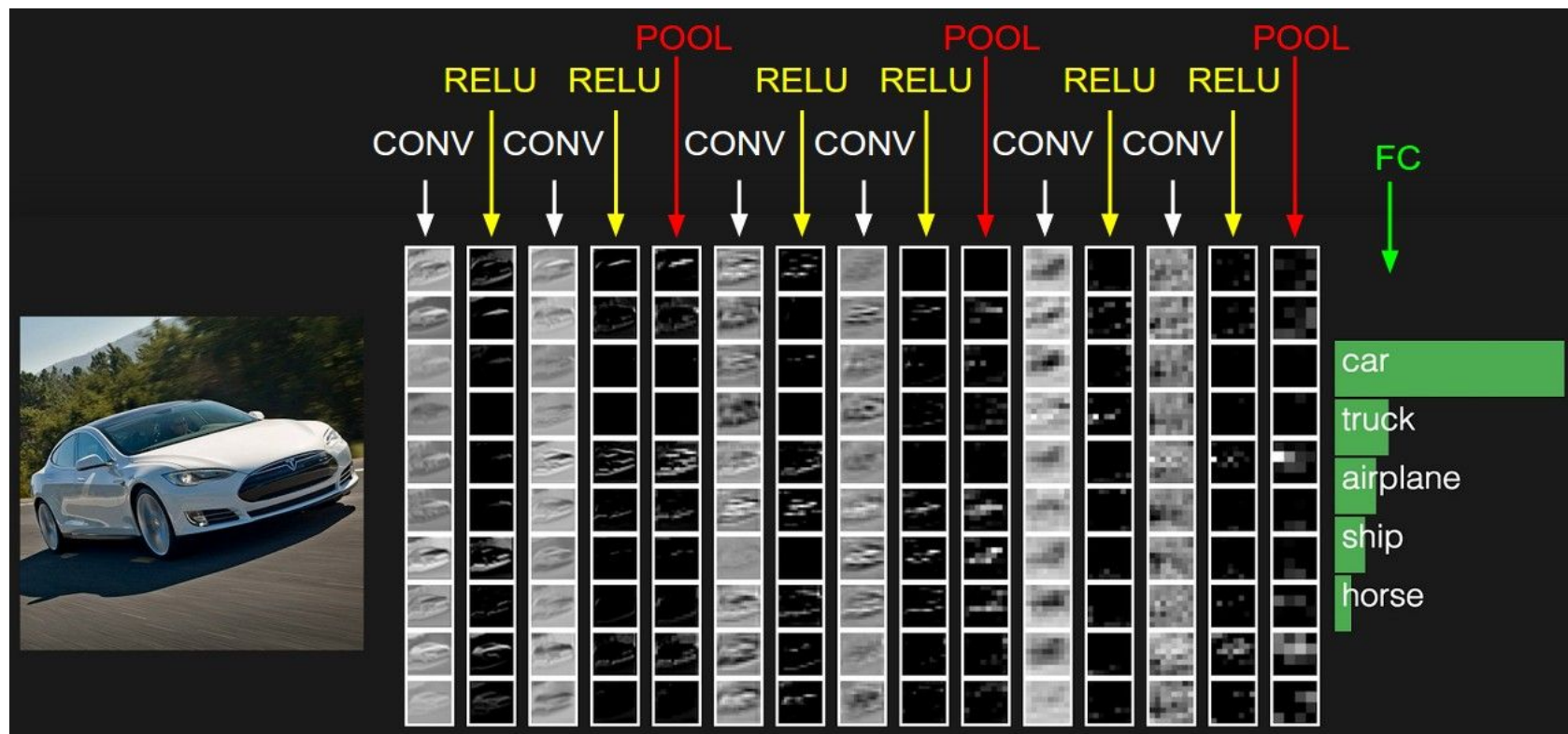
2-layer Neural Network

$$f = W_2 \max(0, W_1 x)$$



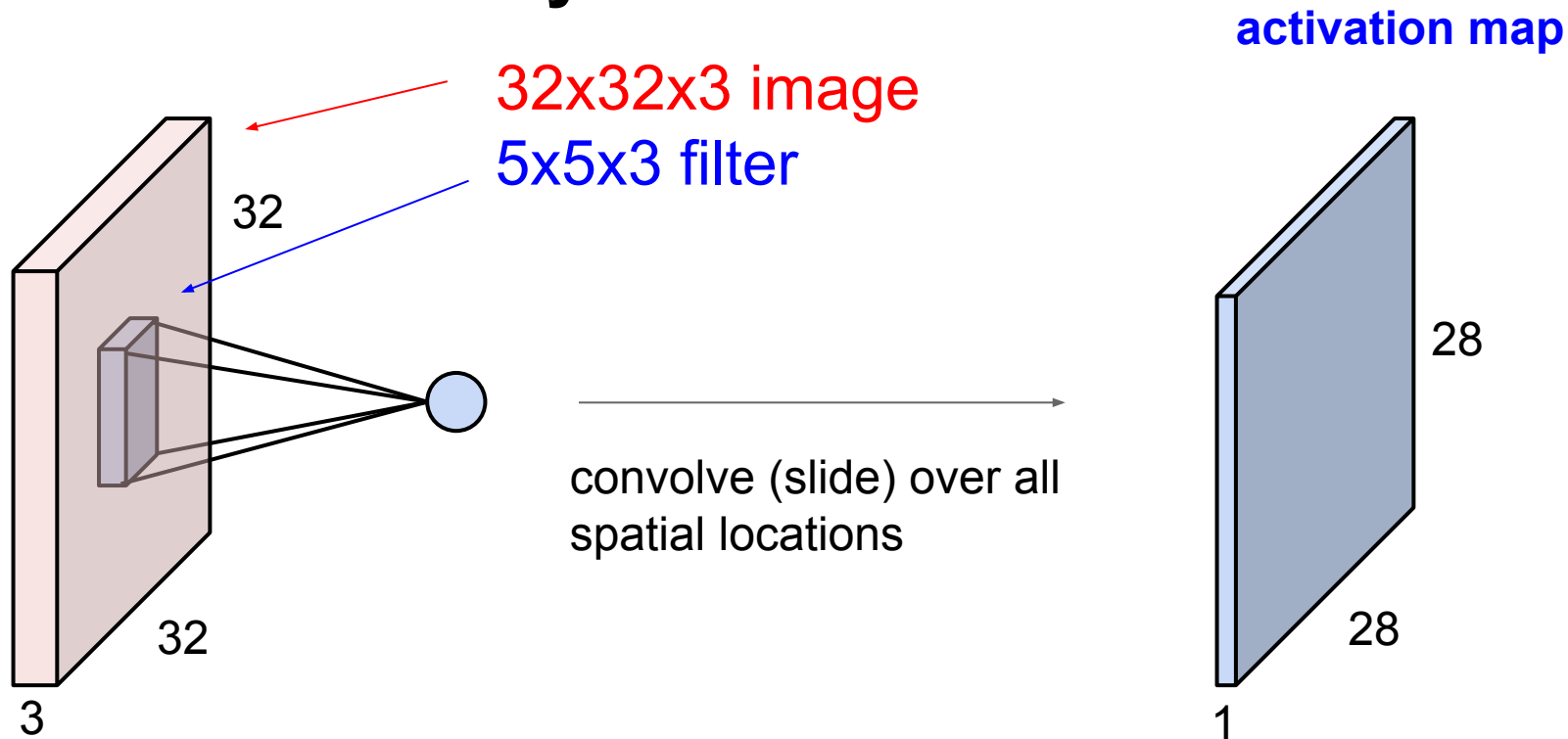
Where we are now...

# Convolutional Neural Networks



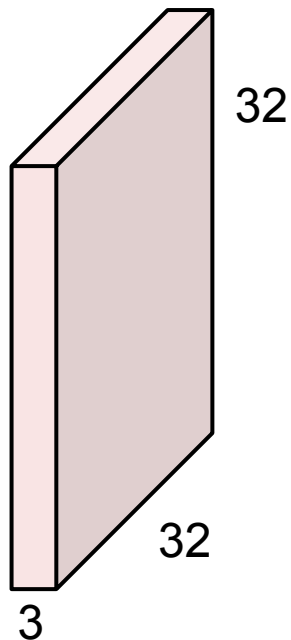
Where we are now...

## Convolutional Layer

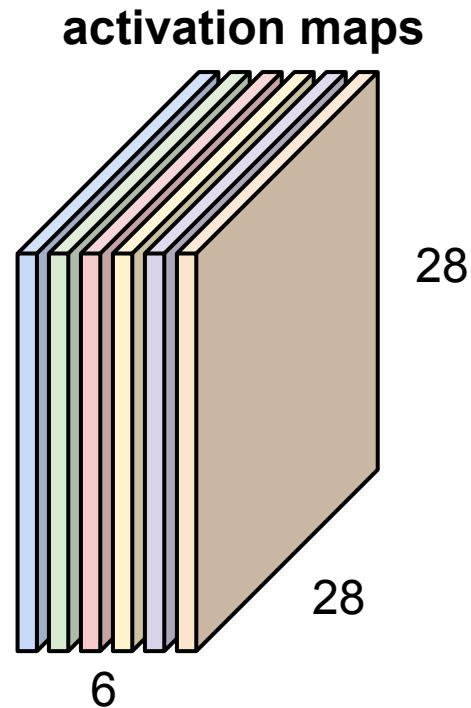


Where we are now...

## Convolutional Layer



Convolution Layer



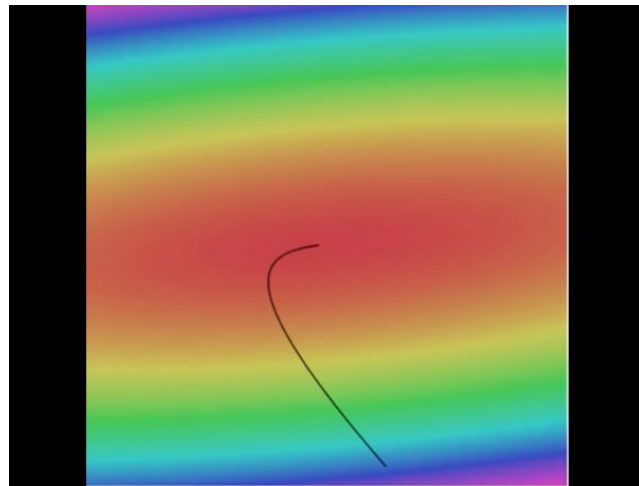
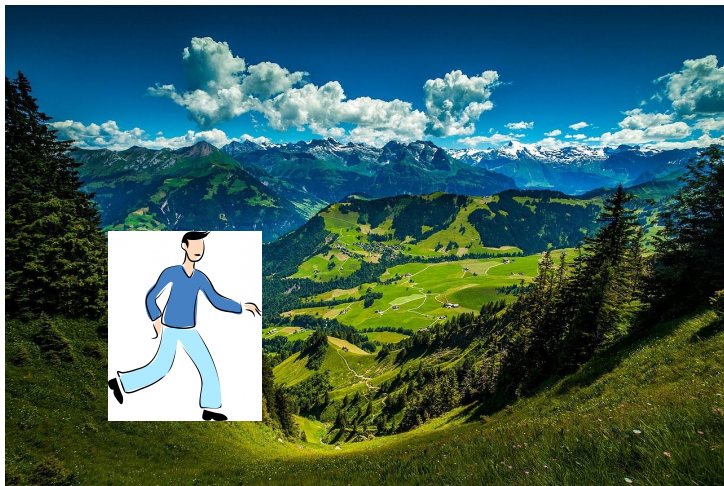
We stack these up to get a “new image” of size 28x28x6!

