Lecture 7: Training Neural Networks

Where we are now...
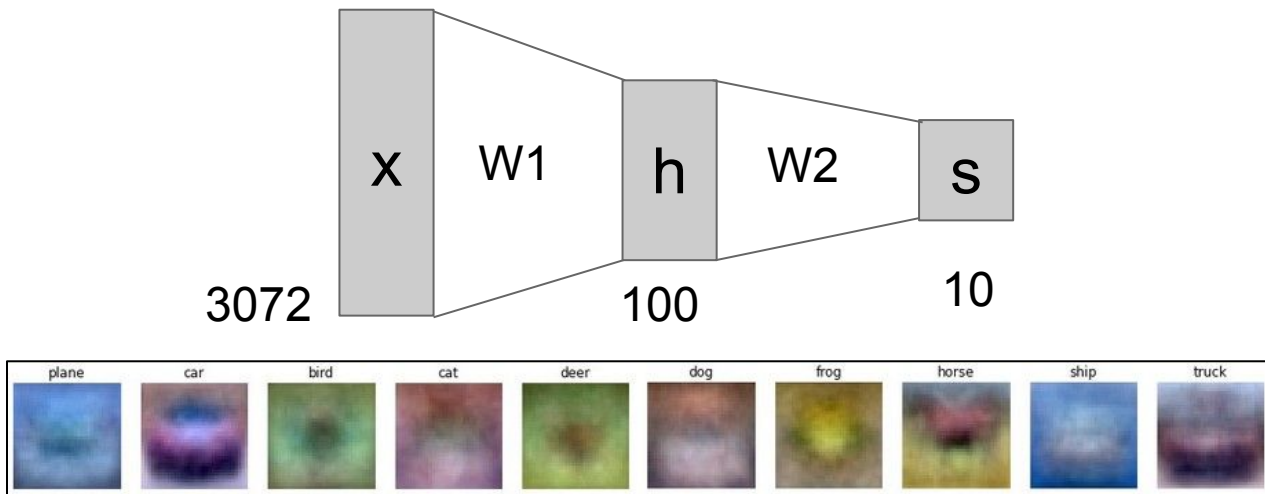
Neural Networks

Linear score function:

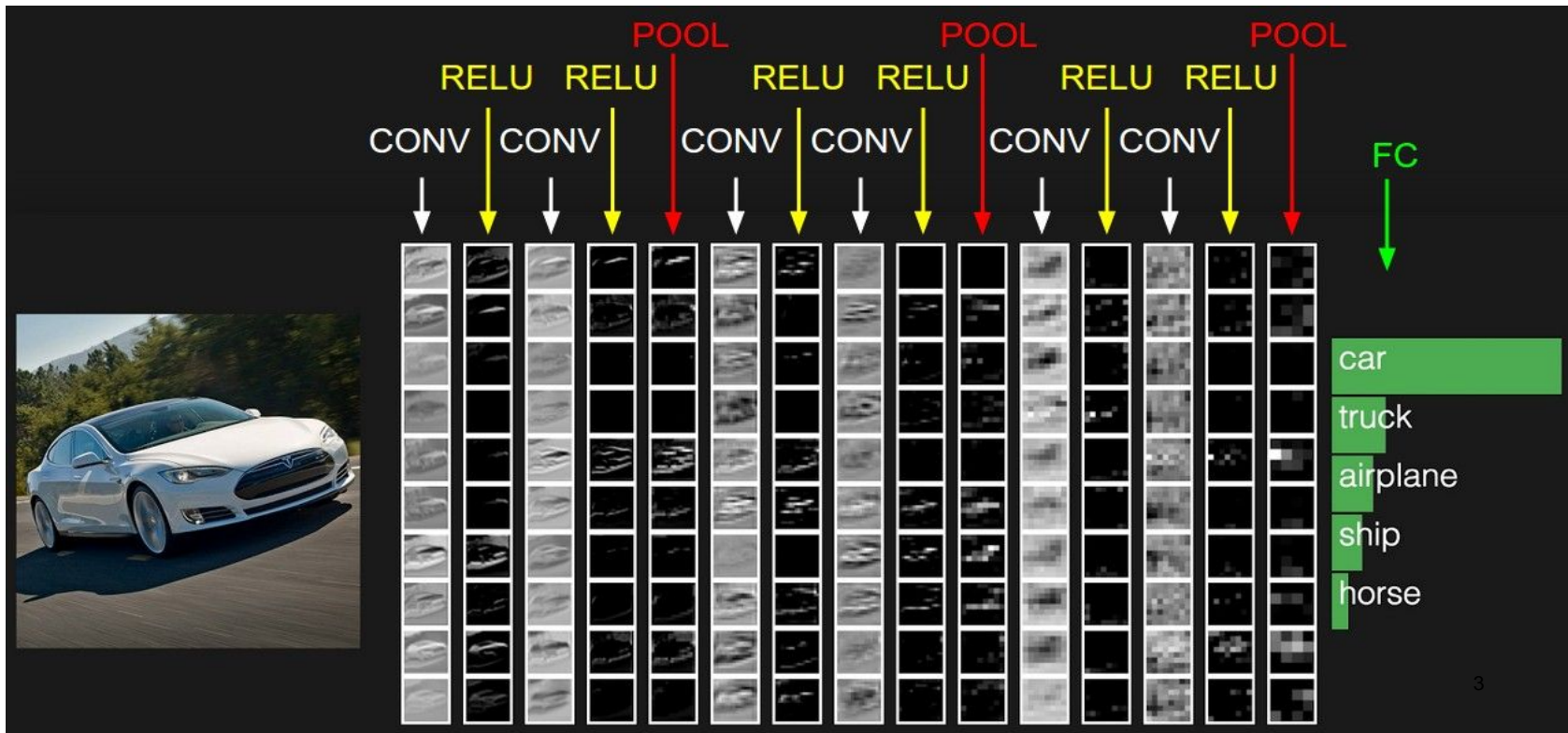$$f = Wx$$

2-layer Neural Network

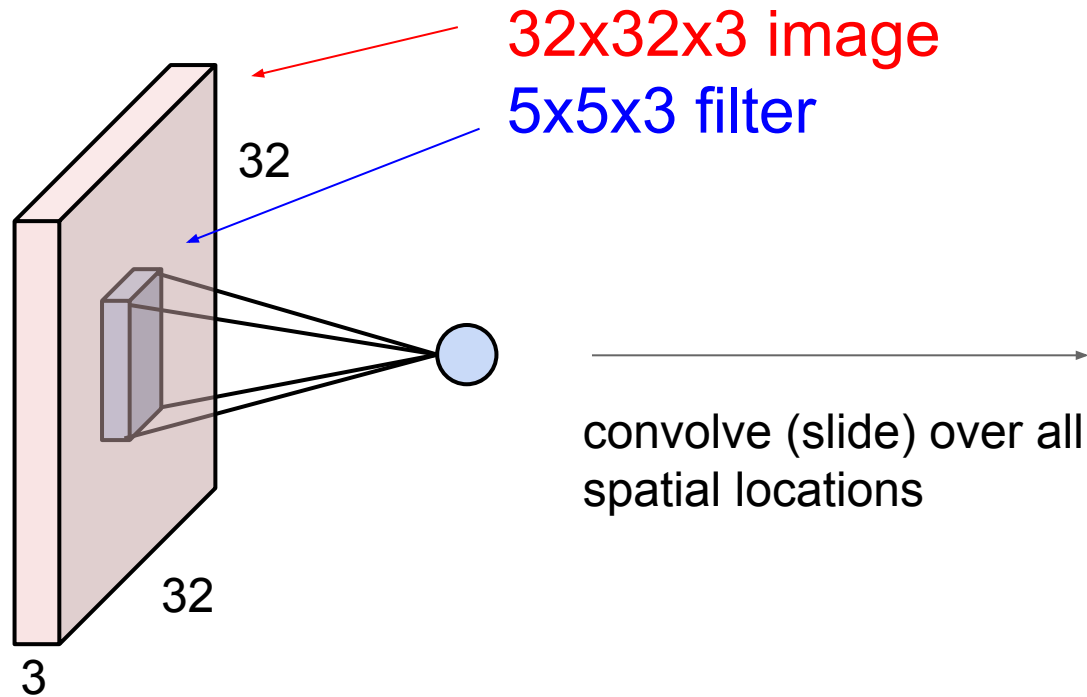$$f = W_2 \max(0, W_1 x)$$

| plane | car | bird | cat | deer | dog | frog | horse | ship | truck |

2

Where we are now...

Convolutional Neural Networks

Where we are now...

Convolutional Layer

32x32x3 image

5x5x3 filter

32

32

3

convolve (slide) over all
spatial locations

activation map

28

28

1

Where we are now...
Convolutional Layer

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

activation maps

32

32

3
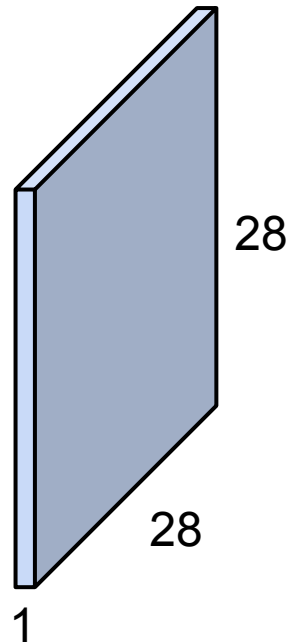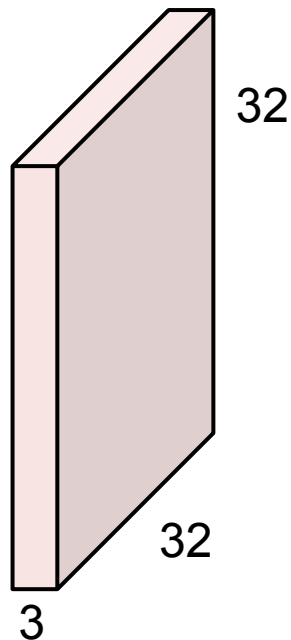
Convolution Layer

28

28

6
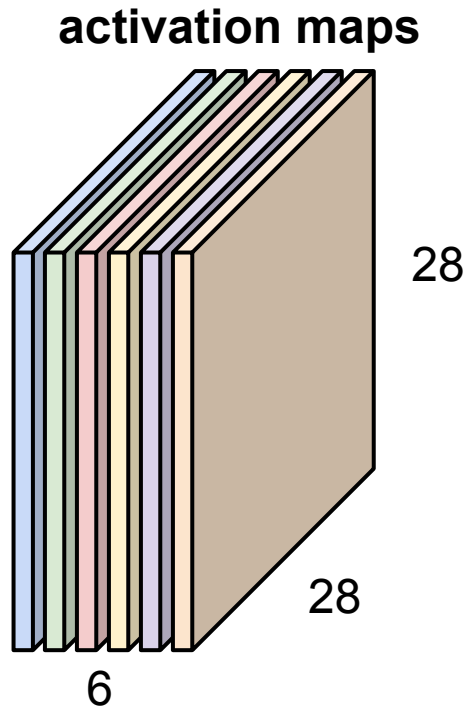
We stack these up to get a "new image" of size 28x28x6!

