# Lecture 7:
# Training Neural Networks

# Administrative: A2

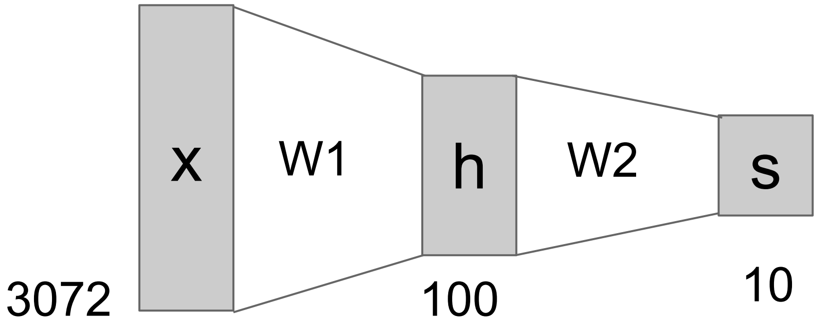
A2 is out, due Monday May 2nd, 11:59pm

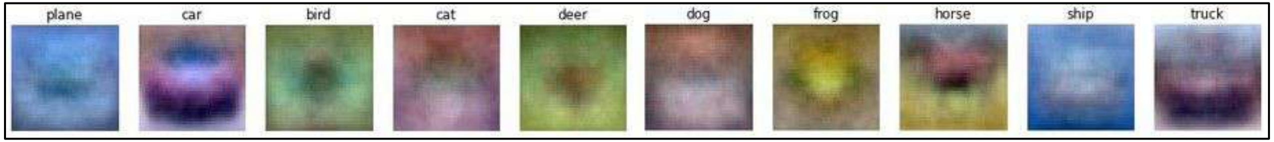
Where we are now...

# Neural Networks

Linear score function: $f = Wx$

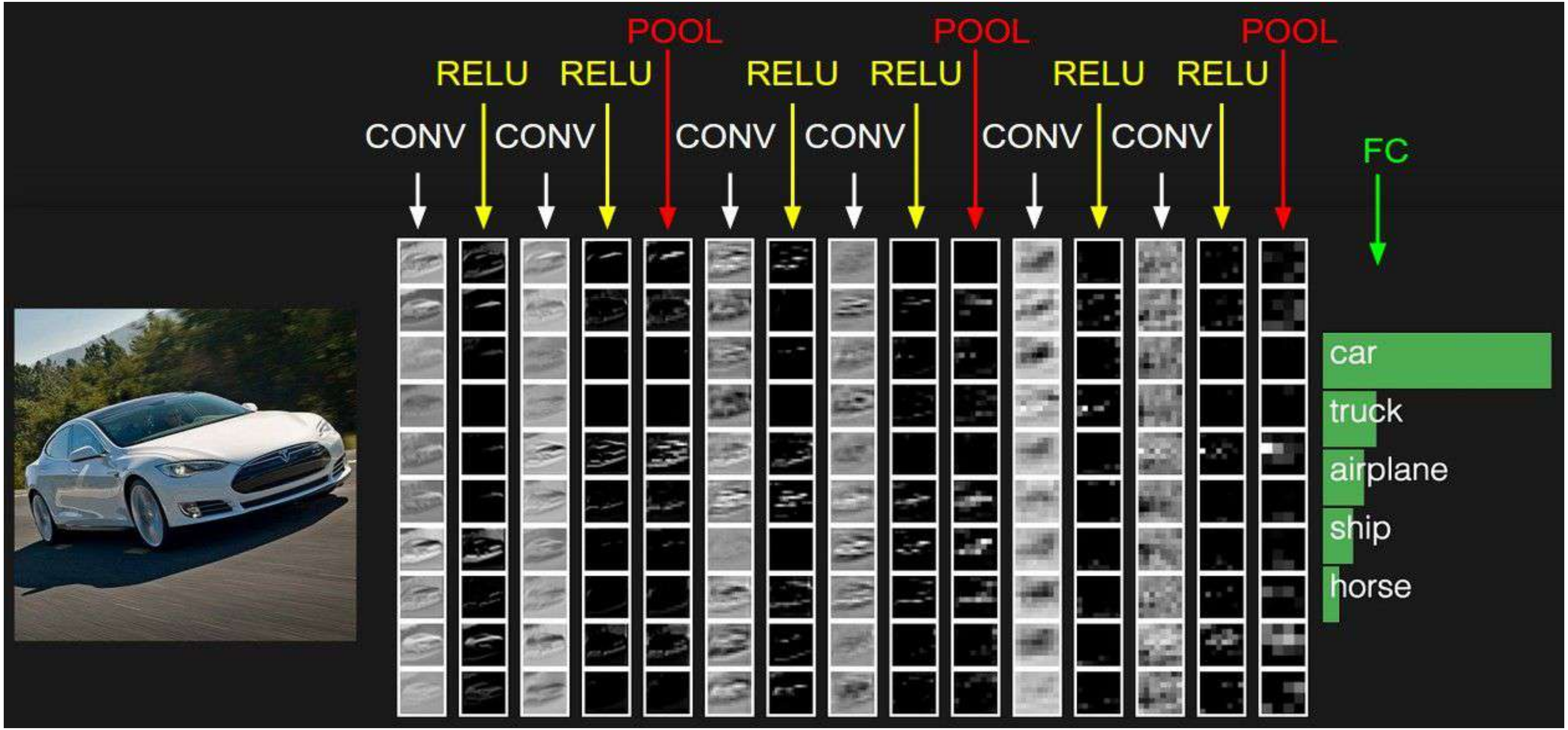
2-layer Neural Network $f = W_2 \max(0, W_1 x)$



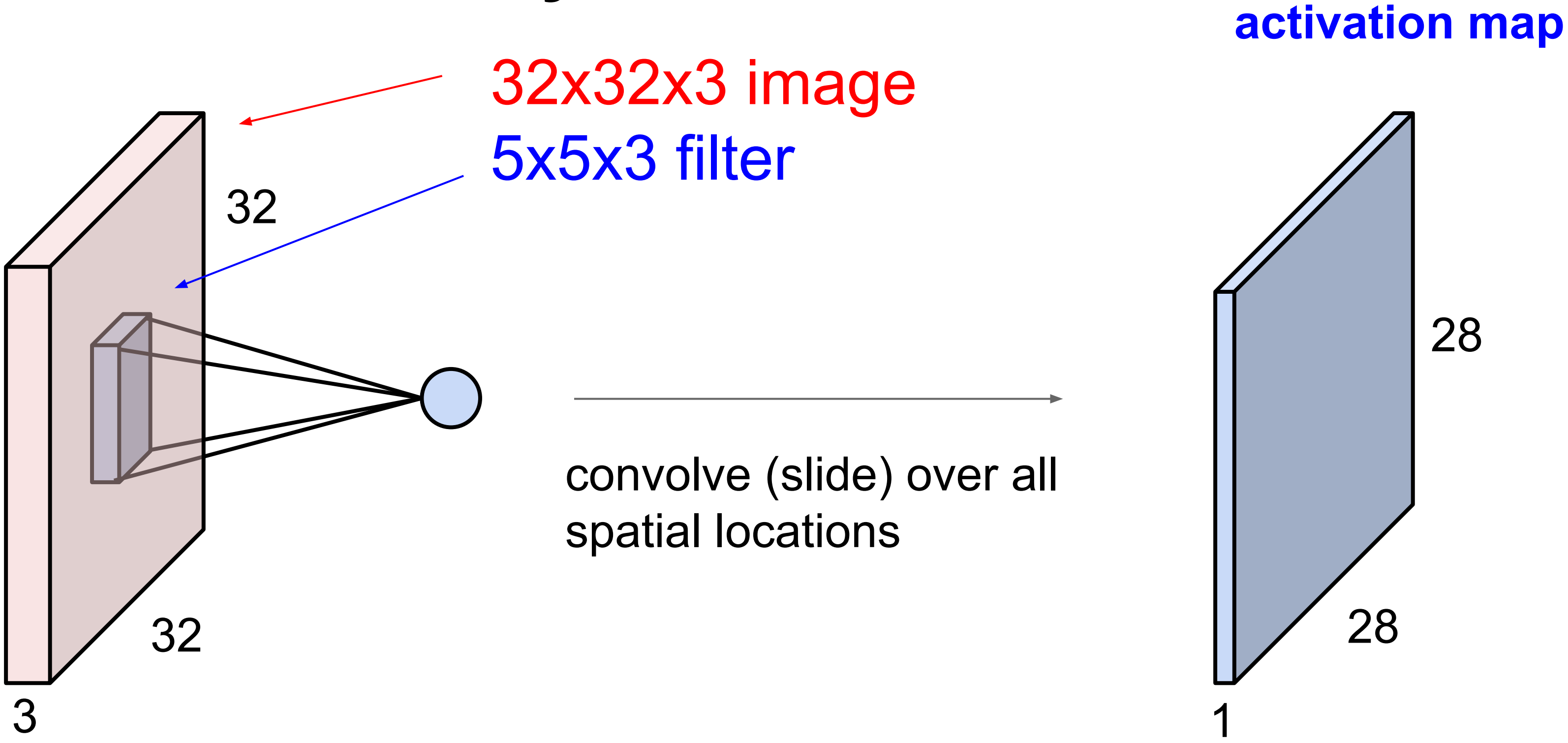
Where we are now...

# Convolutional Neural Networks



Where we are now...

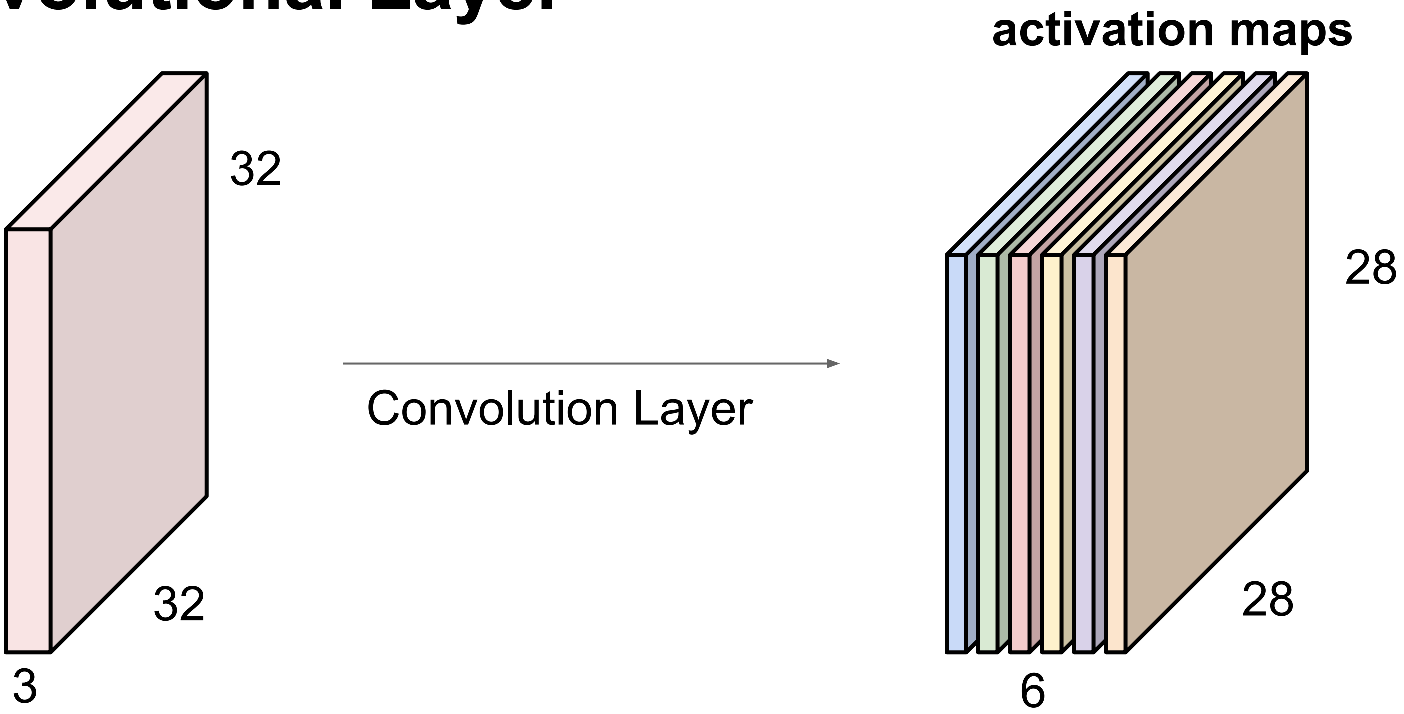
# Convolutional Layer



Where we are now...

# Convolutional Layer

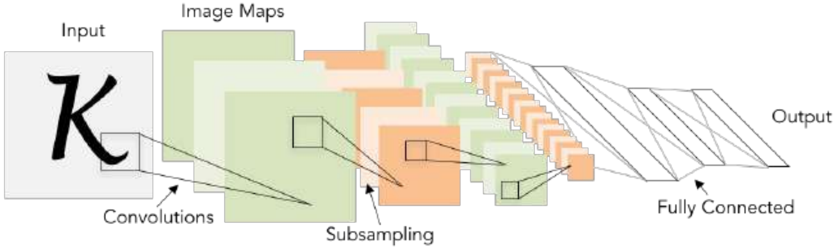
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:

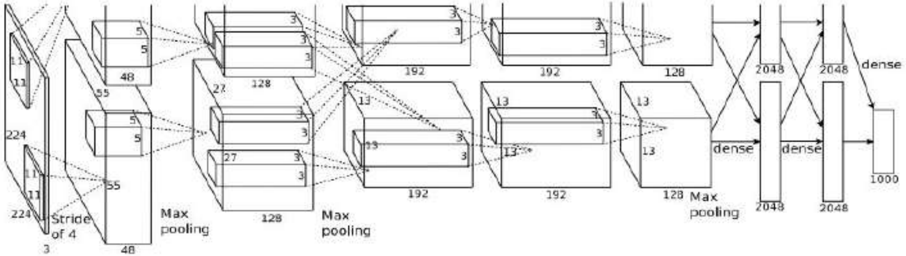


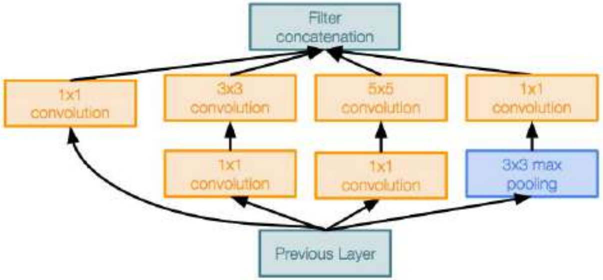

We stack these up to get a "new image" of size 28x28x6!

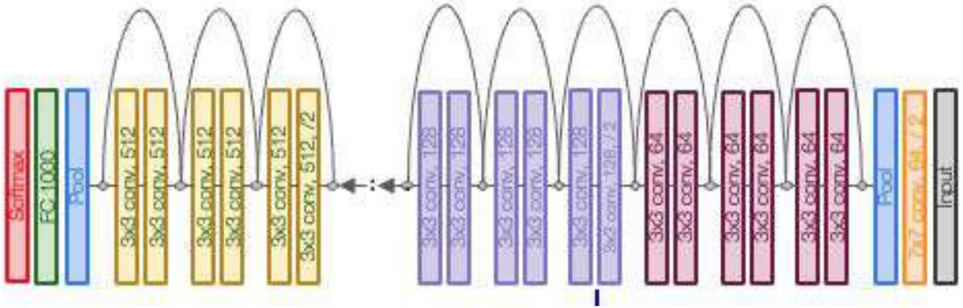
Where we are now...

# CNN Architectures



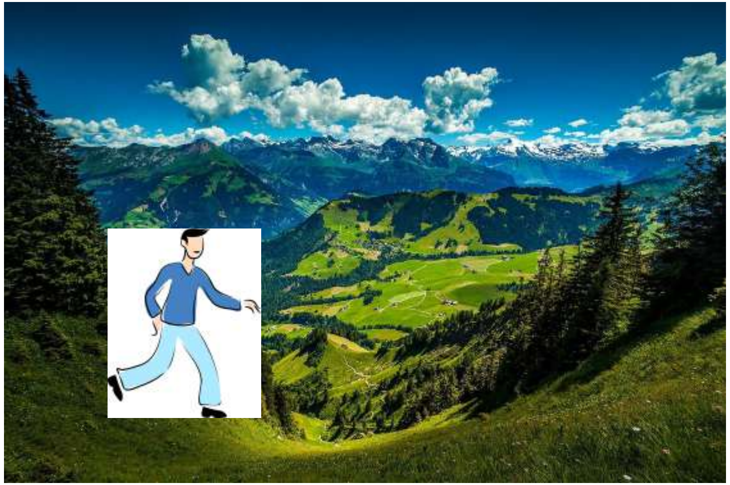



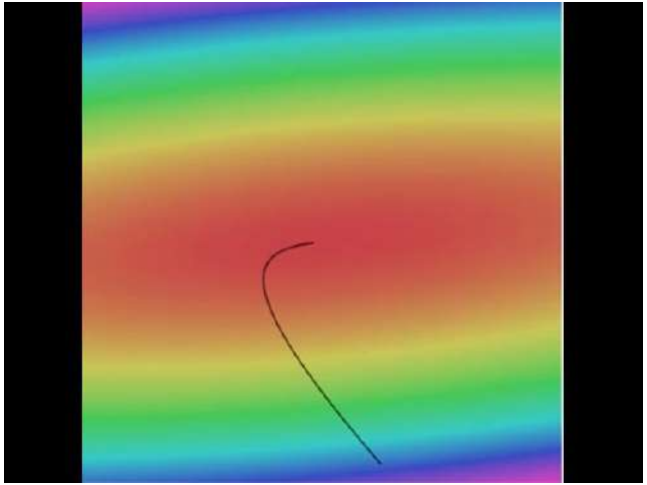



# Where we are now...

## 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

# Today: Training Neural Networks

# Overview

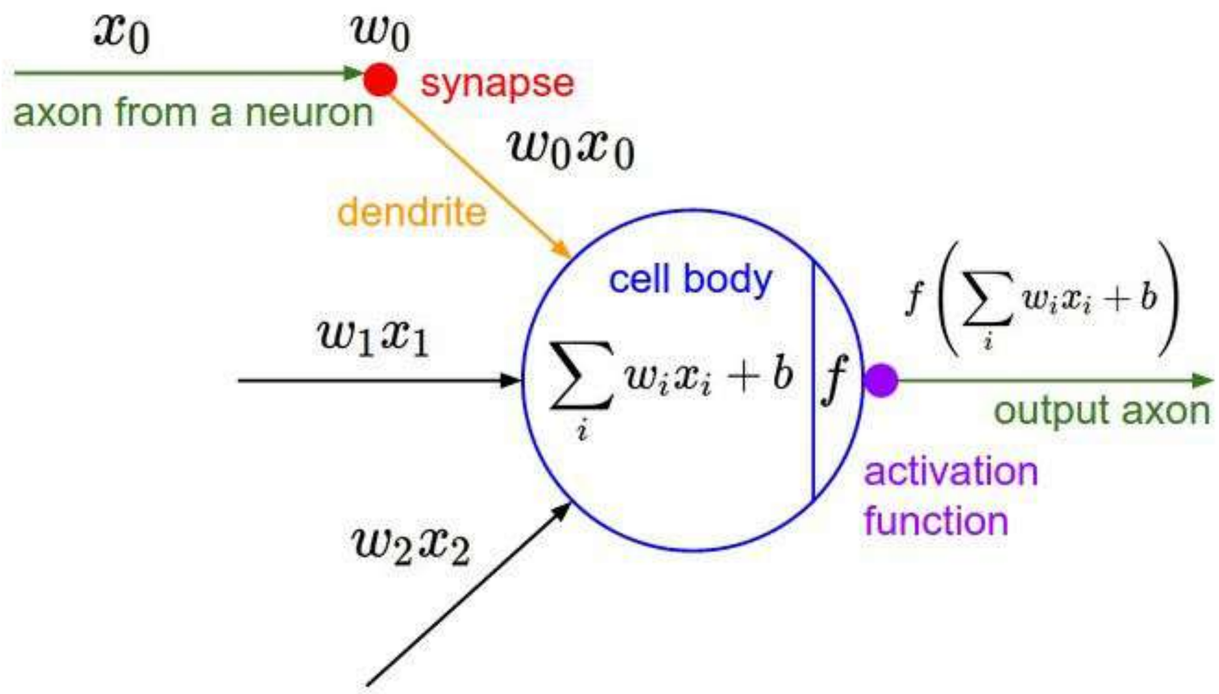
1. **One time set up**: activation functions, preprocessing, weight initialization, regularization, gradient checking