For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



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
```

[Landscape image](#) is [CC0 1.0](#) public domain

[Walking man image](#) is [CC0 1.0](#) public domain



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

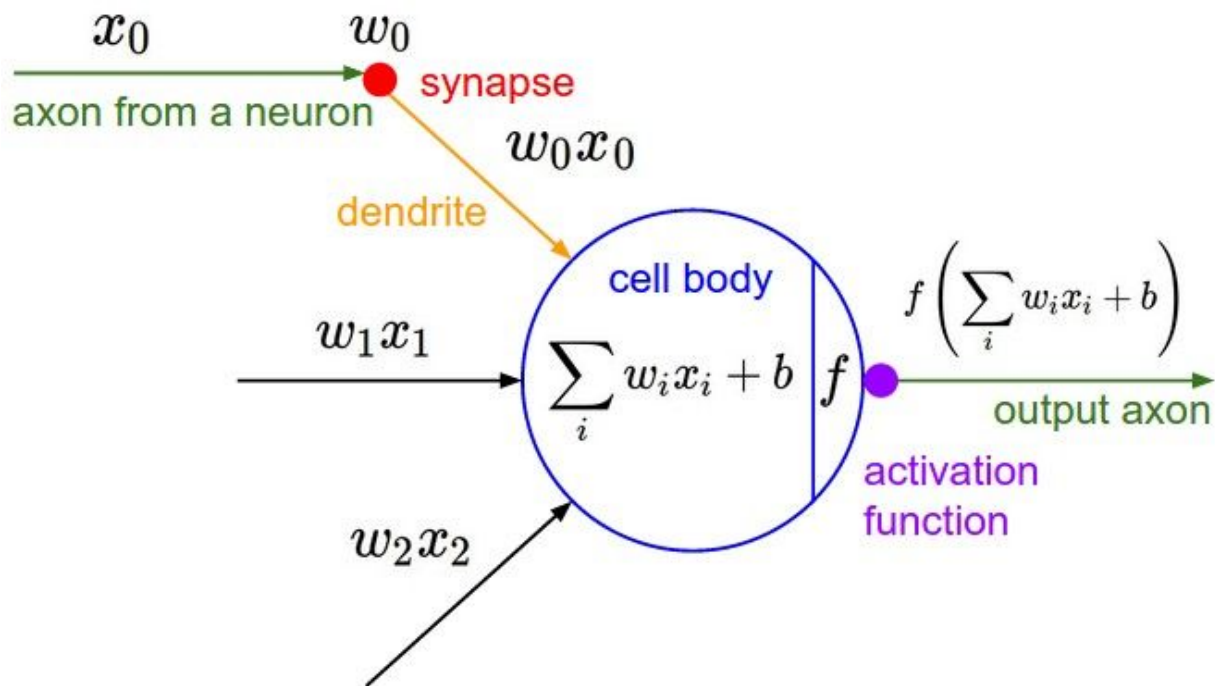
# Today: Training Neural Networks

# Overview

1. **One time set up:** activation functions, preprocessing, weight initialization, regularization, gradient checking
2. **Training dynamics:** babysitting the learning process, parameter updates, hyperparameter optimization
3. **Evaluation:** model ensembles, test-time augmentation, transfer learning

# Activation Functions

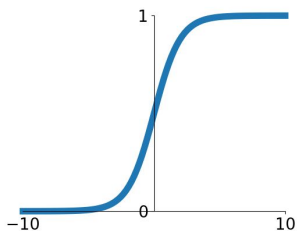
# Activation Functions



# Activation Functions

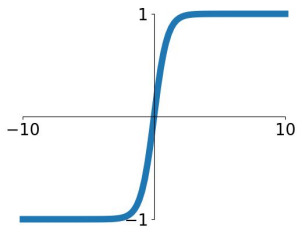
## Sigmoid

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



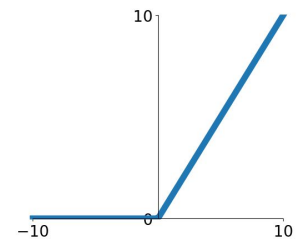
## tanh

$$\tanh(x)$$



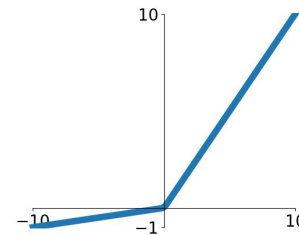
## ReLU

$$\max(0, x)$$



## Leaky ReLU

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

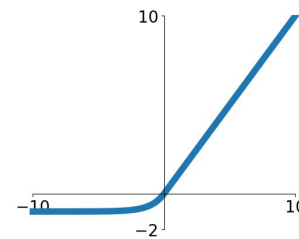


## Maxout

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

## ELU

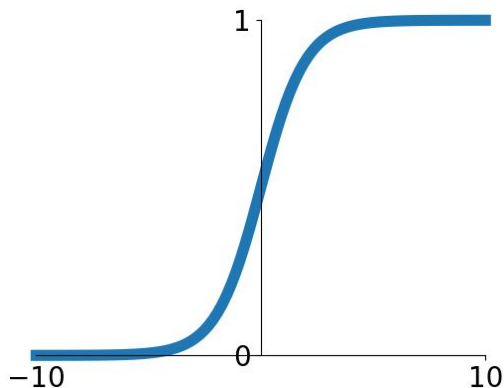
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# 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

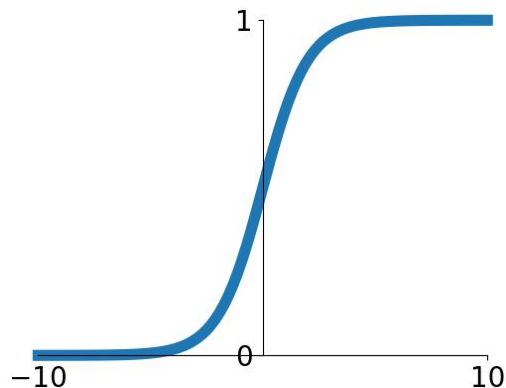


**Sigmoid**

# Activation Functions

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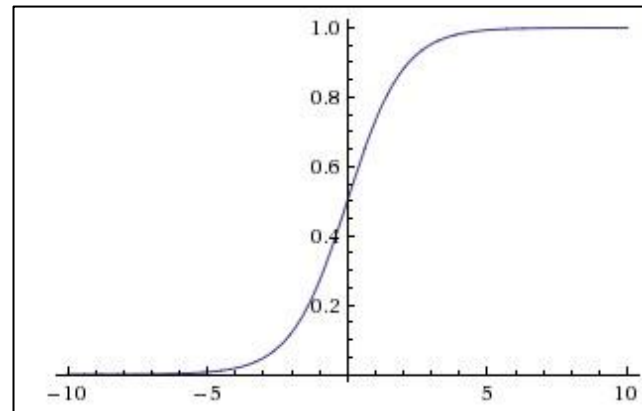
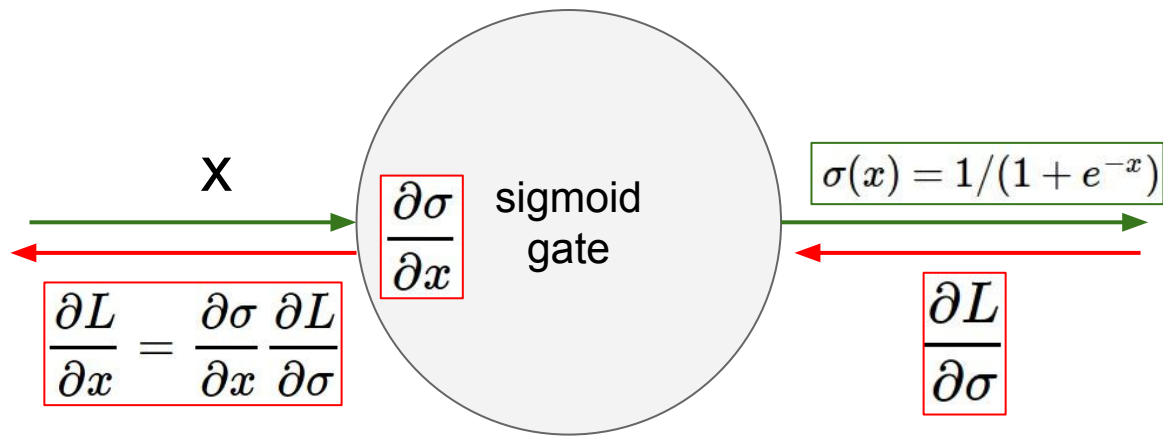


**Sigmoid**

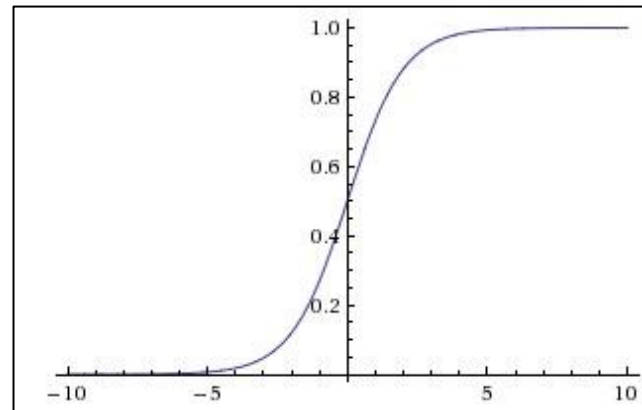
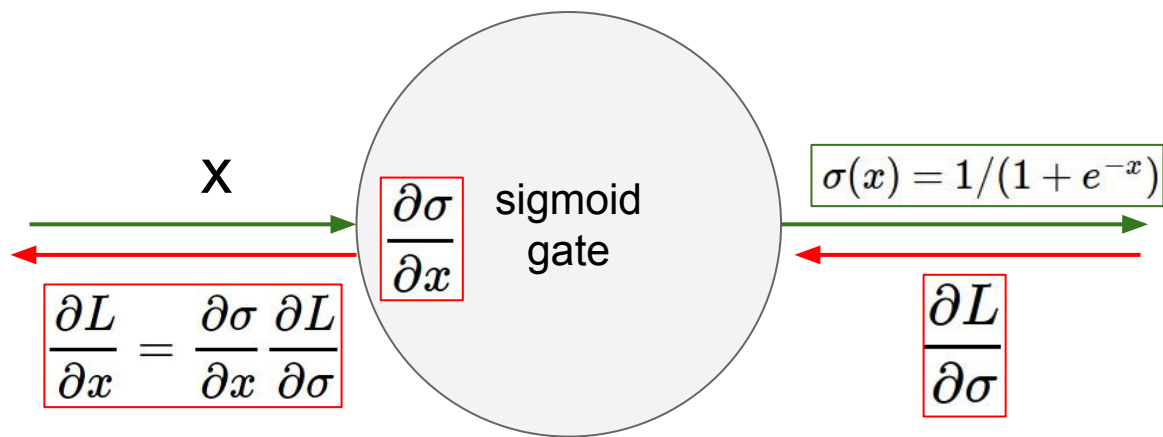
3 problems:

1. Saturated neurons “kill” the gradients



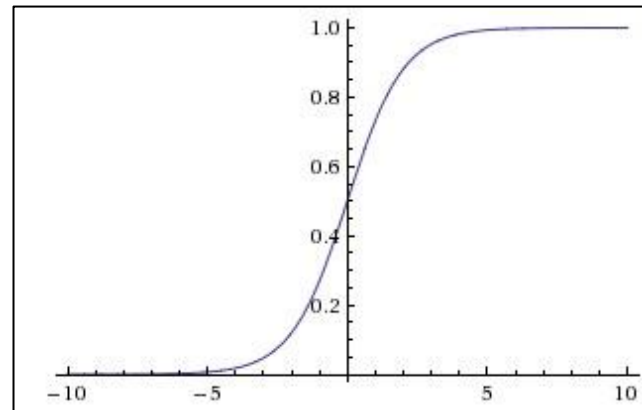
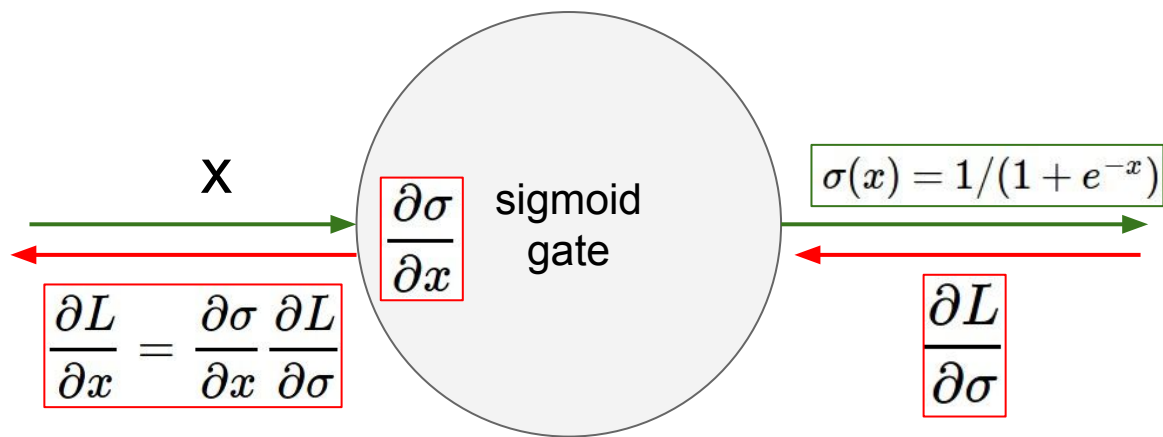


$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x) (1 - \sigma(x))$$



What happens when  $x = -10$ ?

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

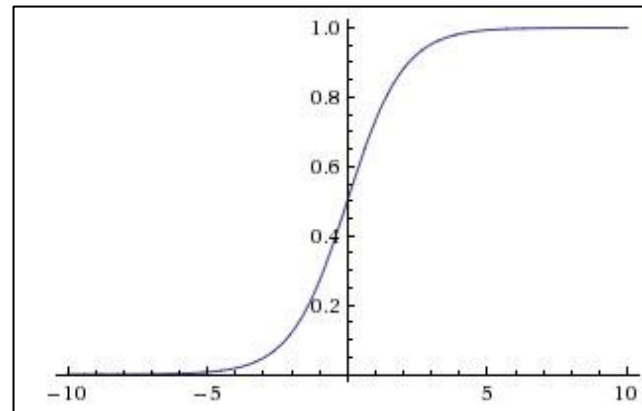
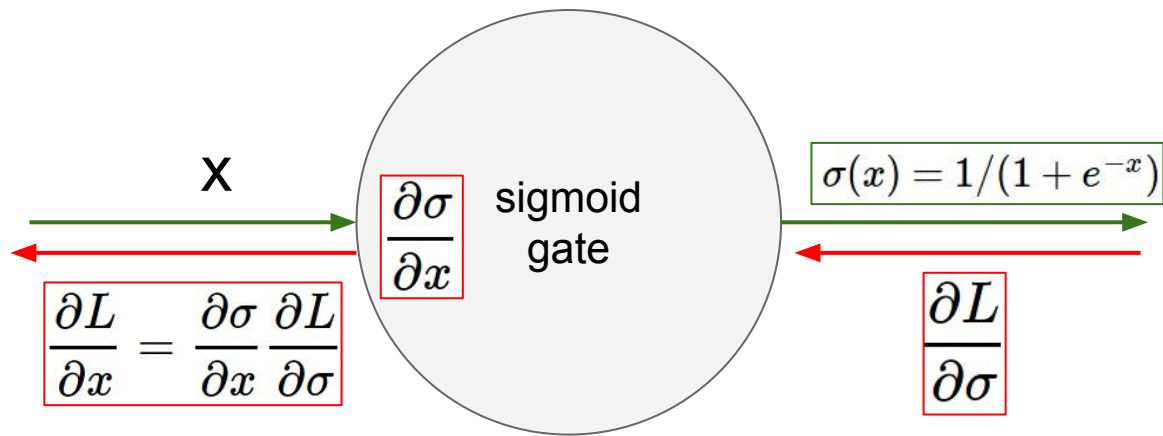


What happens when  $x = -10$ ?

$$\sigma(x) \approx 0$$

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

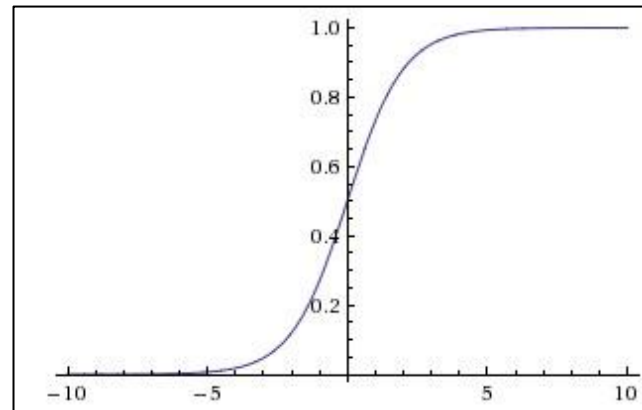
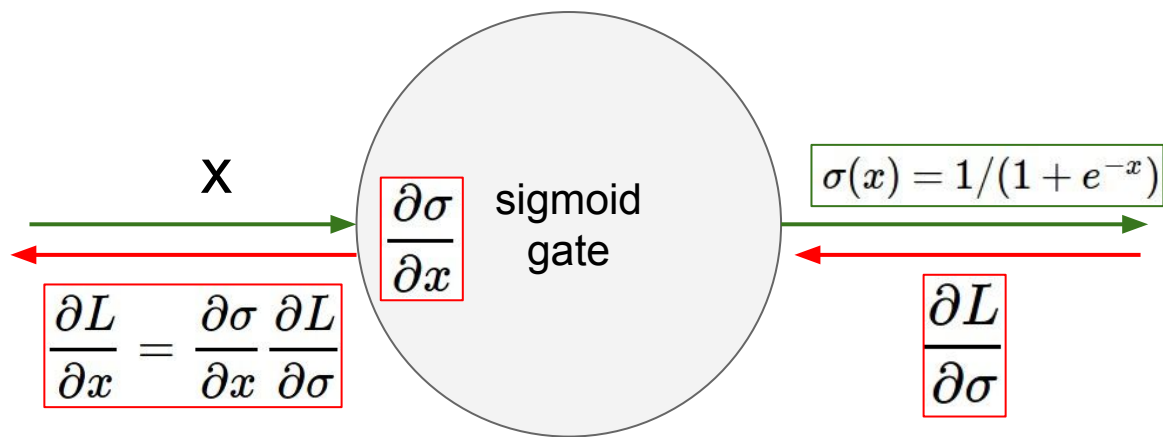
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What happens when  $x = 0$ ?

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



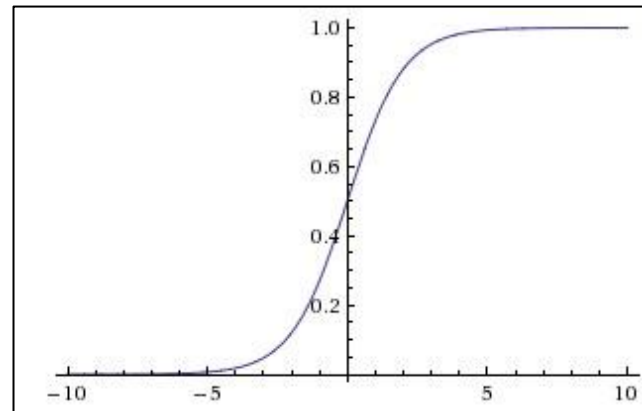
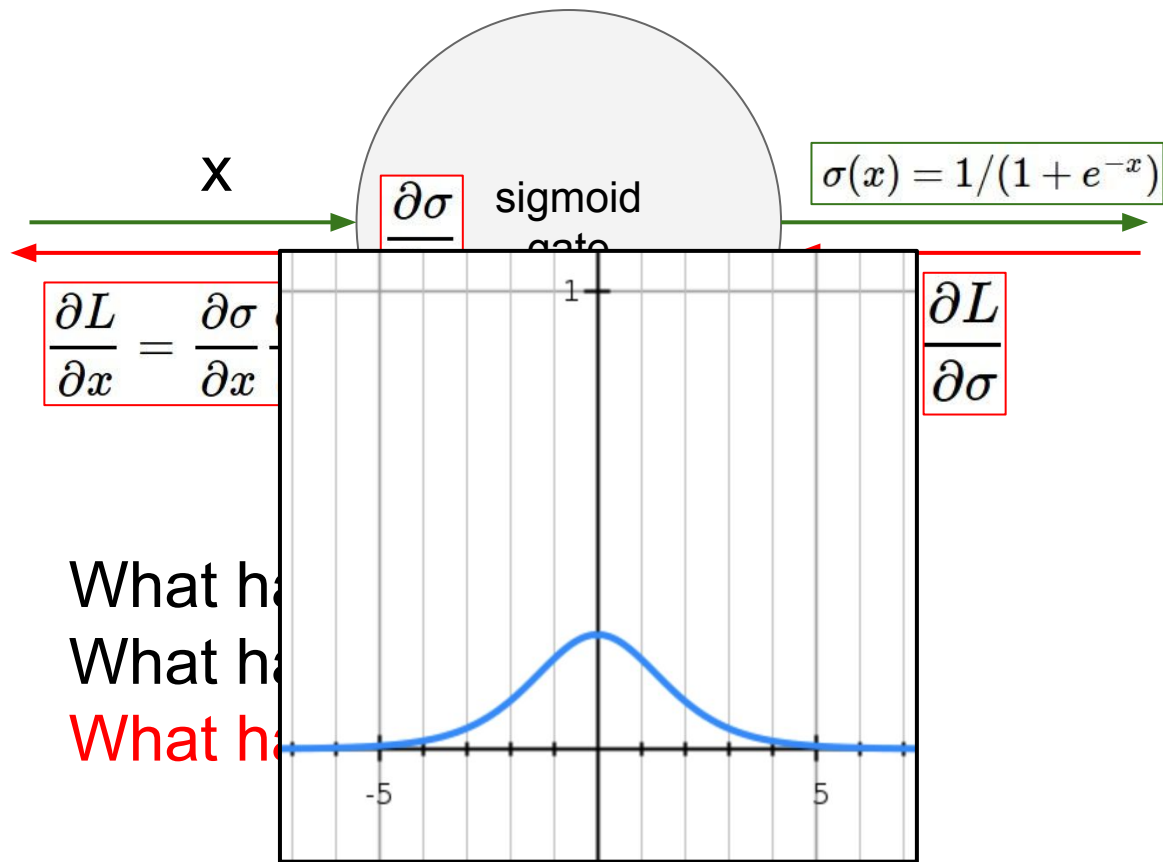
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What happens when  $x = 0$ ?

What happens when  $x = 10$ ?

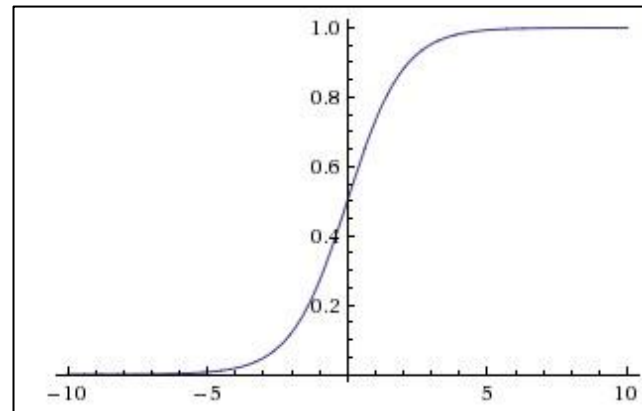
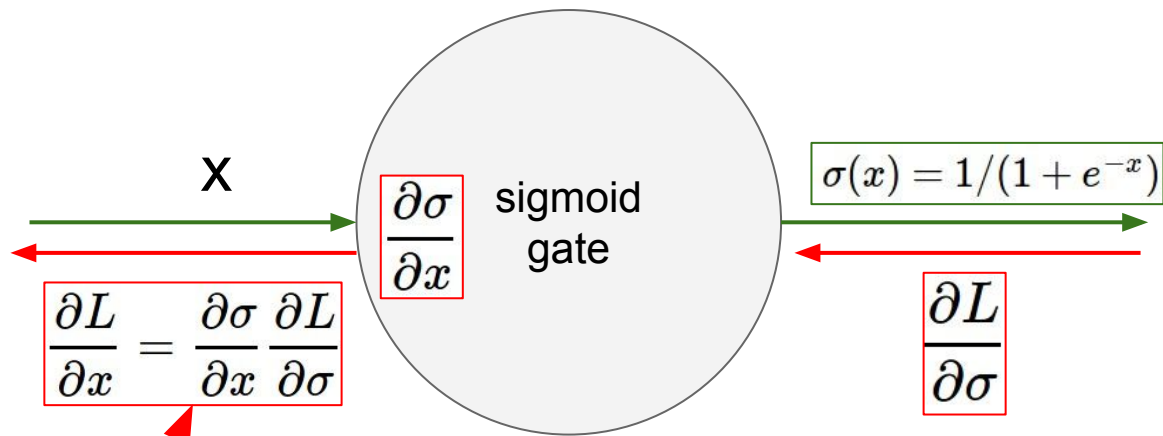
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x) (1 - \sigma(x))$$

$$\sigma(x) \approx 1 \quad \frac{\partial \sigma(x)}{\partial x} = \sigma(x) (1 - \sigma(x)) = 1(1 - 1) = 0$$



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

What has  
 What has  
 What has



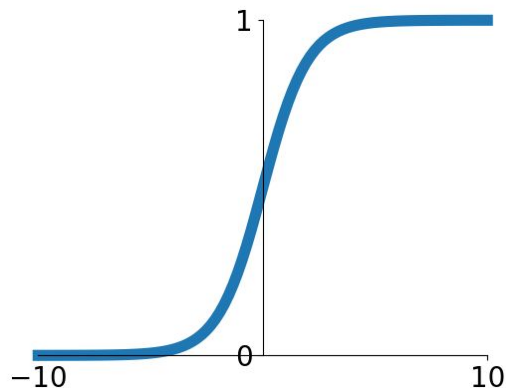
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x) (1 - \sigma(x))$$

Why is this a problem?

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

# Activation Functions

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



**Sigmoid**

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

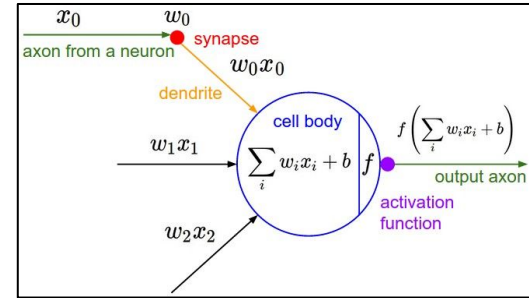
3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered



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

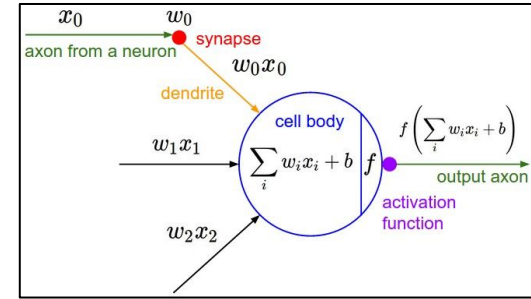
$$f\left(\sum_i w_i x_i + b\right)$$



What can we say about the gradients on  $\mathbf{w}$ ?

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

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

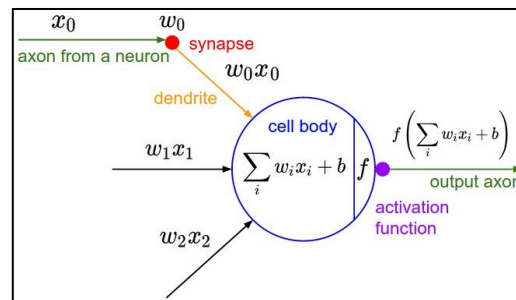


What can we say about the gradients on  $\mathbf{w}$ ?

$$\frac{\partial L}{\partial w} = \sigma\left(\sum_i w_i x_i + b\right)\left(1 - \sigma\left(\sum_i w_i x_i + b\right)\right)x \times \textit{upstream\_gradient}$$

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

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



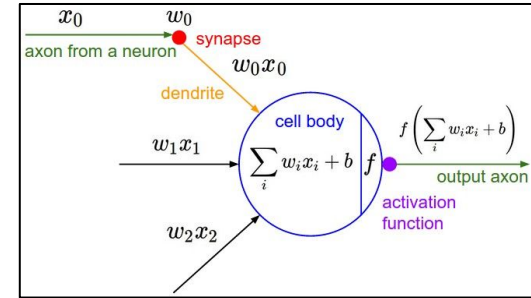
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We know that local gradient of sigmoid is always positive

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What can we say about the gradients on  $\mathbf{w}$ ?

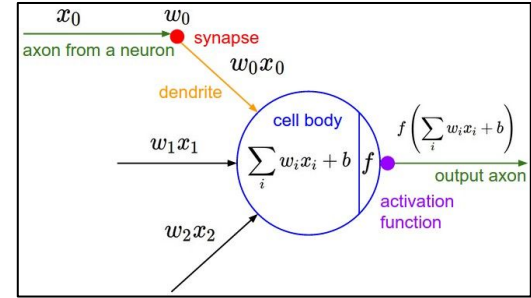
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We are assuming  $x$  is always positive

$$\frac{\partial L}{\partial w} = \sigma\left(\sum_i w_i x_i + b\right) \left(1 - \sigma\left(\sum_i w_i x_i + b\right)\right) x \times \text{upstream\_gradient}$$

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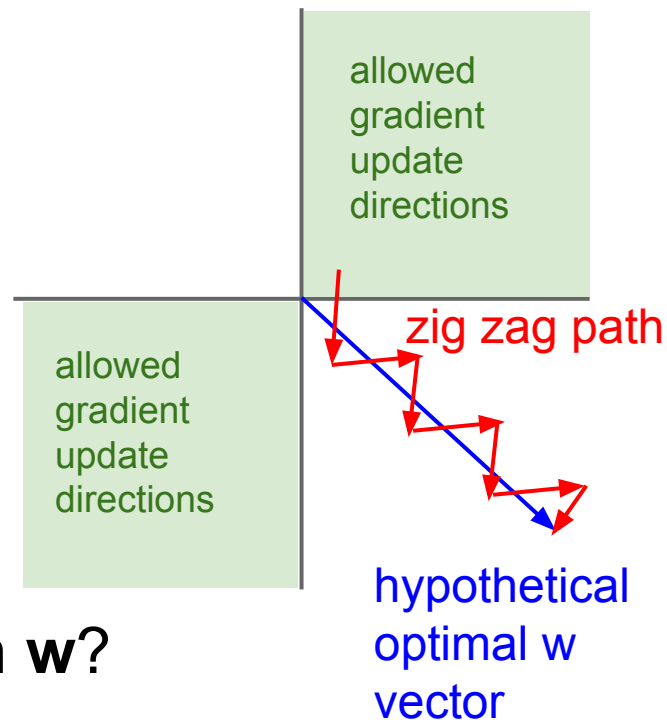
We are assuming  $x$  is always positive

So!! Sign of gradient for all  $w_i$  is the same as the sign of upstream scalar gradient!