Where we are now...

CNN Architectures
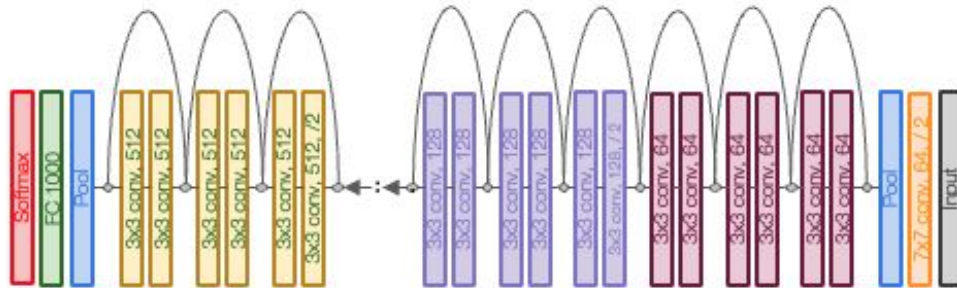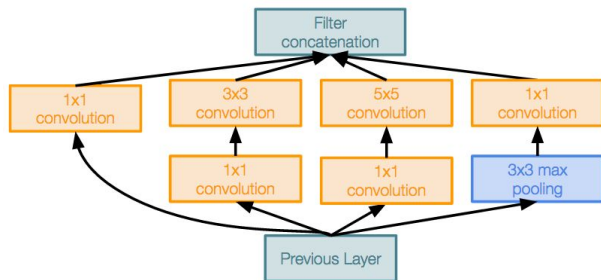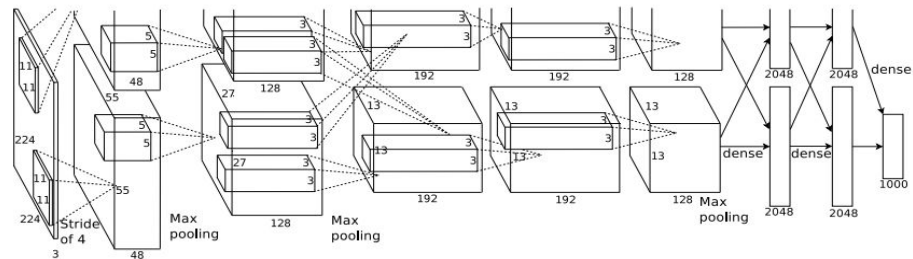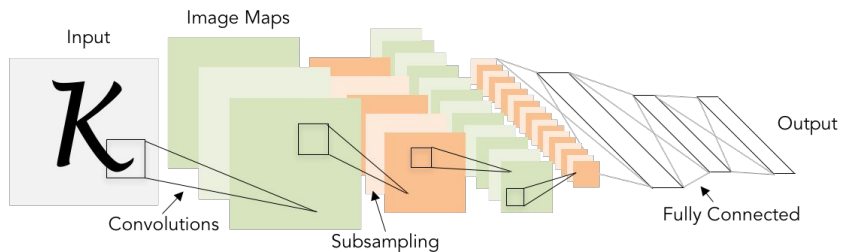
Where we are now...