2. **Training dynamics**: babysitting the learning process, parameter updates, hyperparameter optimization

3. **Evaluation**: model ensembles, test-time augmentation, transfer learning

# Activation Functions

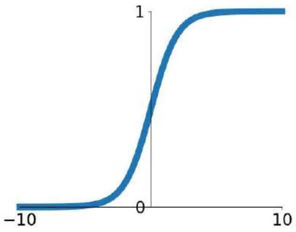
# Activation Functions



# Activation Functions

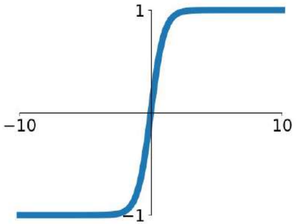
**Sigmoid**

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



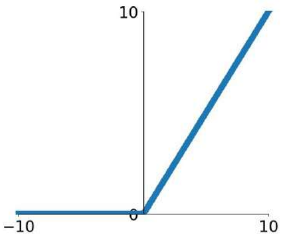

**tanh**

$$\tanh(x)$$



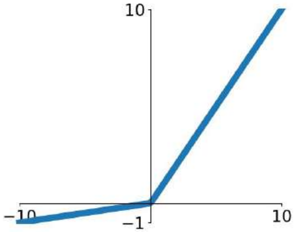

**ReLU**

$$\max(0, x)$$




**Leaky ReLU**

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

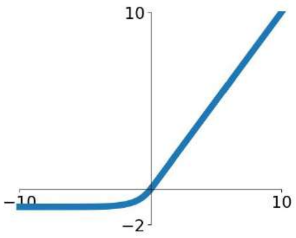



**Maxout**

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

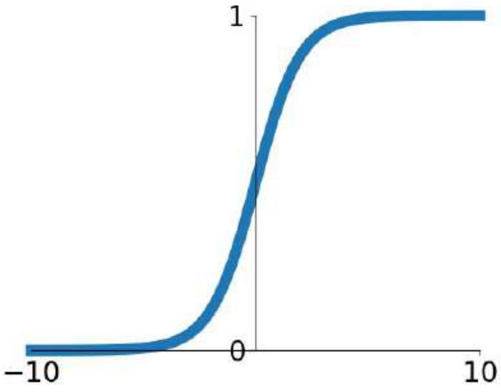
**ELU**

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



# Activation Functions

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




**Sigmoid**

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

# Activation Functions

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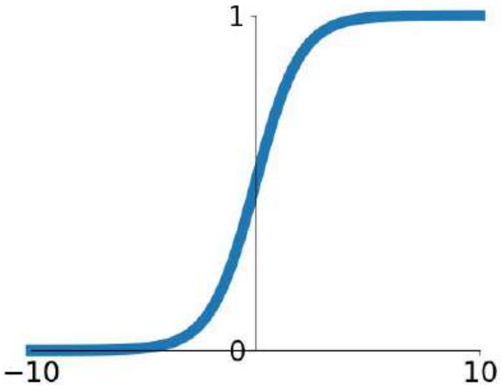


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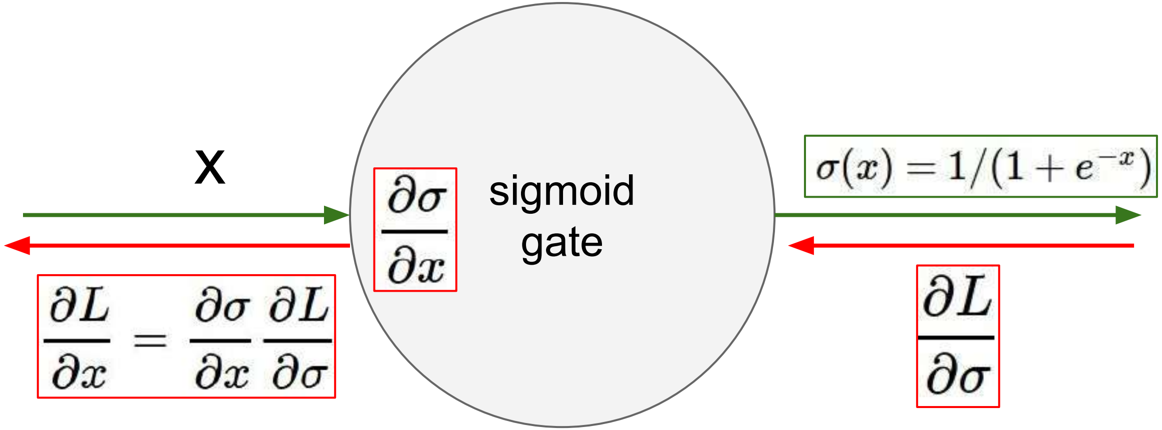
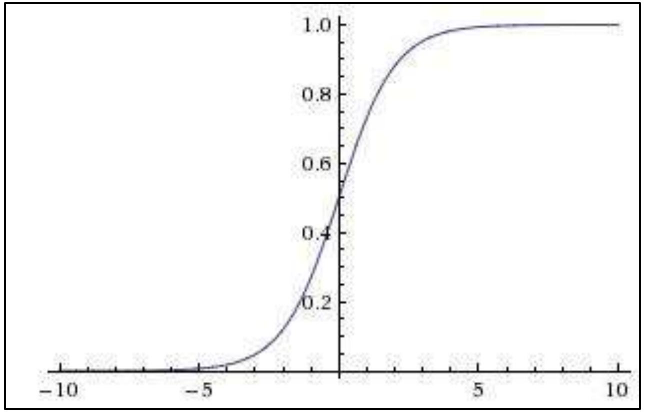
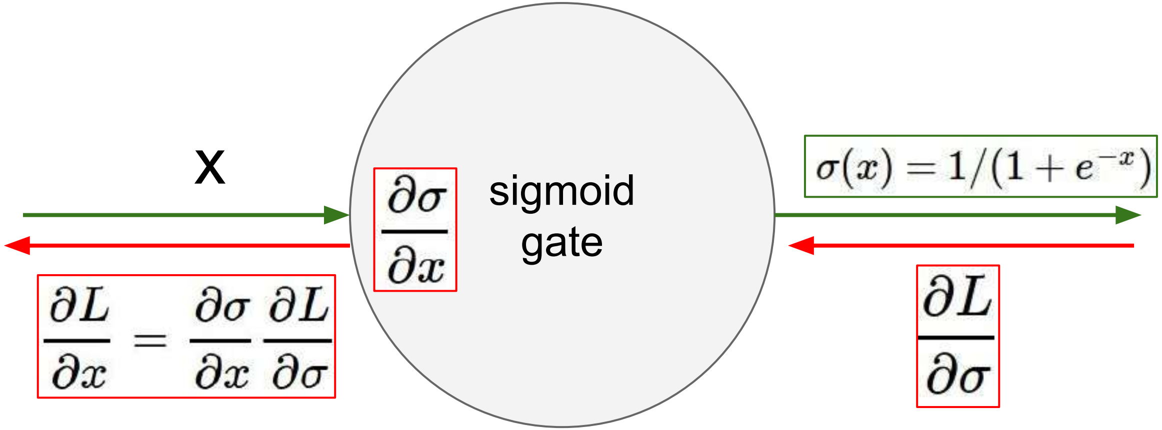
3 problems:

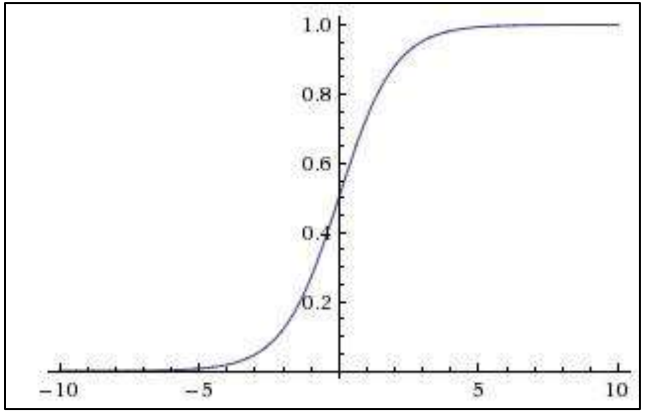
1. Saturated neurons "kill" the gradients



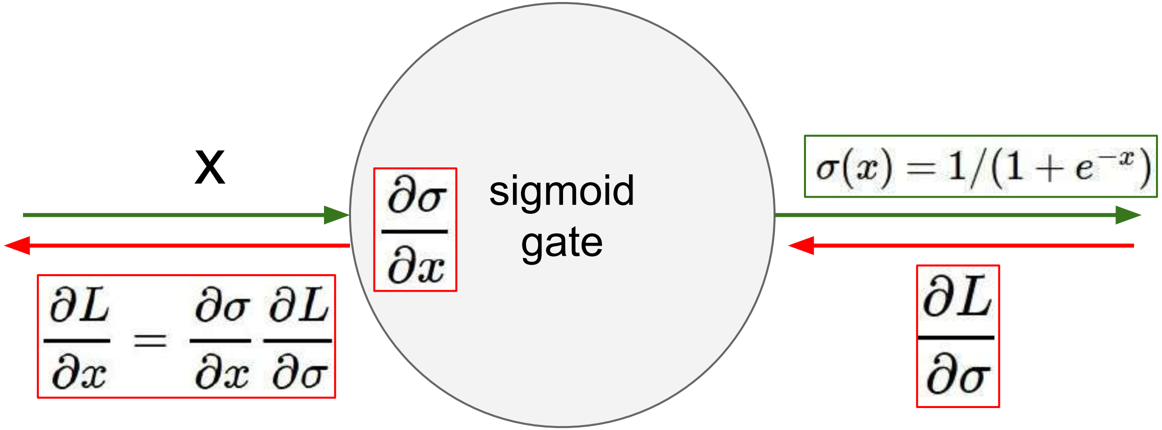

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

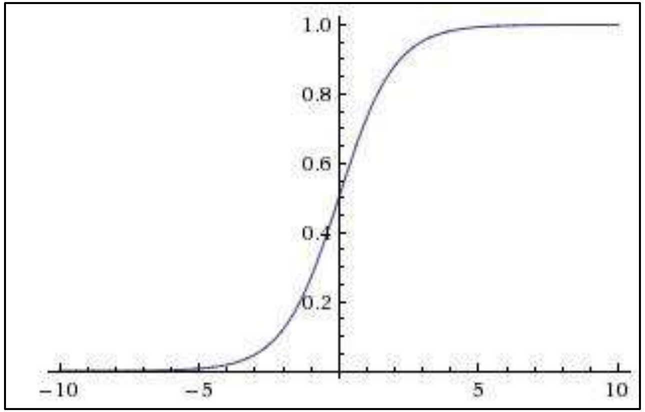



What happens when x = -10?

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



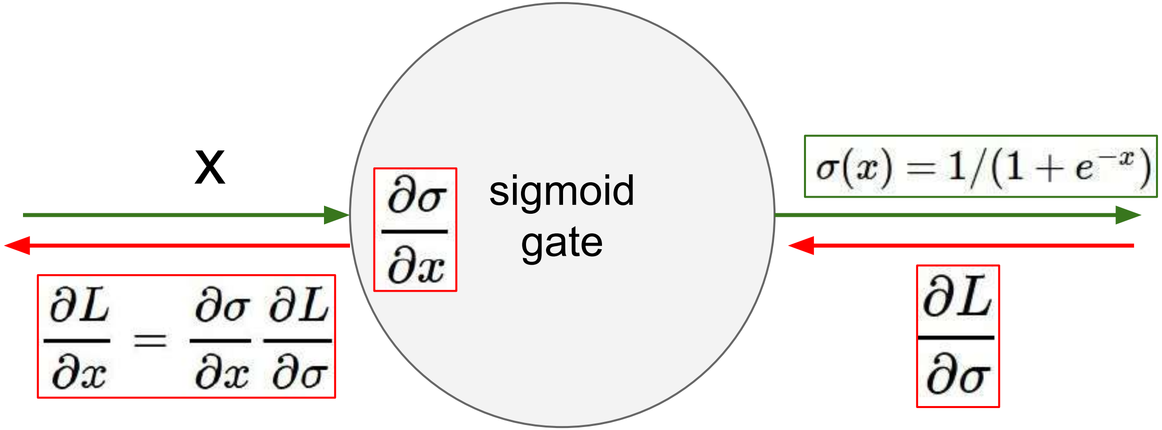



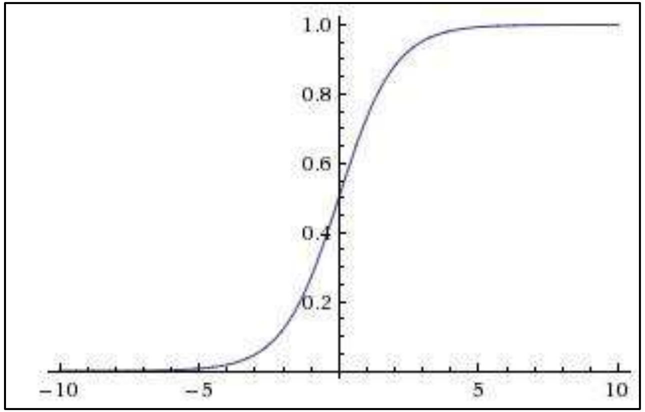

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\left(1 - \sigma(x)\right)$$

What happens when x = -10?

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

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

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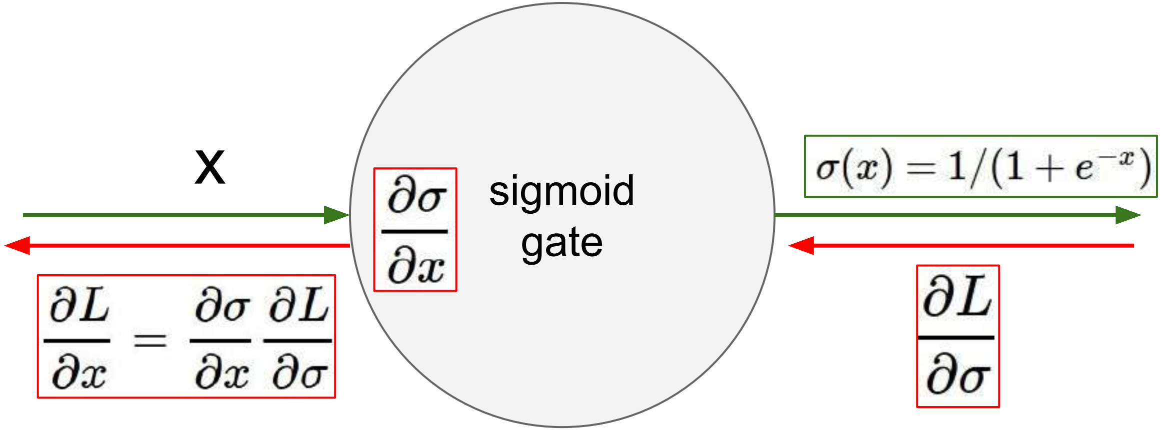
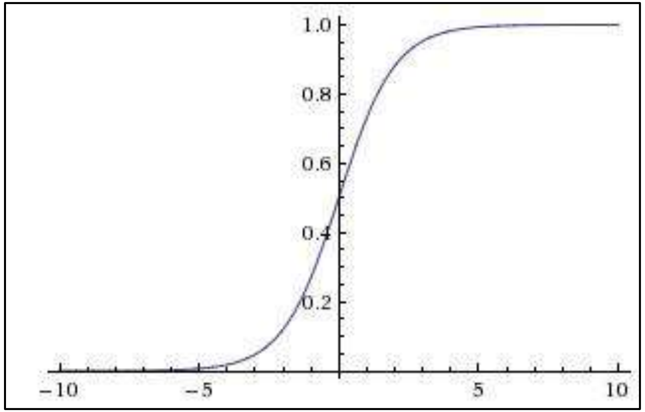
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$




What happens when x = -10?

What happens when x = 0?

What happens when x = 10?