$$\frac{\partial L}{\partial w} = \sigma\left(\sum_i w_i x_i + b\right) \left(1 - \sigma\left(\sum_i w_i x_i + b\right)\right) x \times \text{upstream\_gradient}$$

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

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

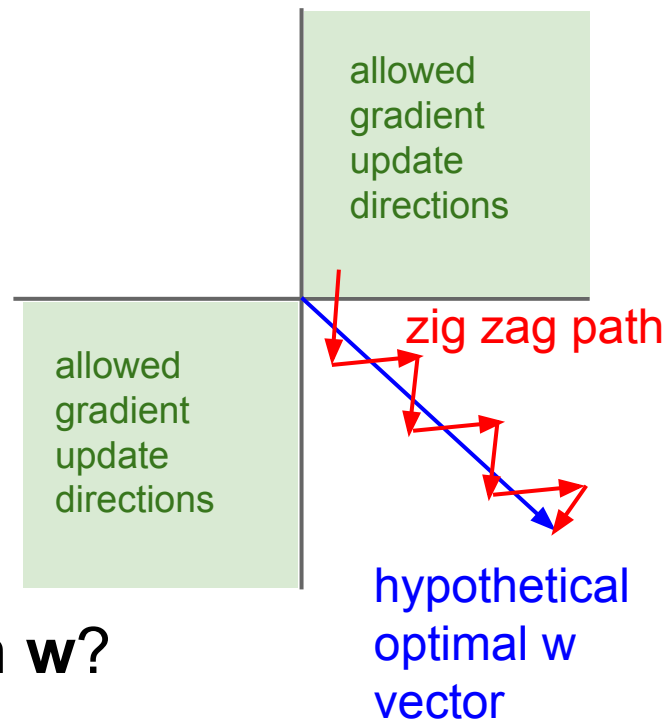


What can we say about the gradients on  $\mathbf{w}$ ?

Always all positive or all negative :(

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

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



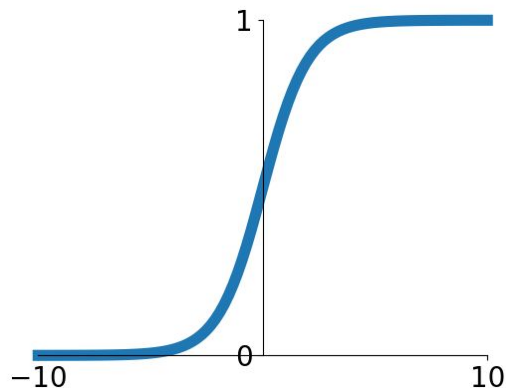
What can we say about the gradients on  $\mathbf{w}$ ?

Always all positive or all negative :(

(For a single element! Minibatches help)

# Activation Functions

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



**Sigmoid**

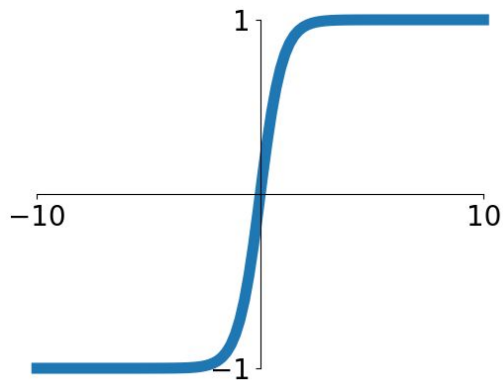
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- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered
3.  $\exp()$  is a bit compute expensive



# Activation Functions

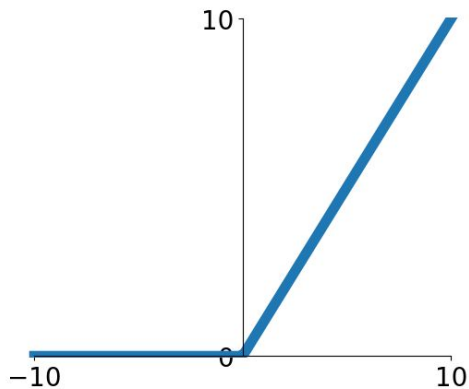


**$\tanh(x)$**

- Squashes numbers to range  $[-1,1]$
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

# Activation Functions

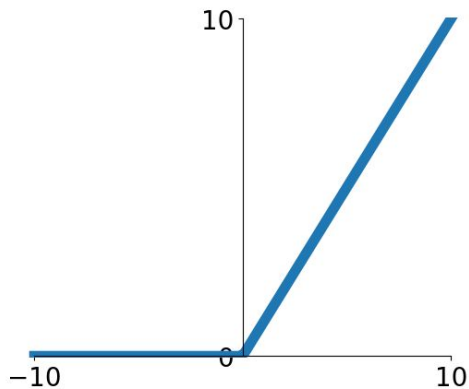


## ReLU (Rectified Linear Unit)

- Computes  $f(x) = \max(0, x)$
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

[Krizhevsky et al., 2012]

# Activation Functions

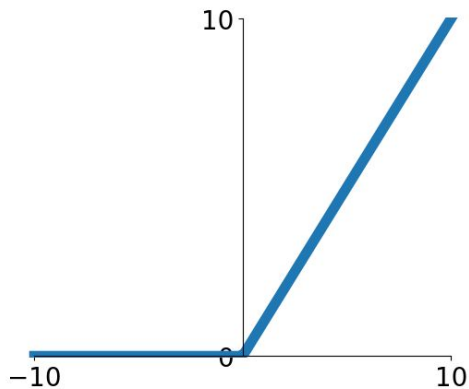


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- Not zero-centered output

# Activation Functions

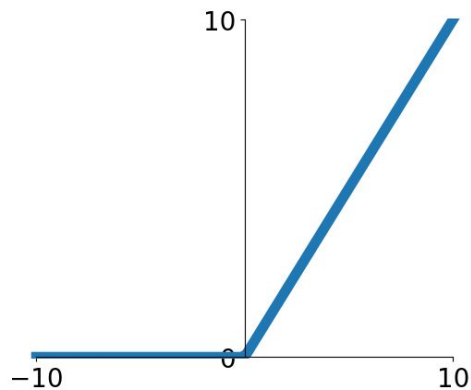
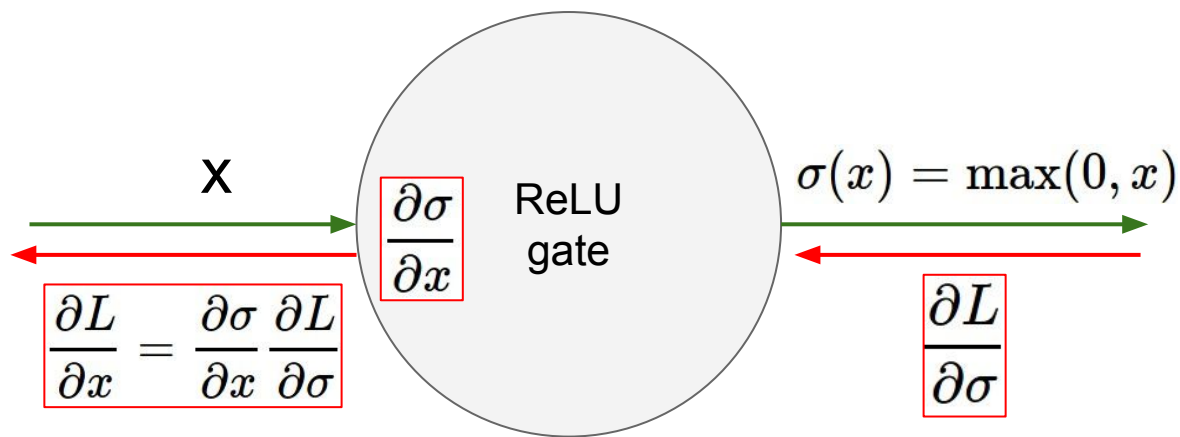


## ReLU (Rectified Linear Unit)

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- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

- Not zero-centered output
- An annoyance:

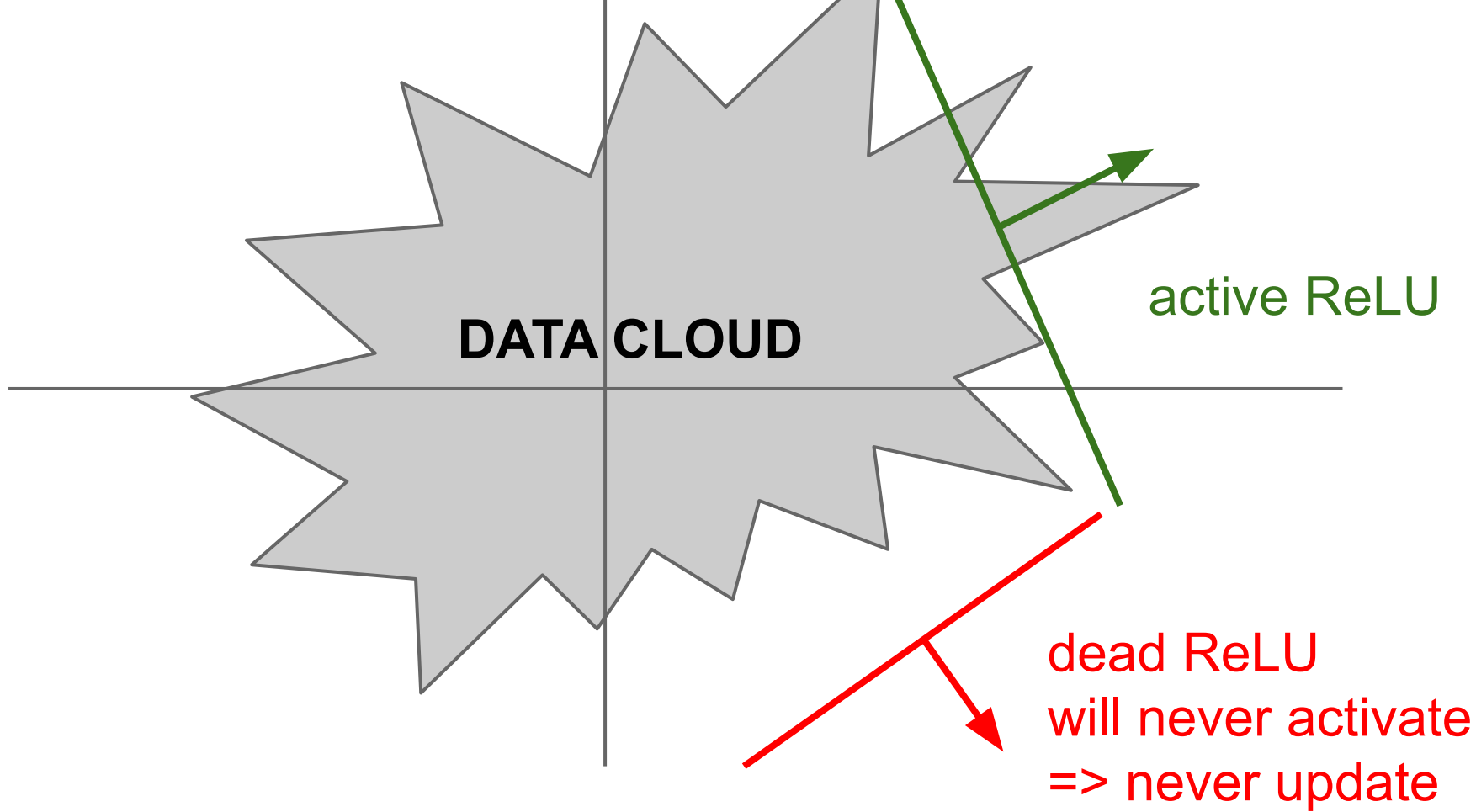
hint: what is the gradient when  $x < 0$ ?

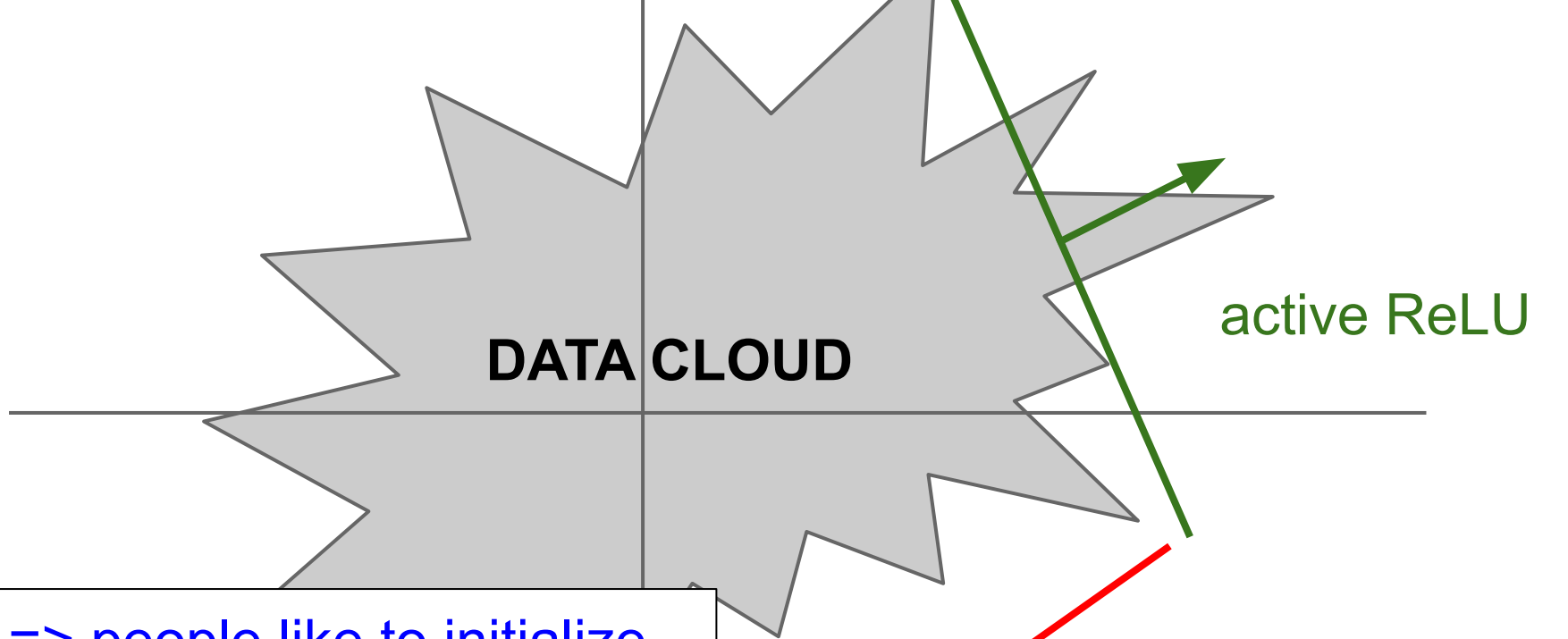


What happens when  $x = -10$ ?

What happens when  $x = 0$ ?

What happens when  $x = 10$ ?





**DATA CLOUD**

active ReLU

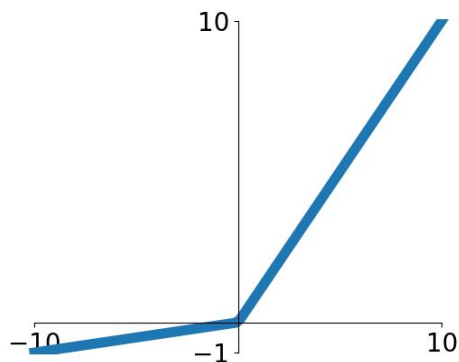
=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

dead ReLU  
will never activate  
=> never update

# Activation Functions

[Mass et al., 2013]

[He et al., 2015]



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

## Leaky ReLU

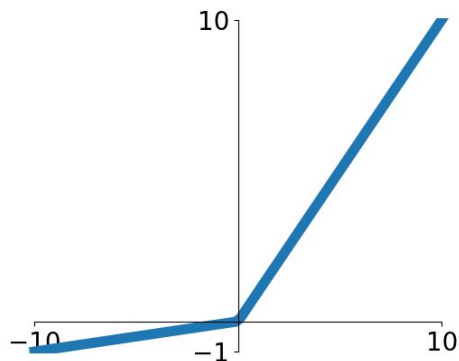
$$f(x) = \max(0.01x, x)$$



# Activation Functions

[Mass et al., 2013]

[He et al., 2015]



## Leaky ReLU

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

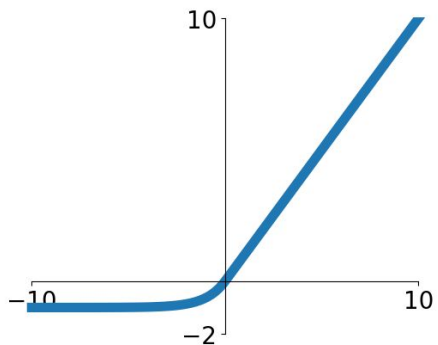
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”**.

## Parametric Rectifier (PReLU)

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

backprop into  $\alpha$  (parameter)

## Exponential Linear Units (ELU)

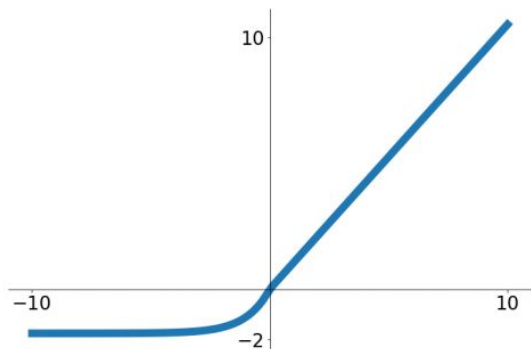


$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha (\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

(Alpha default = 1)

- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise
- Computation requires  $\exp()$

## Scaled Exponential Linear Units (SELU)



- Scaled version of ELU that works better for deep networks
- “Self-normalizing” property;
- Can train deep SELU networks without BatchNorm

$$f(x) = \begin{cases} \lambda x & \text{if } x > 0 \\ \lambda \alpha (e^x - 1) & \text{otherwise} \end{cases}$$

$$\alpha = 1.6732632423543772848170429916717$$

$$\lambda = 1.0507009873554804934193349852946$$

# Maxout “Neuron”

[Goodfellow et al., 2013]

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

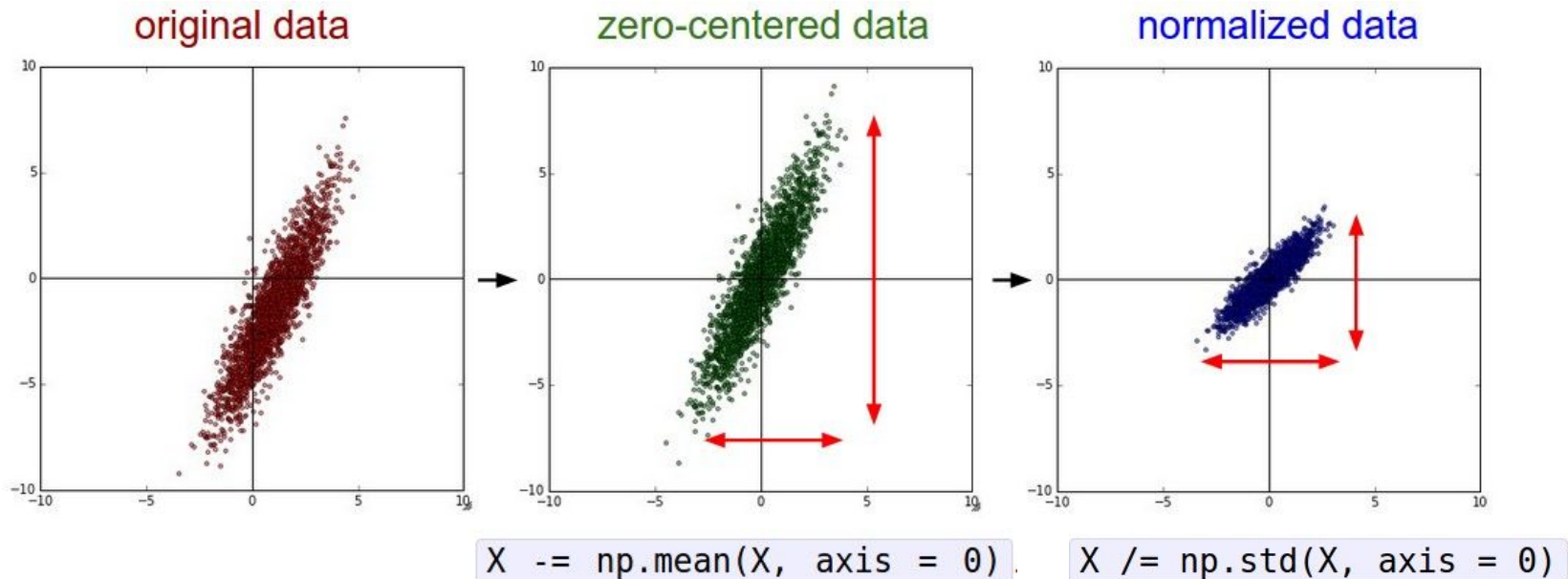
Problem: doubles the number of parameters/neuron :(

## TLDR: In practice:

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

# Data Preprocessing

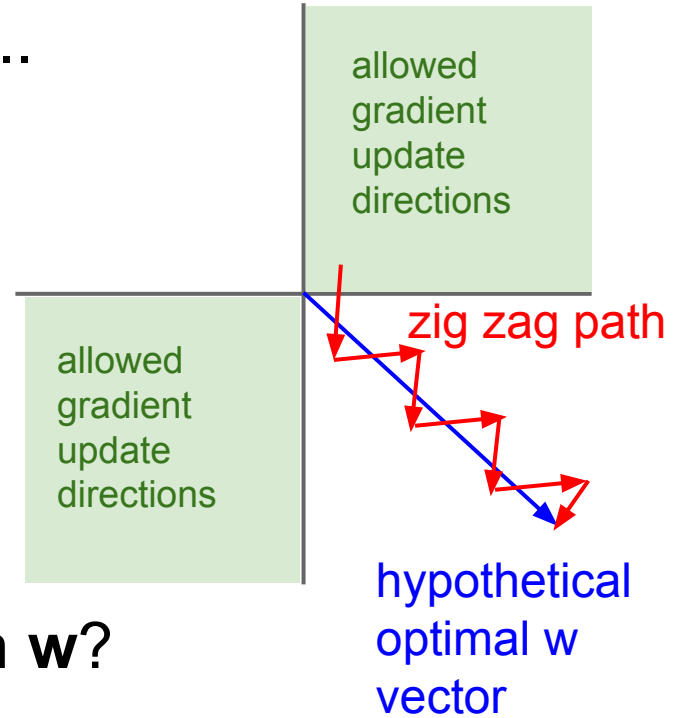
# Data Preprocessing



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

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

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

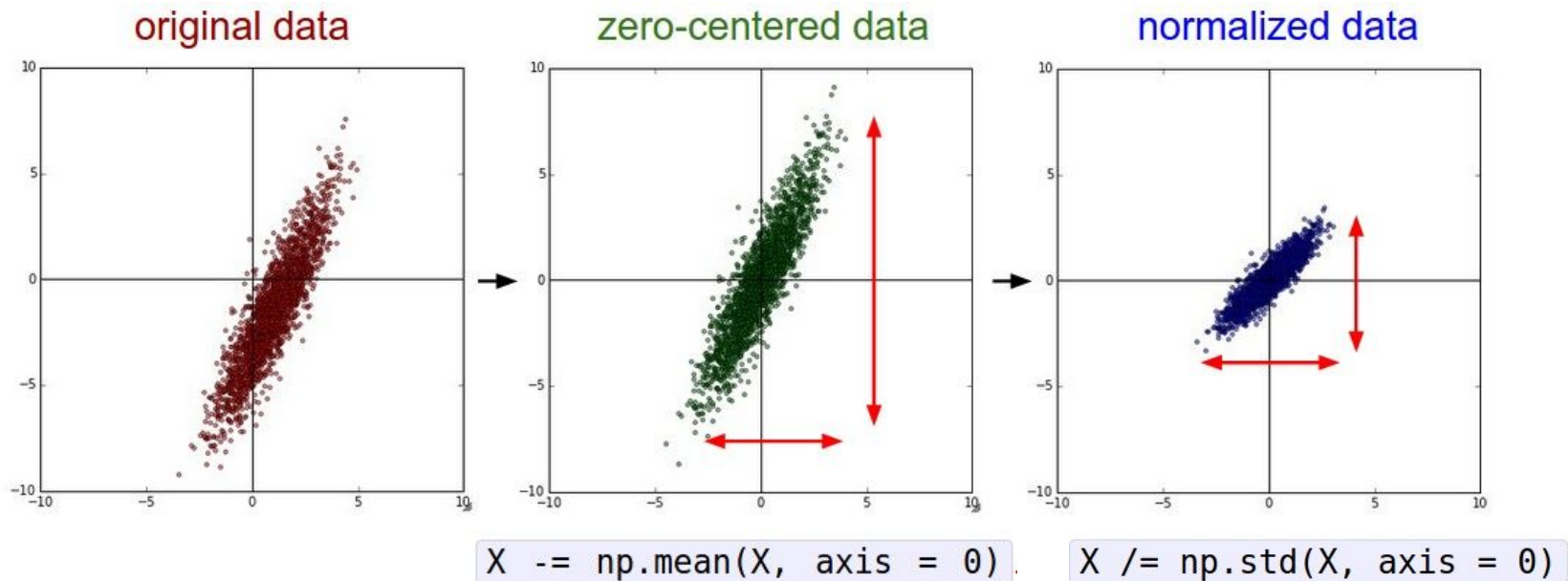


What can we say about the gradients on  $\mathbf{w}$ ?

Always all positive or all negative :(  
(this is also why you want zero-mean data!)



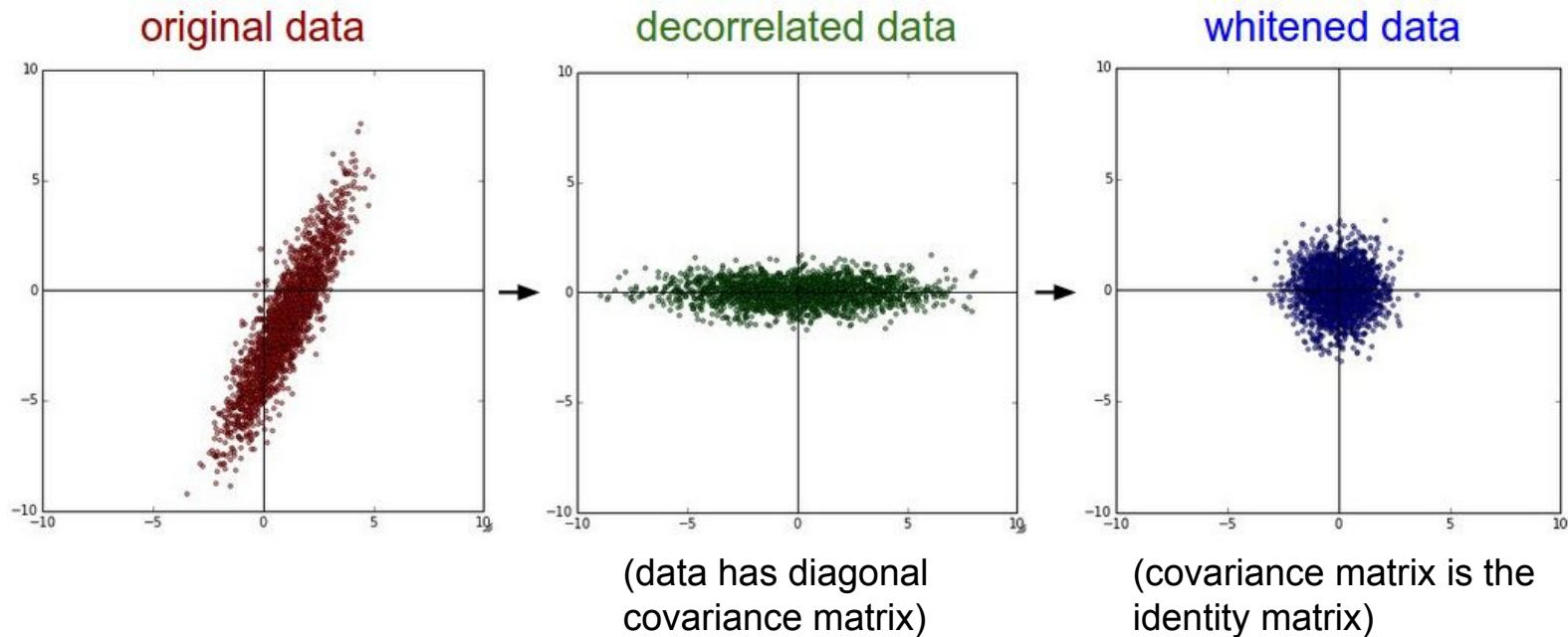
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(Assume  $X$  [NxD] is data matrix, each example in a row)

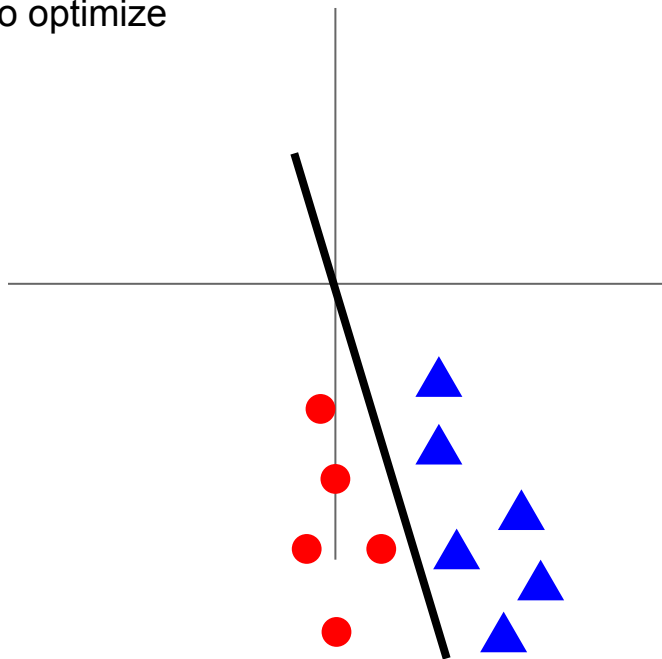
# Data Preprocessing

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

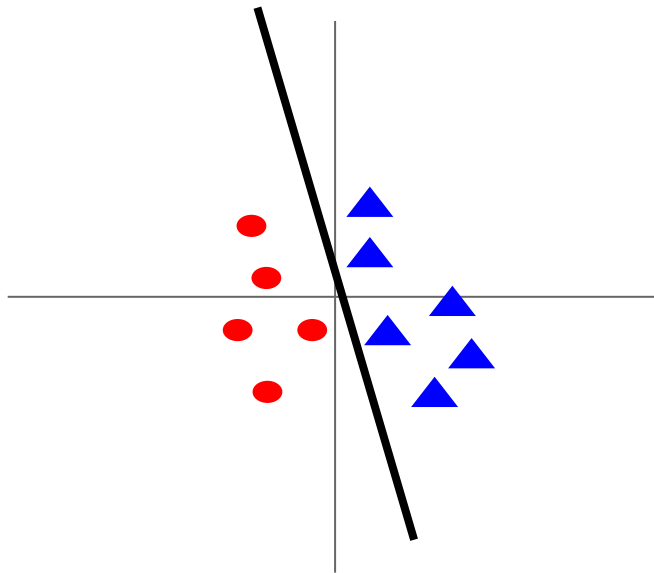


# Data Preprocessing

**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

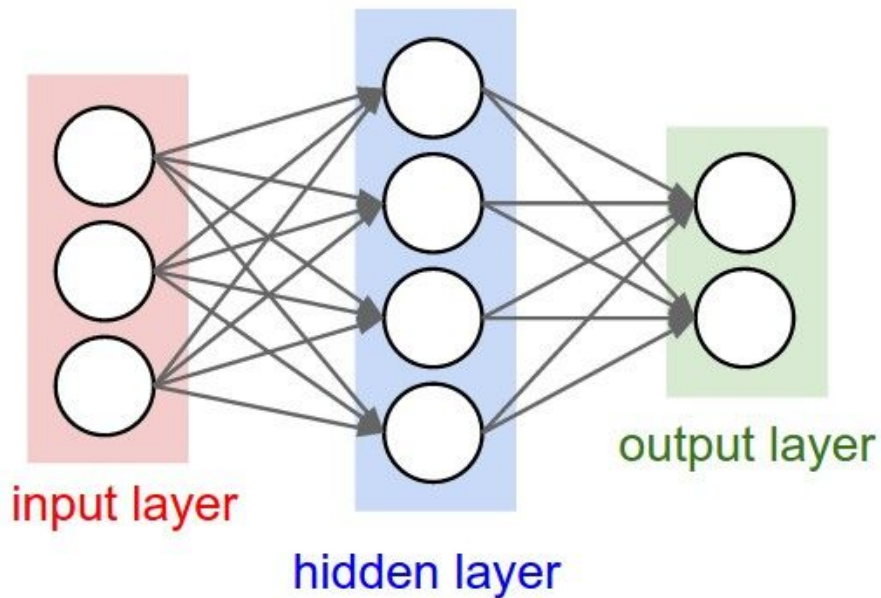
Divide by per-channel std (e.g. ResNet)

(mean along each channel = 3 numbers)

Not common  
to do PCA or  
whitening

# Weight Initialization

- Q: what happens when  $W=\text{constant}$  init is used?



- First idea: **Small random numbers**  
(gaussian with zero mean and  $1e-2$  standard deviation)