Learning network parameters through optimization
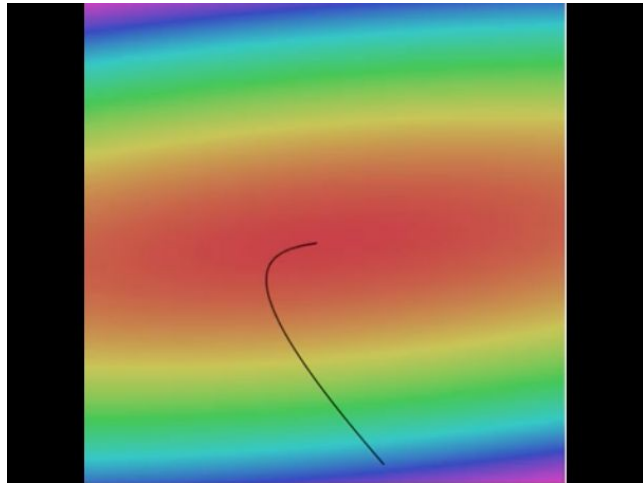

```
# Vanilla Gradient Descent

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
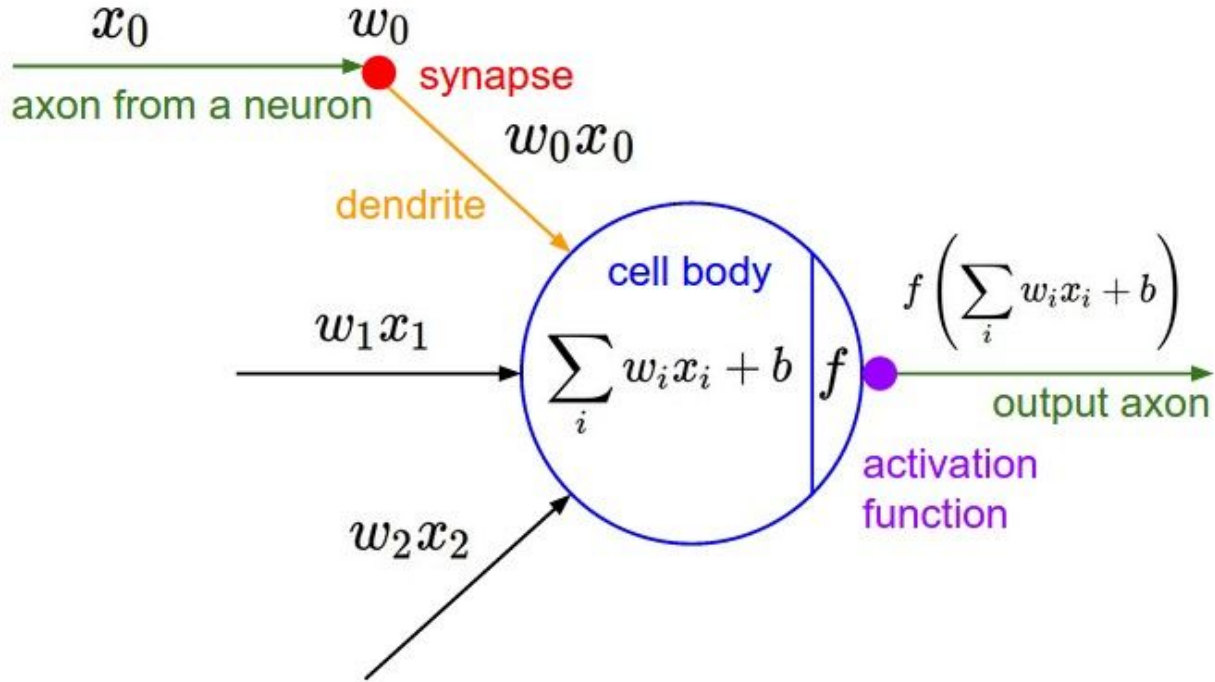
Activation Functions

Sigmoid

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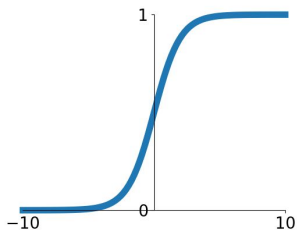
tanh

$$\tanh(x)$$
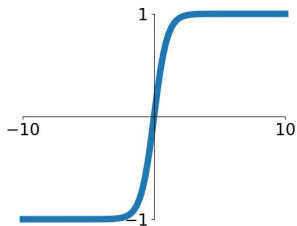
ReLU

$$\max(0, x)$$
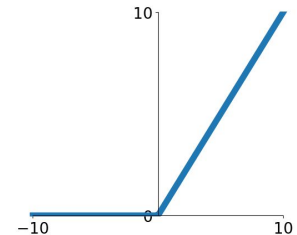
Leaky ReLU

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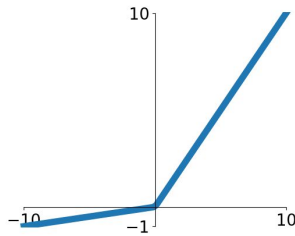
Maxout

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

ELU

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

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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

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Activation Functions

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

Sigmoid

- Squashes numbers to range [0,1]
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3 problems:

1. Saturated neurons "kill" the gradients

$$x$$

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

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

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

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

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

x

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

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

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

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

What happens when x = -10?

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

x

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

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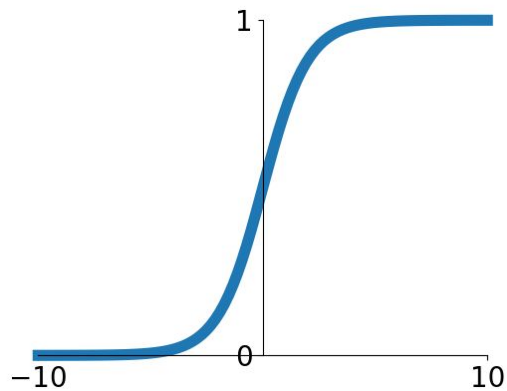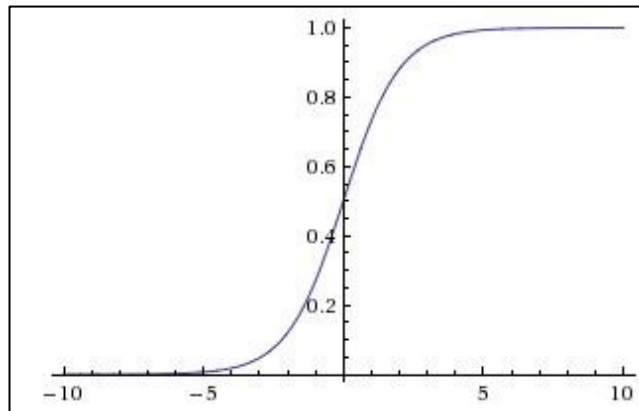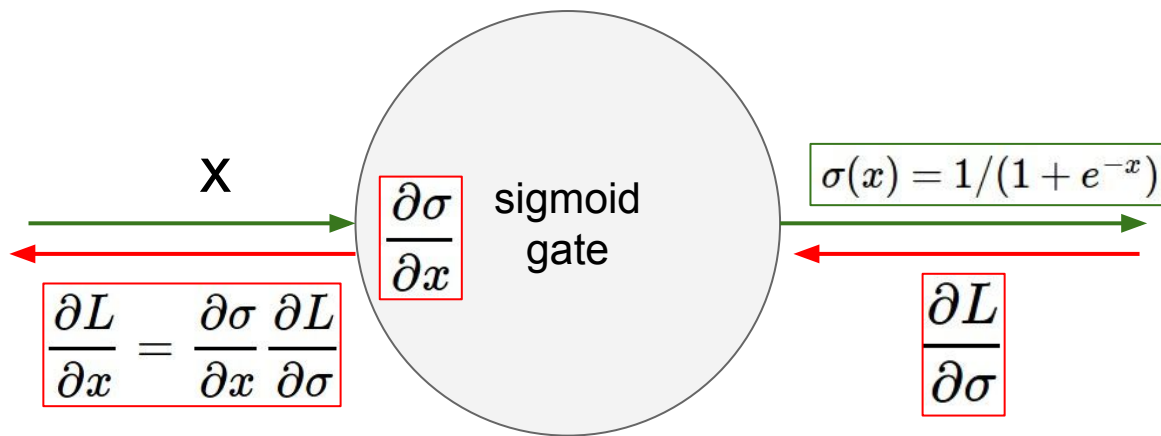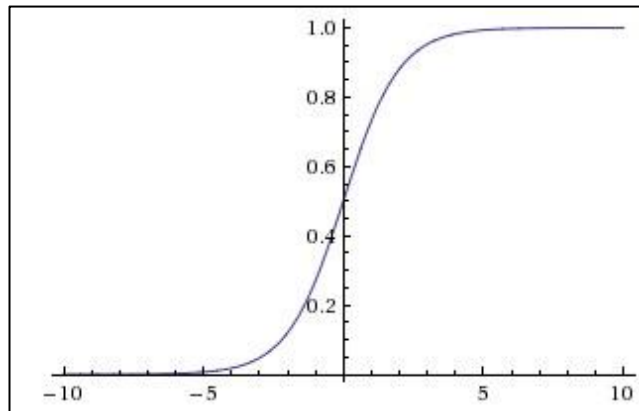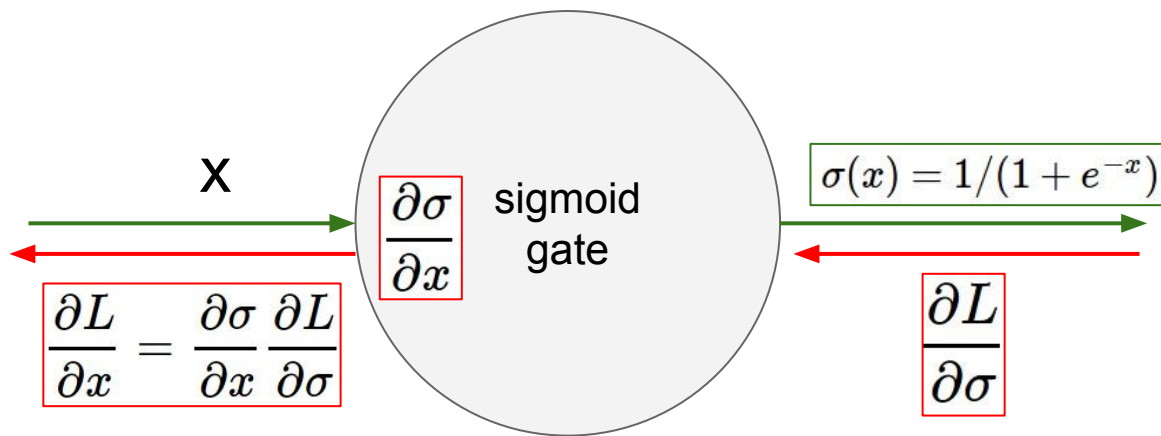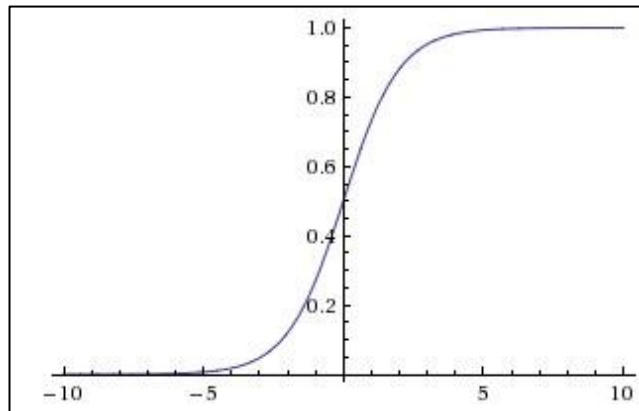
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

What happens when x = -10?

$$\sigma(x) = {\sim}\,0$$

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,) = 0(1 - 0) = 0$$
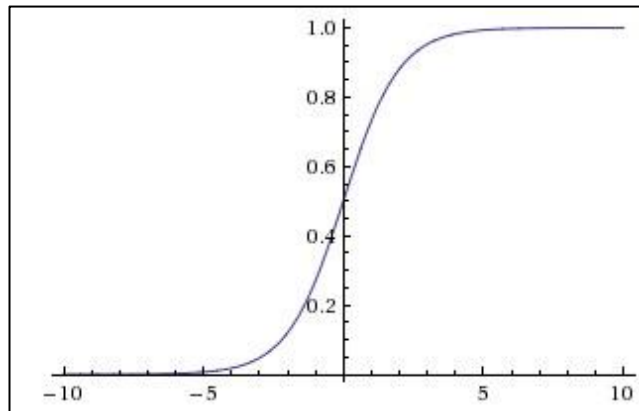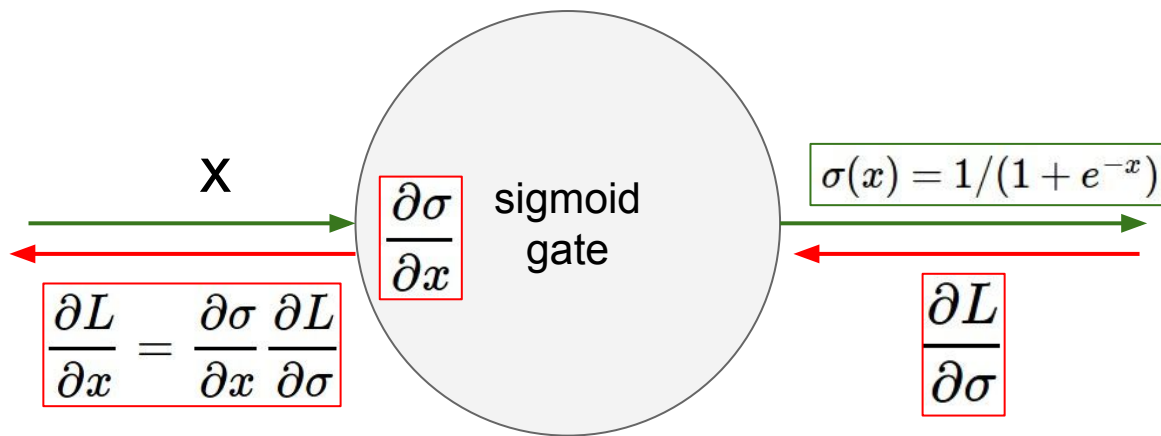
18

x

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

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