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

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

x

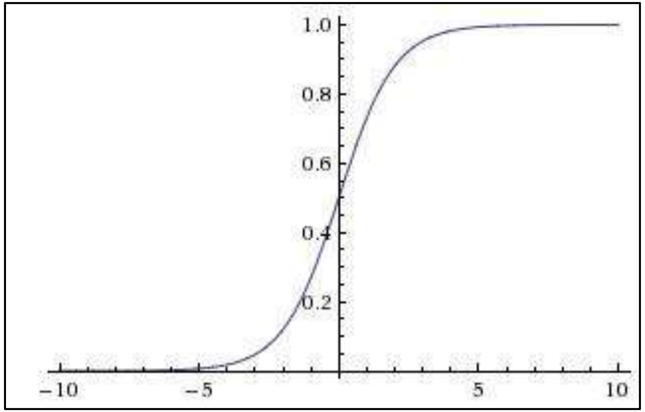
sigmoid gate

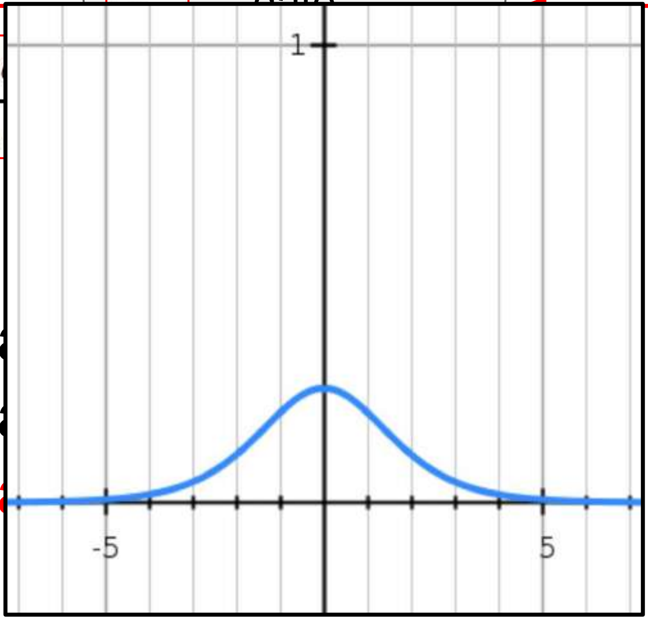
$\frac{\partial \sigma}{}$

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

$\frac{\partial L}{\partial x} = \frac{\partial \sigma}{\partial x}$ ...

$\frac{\partial L}{\partial \sigma}$




What ha

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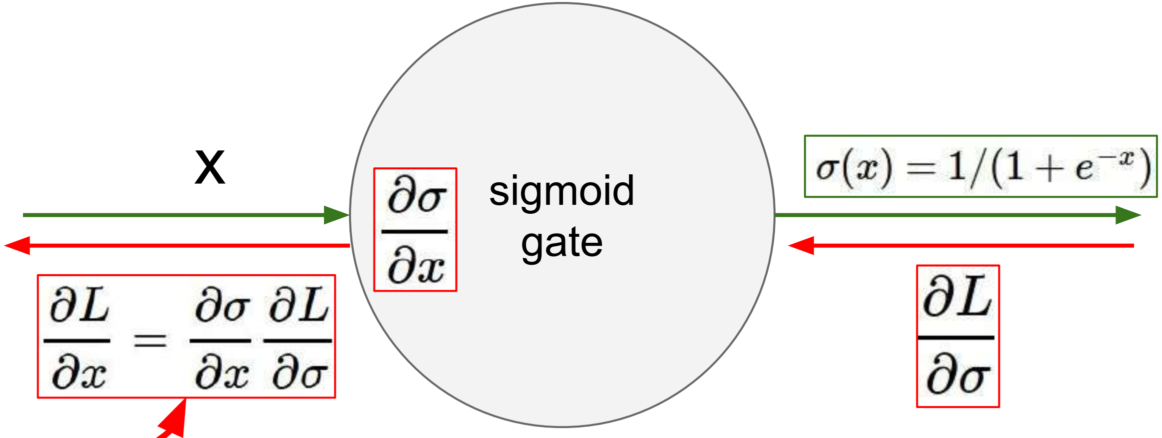
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

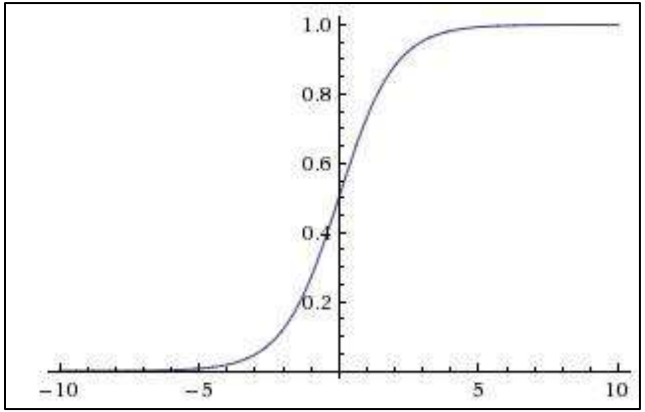



$$\frac{\partial \sigma}{\partial x}$$

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

$$\frac{\partial L}{\partial \sigma}$$

$$\frac{\partial L}{\partial x} = \frac{\partial \sigma}{\partial x}\frac{\partial L}{\partial \sigma}$$



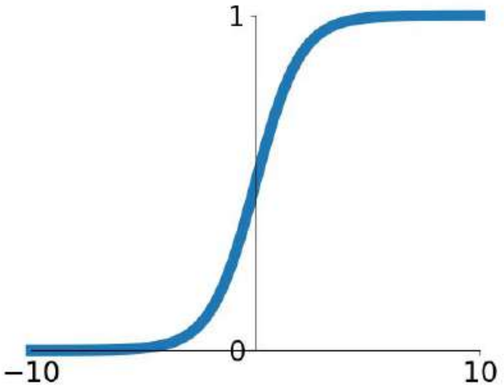

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

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**

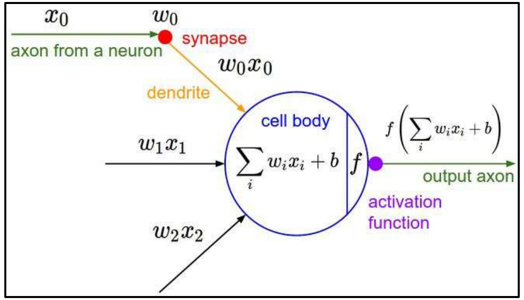
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

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 **w**?

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

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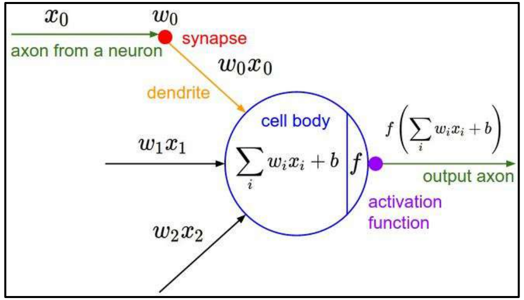
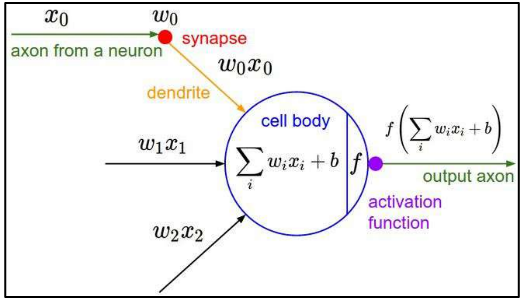



What can we say about the gradients on **w**?

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

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 **w**?

We know that local gradient of sigmoid is always positive

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

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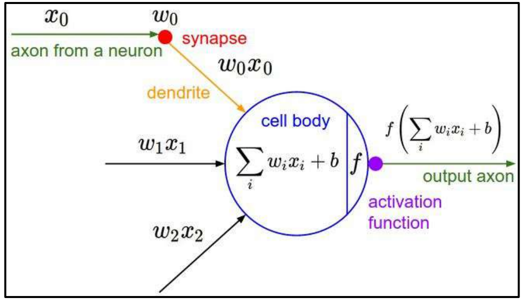


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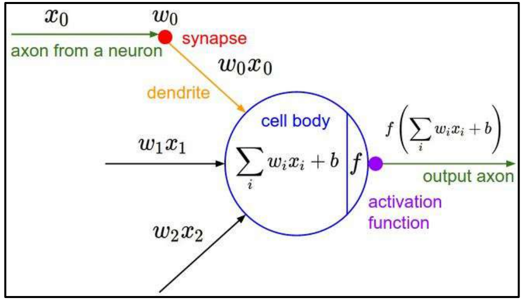
We are assuming x is always positive

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

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 **w**?

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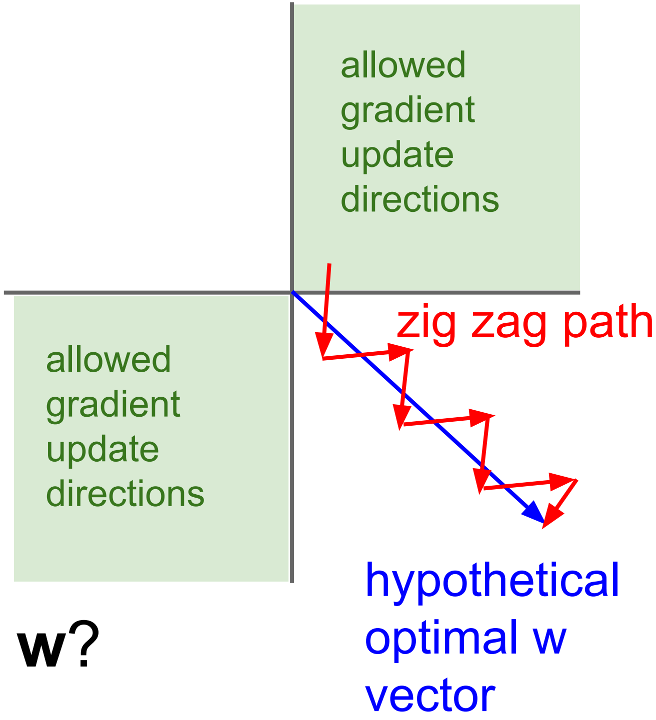
So!! Sign of gradient **for all** $\mathbf{w}_i$ is the same as the sign of upstream scalar gradient!

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

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

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

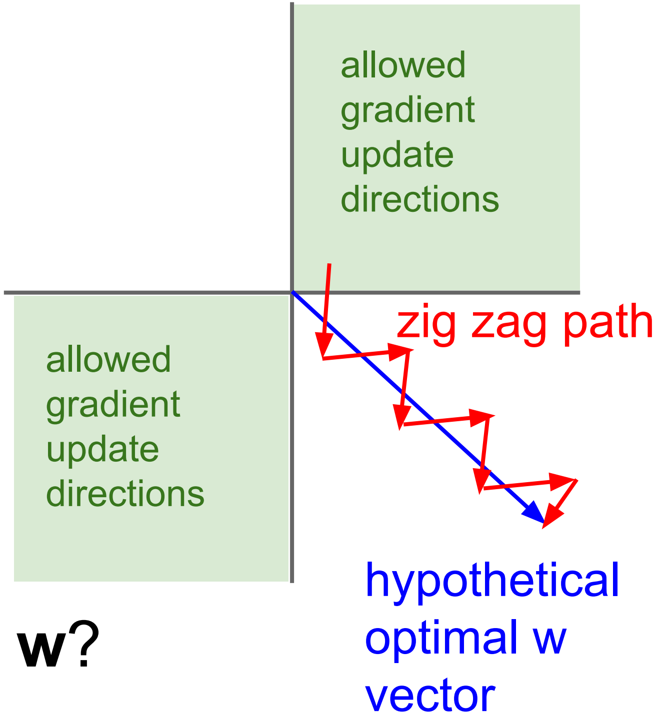



What can we say about the gradients on **w**?

Always all positive or all negative :(

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

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



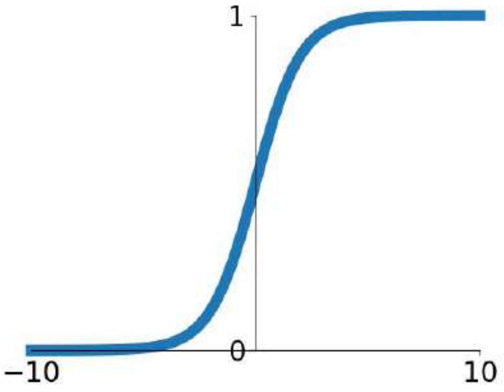

What can we say about the gradients on **w**?

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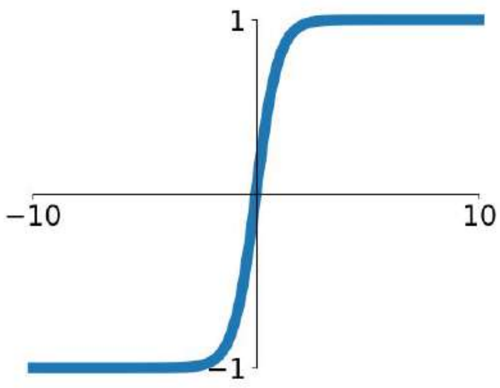
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

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

# Activation Functions

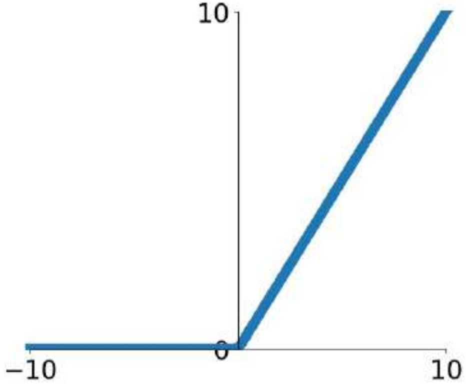



**tanh(x)**

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

[LeCun et al., 1991]

# Activation Functions



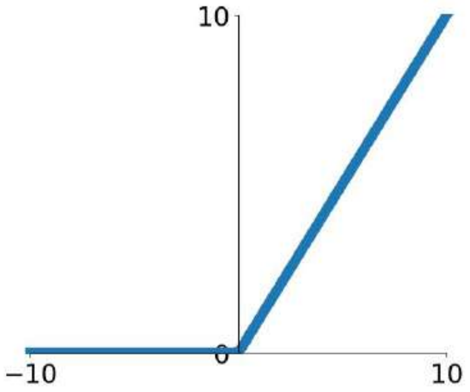

**ReLU**
(Rectified Linear Unit)

- 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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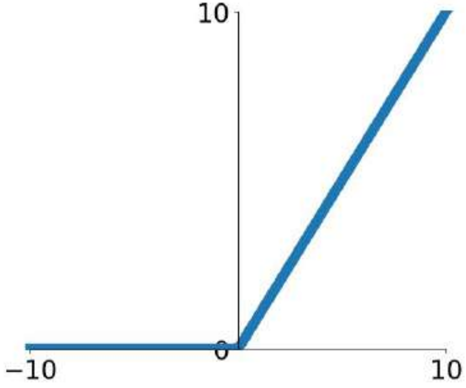
# Activation Functions

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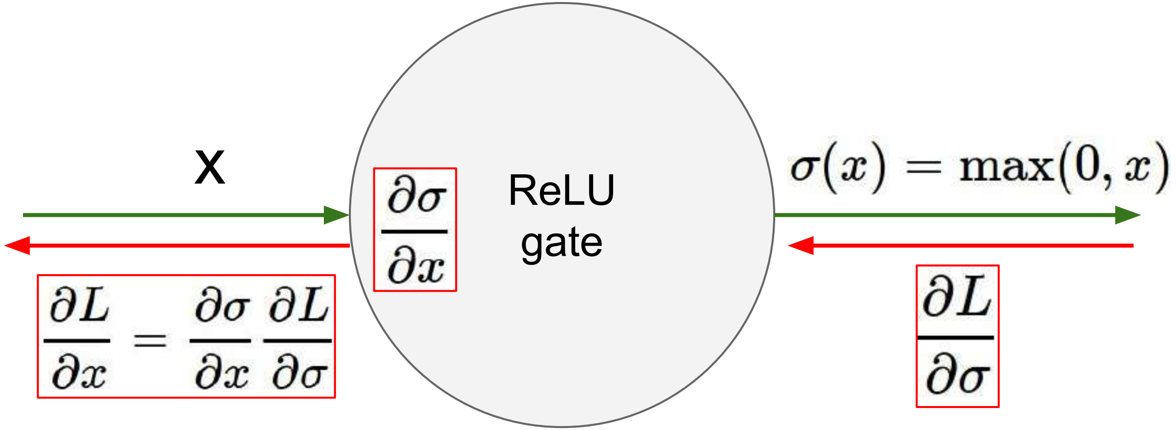
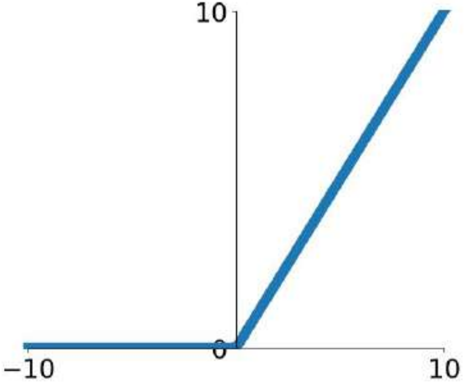
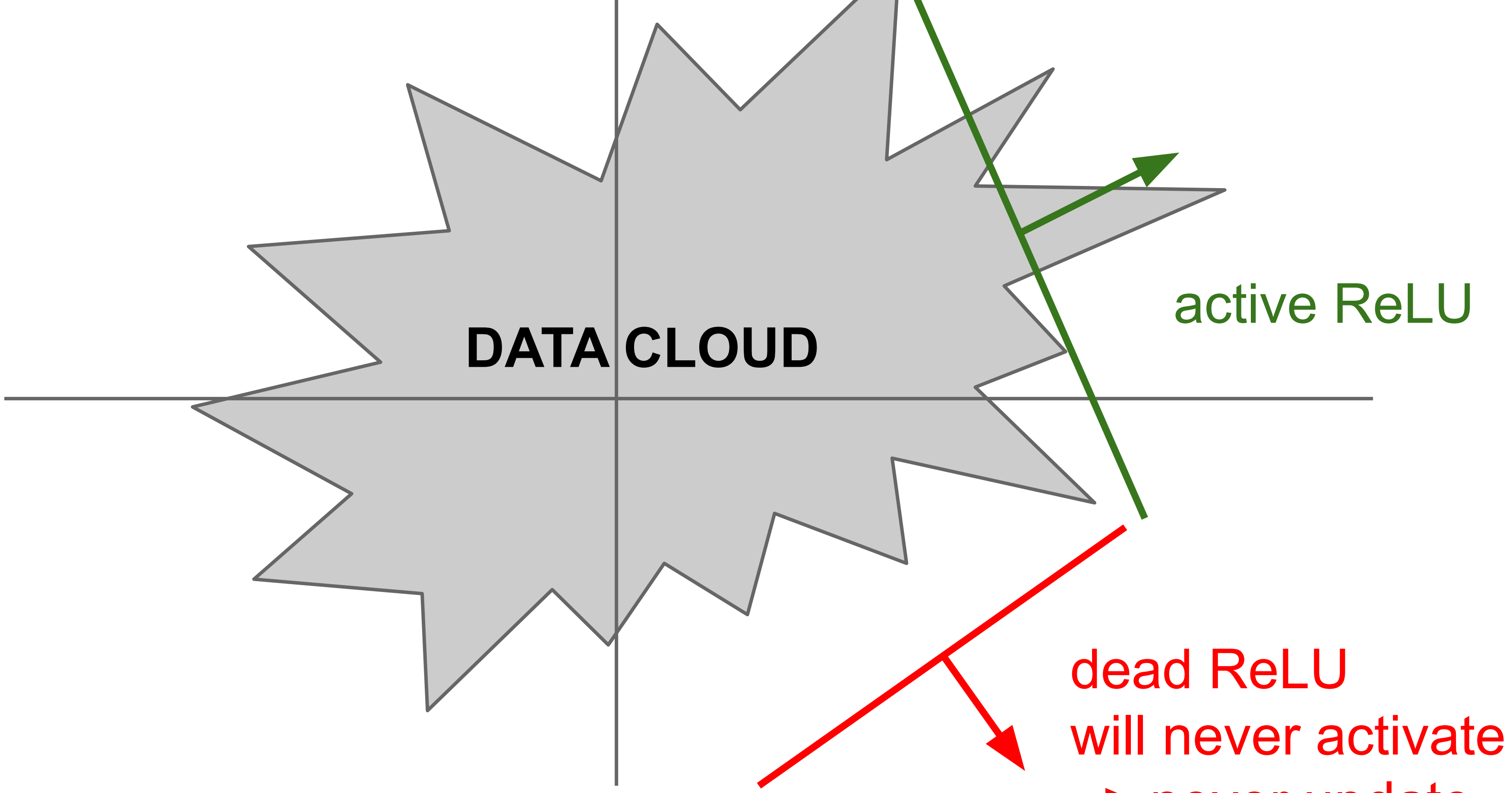
- Not zero-centered output
- An annoyance:

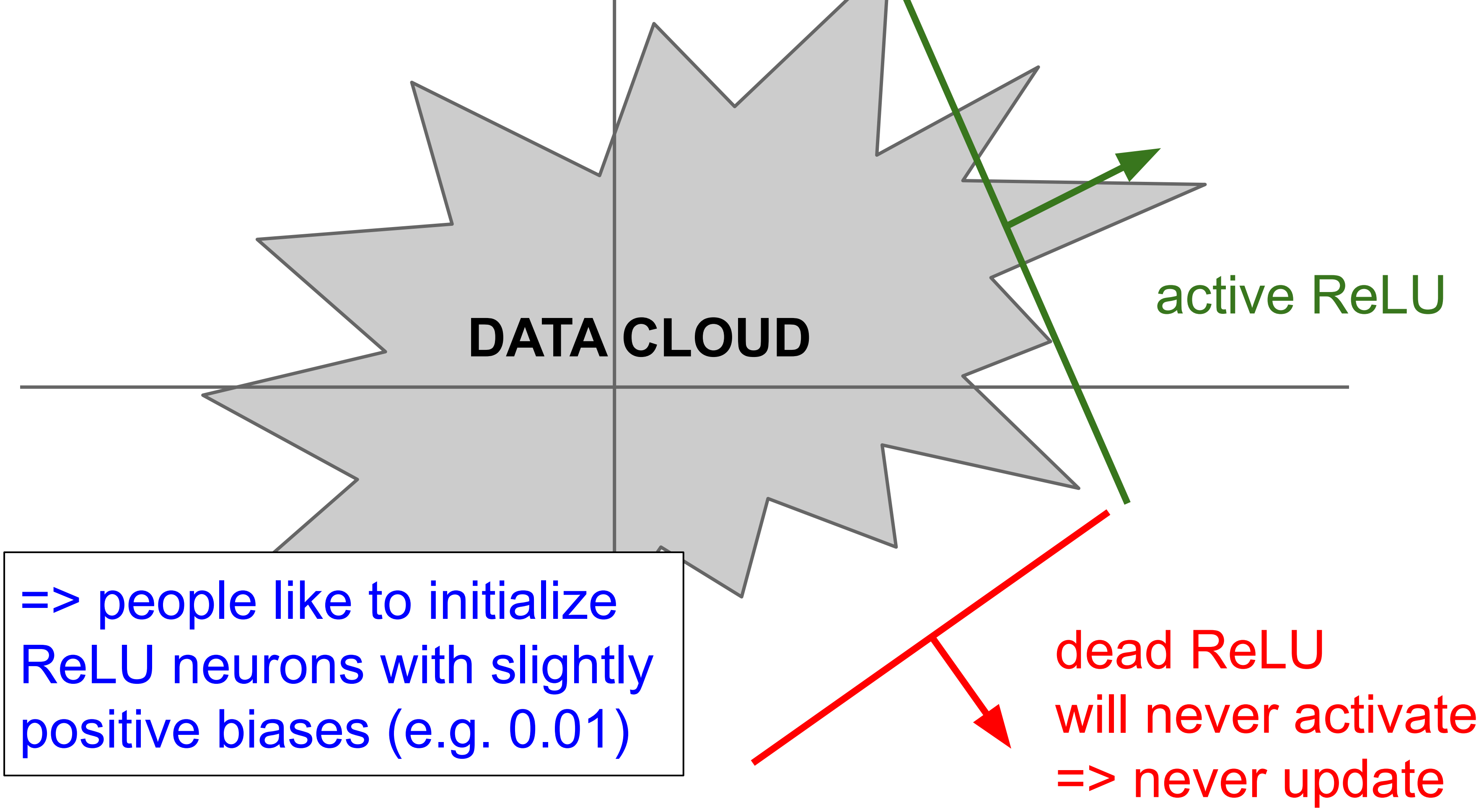
hint: what is the gradient when x < 0?




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

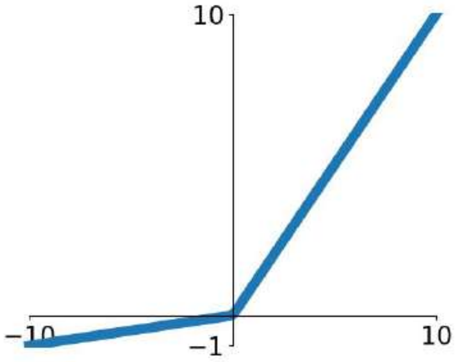

DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update




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

# Activation Functions

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



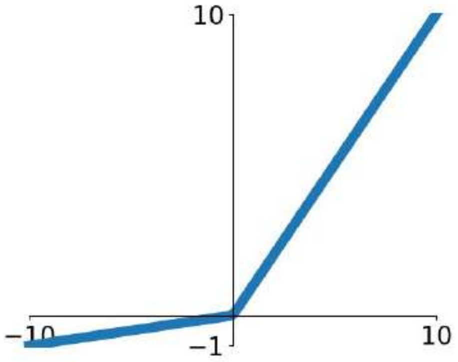

**Leaky ReLU**

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

- 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)**

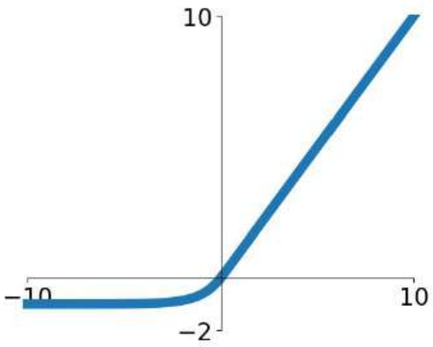
$$f(x) = \max(\alpha x, x)$$

backprop into $\alpha$ (parameter)

# Activation Functions

[Clevert et al., 2015]

## Exponential Linear Units (ELU)




- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

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

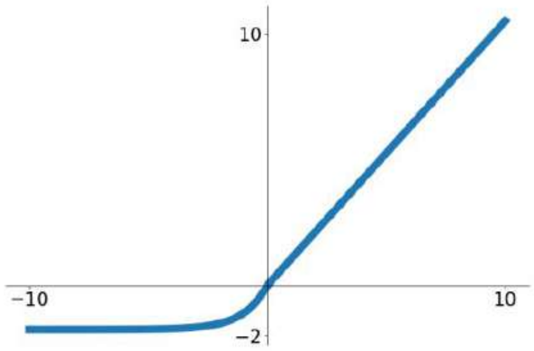
(Alpha default = 1)

- Computation requires exp()

# Activation Functions

[Klambauer et al. ICLR 2017]

## 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!

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

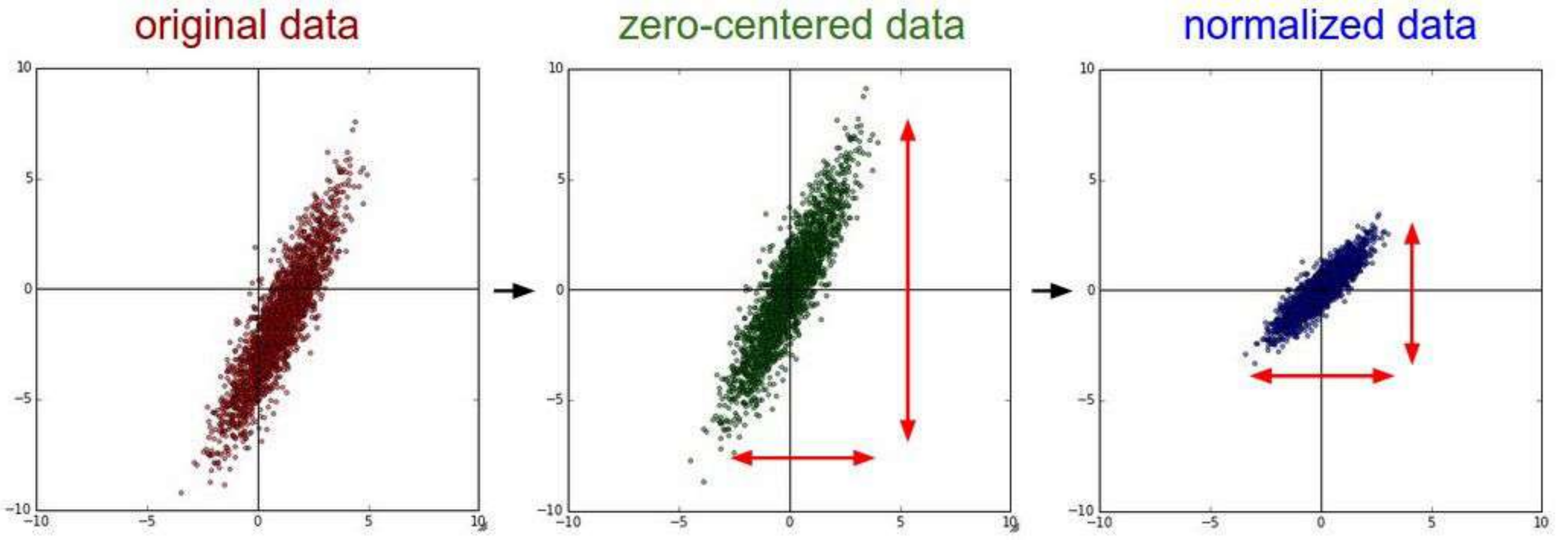
Problem: doubles the number of parameters/neuron :(

# 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



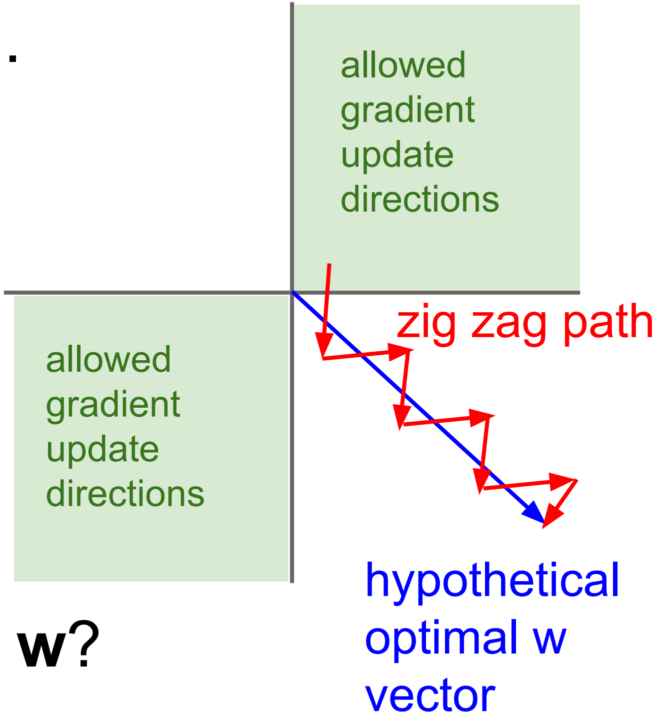

```
X -= np.mean(X, axis = 0)
```

```
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...

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

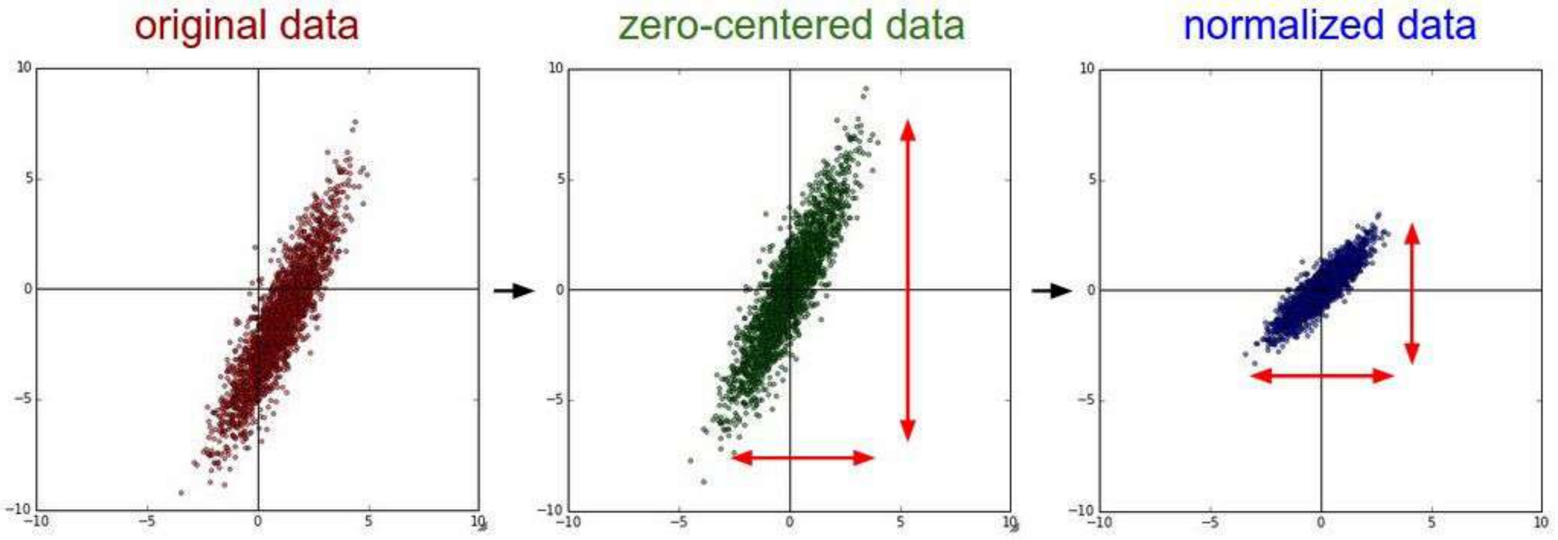



What can we say about the gradients on **w**?

Always all positive or all negative :(

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

# Data Preprocessing



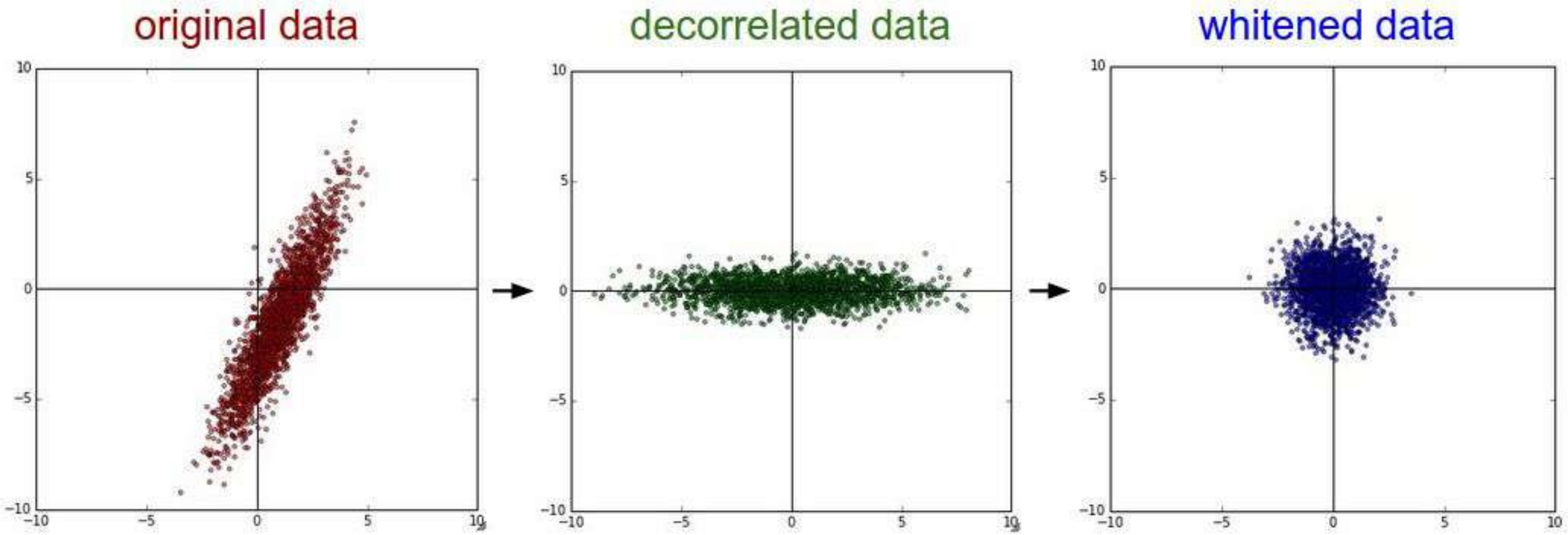

```
X -= np.mean(X, axis = 0)
```

```
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

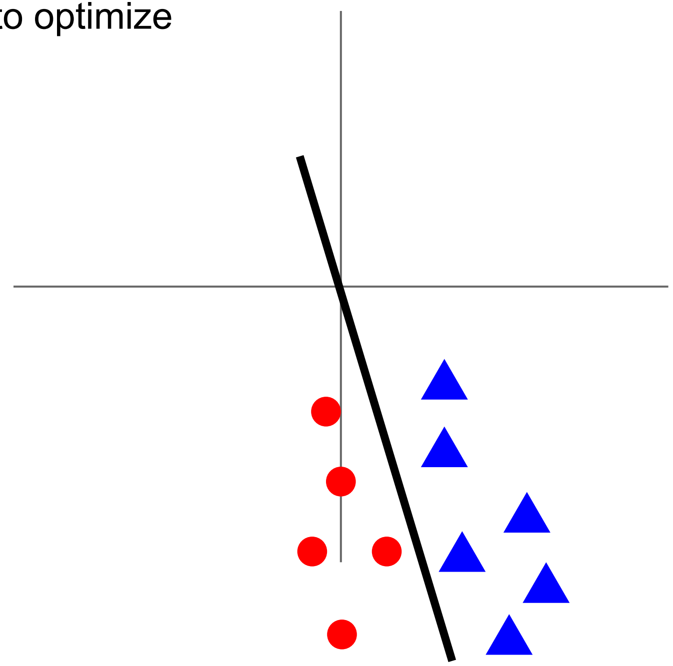



(data has diagonal covariance matrix)