```
W = 0.01 * np.random.randn(Din, Dout)
```

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```
W = 0.01 * np.random.randn(Din, Dout)
```

Works ~okay for small networks, but problems with deeper networks.



# Weight Initialization: Activation statistics

```
dims = [4096] * 7      Forward pass for a 6-layer
hs = []               net with hidden size 4096
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

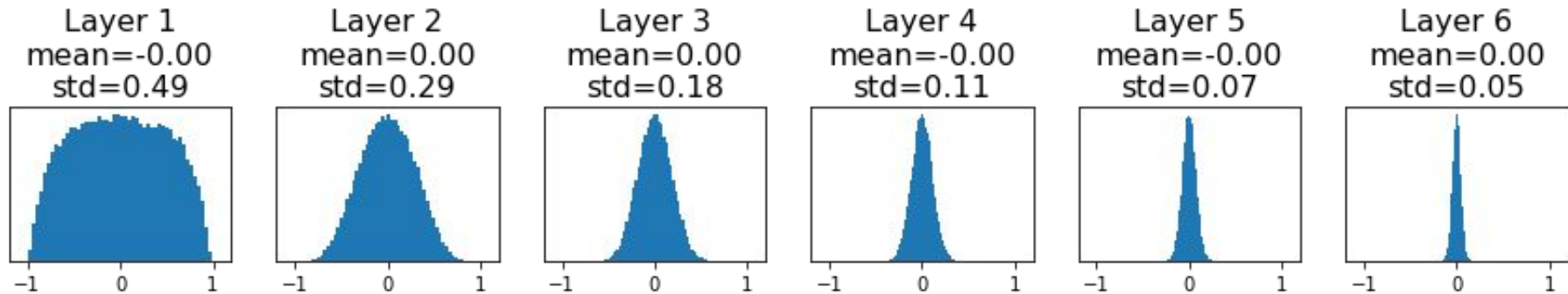
What will happen to the activations for the last layer?

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```

All activations tend to zero for deeper network layers

**Q:** What do the gradients  $dL/dW$  look like?



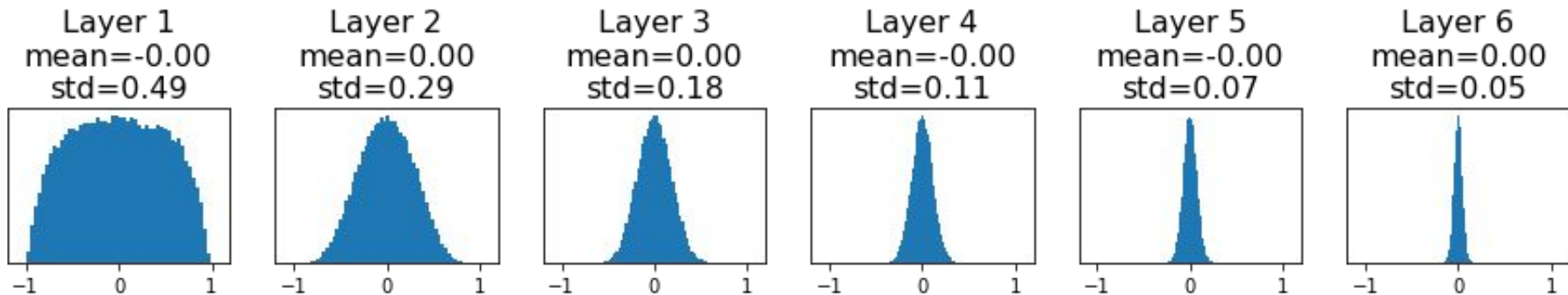
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All activations tend to zero for deeper network layers

**Q:** What do the gradients  $dL/dW$  look like?

**A:** All zero, no learning = (



# Weight Initialization: Activation statistics

```
dims = [4096] * 7    Increase std of initial
hs = []             weights from 0.01 to 0.05
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

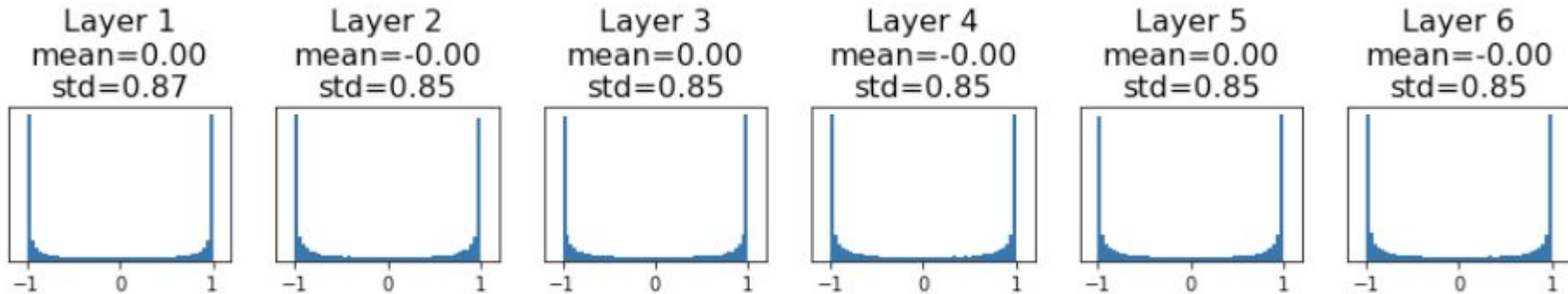
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All activations saturate