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

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

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

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

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x

$$\frac{\partial \sigma}{\partial x} \quad \text{sigmoid gate}$$

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

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

$$\frac{\partial L}{\partial \sigma}$$
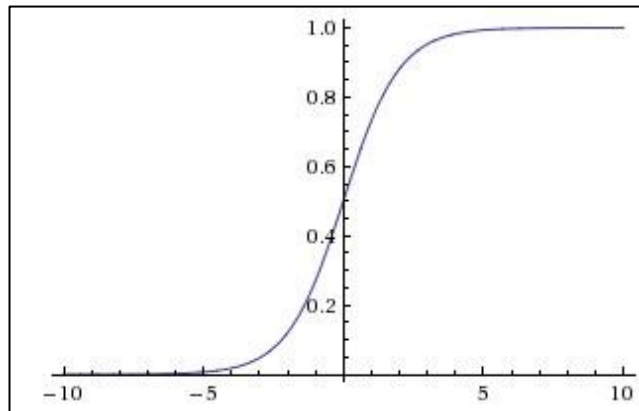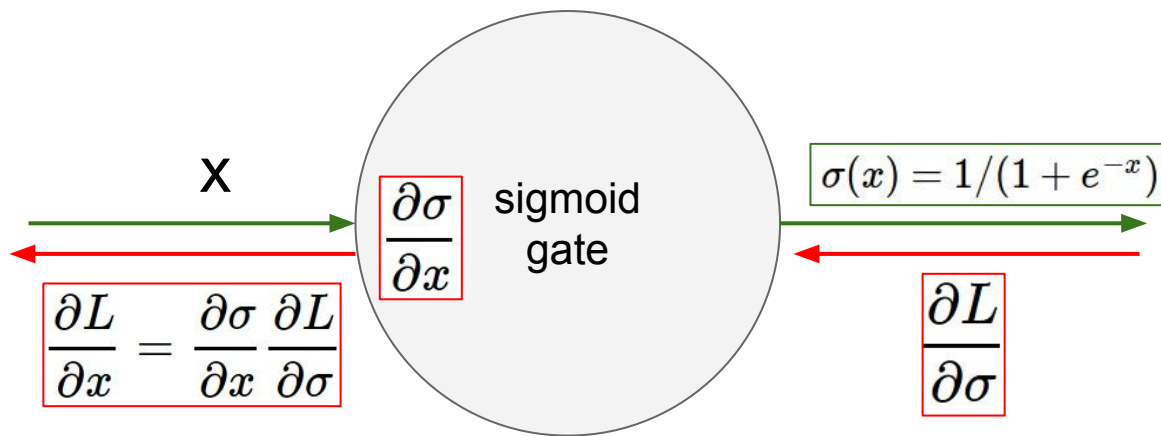
What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

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

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

x

$\dfrac{\partial \sigma}{\partial x}$ sigmoid gate

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

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

$\dfrac{\partial L}{\partial \sigma}$

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

What ha
What ha
What ha

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x

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

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

sigmoid gate

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

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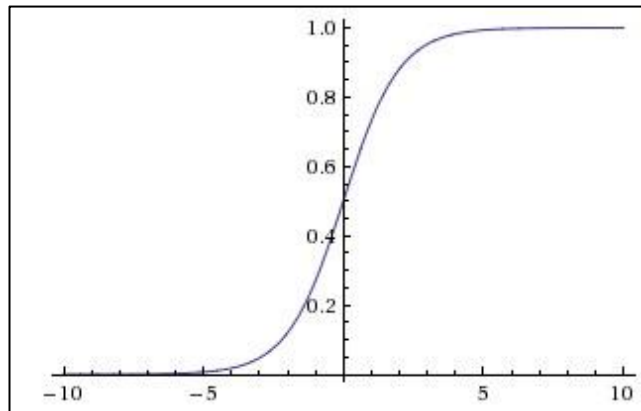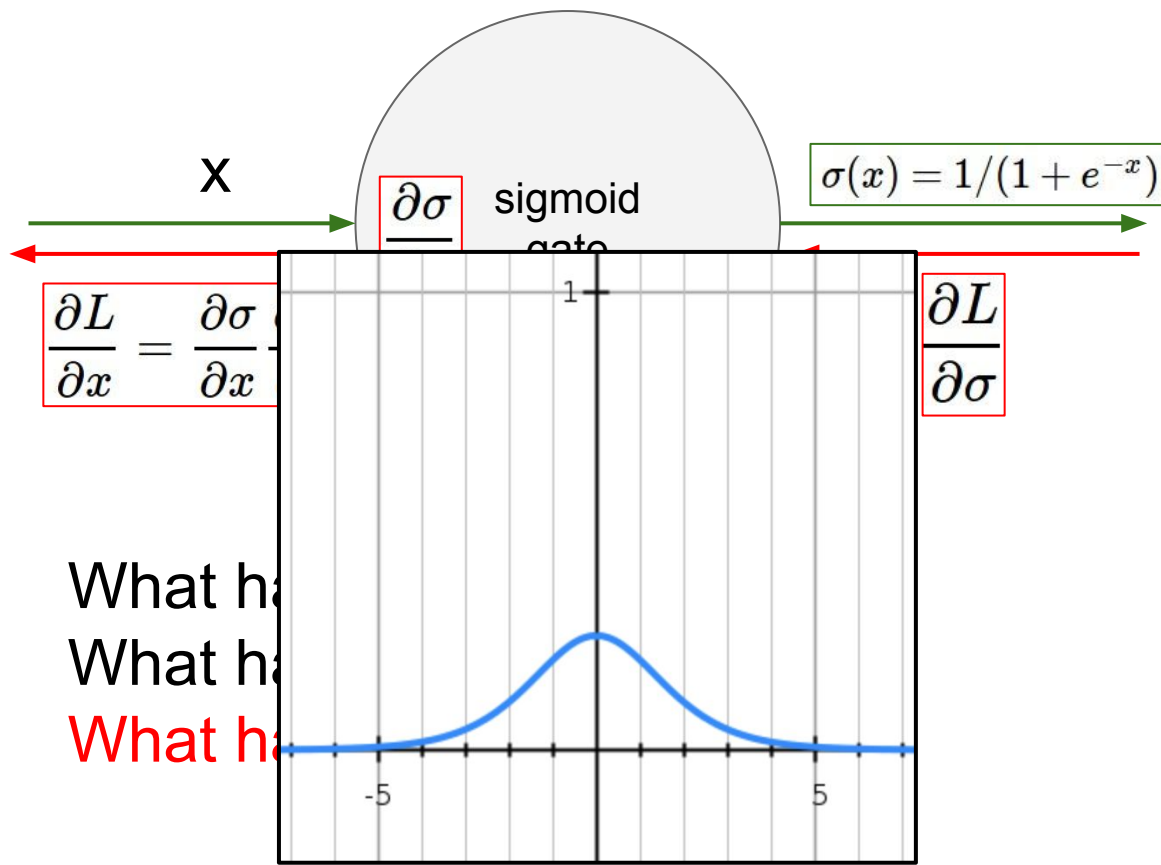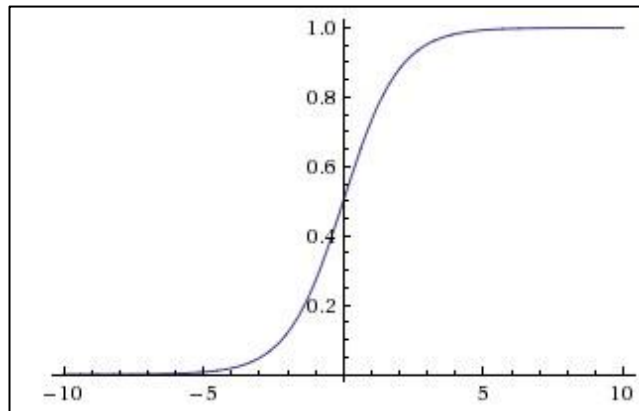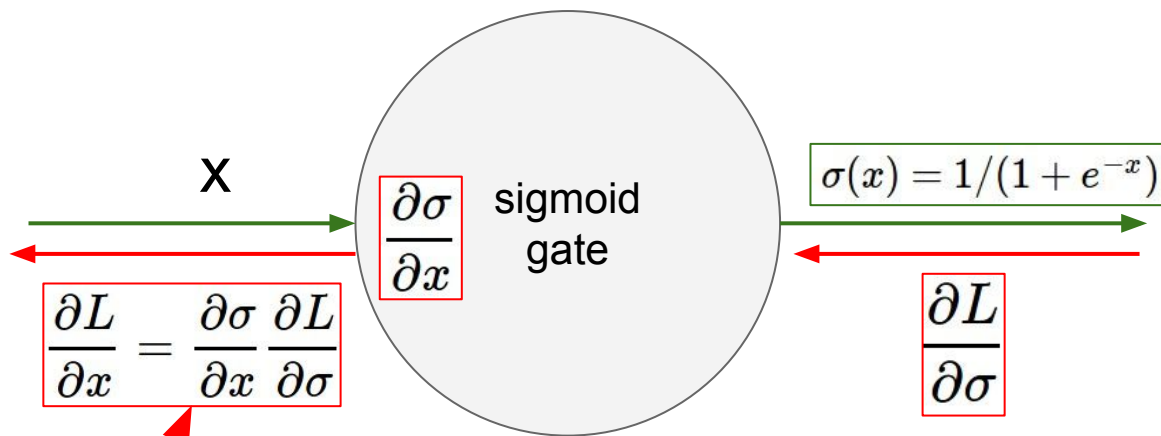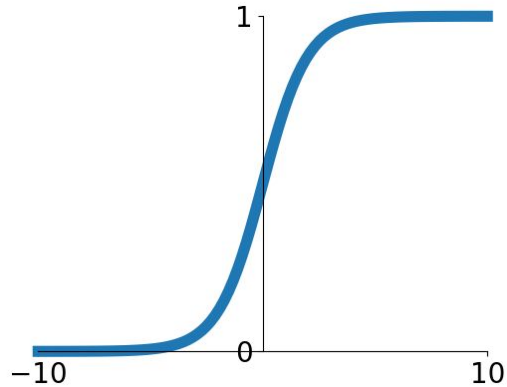
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

Why is this a problem?
If all the gradients flowing back will be zero and weights will never change

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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

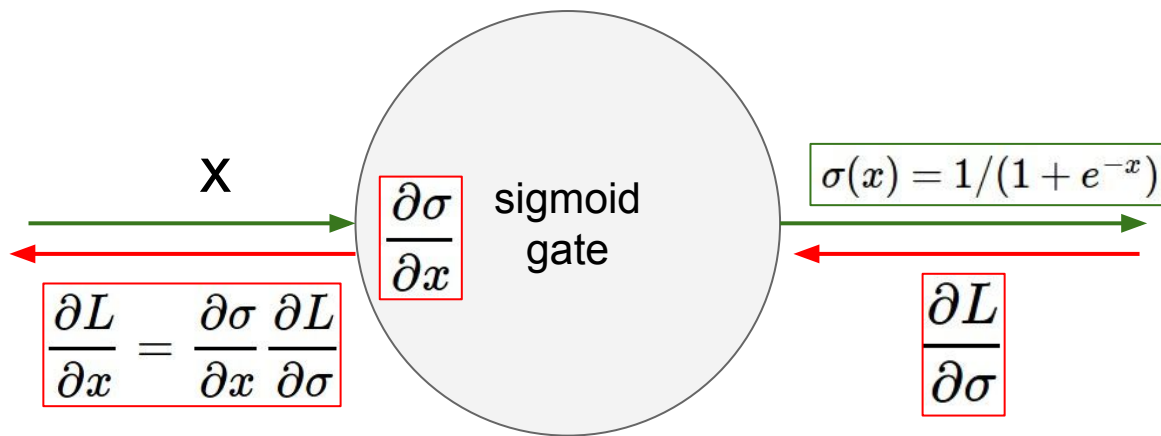3 problems:

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

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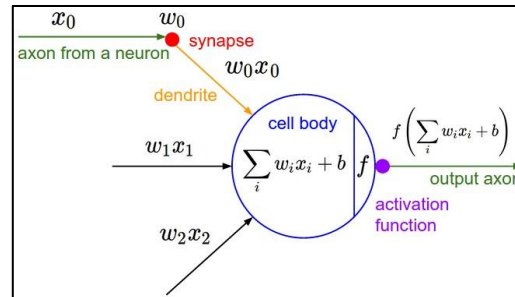
$$f \left(\sum_i w_i x_i + b \right)$$

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

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

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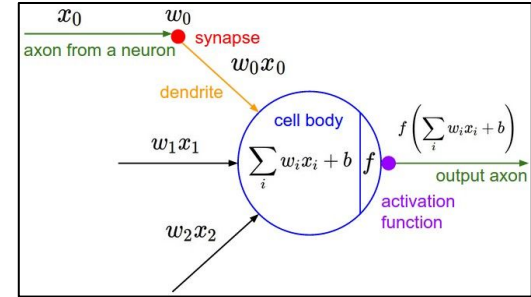
$$f\left(\sum_i w_i x_i + b\right)$$

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

We know that local gradient of sigmoid is always positive