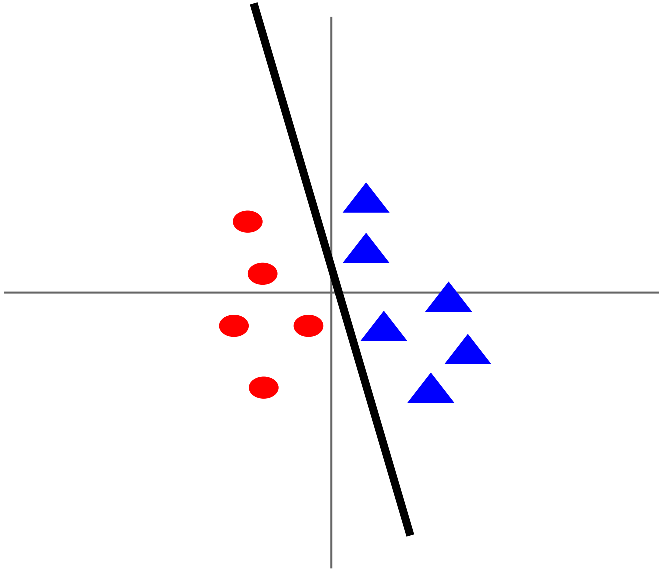
(covariance matrix is the identity matrix)

# 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

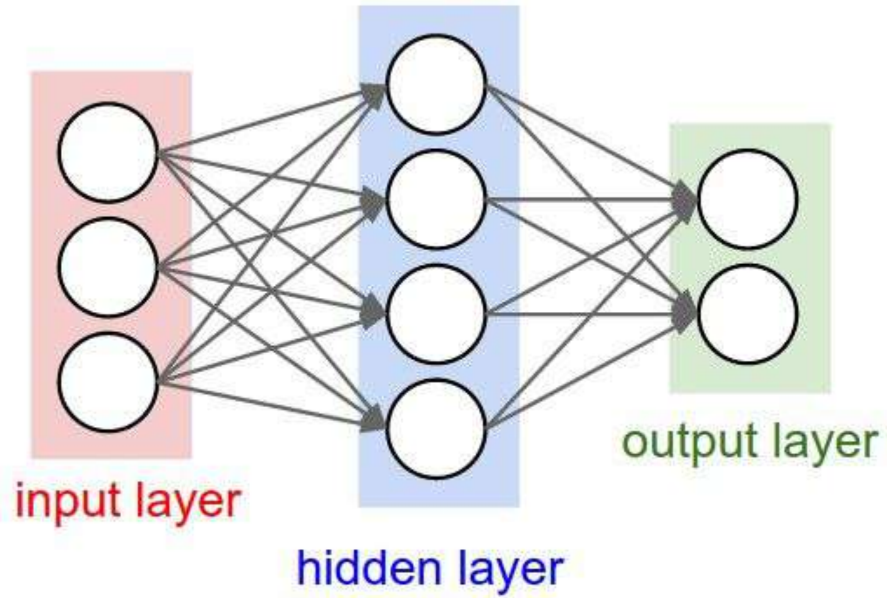
e.g. consider CIFAR-10 example with [32,32,3] images

- 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

# Weight Initialization

- Q: what happens when W=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)
```

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

```
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
hs = []
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)
```

Forward pass for a 6-layer net with hidden size 4096

What will happen to the activations for the last layer?

# Weight Initialization: Activation statistics

```
dims = [4096] * 7
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```
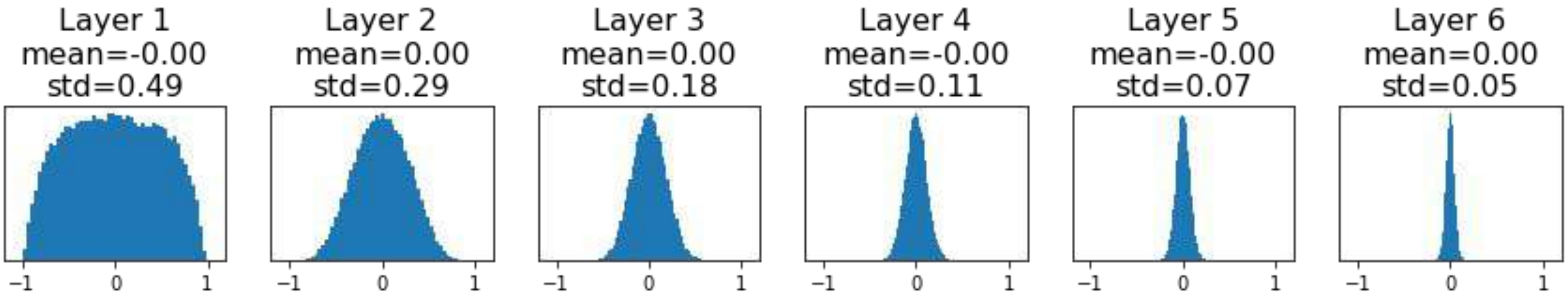

Forward pass for a 6-layer net with hidden size 4096

All activations tend to zero for deeper network layers

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



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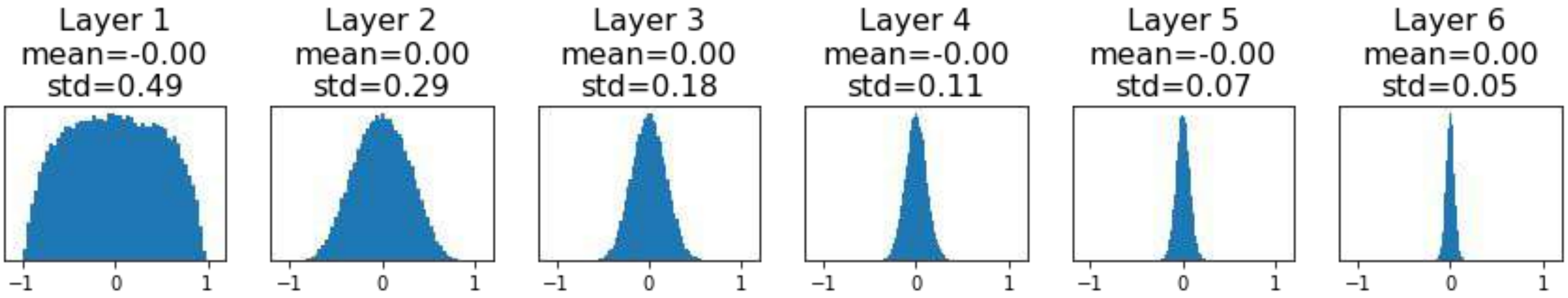
```

Forward pass for a 6-layer net with hidden size 4096

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
hs = []
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)
```

Increase std of initial weights from 0.01 to 0.05

What will happen to the activations for the last layer?

# Weight Initialization: Activation statistics

```
dims = [4096] * 7
hs = []
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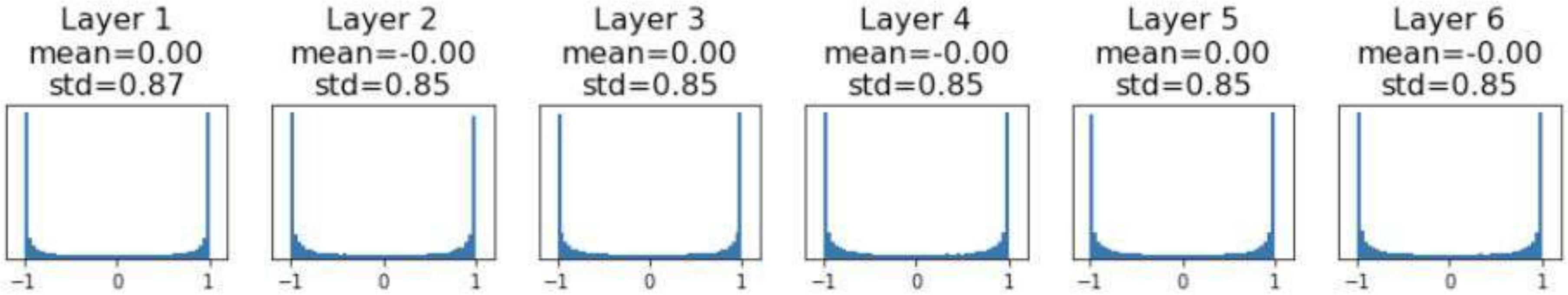
```

Increase std of initial weights from 0.01 to 0.05

All activations saturate

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



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```
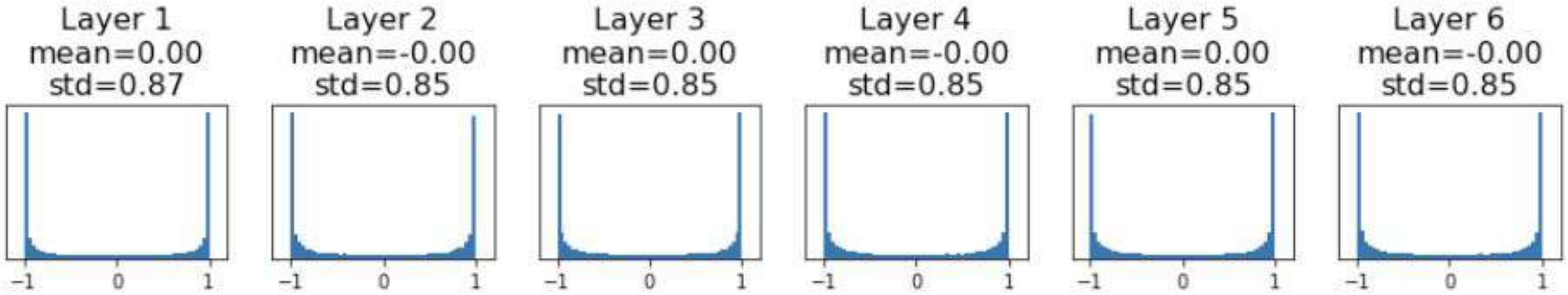

Increase std of initial weights from 0.01 to 0.05

All activations saturate

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

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



# Weight Initialization: “Xavier” 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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

“Xavier” initialization:
std = 1/sqrt(Din)

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

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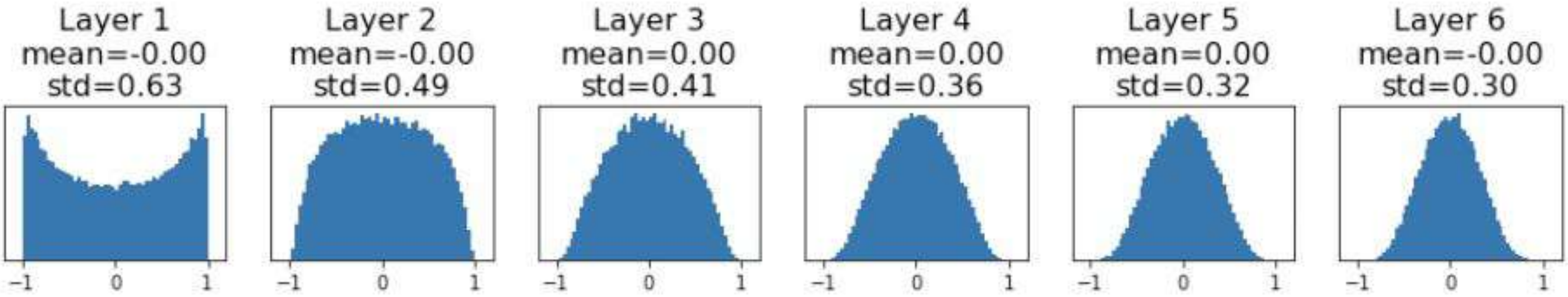
"Xavier" initialization:
std = 1/sqrt(Din)

"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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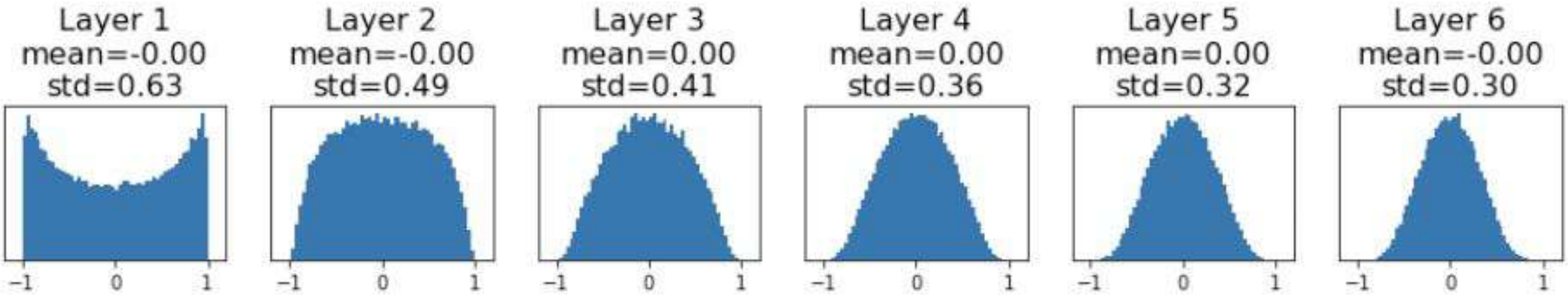
For conv layers, Din is filter_size$^2$ * input_channels

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For conv layers, Din is filter_size$^2$ * input_channels

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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

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```
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    x = np.tanh(x.dot(W))
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```

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For conv layers, Din is filter_size$^2$ * input_channels

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

**Assume:** $Var(x_1) = Var(x_2) = ... = Var(x_{Din})$

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    x = np.tanh(x.dot(W))
    hs.append(x)
```

“Xavier” initialization:
std = 1/sqrt(Din)

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

For conv layers, Din is filter_size$^2$ * input_channels

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

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

**We want:** $Var(y) = Var(x_i)$

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

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dims = [4096] * 7
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x = np.random.randn(16, dims[0])
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    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

"Xavier" initialization:
std = 1/sqrt(Din)

"Just right": Activations are nicely scaled for all layers!

For conv layers, Din is filter_size$^2$ * input_channels

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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

**We want:** $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$
[substituting value of y]

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

# Weight Initialization: "Xavier" Initialization

```python
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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

"Xavier" initialization:
std = 1/sqrt(Din)

"Just right": Activations are nicely scaled for all layers!

For conv layers, Din is $filter\_size^2$ * input_channels

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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

**We want:** $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$
$= Din\ Var(x_iw_i)$
[Assume all $x_i$, $w_i$ are iid]

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

# Weight Initialization: "Xavier" 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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

"Xavier" initialization:
std = 1/sqrt(Din)

"Just right": Activations are nicely scaled for all layers!

For conv layers, Din is $\text{filter\_size}^2$ * input_channels

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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

**We want:** $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$
$= Din\ Var(x_iw_i)$
$= Din\ Var(x_i)\ Var(w_i)$

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

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

# Weight Initialization: “Xavier” 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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

“Xavier” initialization:
std = 1/sqrt(Din)

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

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

**Let:** $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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

**We want:** $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$
$= Din\ Var(x_iw_i)$
$= Din\ Var(x_i)\ Var(w_i)$
[Assume all $x_i$, $w_i$ are iid]

So, $Var(y) = Var(x_i)$ only when $Var(w_i) = 1/Din$

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

# Weight Initialization: What about ReLU?

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

Change from tanh to ReLU

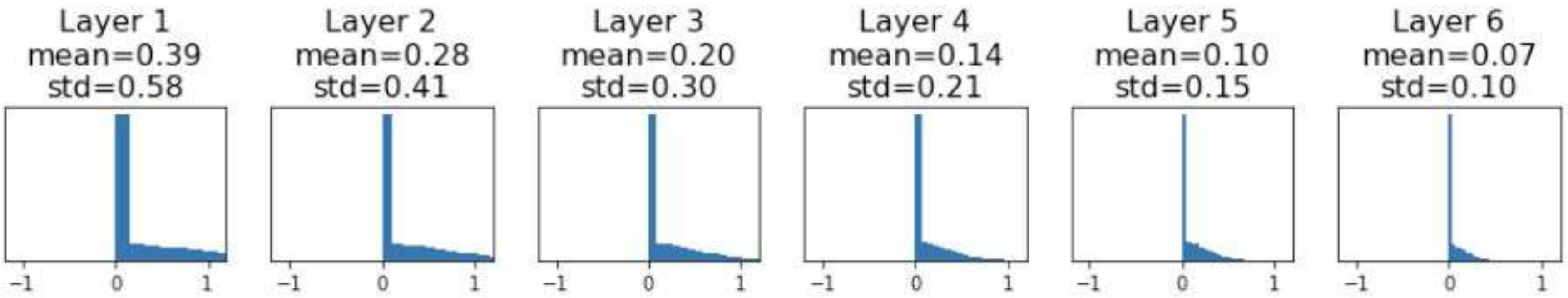
# Weight Initialization: What about ReLU?