**Q:** What do the gradients look like?



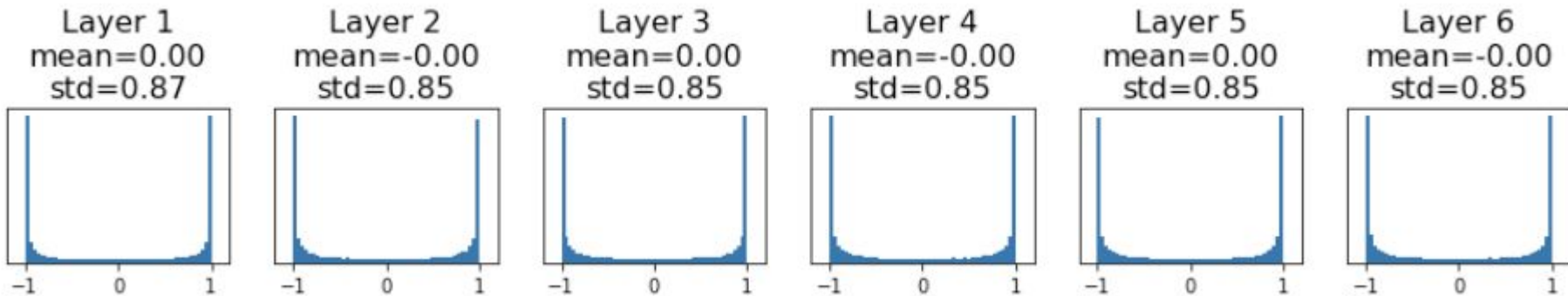
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All activations saturate

**Q:** What do the gradients look like?

**A:** Local gradients all zero, no learning =(



# Weight Initialization: “Xavier” Initialization

```
dims = [4096] * 7          “Xavier” initialization:
hs = []                   std = 1/sqrt(Din)
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

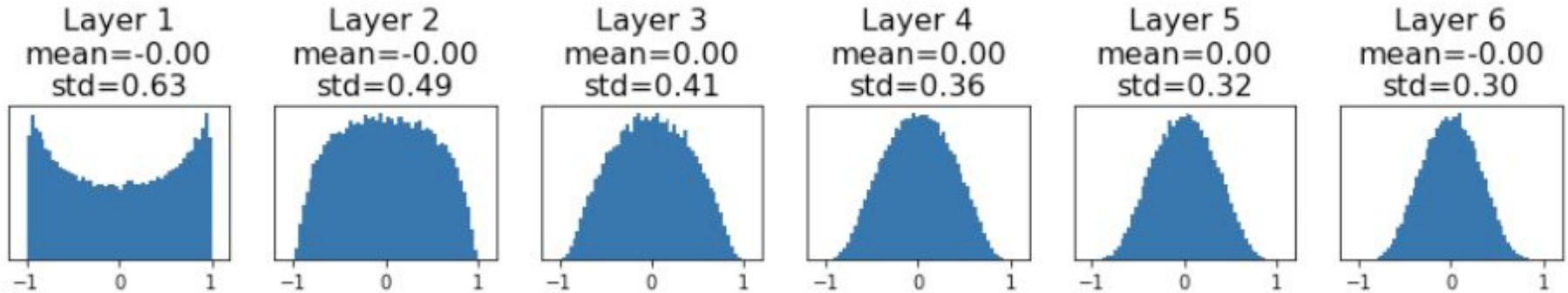
Glorot and Bengio, “Understanding the difficulty of training deep feedforward neural networks”, AISTAT 2010

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```

“Xavier” initialization:  
std =  $1/\sqrt{D_{in}}$

“Just right”: Activations are nicely scaled for all layers!



Glorot and Bengio, “Understanding the difficulty of training deep feedforward neural networks”, AISTAT 2010



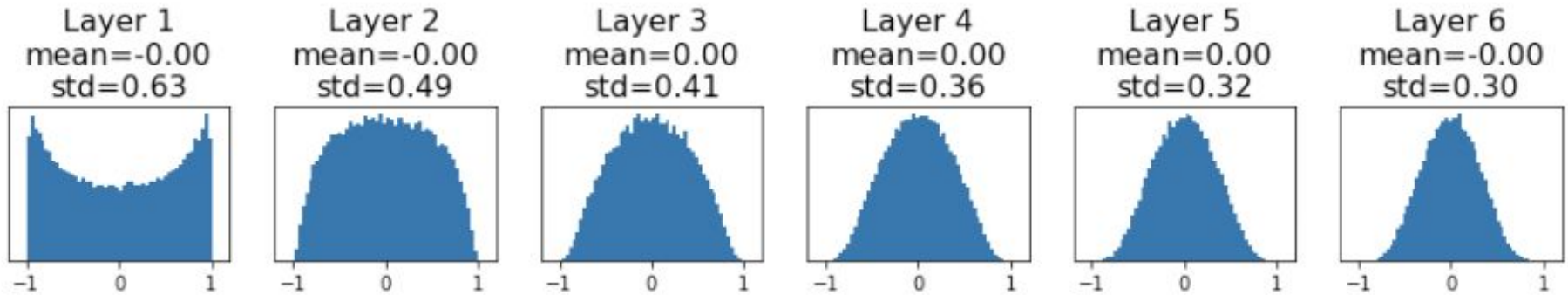
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For conv layers,  $D_{in}$  is  $\text{filter\_size}^2 * \text{input\_channels}$



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For conv layers, Din is filter\_size<sup>2</sup> \* input\_channels

**Let:**  $y = x_1 w_1 + x_2 w_2 + \dots + x_{Din} w_{Din}$

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**Assume:**  $\text{Var}(x_1) = \text{Var}(x_2) = \dots = \text{Var}(x_{D_{in}})$

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**We want:**  $\text{Var}(y) = \text{Var}(x_i)$

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**Assume:**  $\text{Var}(x_1) = \text{Var}(x_2) = \dots = \text{Var}(x_{D_{in}})$

**We want:**  $\text{Var}(y) = \text{Var}(x_i)$

$\text{Var}(y) = \text{Var}(x_1 w_1 + x_2 w_2 + \dots + x_{D_{in}} w_{D_{in}})$   
[substituting value of  $y$ ]

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For conv layers, Din is filter\_size<sup>2</sup> \* input\_channels

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$$\begin{aligned}\text{Var}(y) &= \text{Var}(x_1 w_1 + x_2 w_2 + \dots + x_{Din} w_{Din}) \\ &= \text{Din} \text{Var}(x_i w_i)\end{aligned}$$

[Assume all  $x_i, w_i$  are iid]

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**Let:**  $y = x_1 w_1 + x_2 w_2 + \dots + x_{D_{in}} w_{D_{in}}$

**Assume:**  $\text{Var}(x_1) = \text{Var}(x_2) = \dots = \text{Var}(x_{D_{in}})$

**We want:**  $\text{Var}(y) = \text{Var}(x_i)$

$$\begin{aligned}\text{Var}(y) &= \text{Var}(x_1 w_1 + x_2 w_2 + \dots + x_{D_{in}} w_{D_{in}}) \\ &= D_{in} \text{Var}(x_i w_i) \\ &= D_{in} \text{Var}(x_i) \text{Var}(w_i)\end{aligned}$$

[Assume all  $x_i, w_i$  are zero mean]

# Weight Initialization: “Xavier” Initialization

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for Din, Dout in zip(dims[:-1], dims[1:]):
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“Xavier” initialization:  
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For conv layers, Din is  $\text{filter\_size}^2 * \text{input\_channels}$

**Let:**  $y = x_1 w_1 + x_2 w_2 + \dots + x_{\text{Din}} w_{\text{Din}}$

**Assume:**  $\text{Var}(x_1) = \text{Var}(x_2) = \dots = \text{Var}(x_{\text{Din}})$

**We want:**  $\text{Var}(y) = \text{Var}(x_i)$

$$\begin{aligned}\text{Var}(y) &= \text{Var}(x_1 w_1 + x_2 w_2 + \dots + x_{\text{Din}} w_{\text{Din}}) \\ &= \text{Din} \text{Var}(x_i w_i) \\ &= \text{Din} \text{Var}(x_i) \text{Var}(w_i) \\ &[\text{Assume all } x_i, w_i \text{ are iid}]\end{aligned}$$

So,  $\text{Var}(y) = \text{Var}(x_i)$  only when  $\text{Var}(w_i) = 1/\text{Din}$

Glort and Bengio, “Understanding the difficulty of training deep feedforward neural networks”, AISTAT 2010



# Weight Initialization: What about ReLU?

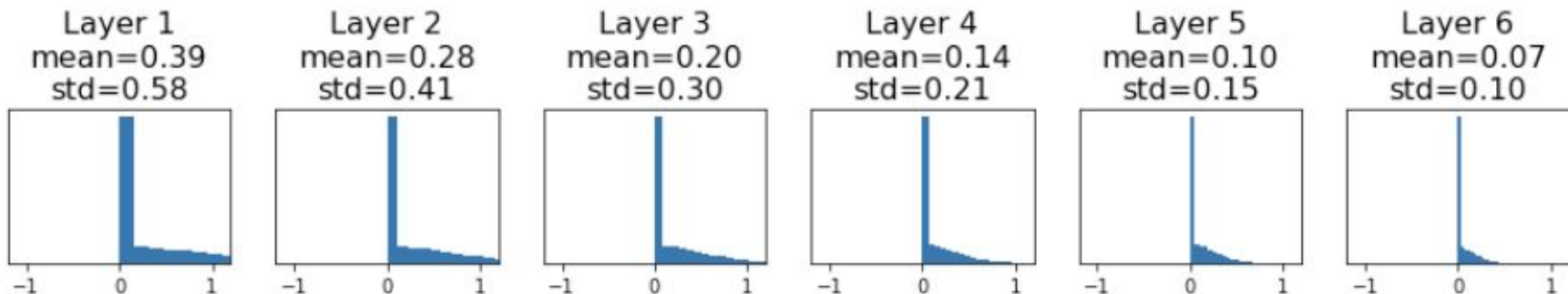
```
dims = [4096] * 7      Change from tanh to ReLU
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

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    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning =(

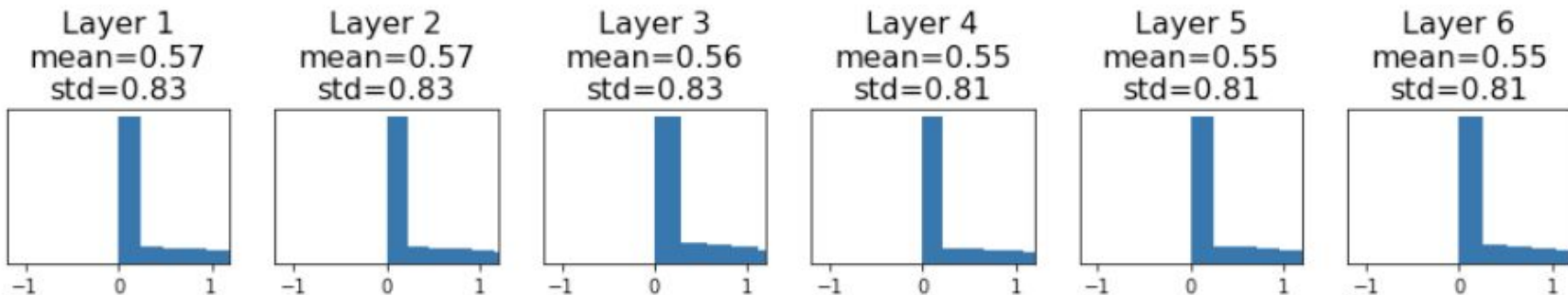


# Weight Initialization: Kaiming / MSRA Initialization

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) * np.sqrt(2/Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

ReLU correction:  $\text{std} = \sqrt{2 / \text{Din}}$

“Just right”: Activations are nicely scaled for all layers!



He et al, “Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification”, ICCV 2015

# Proper initialization is an active area of research...

***Understanding the difficulty of training deep feedforward neural networks***

by Glorot and Bengio, 2010

***Exact solutions to the nonlinear dynamics of learning in deep linear neural networks*** by Saxe et al, 2013

***Random walk initialization for training very deep feedforward networks*** by Sussillo and Abbott, 2014

***Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification*** by He et al., 2015

***Data-dependent Initializations of Convolutional Neural Networks*** by Krähenbühl et al., 2015

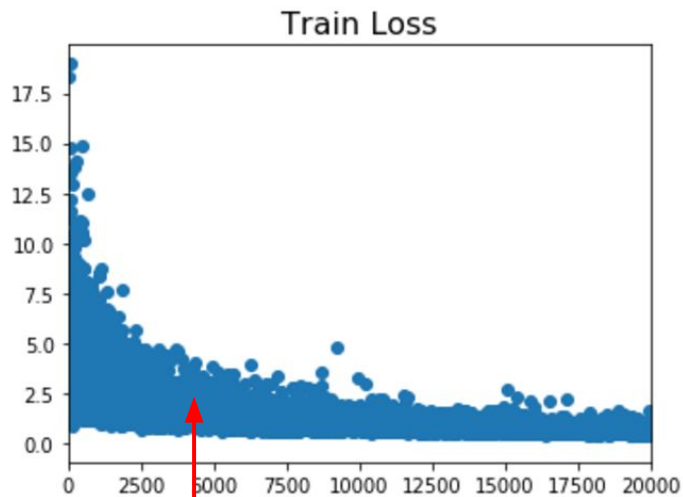
***All you need is a good init***, Mishkin and Matas, 2015

***Fixup Initialization: Residual Learning Without Normalization***, Zhang et al, 2019

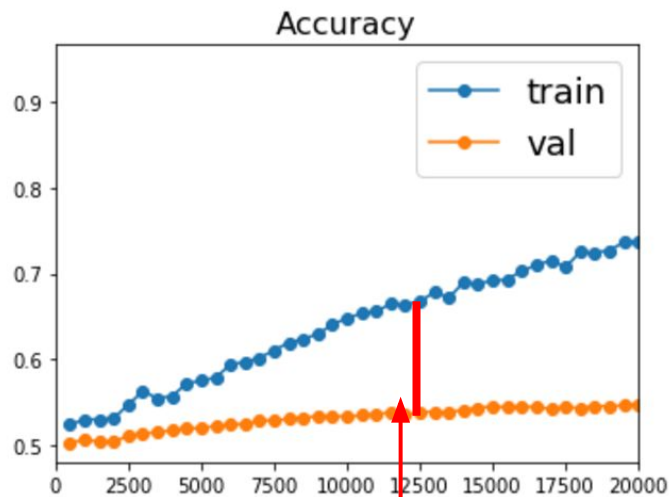
***The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks***, Frankle and Carbin, 2019

# Training vs. Testing Error

# Beyond Training Error

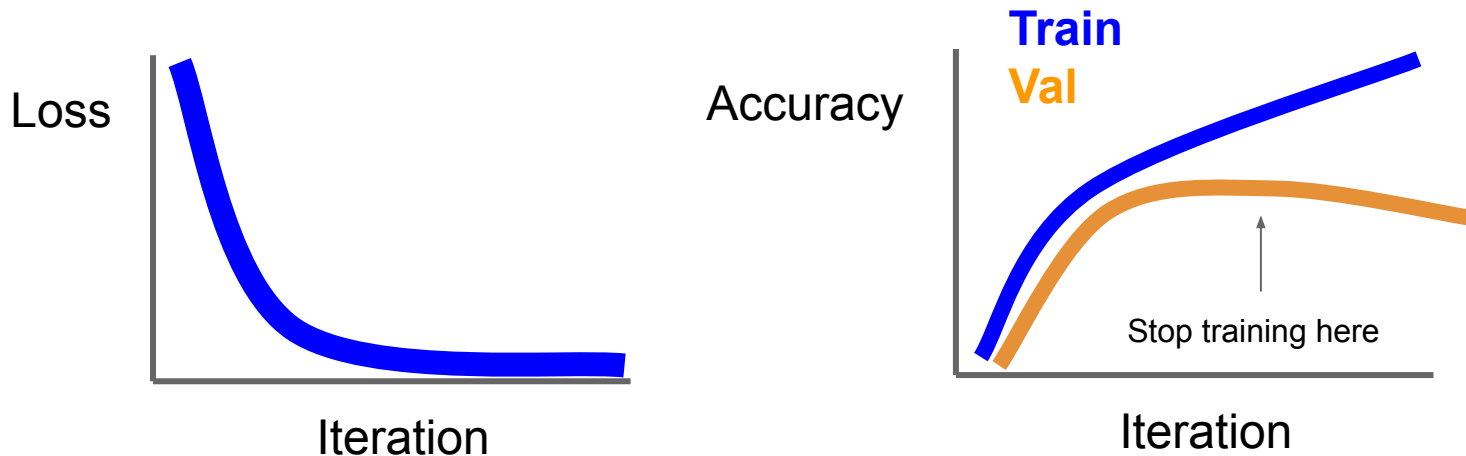


Better optimization algorithms help reduce training loss



But we really care about error on new data - how to reduce the gap?

# Early Stopping: Always do this



Stop training the model when accuracy on the validation set decreases  
Or train for a long time, but always keep track of the model snapshot  
that worked best on val

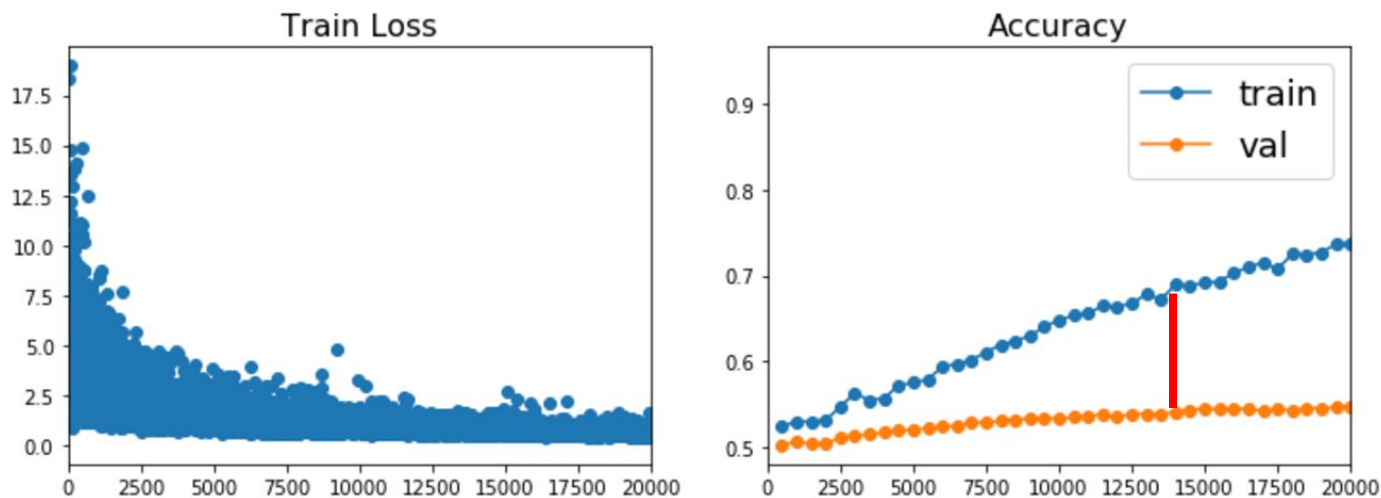
# Model Ensembles

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



# How to improve single-model performance?



Regularization

# Regularization: Add term to loss

$$L = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1) + \lambda R(W)$$

In common use:

L2 regularization

$$R(W) = \sum_k \sum_l W_{k,l}^2 \quad (\text{Weight decay})$$

L1 regularization

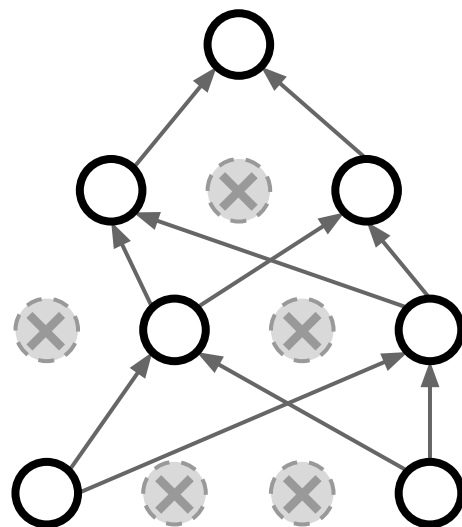
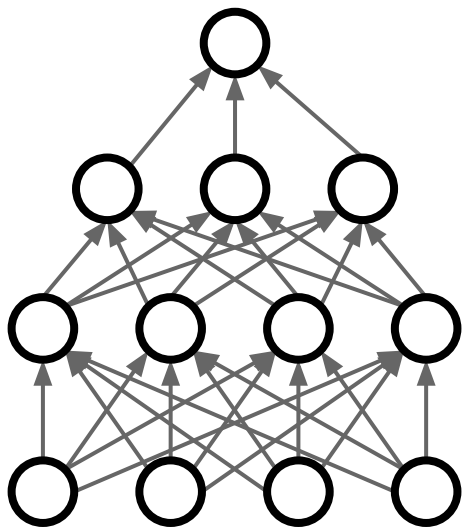
$$R(W) = \sum_k \sum_l |W_{k,l}|$$