We are assuming x is always positive

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

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**?

We know that local gradient of sigmoid is always positive
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!

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

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

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

allowed gradient update directions

allowed gradient update directions

zig zag path

hypothetical optimal w vector
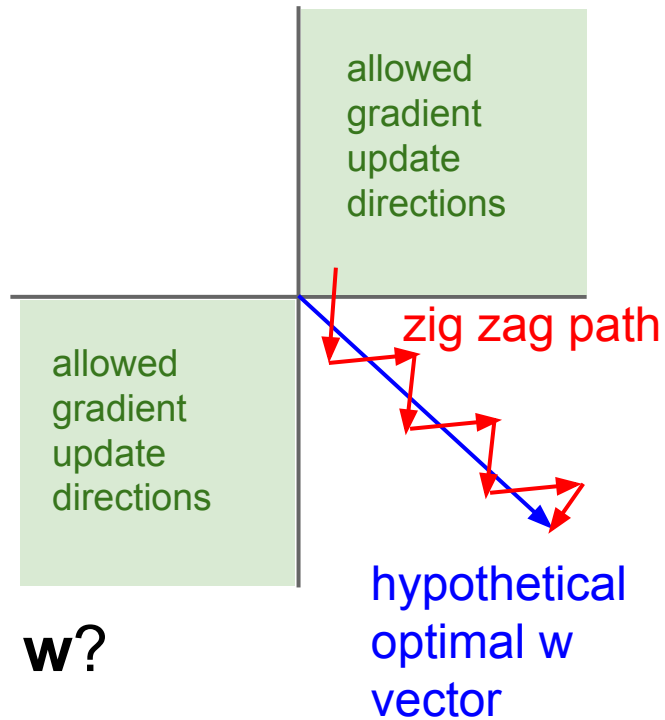
What can we say about the gradients on **w**?
Always all positive or all negative :(

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

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

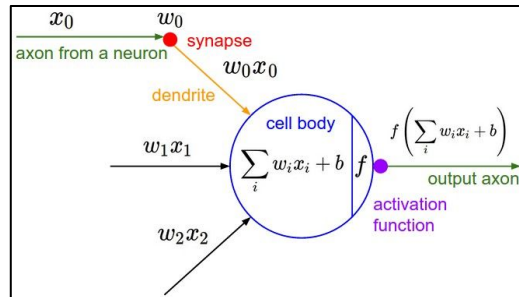allowed gradient update directions

zig zag path

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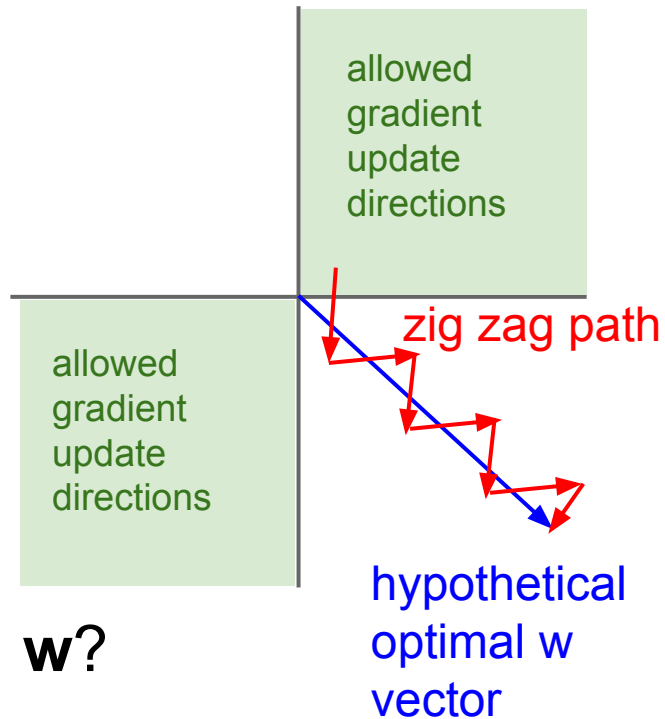
What can we say about the gradients on **w**?
Always all positive or all negative :(
(For a single element! Minibatches help)

Activation Functions

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

Sigmoid

- 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
3. exp() is a bit compute expensive

Activation Functions
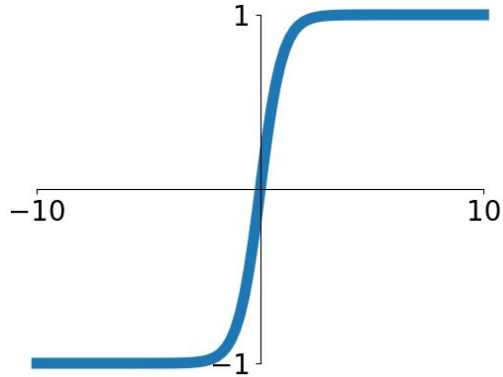
tanh(x)

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

Activation Functions
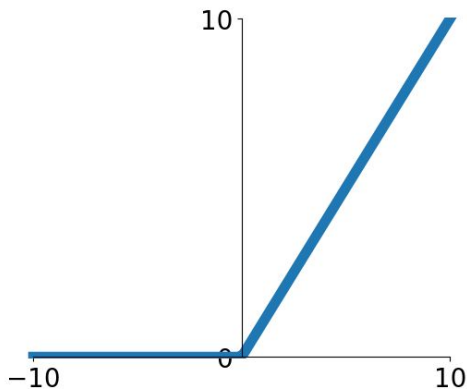
- Computes **f(x) = max(0,x)**

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

ReLU
(Rectified Linear Unit)

[Krizhevsky et al., 2012]

Activation Functions
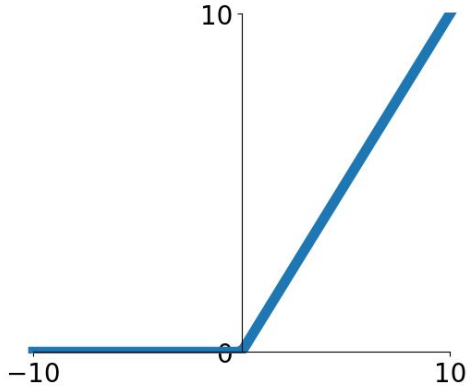
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- Not zero-centered output

Activation Functions
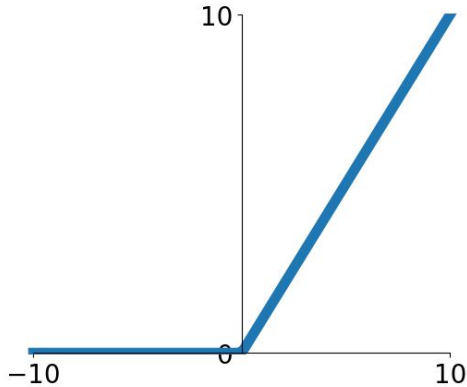
ReLU
(Rectified Linear Unit)

- 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)

- Not zero-centered output
- An annoyance:

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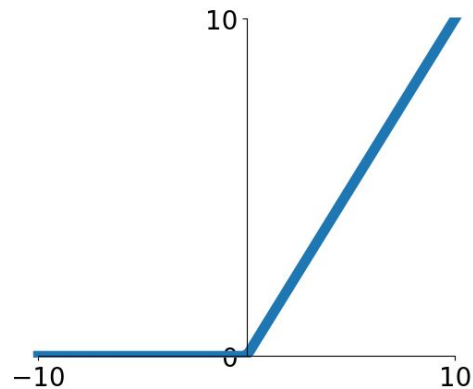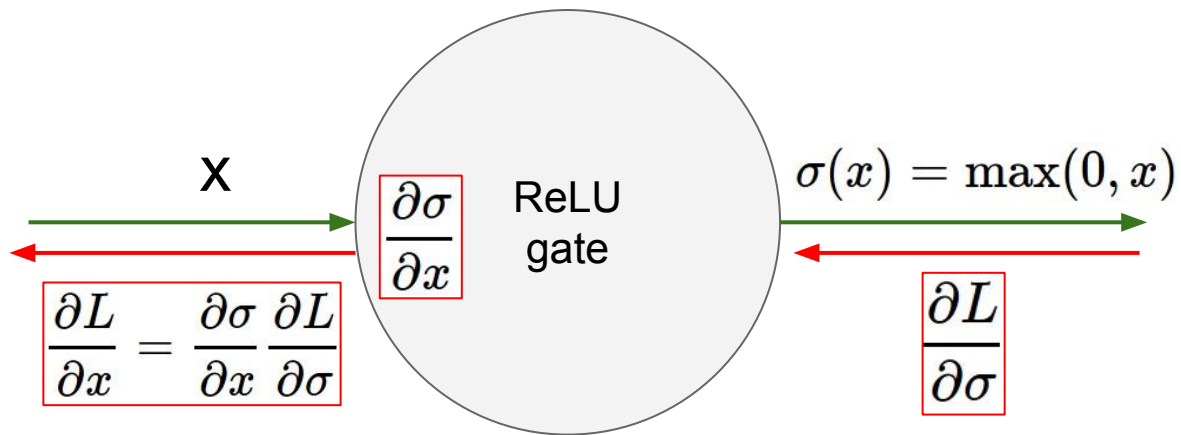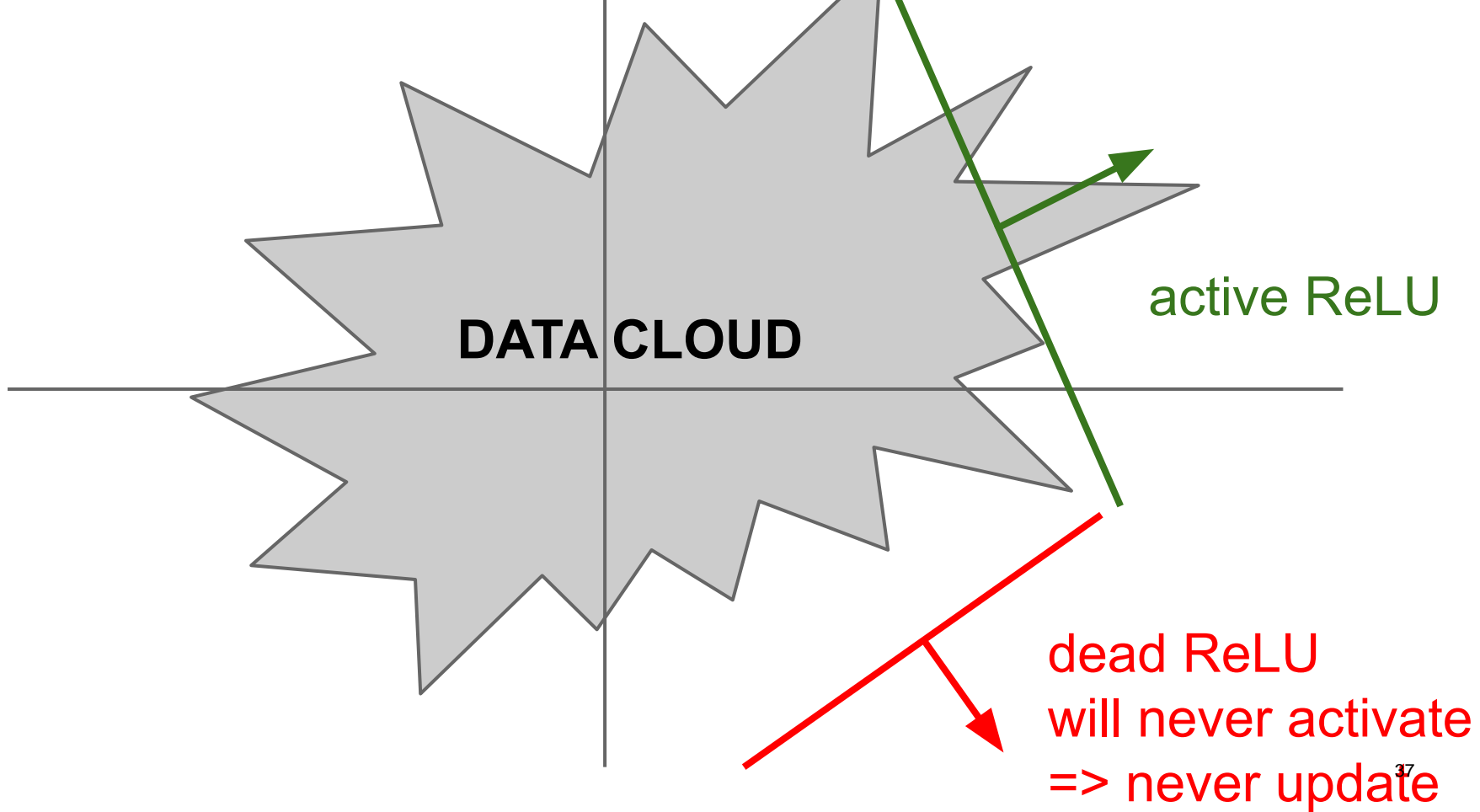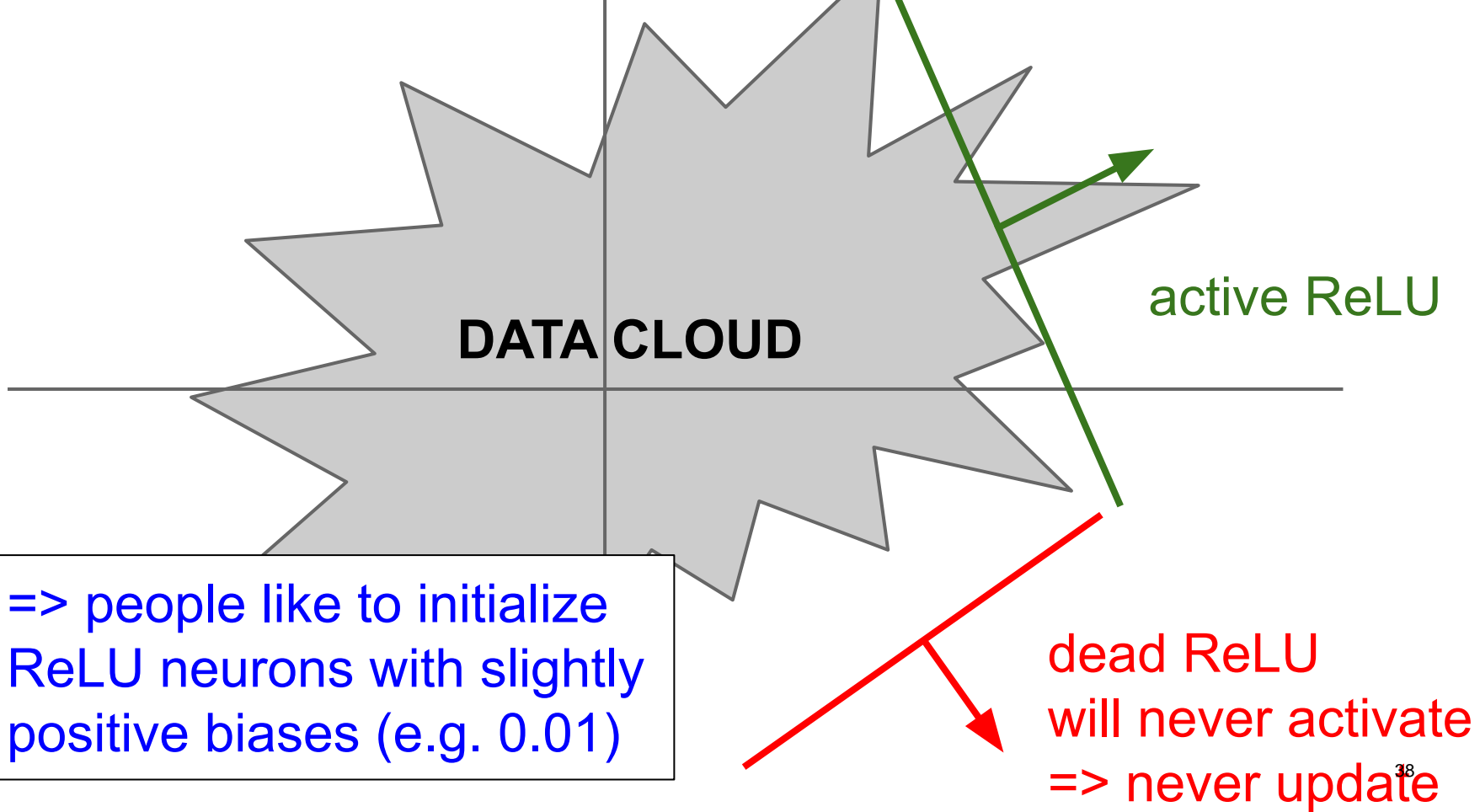
x

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

$$\sigma(x) = \max(0, x)$$

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

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