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

Change from tanh to ReLU

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning =(

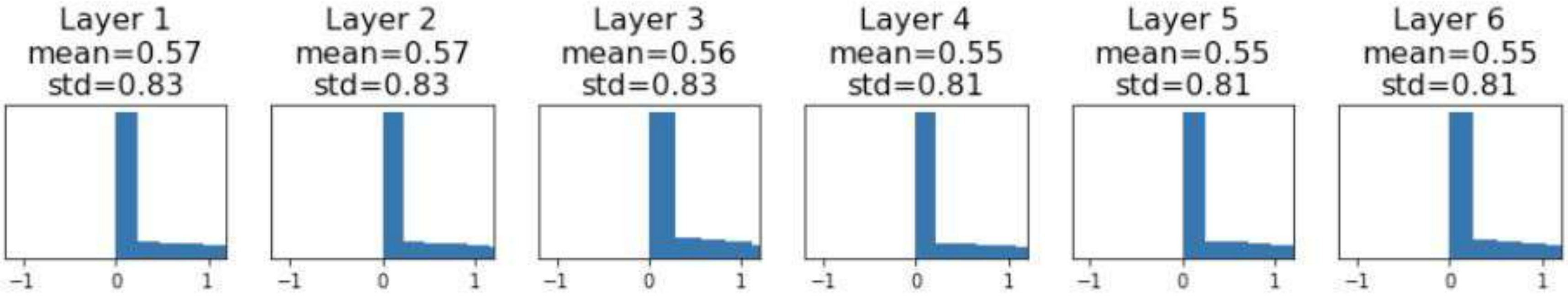


# Weight Initialization: Kaiming / MSRA Initialization

```python
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: std = sqrt(2 / 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

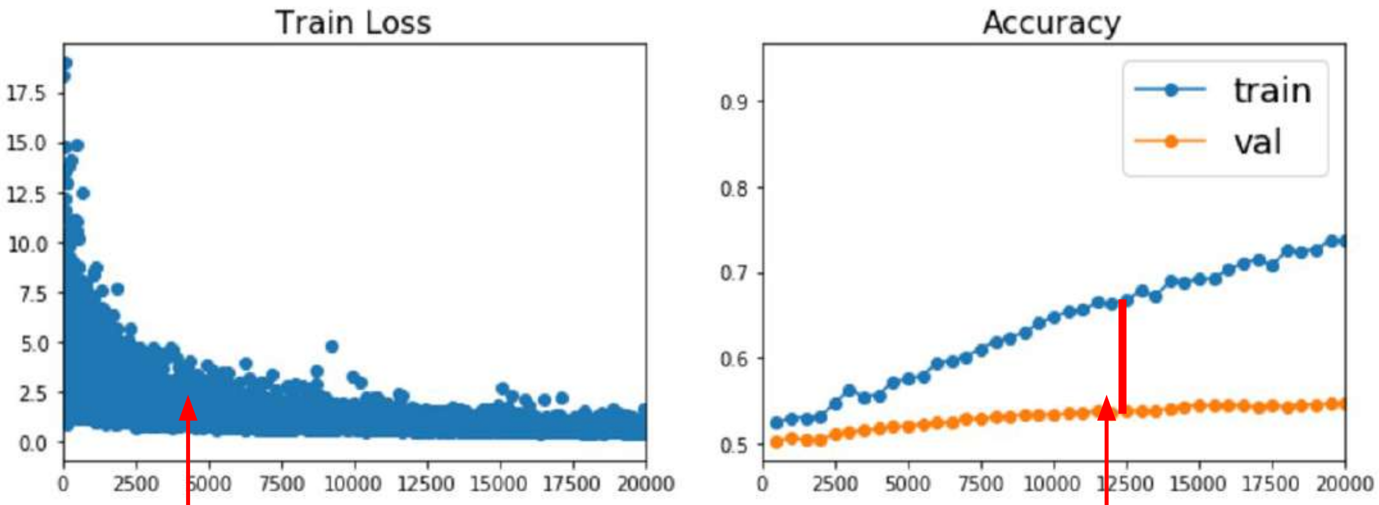
***All you need is a good init***, Mishkin and Matas, 2015

***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

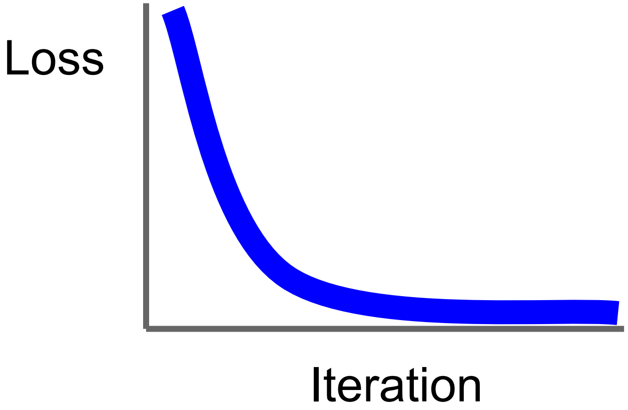
# Beyond Training Error

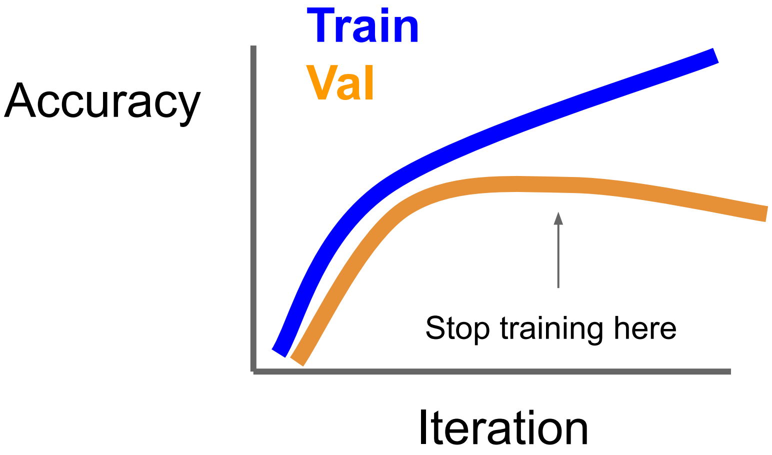



Better optimization algorithms help reduce training loss

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

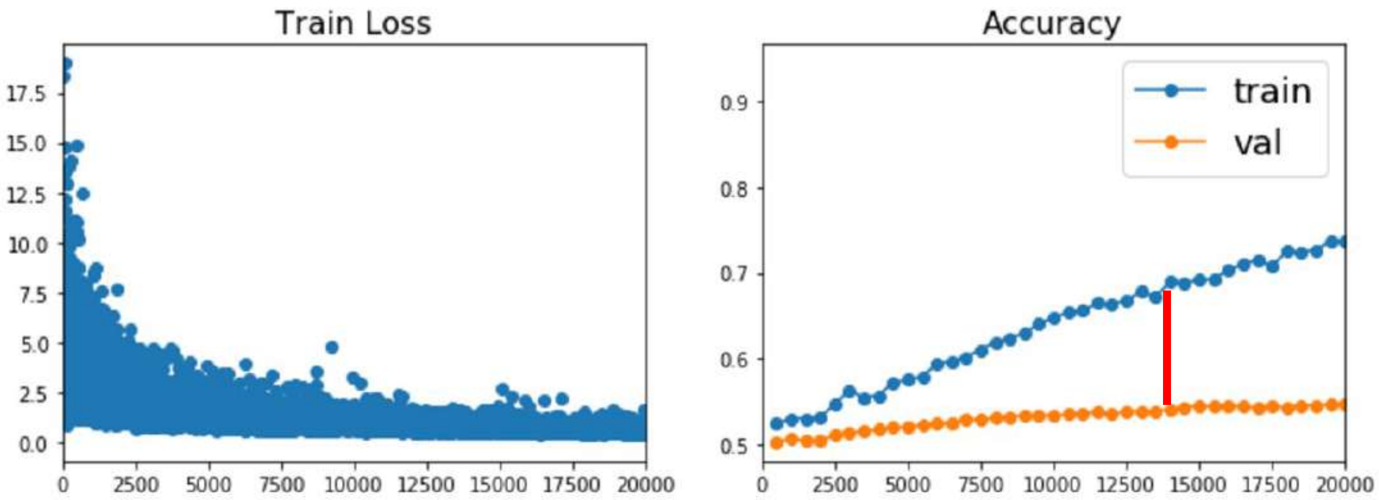
# Model Ensembles

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

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

In common use:

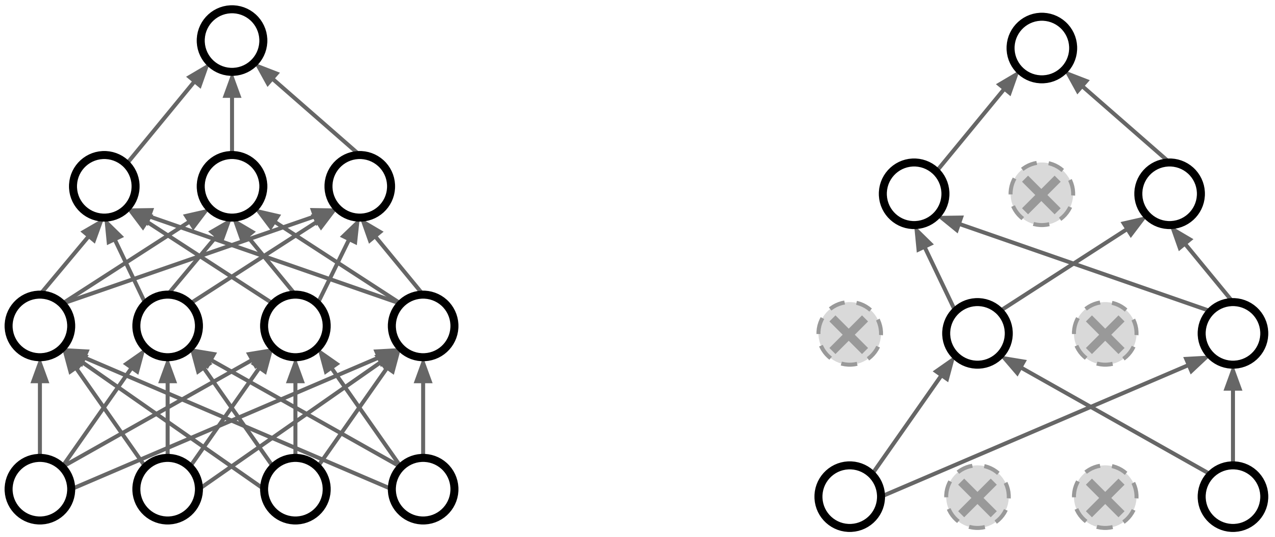
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

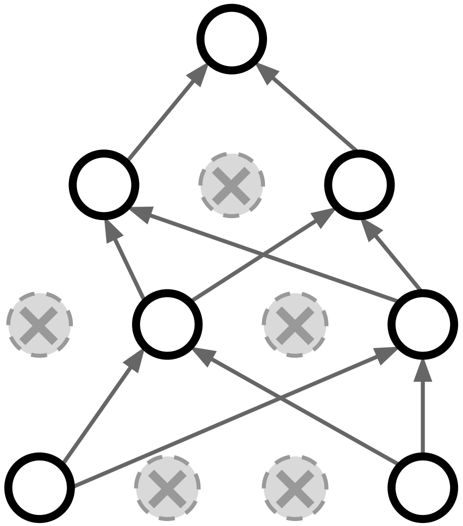


Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

# Regularization: Dropout

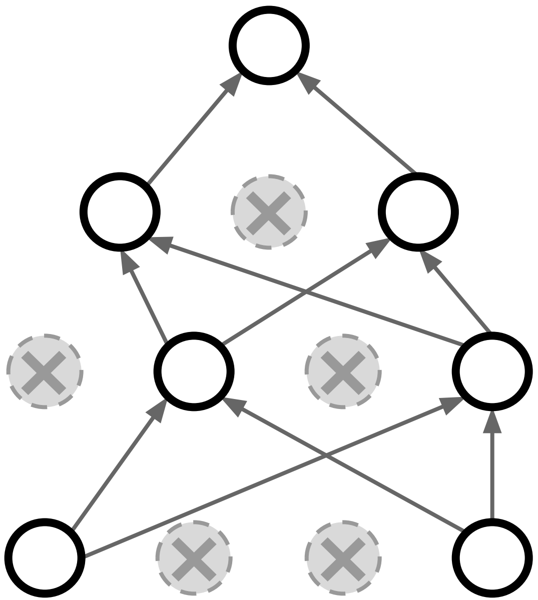
```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

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

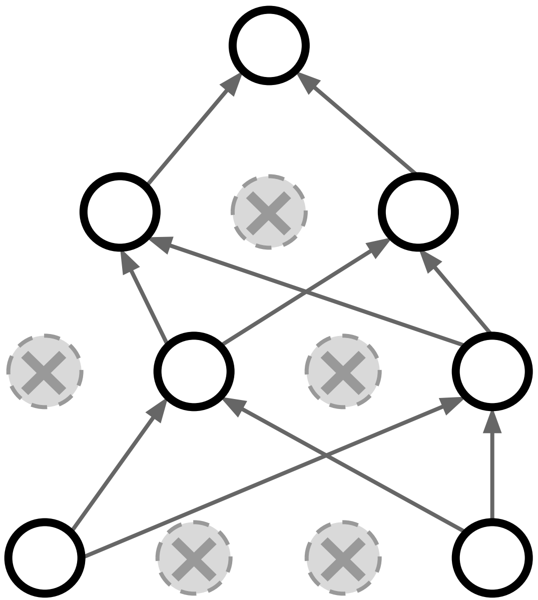
How can this possibly be a good idea?



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!

$$\underbrace{\boxed{y}}_{\text{Output (label)}} = f_W(\underbrace{\boxed{x}}_{\text{Input (image)}}, \underbrace{\boxed{z}}_{\text{Random mask}})$$

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

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

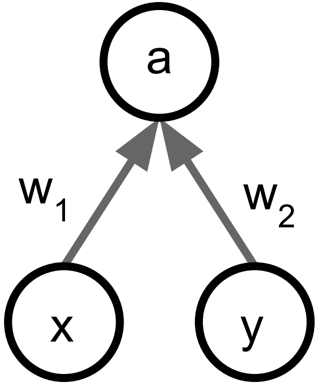
But this integral seems hard …

# Dropout: Test time

Want to approximate the integral

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

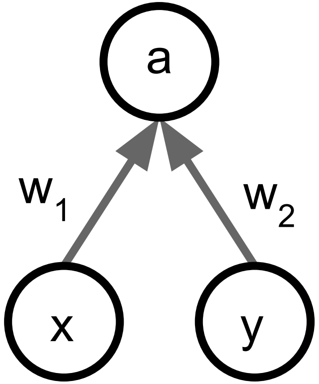
Consider a single neuron.



# Dropout: Test time

Want to approximate the integral

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



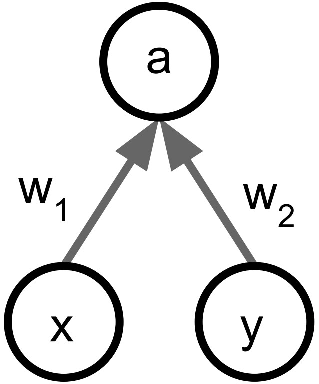

Consider a single neuron.

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

# Dropout: Test time

Want to approximate the integral

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




Consider a single neuron.

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

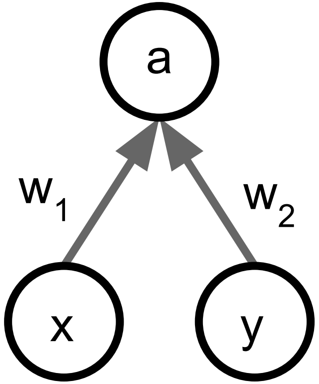
During training we have:

$$\begin{aligned} E\big[a\big] =& \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) \\ &+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) \\ =& \frac{1}{2}(w_1x + w_2y) \end{aligned}$$

# Dropout: Test time

Want to approximate the integral

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




Consider a single neuron.

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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:
<u>output at test time</u> = <u>expected output at training time</u>