Elastic net (L1 + L2)

$$R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$$

# Regularization: Dropout

In each forward pass, randomly set some neurons to zero  
Probability of dropping is a hyperparameter; 0.5 is common



Srivastava et al, "Dropout: A simple way to prevent neural networks from overfitting", JMLR 2014

# Regularization: Dropout

```
p = 0.5 # probability of keeping a unit active. higher = less dropout
```

```
def train_step(X):
```

```
    """ X contains the data """
```

```
    # forward pass for example 3-layer neural network
```

```
    H1 = np.maximum(0, np.dot(W1, X) + b1)
```

```
    U1 = np.random.rand(*H1.shape) < p # first dropout mask
```

```
    H1 *= U1 # drop!
```

```
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
```

```
    U2 = np.random.rand(*H2.shape) < p # second dropout mask
```

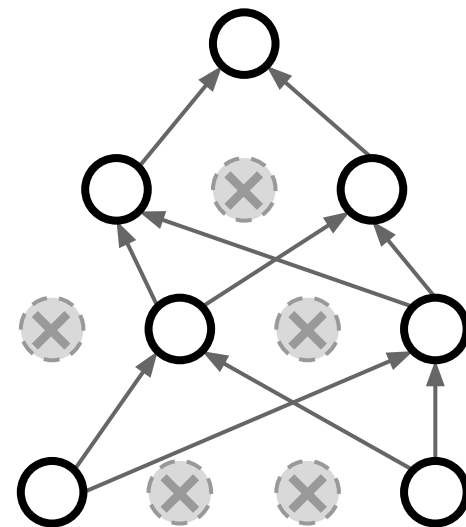
```
    H2 *= U2 # drop!
```

```
    out = np.dot(W3, H2) + b3
```

```
    # backward pass: compute gradients... (not shown)
```

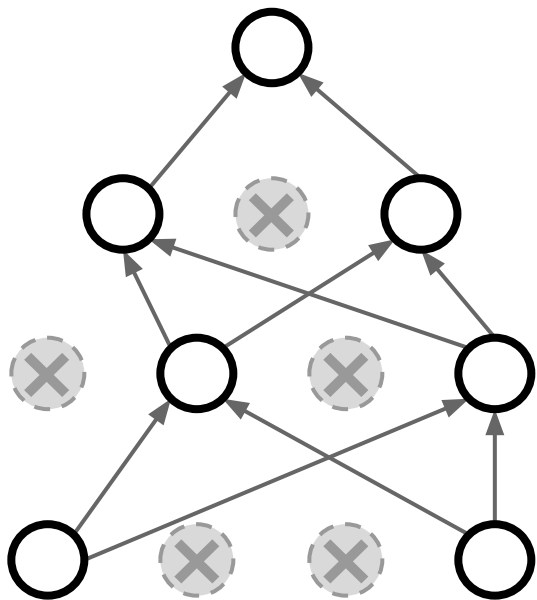
```
    # perform parameter update... (not shown)
```

Example forward pass with a 3-layer network using dropout

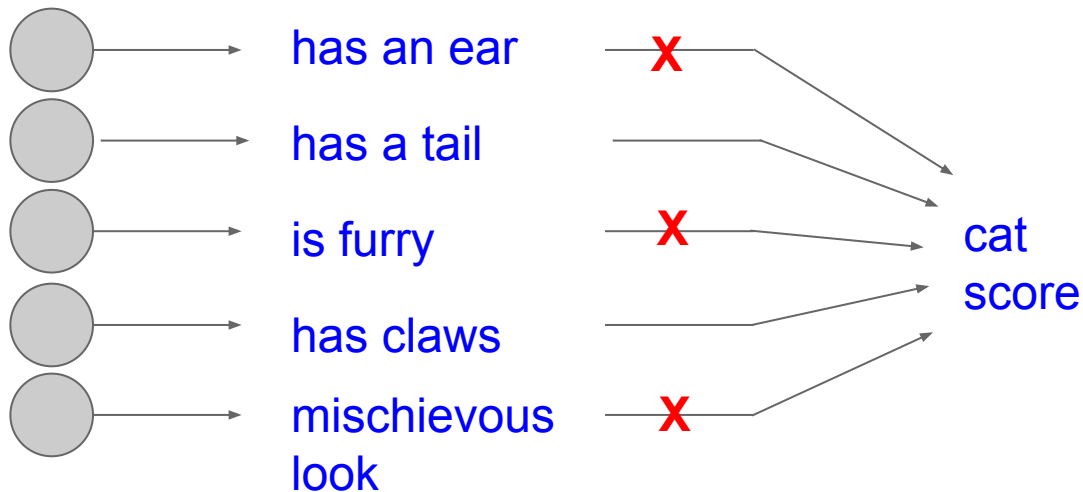


# Regularization: Dropout

How can this possibly be a good idea?

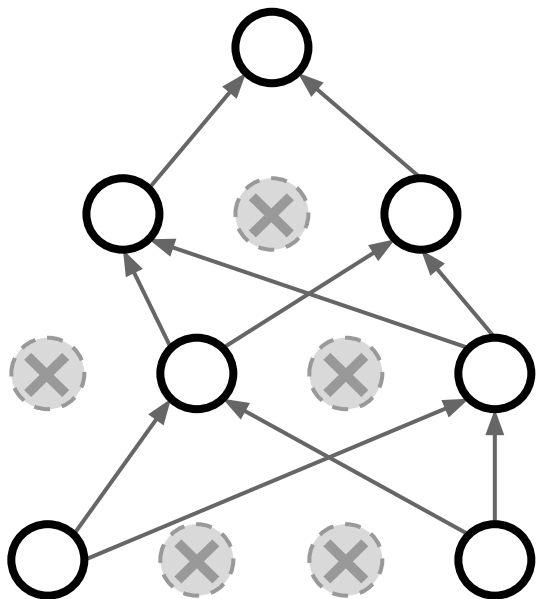


Forces the network to have a redundant representation;  
Prevents co-adaptation of features



# Regularization: Dropout

How can this possibly be a good idea?



Another interpretation:

Dropout is training a large **ensemble** of models (that share parameters).

Each binary mask is one model

An FC layer with 4096 units has  $2^{4096} \sim 10^{1233}$  possible masks!

Only  $\sim 10^{82}$  atoms in the universe...

# Dropout: Test time

Dropout makes our output random!

$$\begin{array}{l} \text{Output} \\ \text{(label)} \end{array} \quad \begin{array}{l} \text{Input} \\ \text{(image)} \end{array} \quad \begin{array}{l} \text{Random} \\ \text{mask} \end{array}$$
$$y = f_W(x, z)$$

The diagram shows the equation  $y = f_W(x, z)$  with color-coded boxes: a red box around  $y$ , a blue box around  $x$ , and a green box around  $z$ . The labels "Output (label)", "Input (image)", and "Random mask" are positioned above their respective variables.

Want to “average out” the randomness at test-time

$$y = f(x) = E_z[f(x, z)] = \int p(z) f(x, z) dz$$

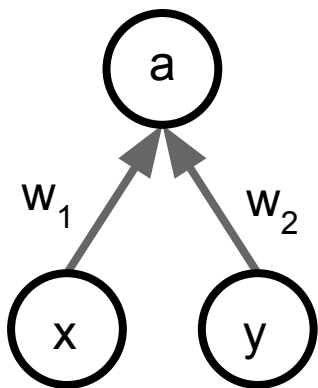
But this integral seems hard ...

# Dropout: Test time

Want to approximate  
the integral

$$y = f(x) = E_z [f(x, z)] = \int p(z) f(x, z) dz$$

Consider a single neuron.





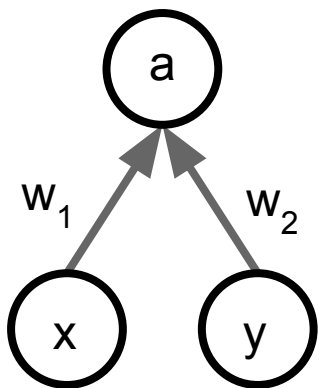
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Consider a single neuron.

At test time we have:  $E[a] = w_1 x + w_2 y$

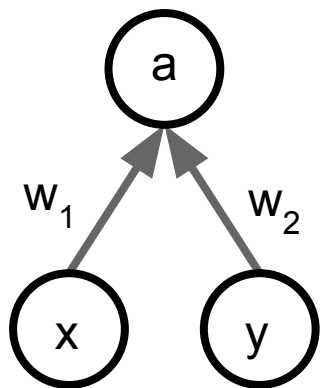


# Dropout: Test time

Want to approximate the integral

$$y = f(x) = E_z [f(x, z)] = \int p(z) f(x, z) dz$$

Consider a single neuron.



At test time we have:  $E[a] = w_1x + w_2y$

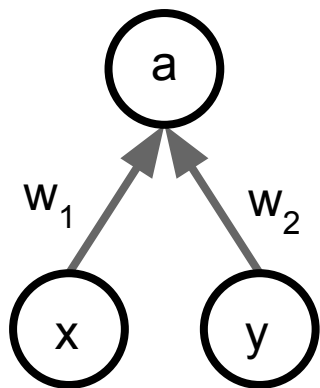
During training we have: 
$$\begin{aligned} E[a] &= \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) \\ &\quad + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) \\ &= \frac{1}{2}(w_1x + w_2y) \end{aligned}$$

# Dropout: Test time

Want to approximate the integral

$$y = f(x) = E_z [f(x, z)] = \int p(z) f(x, z) dz$$

Consider a single neuron.



At test time we have:  $E[a] = w_1x + w_2y$

During training we have:  $E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) = \frac{1}{2}(w_1x + w_2y)$

**At test time, multiply by dropout probability**

# Dropout: Test time

```
def predict(X):  
    # ensembled forward pass  
    H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations  
    H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations  
    out = np.dot(W3, H2) + b3
```

At test time all neurons are active always

=> We must scale the activations so that for each neuron:

output at test time = expected output at training time

# Dropout Summary

```
""" Vanilla Dropout: Not recommended implementation (see notes below) """
```

```
p = 0.5 # probability of keeping a unit active. higher = less dropout
```

```
def train_step(X):
```

```
    """ X contains the data """
```

```
    # forward pass for example 3-layer neural network:
```

```
    H1 = np.maximum(0, np.dot(W1, X) + b1)
```

```
    U1 = np.random.rand(*H1.shape) < p # first dropout mask
```

```
    H1 *= U1 # drop!
```

```
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
```

```
    U2 = np.random.rand(*H2.shape) < p # second dropout mask
```

```
    H2 *= U2 # drop!
```

```
    out = np.dot(W3, H2) + b3
```

```
    # backward pass: compute gradients... (not shown)
```

```
    # perform parameter update... (not shown)
```

```
def predict(X):
```

```
    # ensembled forward pass
```

```
    H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
```

```
    H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
```

```
    out = np.dot(W3, H2) + b3
```

drop in train time

scale at test time

# More common: “Inverted dropout”

```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
    # forward pass for example 3-layer neural network
    H1 = np.maximum(0, np.dot(W1, X) + b1)
    U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
    H1 *= U1 # drop!
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
    U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
    H2 *= U2 # drop!
    out = np.dot(W3, H2) + b3

    # backward pass: compute gradients... (not shown)
    # perform parameter update... (not shown)

def predict(X):
    # ensembled forward pass
    H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
    H2 = np.maximum(0, np.dot(W2, H1) + b2)
    out = np.dot(W3, H2) + b3
```

test time is unchanged!



# Regularization: A common pattern

**Training:** Add some kind of randomness

$$y = f_W(x, z)$$

**Testing:** Average out randomness (sometimes approximate)

$$y = f(x) = E_z [f(x, z)] = \int p(z) f(x, z) dz$$

# Regularization: A common pattern

**Training:** Add some kind of randomness

$$y = f_W(x, z)$$

**Testing:** Average out randomness (sometimes approximate)

$$y = f(x) = E_z[f(x, z)] = \int p(z)f(x, z)dz$$

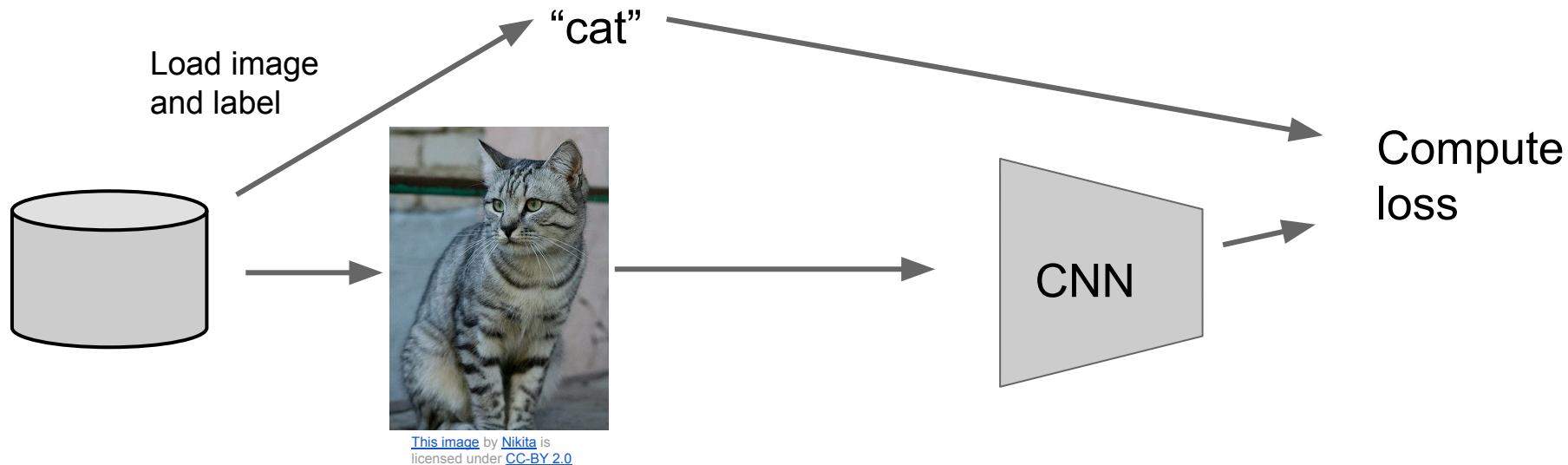
**Example:** Batch Normalization

**Training:** Normalize using stats from random minibatches

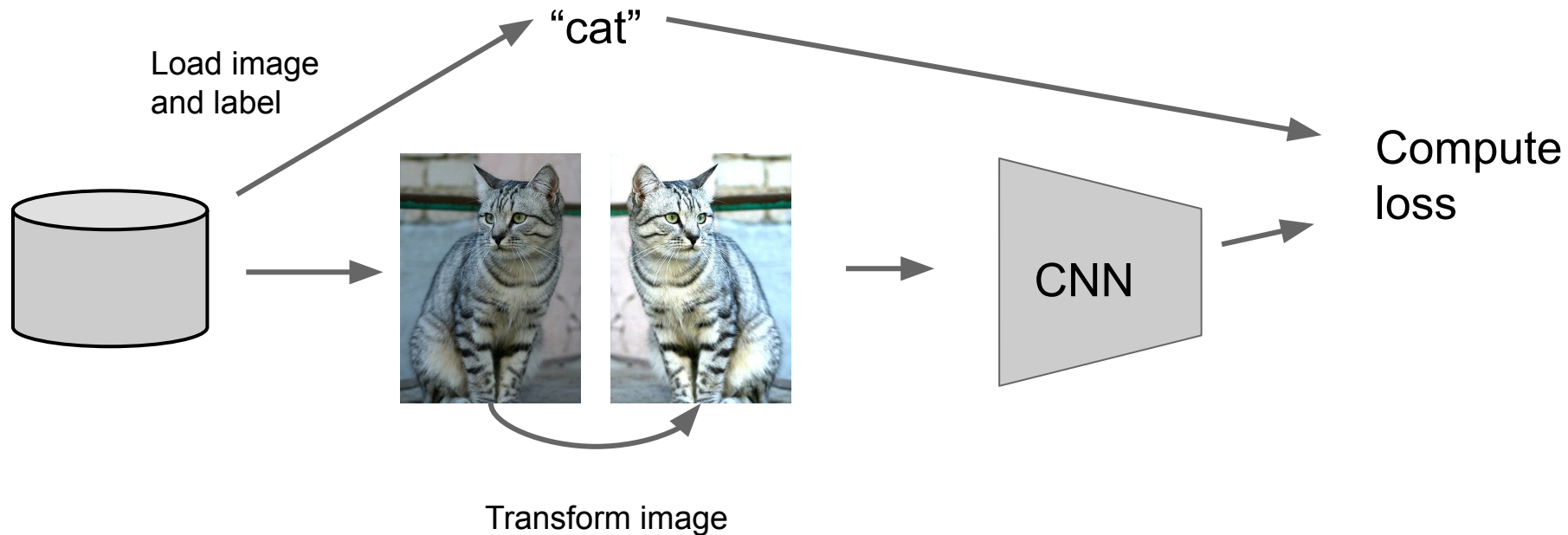
**Testing:** Use fixed stats to normalize



# Regularization: Data Augmentation



# Regularization: Data Augmentation



# Data Augmentation

## Horizontal Flips



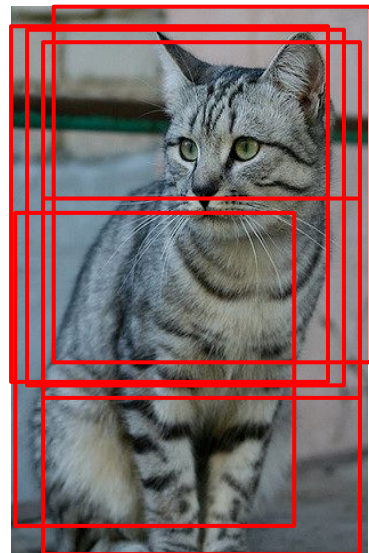
# Data Augmentation

## Random crops and scales

**Training:** sample random crops / scales

ResNet:

1. Pick random  $L$  in range  $[256, 480]$
2. Resize training image, short side =  $L$
3. Sample random  $224 \times 224$  patch



# Data Augmentation

## Random crops and scales

**Training:** sample random crops / scales

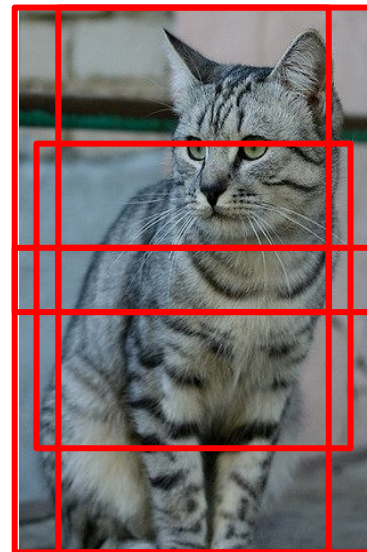
ResNet:

1. Pick random  $L$  in range  $[256, 480]$
2. Resize training image, short side =  $L$
3. Sample random  $224 \times 224$  patch

**Testing:** average a fixed set of crops

ResNet:

1. Resize image at 5 scales:  $\{224, 256, 384, 480, 640\}$
2. For each size, use 10  $224 \times 224$  crops: 4 corners + center, + flips



# Data Augmentation

## Color Jitter

Simple: Randomize  
contrast and brightness



# Data Augmentation

## Color Jitter

Simple: Randomize  
contrast and brightness



## More Complex:

1. Apply PCA to all [R, G, B] pixels in training set
2. Sample a “color offset” along principal component directions
3. Add offset to all pixels of a training image

(As seen in *[Krizhevsky et al. 2012]*, ResNet, etc)

# Data Augmentation

Get creative for your problem!