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

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)

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Activation Functions

[Mass et al., 2013]
[He et al., 2015]
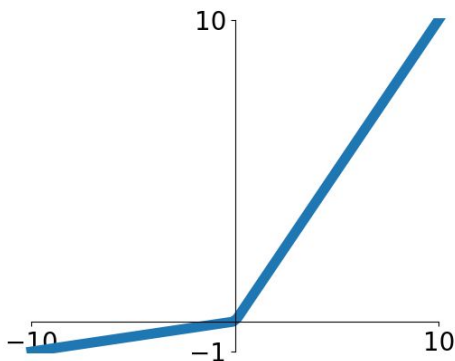
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

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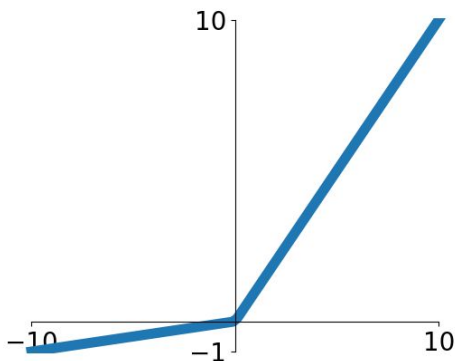
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- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

Parametric Rectifier (PReLU)

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

backprop into α (parameter)

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Activation Functions

Exponential Linear Units (ELU)
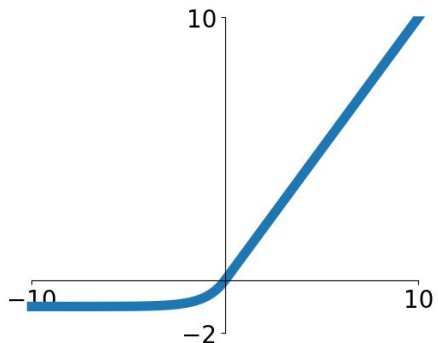
- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

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

(Alpha default = 1)

- Computation requires exp()

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Activation Functions

Scaled Exponential Linear Units (SELU)
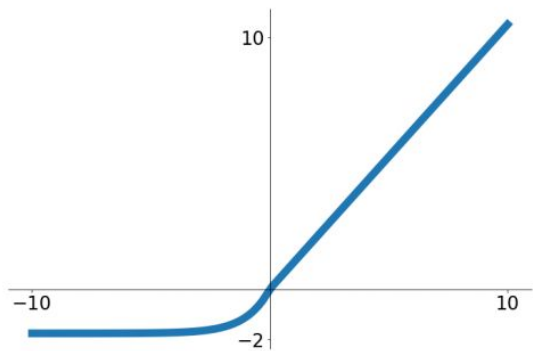
- Scaled version of ELU that works better for deep networks
- "Self-normalizing" property;
- Can train deep SELU networks without BatchNorm

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

$$\alpha = 1.6732632423543772848170429916717$$
$$\lambda = 1.0507009873554804934193349852946$$

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Maxout "Neuron"

- 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

original data   zero-centered data   normalized data

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

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

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

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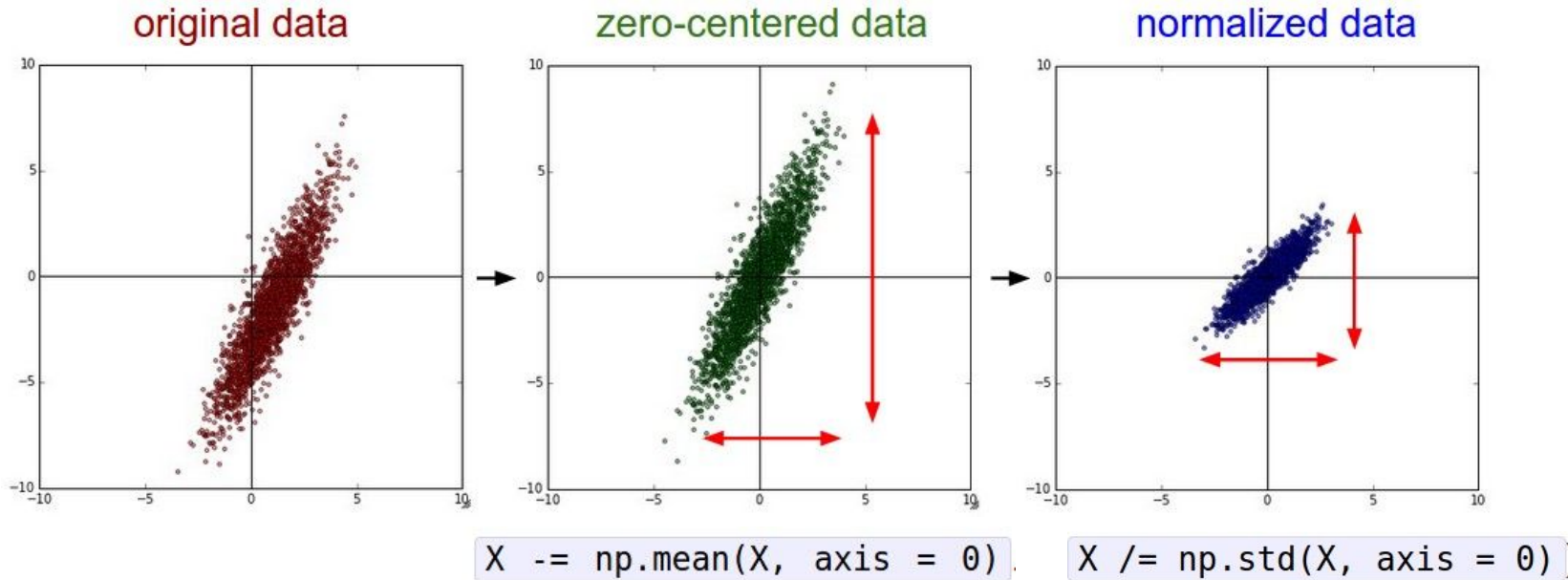
Remember: Consider what happens when the input to a neuron is always positive...

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

allowed gradient update directions

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zig zag path

hypothetical optimal w vector
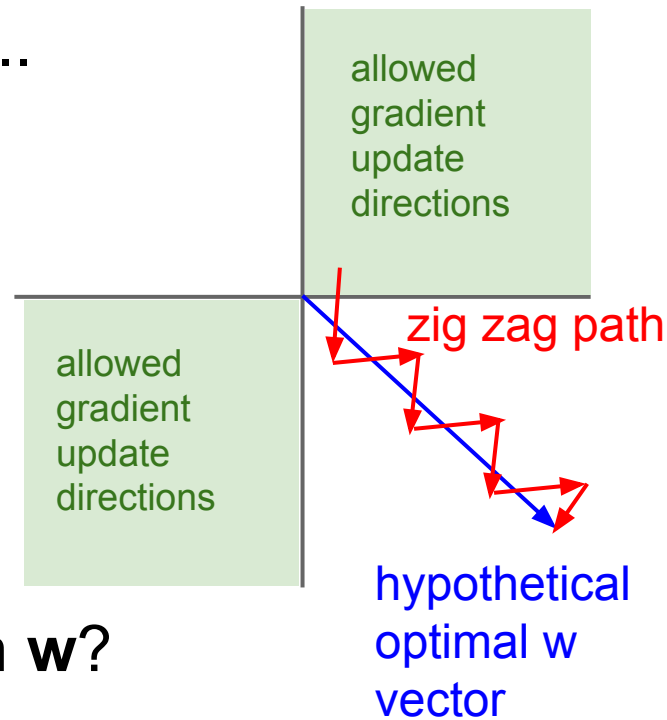
What can we say about the gradients on **w**?
Always all positive or all negative :(
(this is also why you want zero-mean data!)

Data Preprocessing

original data   zero-centered data   normalized data

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