# 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”

```python
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)

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

# Regularization: A common pattern

**Training**: Add some kind of randomness

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

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

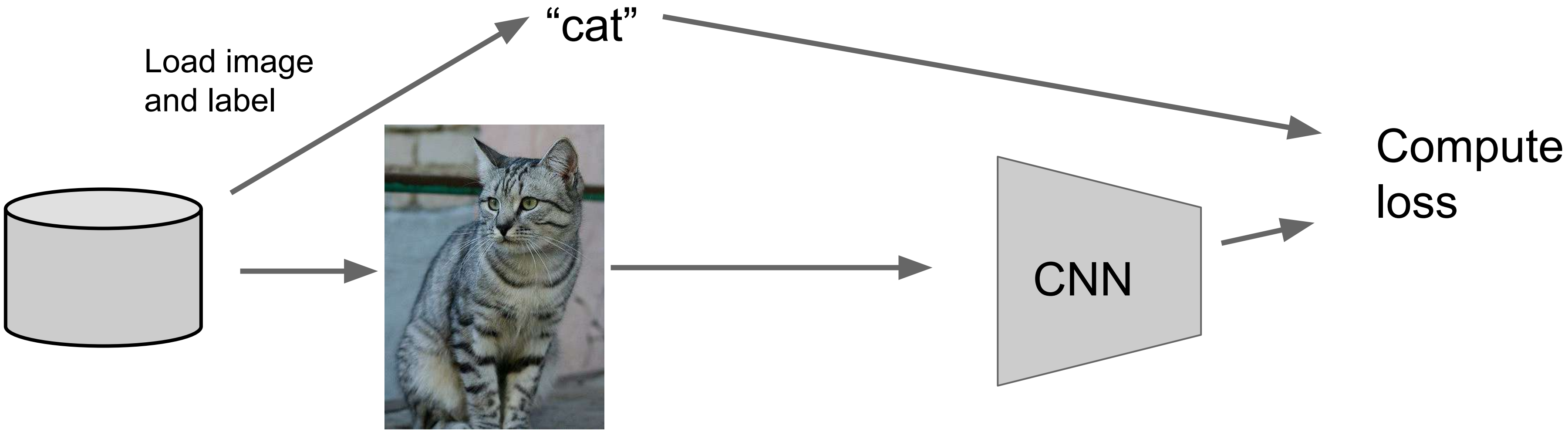
$$y = f(x) = E_z\big[f(x, z)\big] = \int p(z) f(x, z) dz$$

**Example**: Batch Normalization

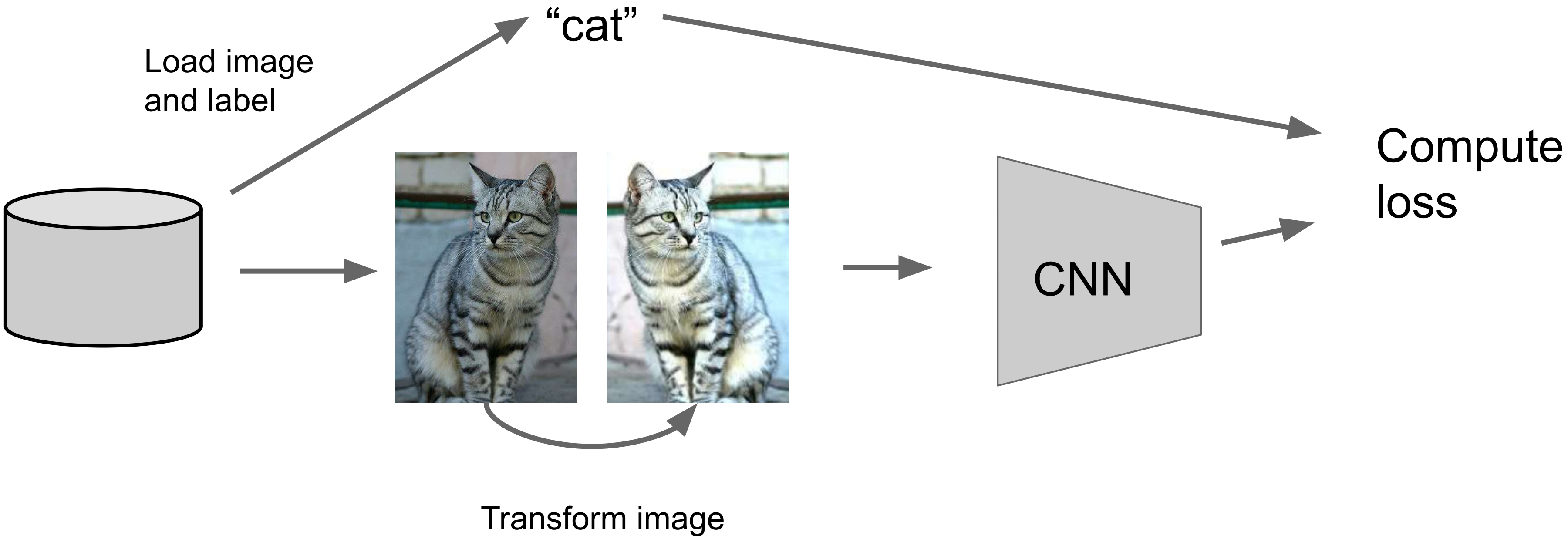
**Training**: Normalize using stats from random minibatches

**Testing**: Use fixed stats to normalize

# Regularization: Data Augmentation



# Regularization: Data Augmentation



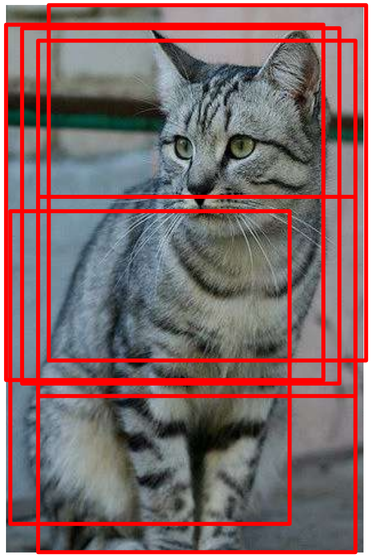
# Data Augmentation
## Horizontal Flips

# 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 x 224 patch



# Data Augmentation

## Random crops and scales

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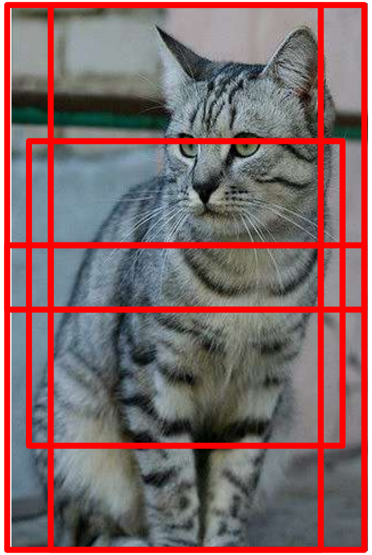


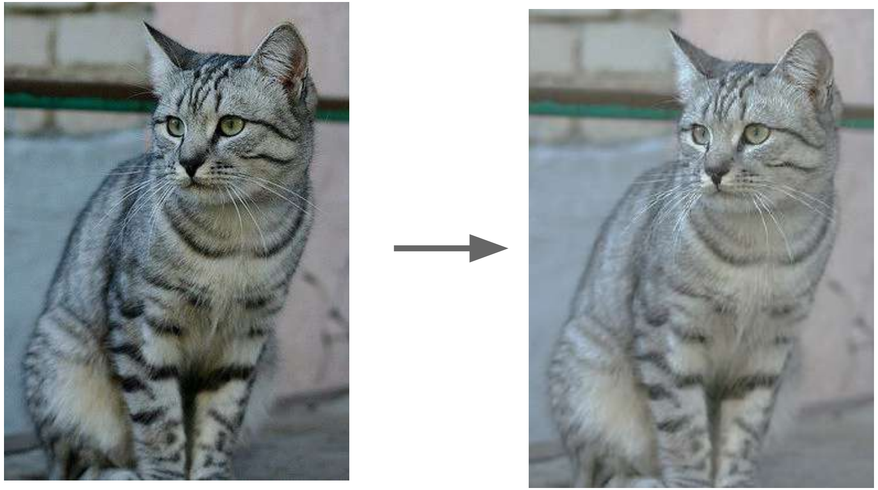
**Testing**: average a fixed set of crops

ResNet:

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

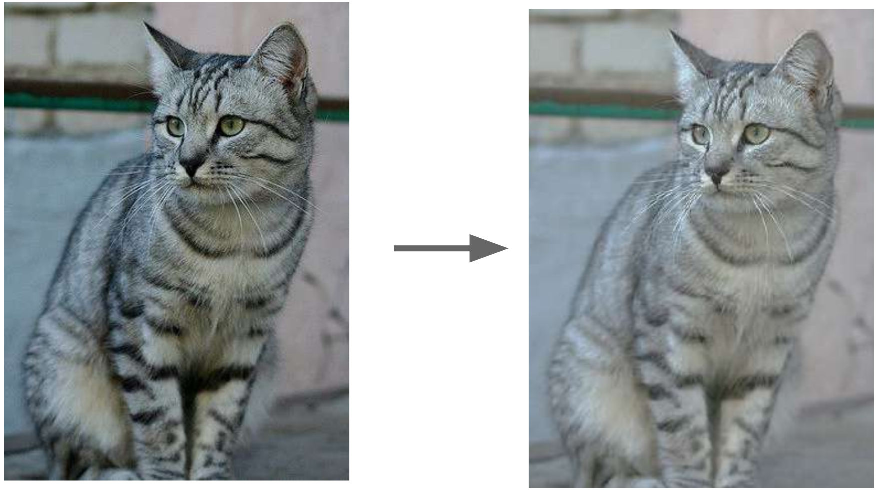
# Data Augmentation
## Color Jitter

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)

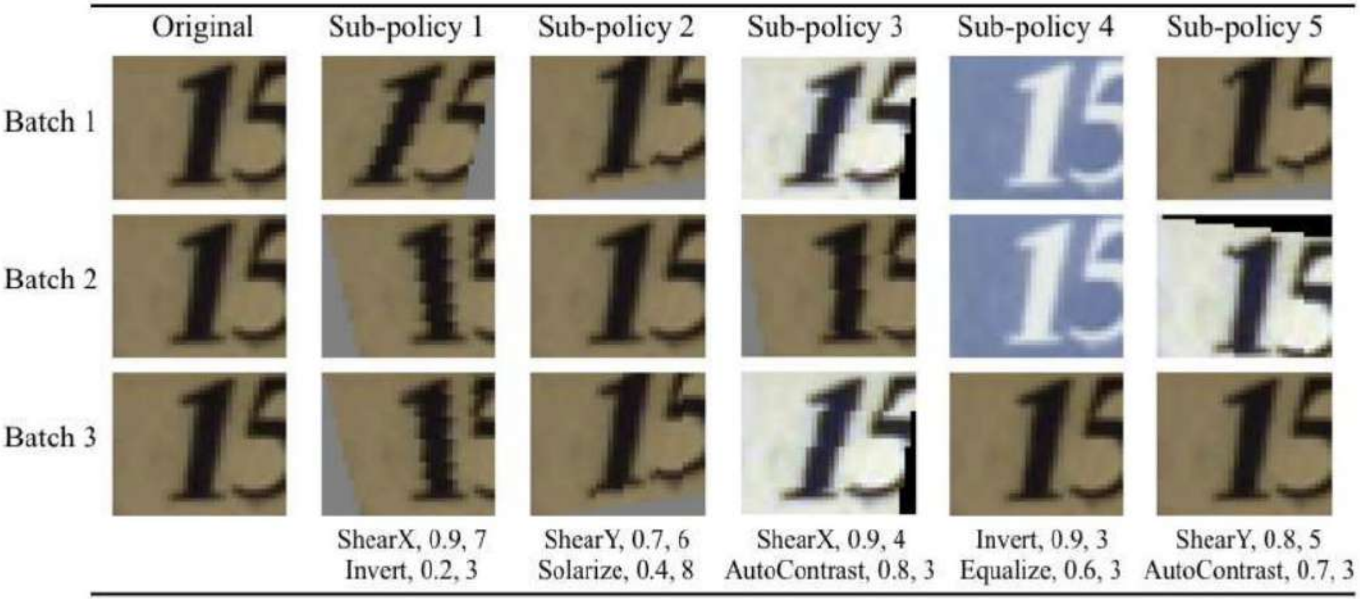
# Data Augmentation

## Get creative for your problem!

Examples of data augmentations:

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

# Automatic Data Augmentation




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

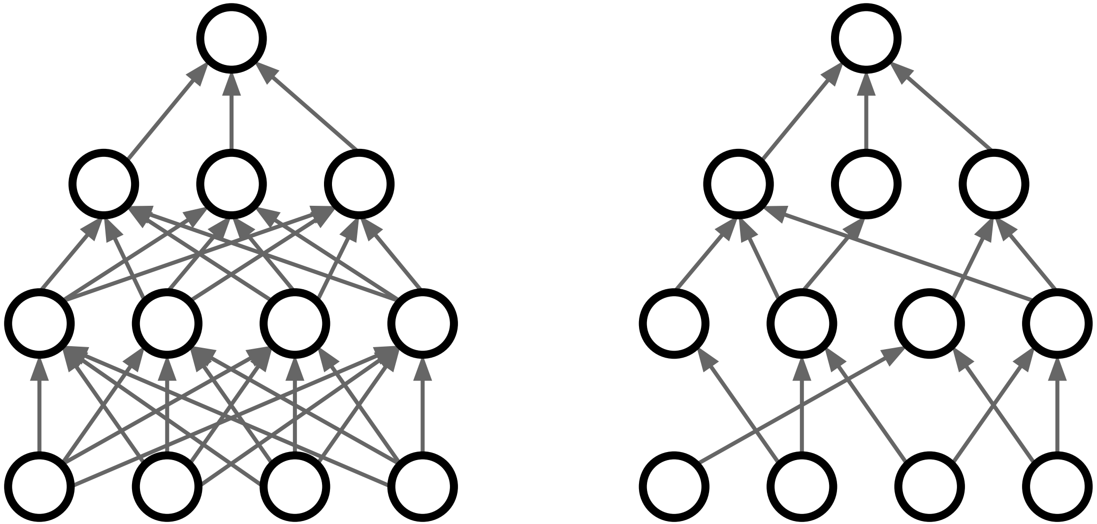
# Regularization: DropConnect

**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**:

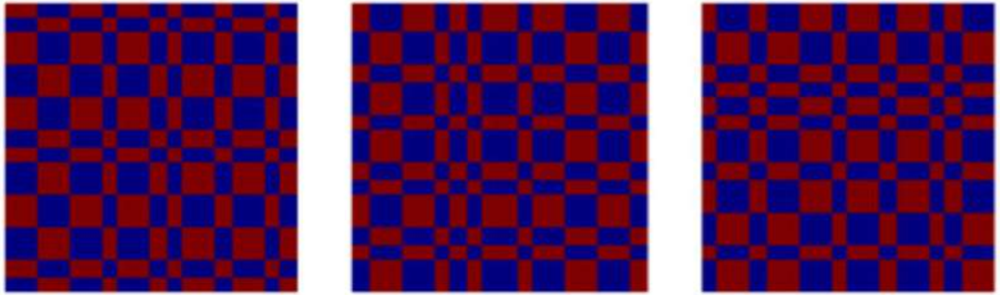
Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

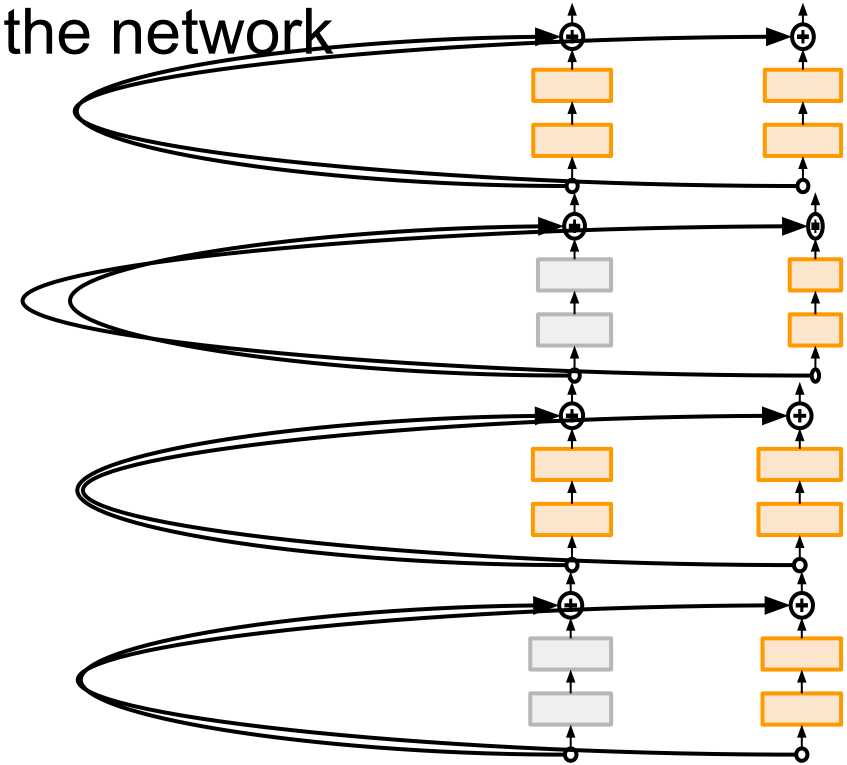


Graham, “Fractional Max Pooling”, arXiv 2014

# Regularization: Stochastic Depth

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