Examples of data augmentations:

- translation
- rotation
- stretching
- shearing,
- lens distortions, ... (go crazy)



# Automatic Data Augmentation

	Original	Sub-policy 1	Sub-policy 2	Sub-policy 3	Sub-policy 4	Sub-policy 5
Batch 1						
Batch 2						
Batch 3						
		ShearX, 0.9, 7 Invert, 0.2, 3	ShearY, 0.7, 6 Solarize, 0.4, 8	ShearX, 0.9, 4 AutoContrast, 0.8, 3	Invert, 0.9, 3 Equalize, 0.6, 3	ShearY, 0.8, 5 AutoContrast, 0.7, 3

Cubuk et al., "AutoAugment: Learning Augmentation Strategies from Data", CVPR 2019

# Regularization: A common pattern

**Training:** Add random noise

**Testing:** Marginalize over the noise

## Examples:

Dropout

Batch Normalization

Data Augmentation

# Regularization: DropConnect

**Training:** Drop connections between neurons (set weights to 0)

**Testing:** Use all the connections

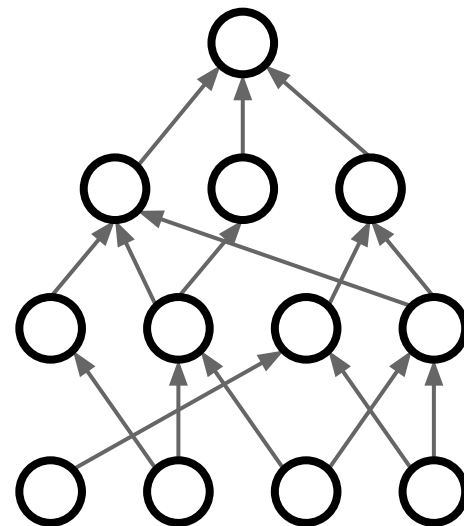
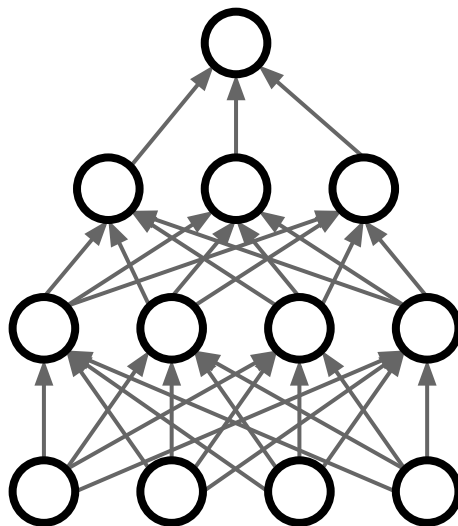
## Examples:

Dropout

Batch Normalization

Data Augmentation

**DropConnect**



Wan et al, "Regularization of Neural Networks using DropConnect", ICML 2013

# Regularization: Fractional Pooling

**Training:** Use randomized pooling regions

**Testing:** Average predictions from several regions

## Examples:

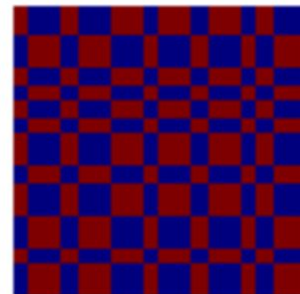
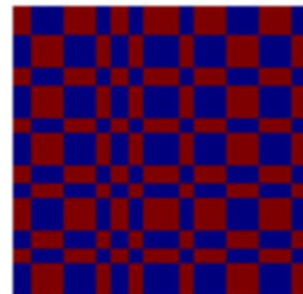
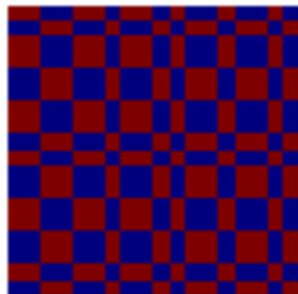
Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling



# Regularization: Stochastic Depth

**Training:** Skip some layers in the network

**Testing:** Use all the layer

## Examples:

Dropout

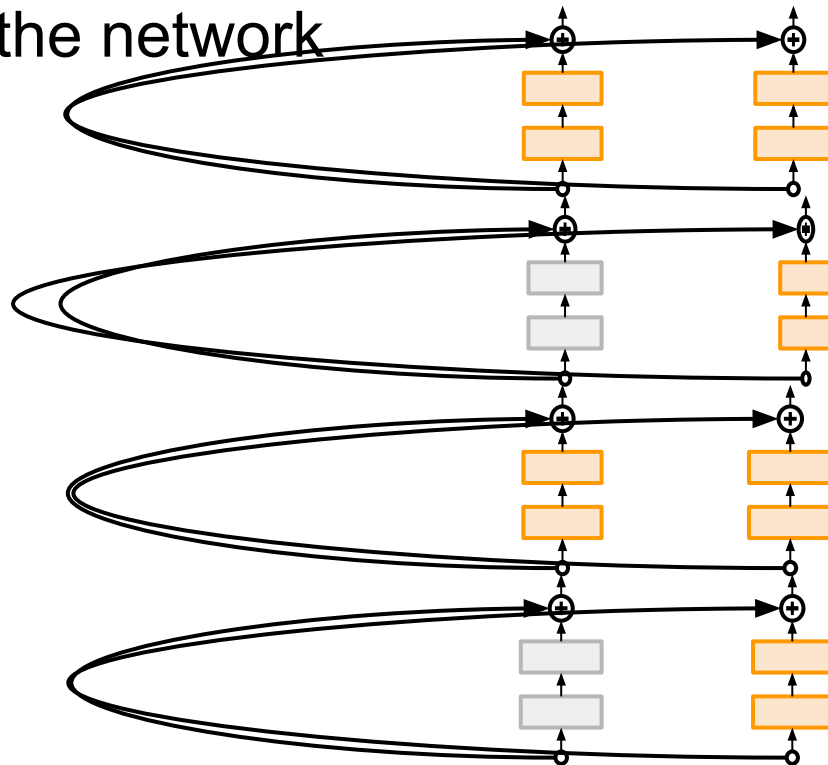
Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

**Stochastic Depth**



Huang et al, "Deep Networks with Stochastic Depth", ECCV 2016

# Regularization: Cutout

**Training:** Set random image regions to zero

**Testing:** Use full image

## Examples:

Dropout

Batch Normalization

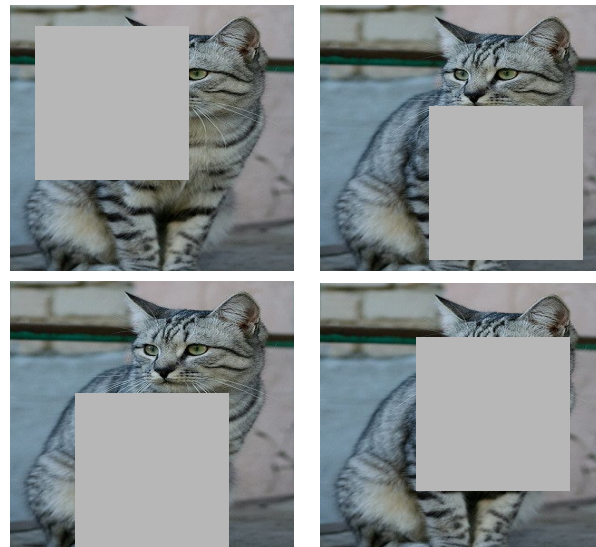
Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth

**Cutout / Random Crop**



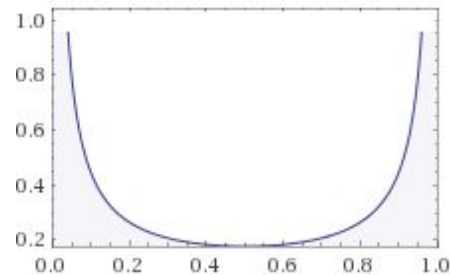
Works very well for small datasets like CIFAR,  
less common for large datasets like ImageNet

DeVries and Taylor, "Improved Regularization of Convolutional Neural Networks with Cutout", arXiv 2017

# Regularization: Mixup

**Training:** Train on random blends of images

**Testing:** Use original images



## Examples:

Dropout

Batch Normalization

Data Augmentation

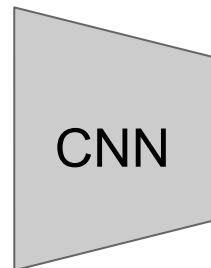
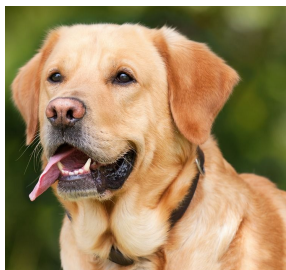
DropConnect

Fractional Max Pooling

Stochastic Depth

Cutout / Random Crop

Mixup



Target label:

cat: 0.4

dog: 0.6

Randomly blend the pixels of pairs of training images, e.g. 40% cat, 60% dog

Zhang et al, "mixup: Beyond Empirical Risk Minimization", ICLR 2018

# Regularization - In practice

**Training:** Add random noise

**Testing:** Marginalize over the noise

## Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth

Cutout / Random Crop

Mixup

- Consider dropout for large fully-connected layers
- Batch normalization and data augmentation almost always a good idea
- Try cutout and mixup especially for small classification datasets



# Choosing Hyperparameters

(without tons of GPUs)

# Choosing Hyperparameters

## Step 1: Check initial loss

Turn off weight decay, sanity check loss at initialization  
e.g.  $\log(C)$  for softmax with  $C$  classes

# Choosing Hyperparameters

**Step 1:** Check initial loss

**Step 2:** Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization

Loss not going down? LR too low, bad initialization

Loss explodes to Inf or NaN? LR too high, bad initialization

# Choosing Hyperparameters

**Step 1:** Check initial loss

**Step 2:** Overfit a small sample

**Step 3:** Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within  $\sim 100$  iterations

Good learning rates to try:  $1e-1$ ,  $1e-2$ ,  $1e-3$ ,  $1e-4$

# Choosing Hyperparameters

**Step 1:** Check initial loss

**Step 2:** Overfit a small sample

**Step 3:** Find LR that makes loss go down

**Step 4:** Coarse grid, train for ~1-5 epochs

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs.

Good weight decay to try:  $1e-4$ ,  $1e-5$ , 0

# Choosing Hyperparameters

**Step 1:** Check initial loss

**Step 2:** Overfit a small sample

**Step 3:** Find LR that makes loss go down

**Step 4:** Coarse grid, train for ~1-5 epochs

**Step 5:** Refine grid, train longer

Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

# Choosing Hyperparameters

**Step 1:** Check initial loss

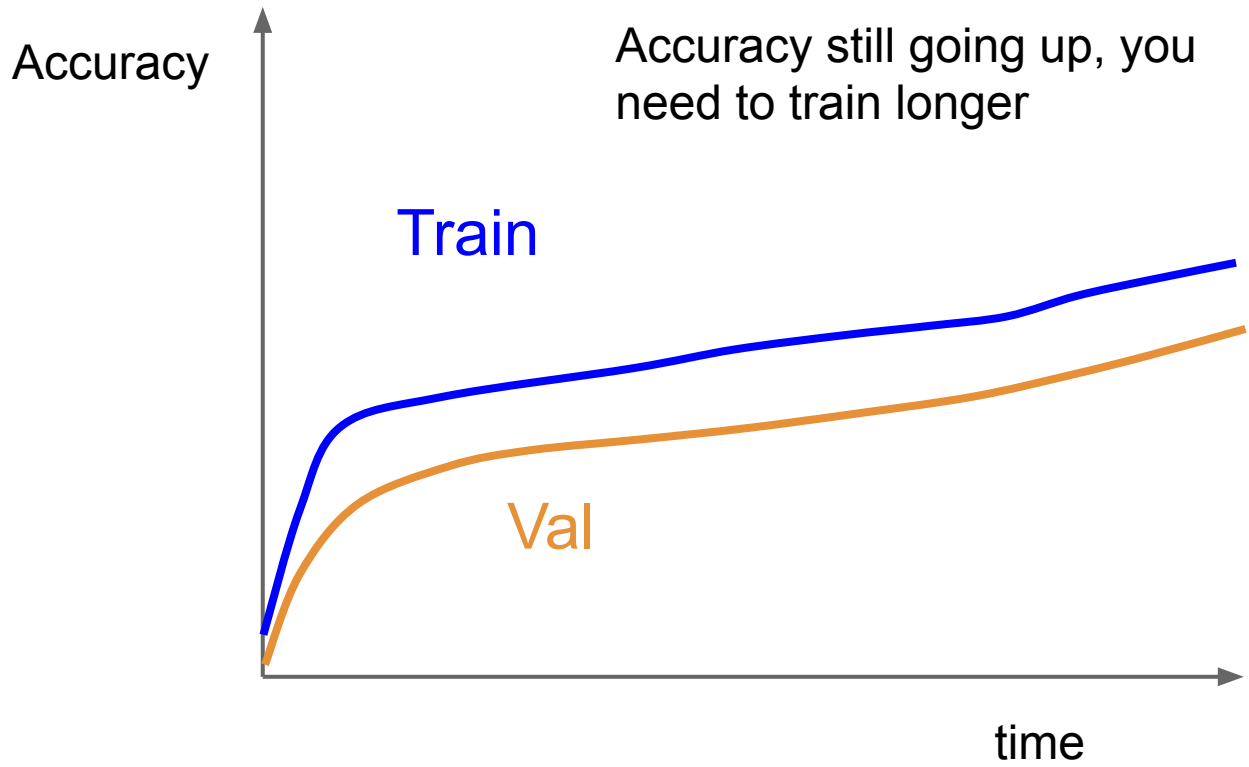
**Step 2:** Overfit a small sample

**Step 3:** Find LR that makes loss go down

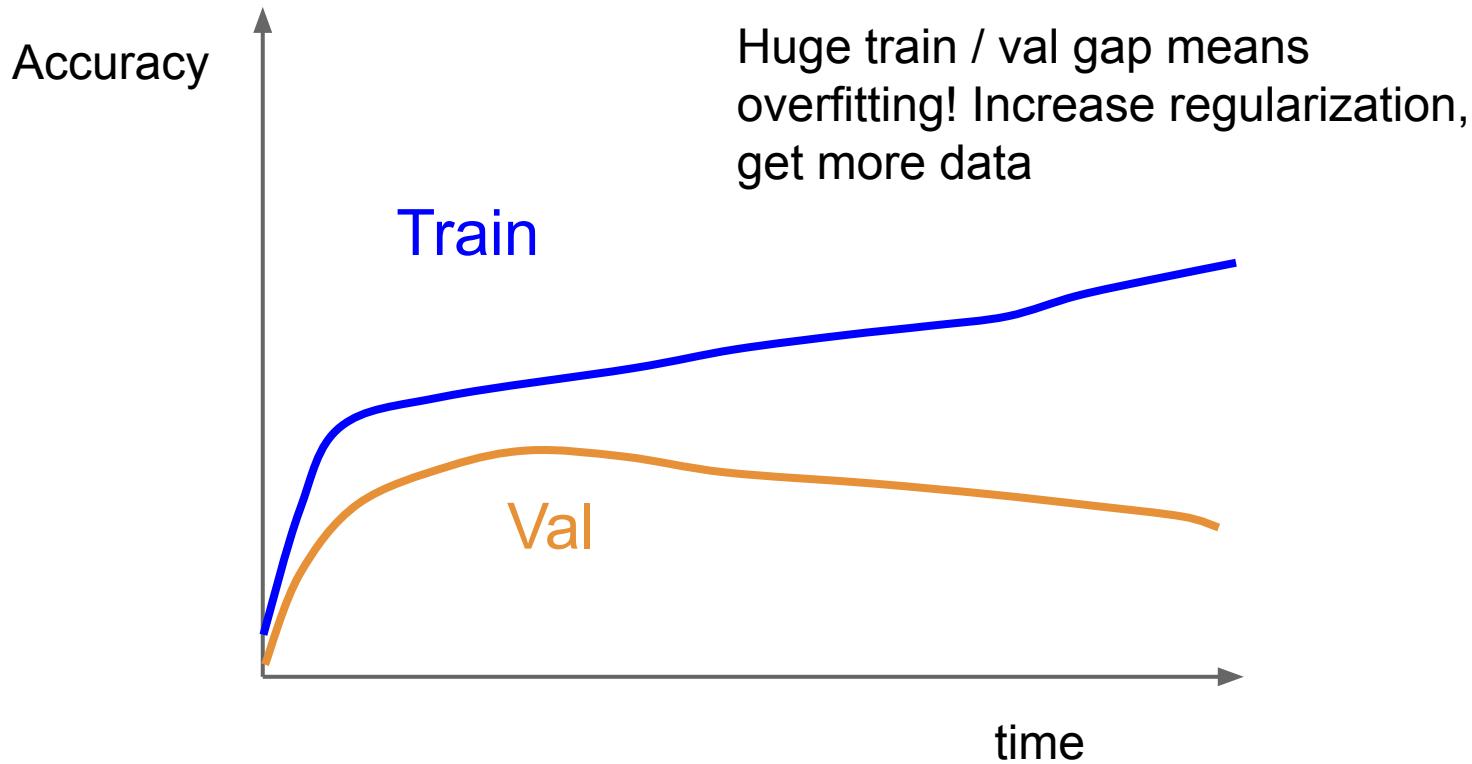
**Step 4:** Coarse grid, train for ~1-5 epochs