```
X /= np.std(X, axis = 0)
```
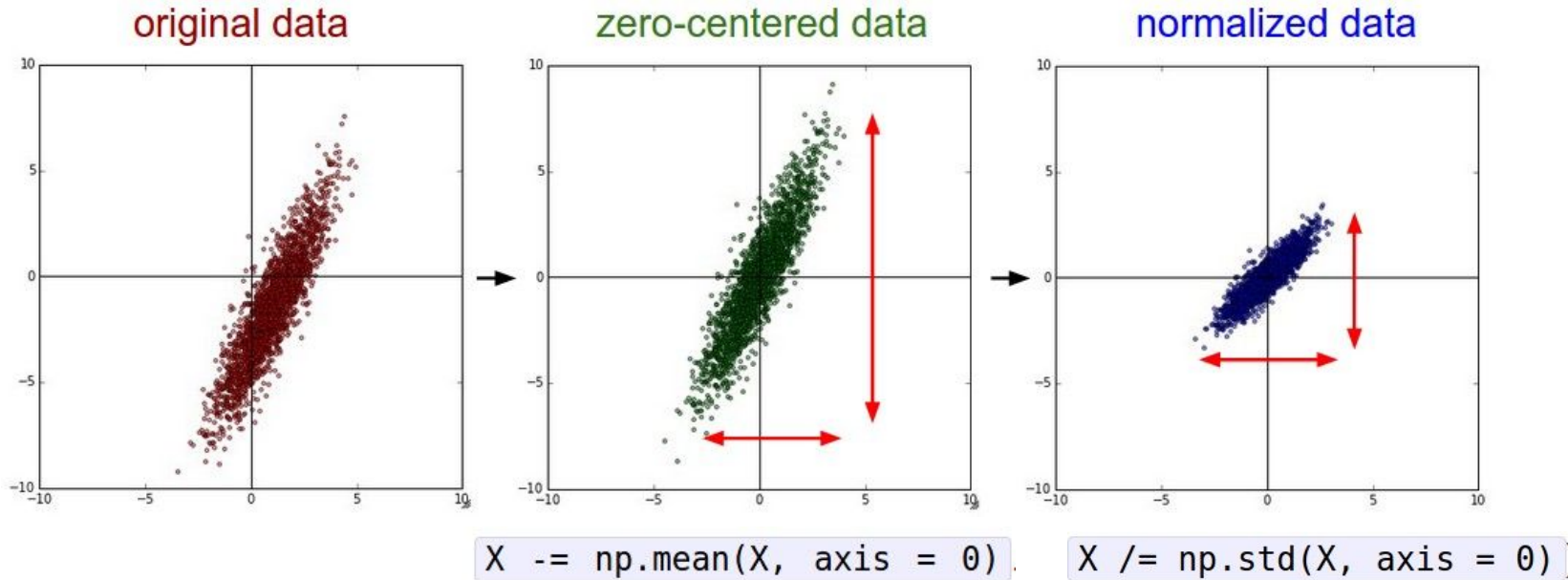
(Assume X [NxD] is data matrix, each example in a row)

Data Preprocessing

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

original data   decorrelated data   whitened data

(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)
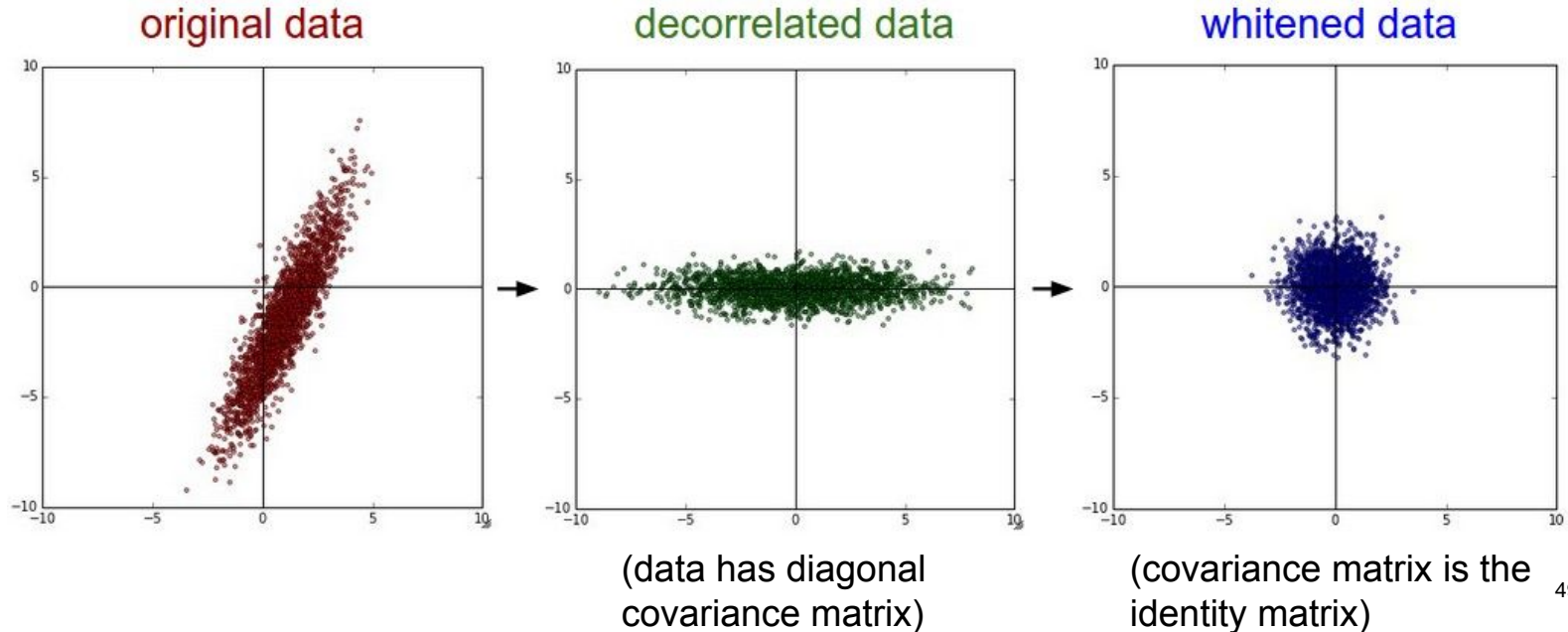
Data Preprocessing

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize
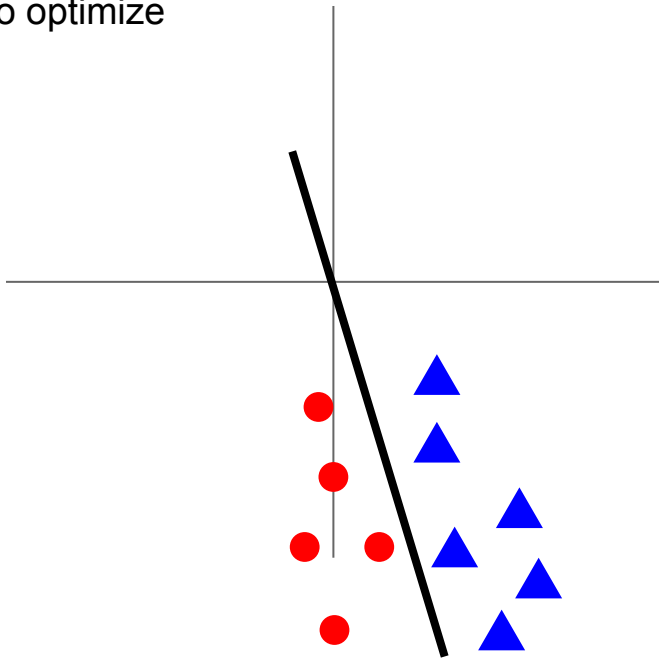
After normalization: less sensitive to small changes in weights; easier to optimize
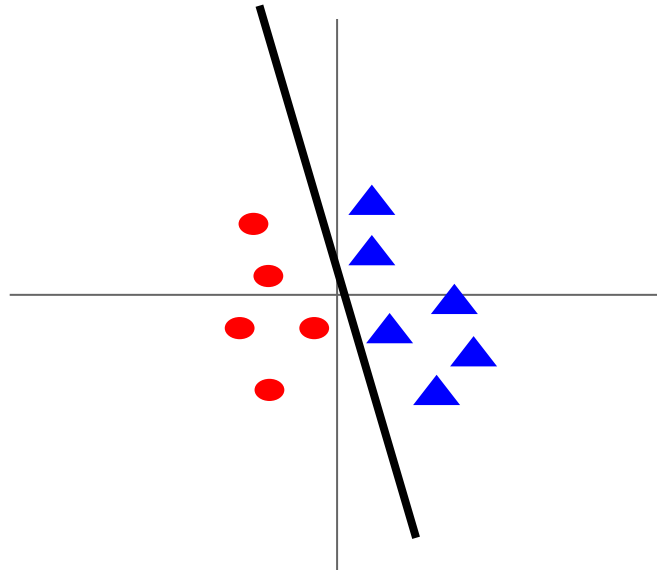
TLDR: In practice for Images: center only

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?
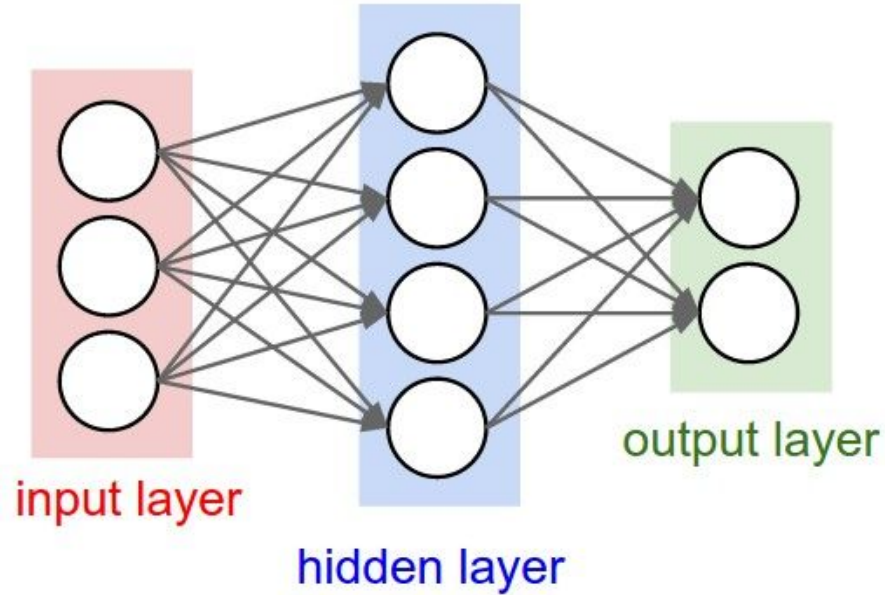
input layer

hidden layer

output layer

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

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

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