**Testing**: Use all the layer



**Examples**:

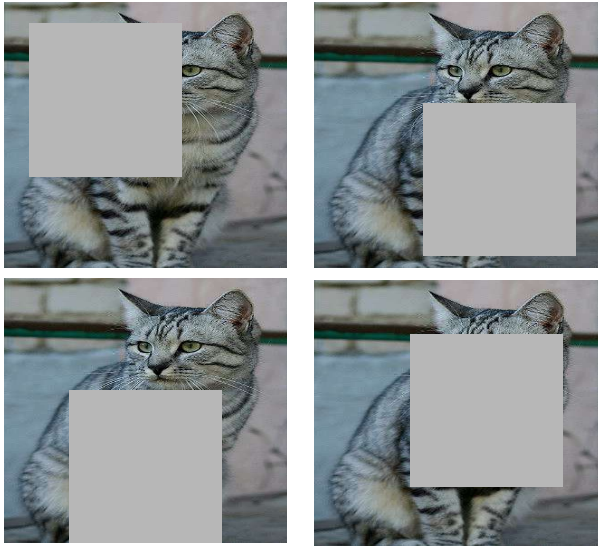
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth

Huang et al, “Deep Networks with Stochastic Depth”, ECCV 2016

# Regularization: Cutout

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

**Testing**: Use full image



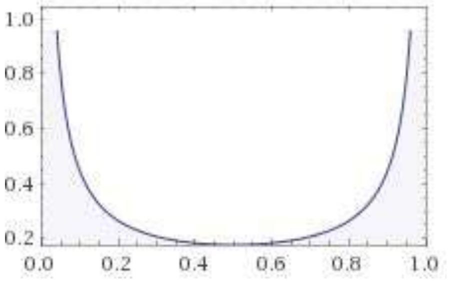
**Examples**:

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

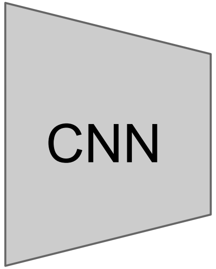



**Training**: Train on random blends of images

**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 ~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

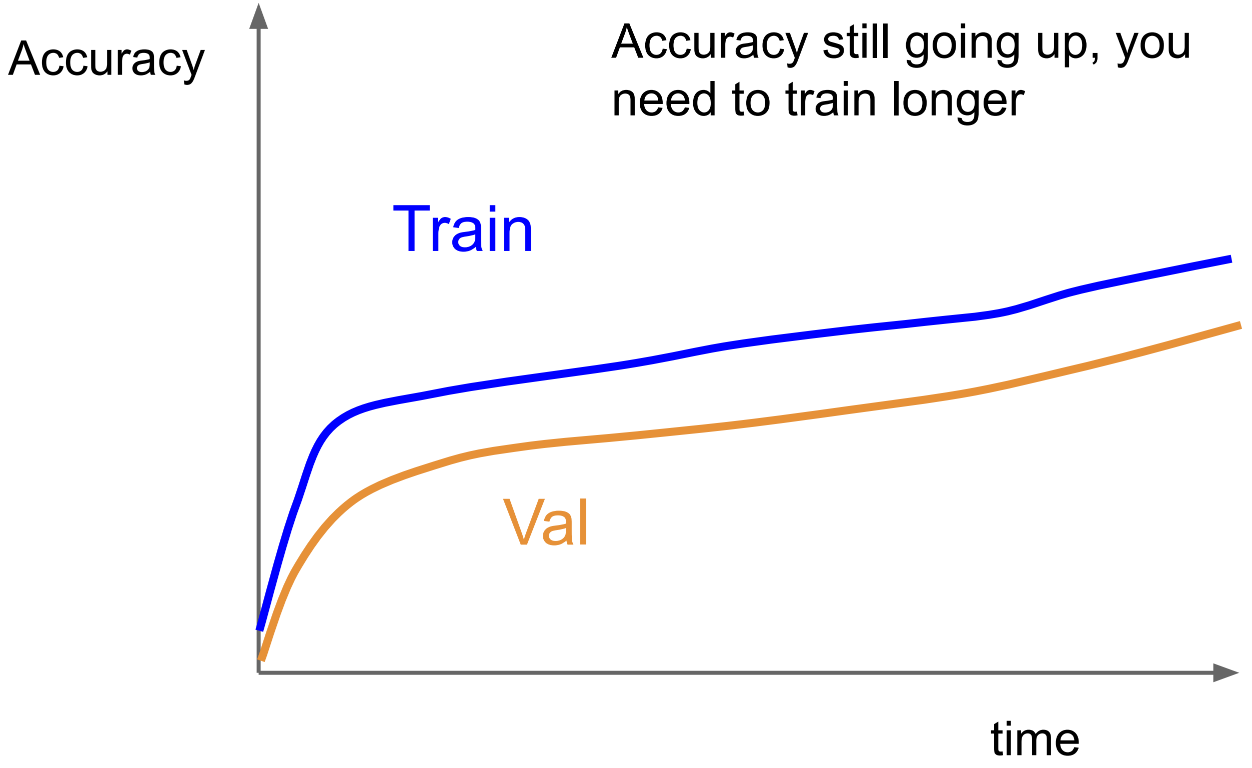
# Choosing Hyperparameters

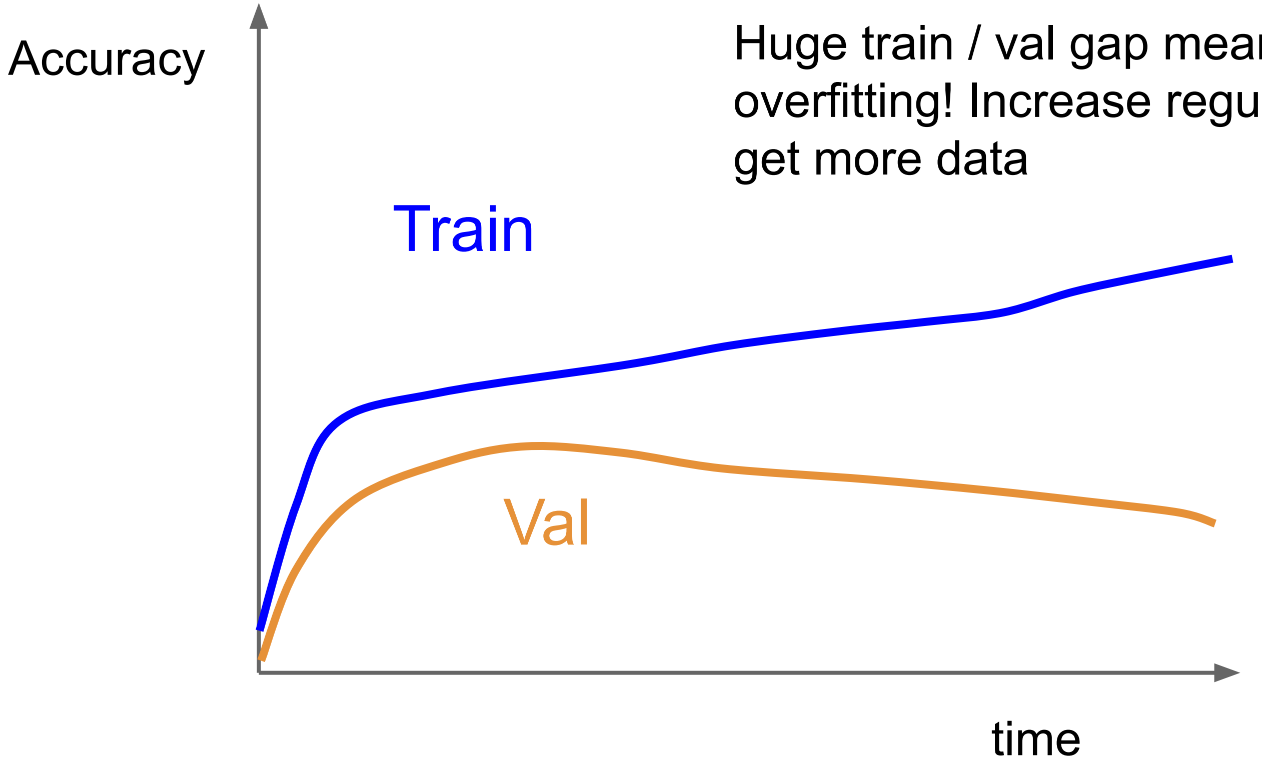
**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down
**Step 4**: Coarse grid, train for ~1-5 epochs
**Step 5**: Refine grid, train longer

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

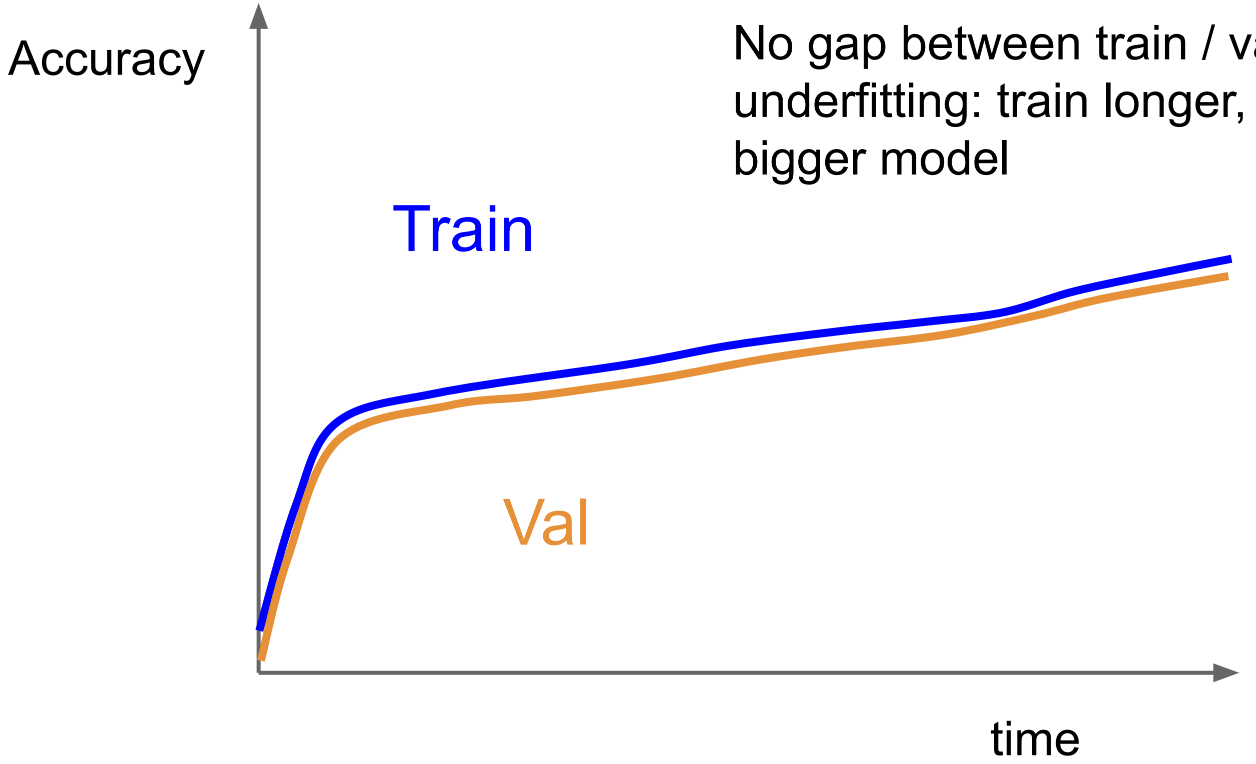
# Choosing Hyperparameters

**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


Accuracy
Accuracy still going up, you need to train longer
Train
Val
time



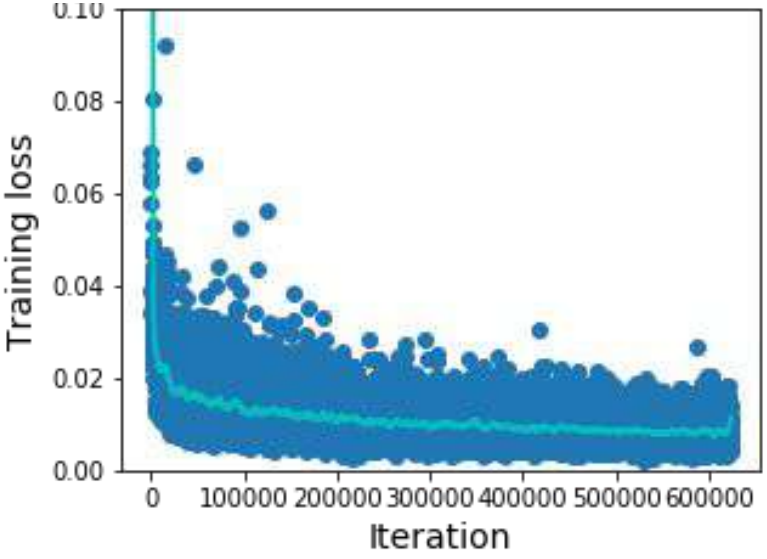

Huge train / val gap means overfitting! Increase regularization, get more data




No gap between train / val means underfitting: train longer, use a bigger model

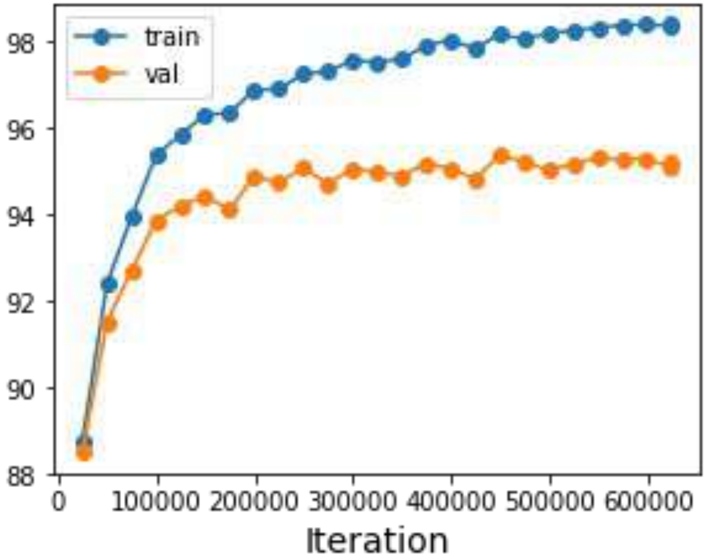
# Look at learning curves!

Training Loss




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

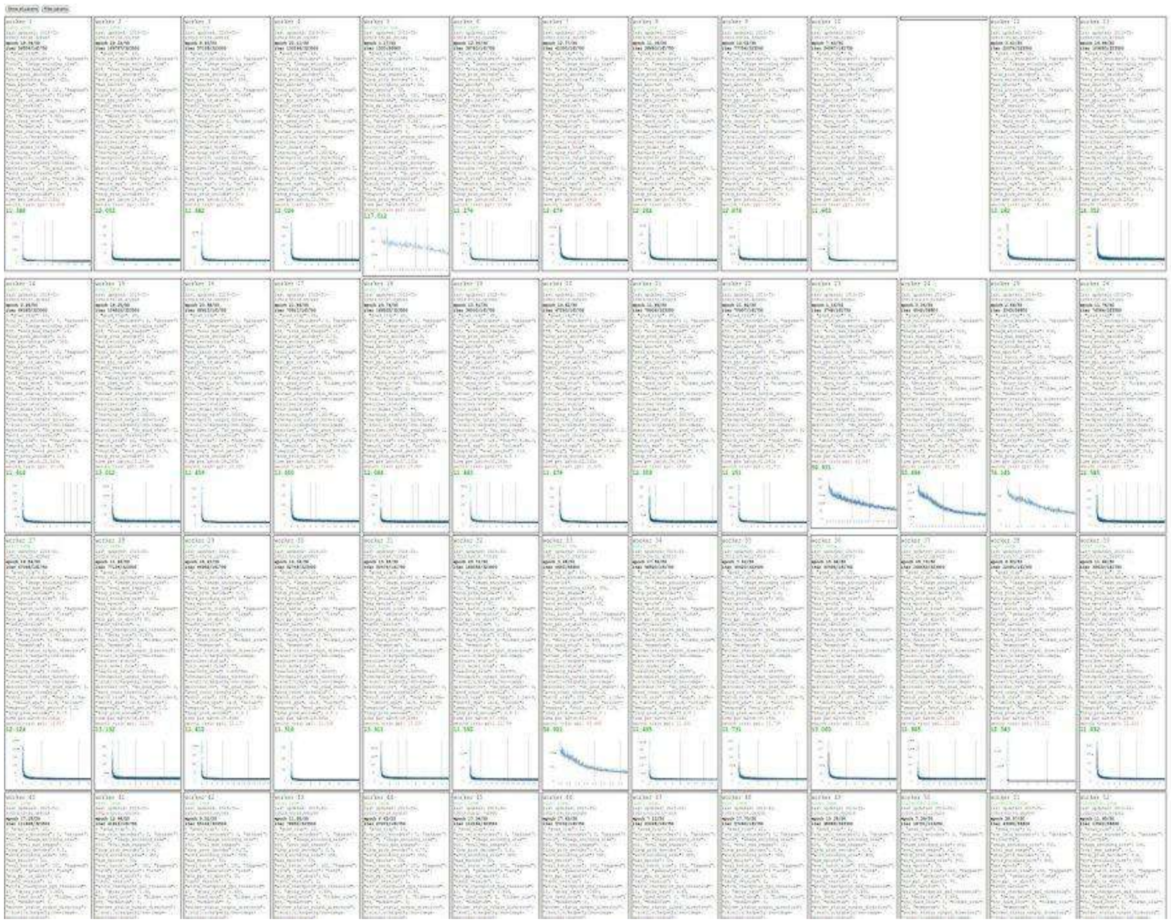
Train / Val Accuracy



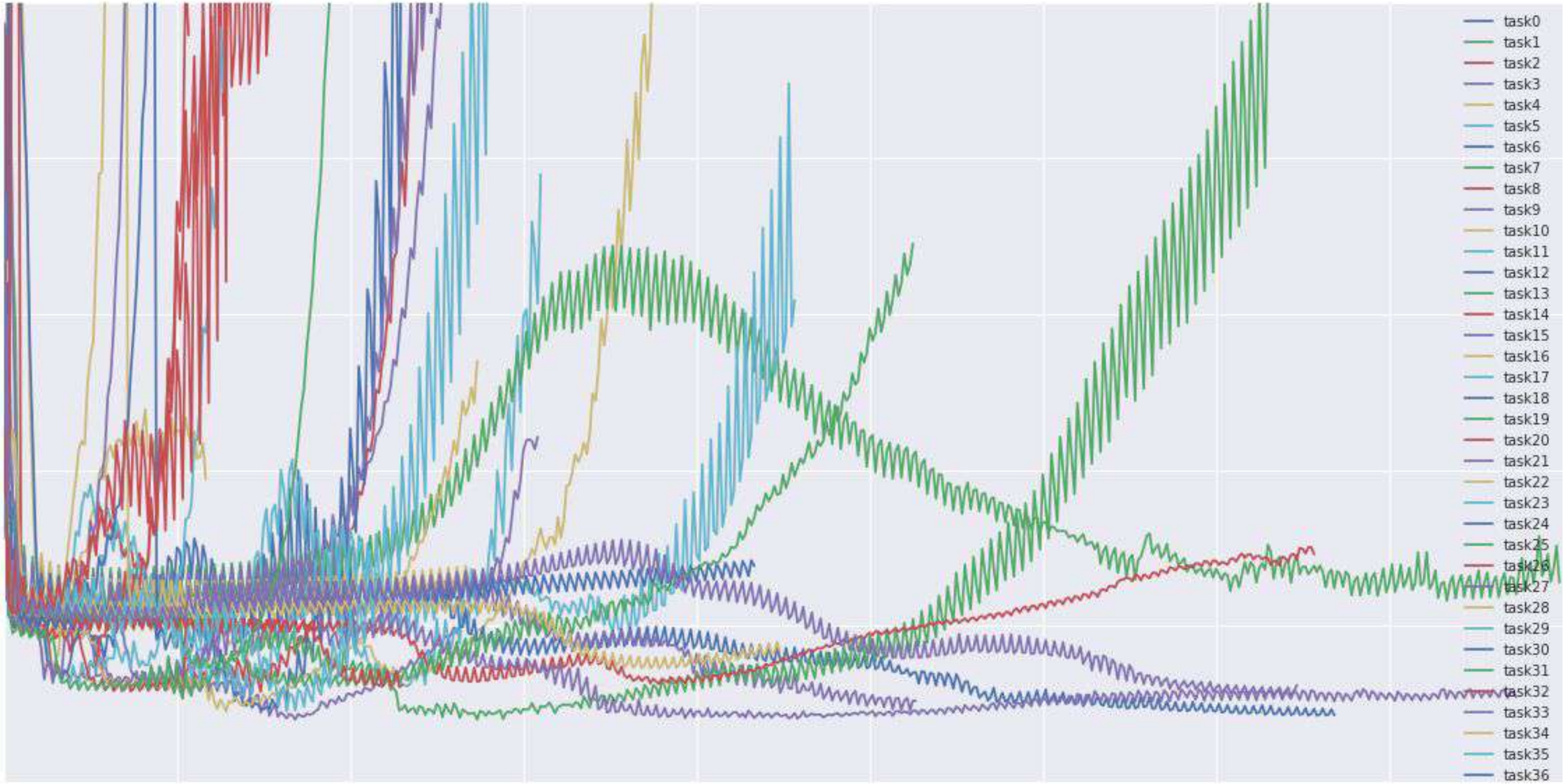
Cross-validation

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

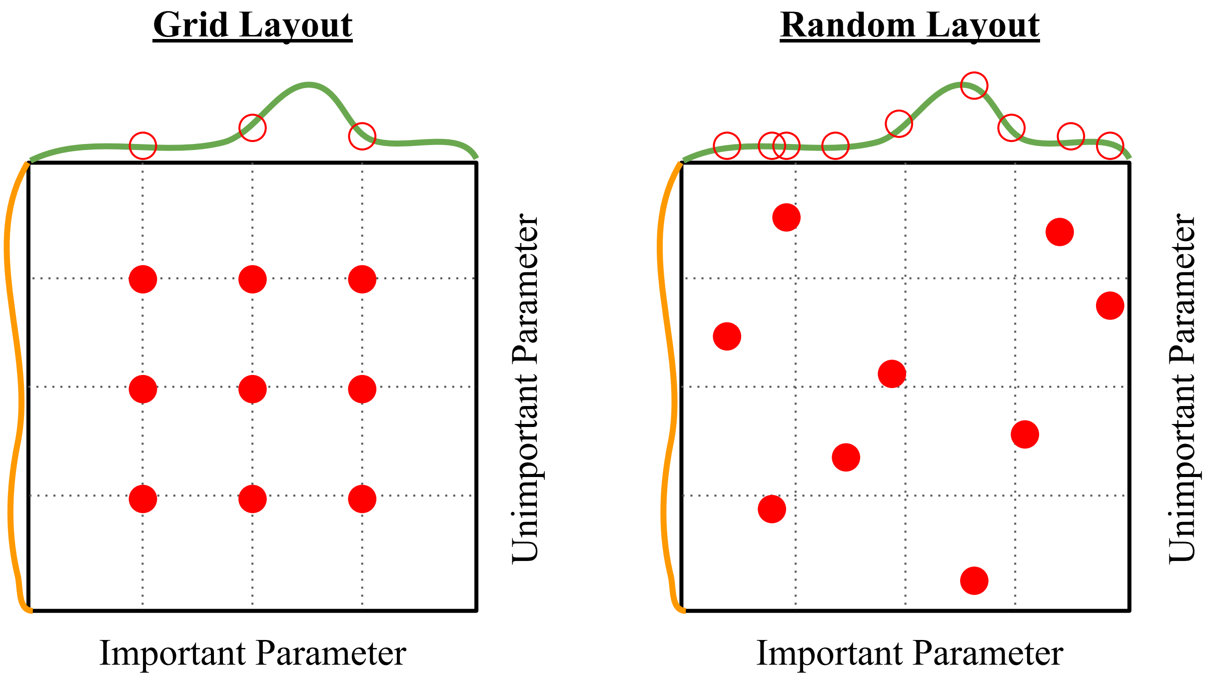



Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

# 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/He init)
- Batch Normalization (use this!)
- Transfer learning (use this if you can!)

# Next time: Visualizing and Understanding