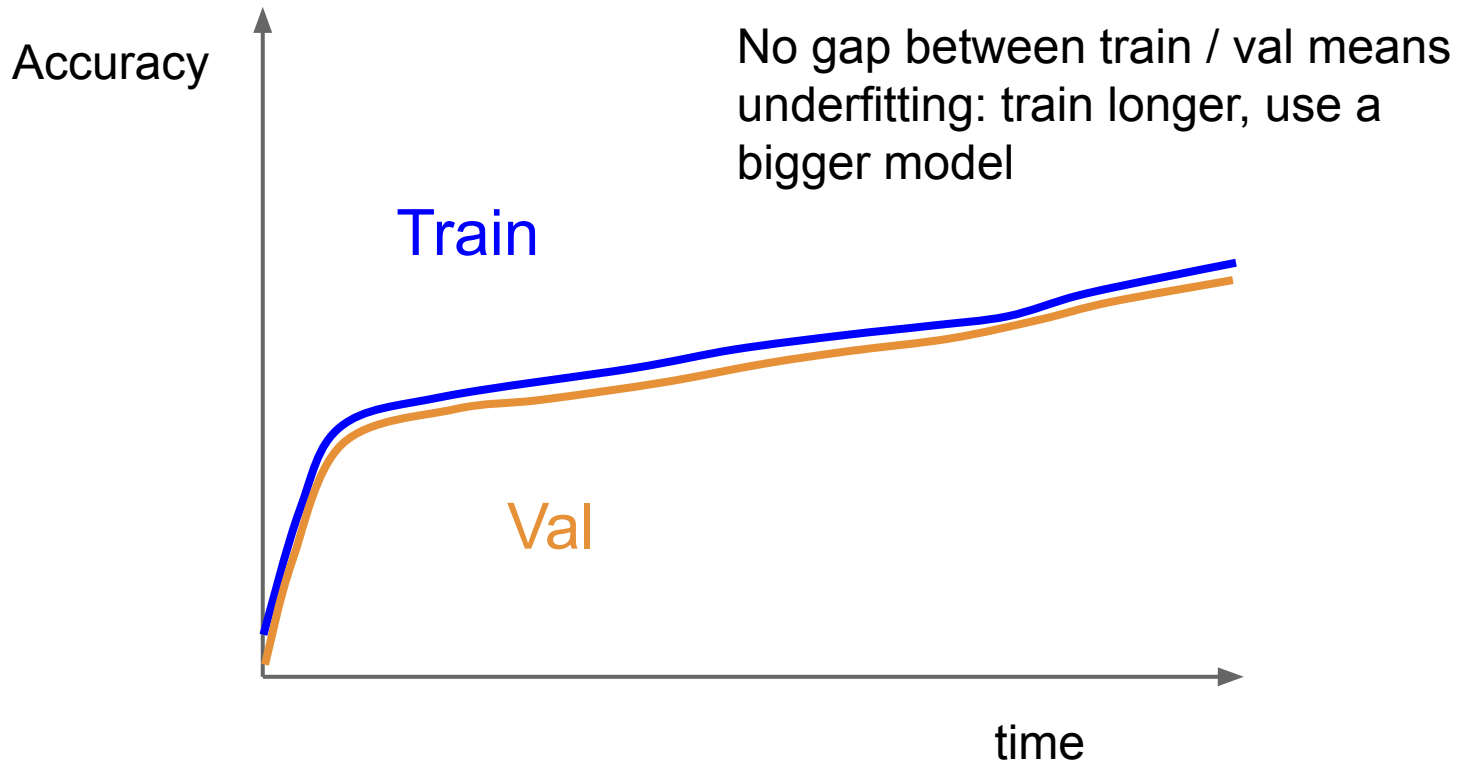
**Step 5:** Refine grid, train longer

**Step 6:** Look at loss and accuracy curves



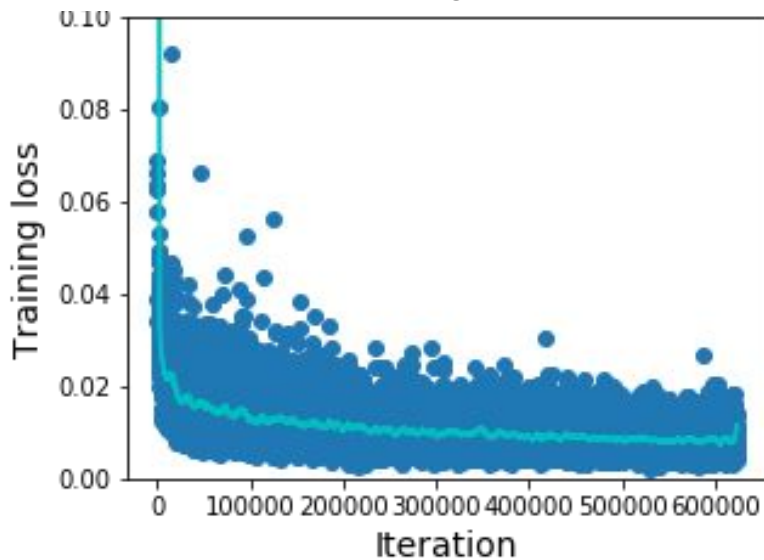




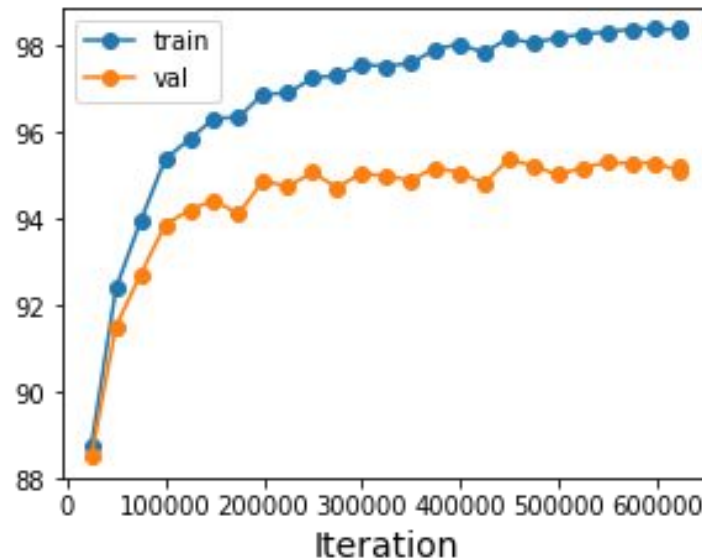


# Look at learning curves!

Training Loss



Train / Val Accuracy

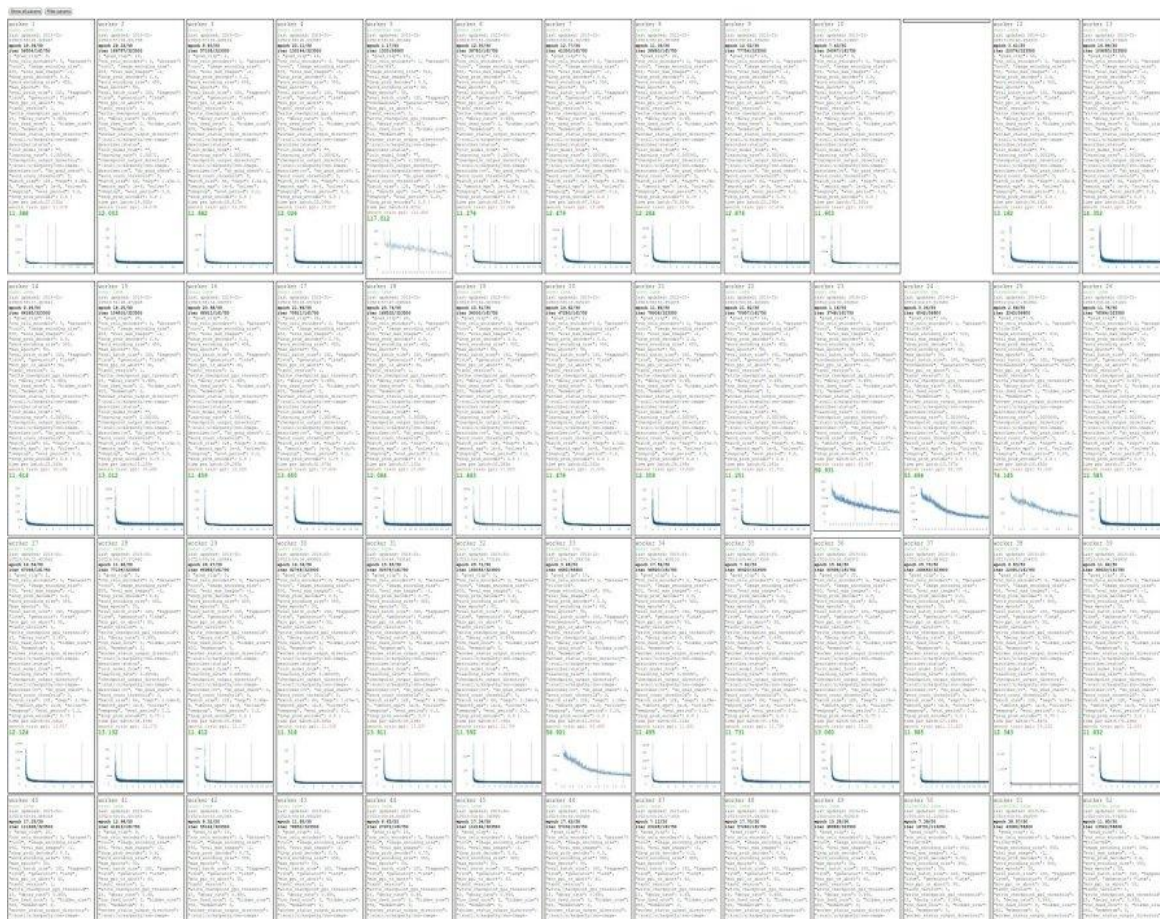


Losses may be noisy, use a scatter plot and also plot moving average to see trends better

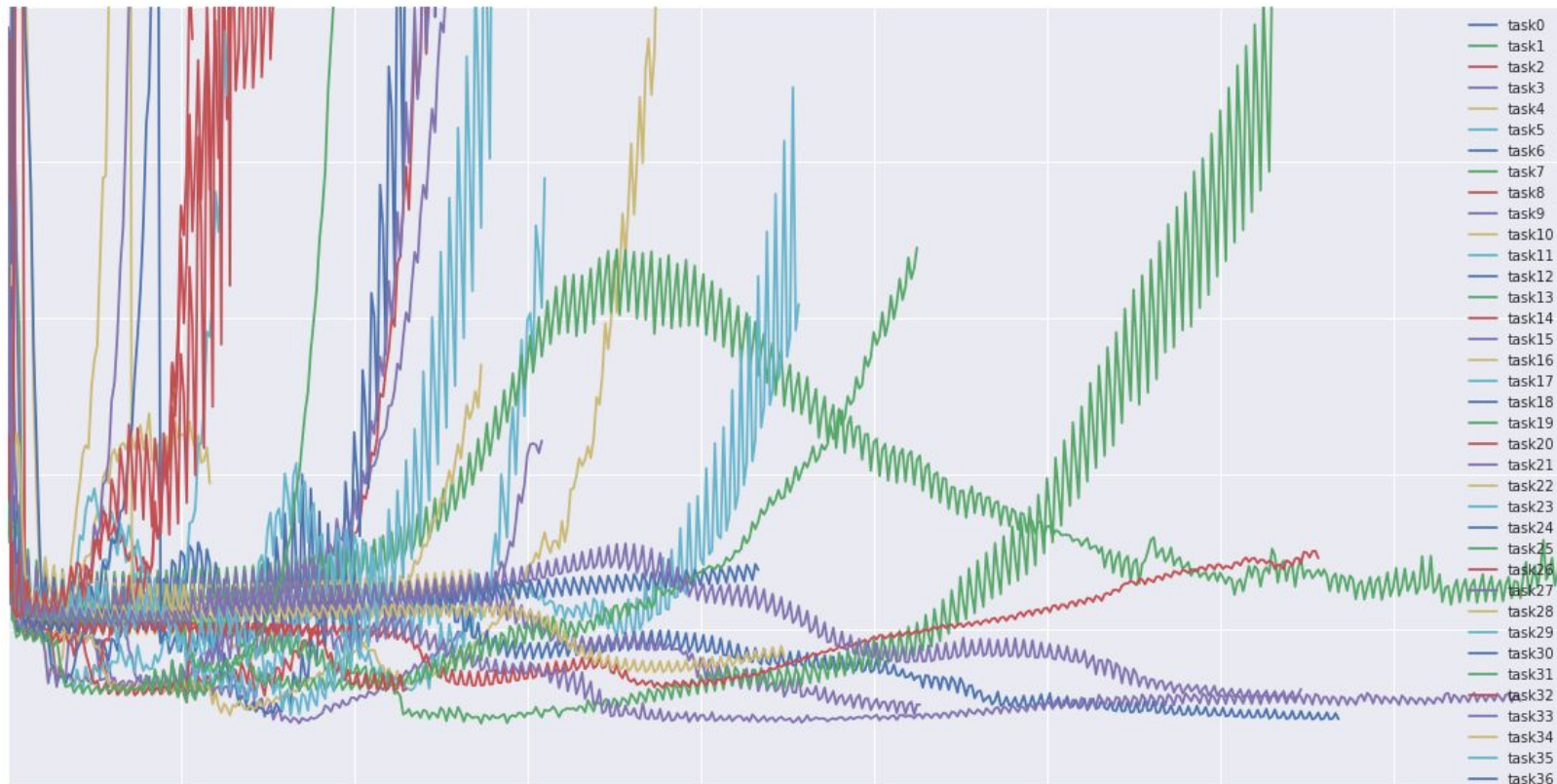
# Cross-validation

We develop "command centers" to visualize all our models training with different hyperparameters

check out [weights and biases](#)



You can plot all your loss curves for different hyperparameters on a single plot



Don't look at accuracy or loss curves for too long!



# Choosing Hyperparameters

**Step 1:** Check initial loss

**Step 2:** Overfit a small sample

**Step 3:** Find LR that makes loss go down

**Step 4:** Coarse grid, train for ~1-5 epochs

**Step 5:** Refine grid, train longer

**Step 6:** Look at loss and accuracy curves

**Step 7:** GOTO step 5

# Random Search vs. Grid Search

*Random Search for  
Hyper-Parameter Optimization*  
Bergstra and Bengio, 2012

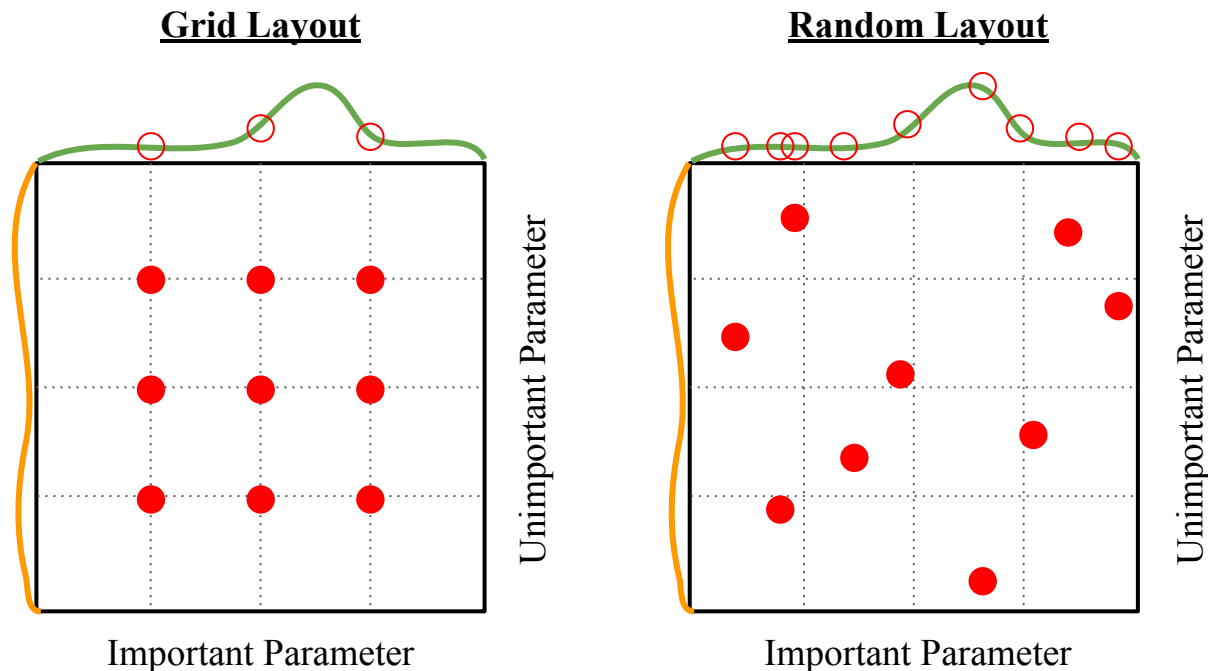


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017



# Transfer learning

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

# 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



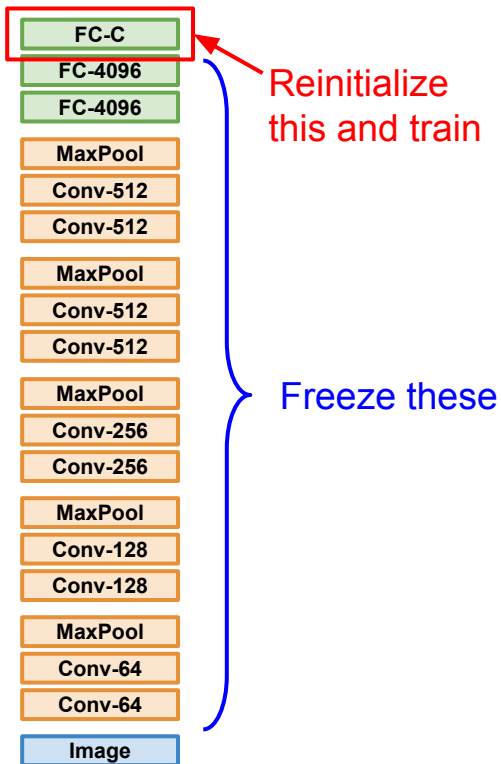
# Transfer Learning with CNNs

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)

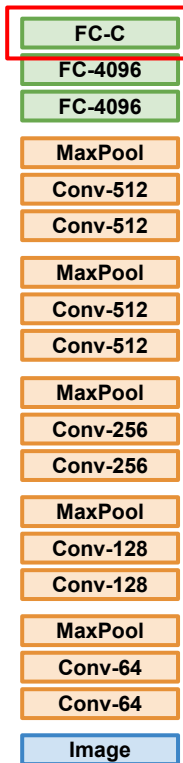


# Transfer Learning with CNNs

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

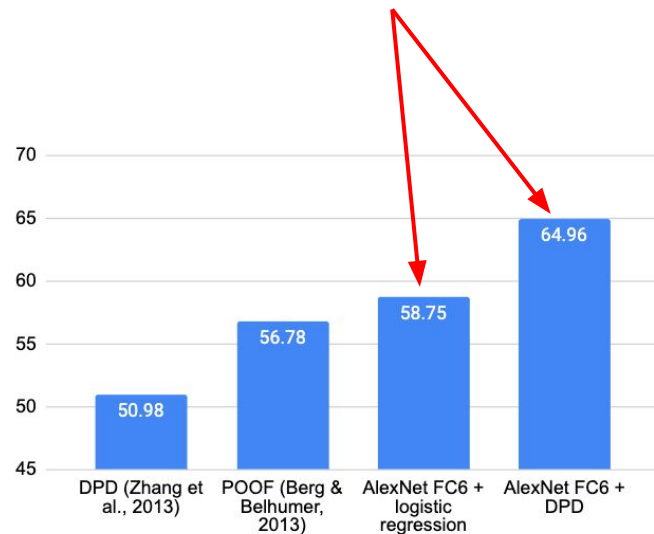
## 2. Small Dataset (C classes)



Reinitialize this and train

Freeze these

Finetuned from AlexNet



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

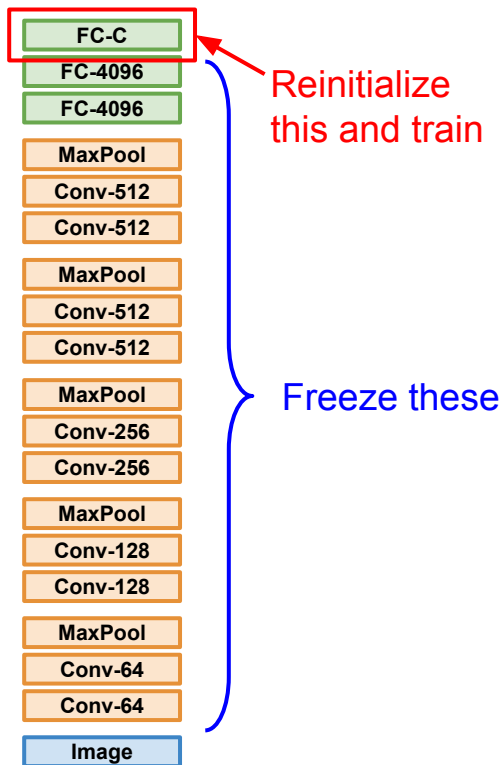
# Transfer Learning with CNNs

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

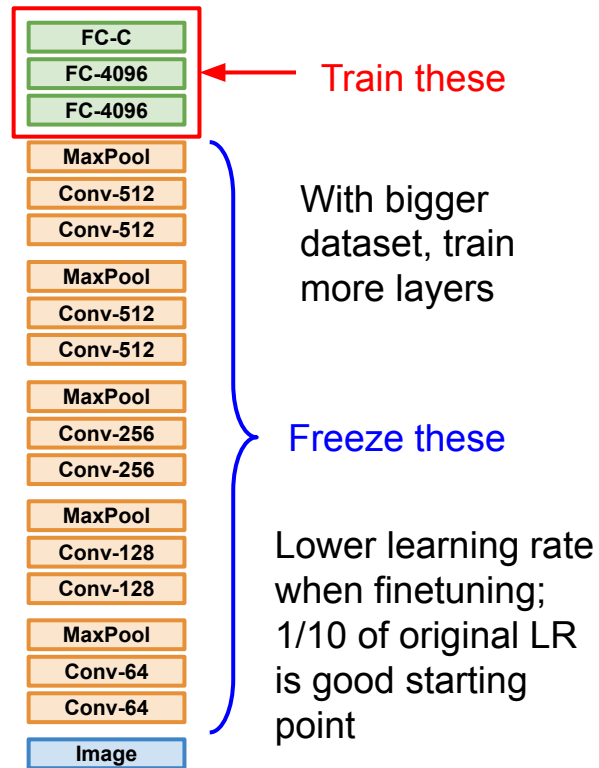
## 1. Train on Imagenet



## 2. Small Dataset (C classes)



## 3. Bigger dataset



# Takeaway for your projects and beyond:

Have some dataset of interest but it has  $< \sim 1\text{M}$  images?

1. Find a very large dataset that has similar data, train a big ConvNet there
2. Transfer learn to your dataset

Deep learning frameworks provide a “Model Zoo” of pretrained models so you don’t need to train your own

TensorFlow: <https://github.com/tensorflow/models>

PyTorch: <https://github.com/pytorch/vision>

# Summary

- Improve your training error:
  - Optimizers
  - Learning rate schedules
- Improve your test error:
  - Regularization
  - Choosing Hyperparameters



# Summary

## TLDRs

We looked in detail at:

- Activation Functions (use ReLU)
- Data Preprocessing (images: subtract mean)
- Weight Initialization (use Xavier/Kaiming init)
- Batch Normalization (use this!)
- Transfer learning (use this if you can!)

Next time: Recurrent Neural Networks