```python
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
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

All activations tend to zero for deeper network layers

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

| Layer 1 mean=-0.00 std=0.49 | Layer 2 mean=0.00 std=0.29 | Layer 3 mean=0.00 std=0.18 | Layer 4 mean=-0.00 std=0.11 | Layer 5 mean=-0.00 std=0.07 | Layer 6 mean=0.00 std=0.05 |

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

All activations tend to zero for deeper network layers

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

A: All zero, no learning =(

| Layer 1 mean=-0.00 std=0.49 | Layer 2 mean=0.00 std=0.29 | Layer 3 mean=0.00 std=0.18 | Layer 4 mean=-0.00 std=0.11 | Layer 5 mean=-0.00 std=0.07 | Layer 6 mean=0.00 std=0.05 |

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 = []
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)
```
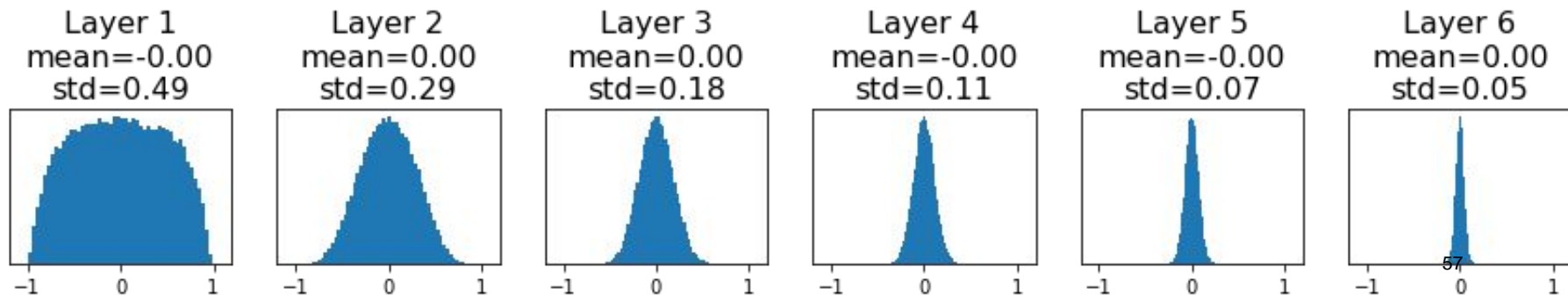
Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
mean=0.00 std=0.87	mean=-0.00 std=0.85	mean=0.00 std=0.85	mean=-0.00 std=0.85	mean=0.00 std=0.85	mean=-0.00 std=0.85

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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

All activations saturate

Q: What do the gradients look like?

A: Local gradients all zero, no learning =(

Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
mean=0.00 std=0.87	mean=-0.00 std=0.85	mean=0.00 std=0.85	mean=-0.00 std=0.85	mean=0.00 std=0.85	mean=-0.00 std=0.85

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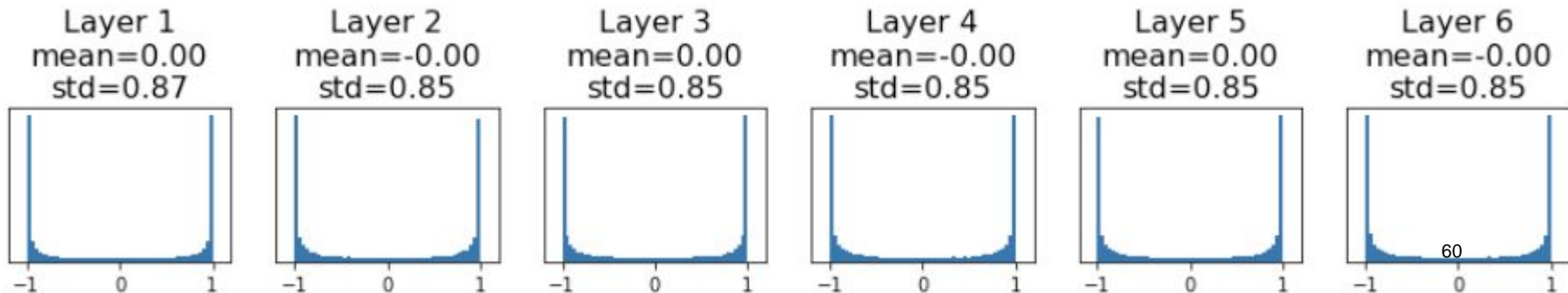
"Xavier" initialization:
std = 1/sqrt(Din)

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

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!

Layer 1
mean=-0.00
std=0.63

Layer 2
mean=-0.00
std=0.49

Layer 3
mean=0.00
std=0.41

Layer 4
mean=0.00
std=0.36

Layer 5
mean=0.00
std=0.32

Layer 6
mean=-0.00
std=0.30

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 filter_size^2 * input_channels

Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
mean=-0.00 std=0.63	mean=-0.00 std=0.49	mean=0.00 std=0.41	mean=0.00 std=0.36	mean=0.00 std=0.32	mean=-0.00 std=0.30

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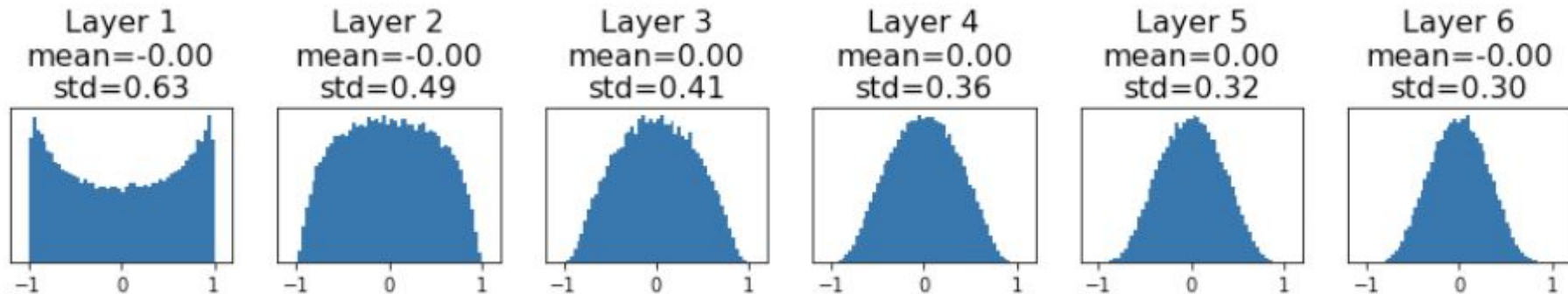
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Weight Initialization: "Xavier" Initialization

```
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 filter_size^2 * input_channels

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

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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 filter_size^2 * input_channels

Let: $y = x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din}$

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

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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 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: $Var(y) = Var(x_i)$

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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: $y = x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din}$

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

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

$Var(y) = Var(x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din})$
[substituting value of y]

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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 filter_size^2 * input_channels

Let: $y = x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din}$

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

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

$Var(y) = Var(x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din})$
$= Din\ Var(x_i w_i)$
[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 filter_size^2 * input_channels

Let: $y = x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din}$

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

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

$Var(y) = Var(x_1 w_1 + x_2 w_2 + ... + x_{Din} w_{Din})$
$\qquad = Din\ Var(x_i w_i)$
$\qquad = Din\ Var(x_i)\ Var(w_i)$
[Assume all x_i, w_i are zero mean]

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

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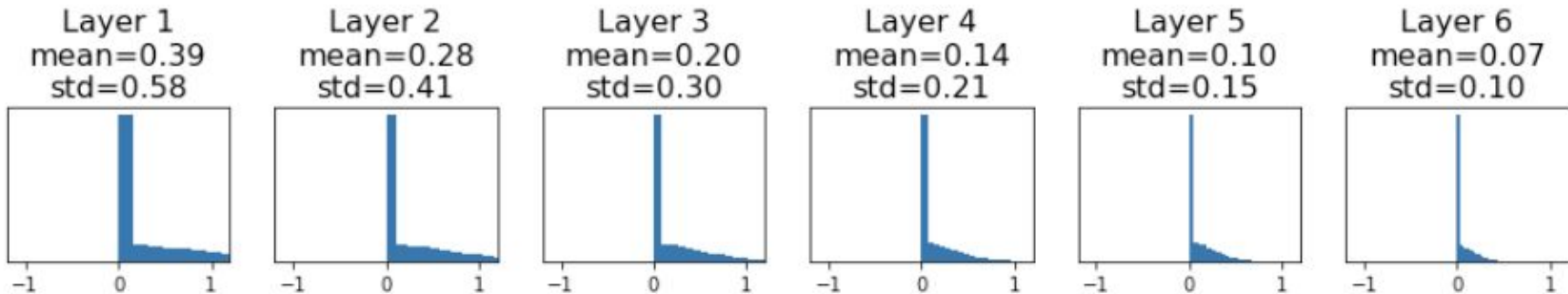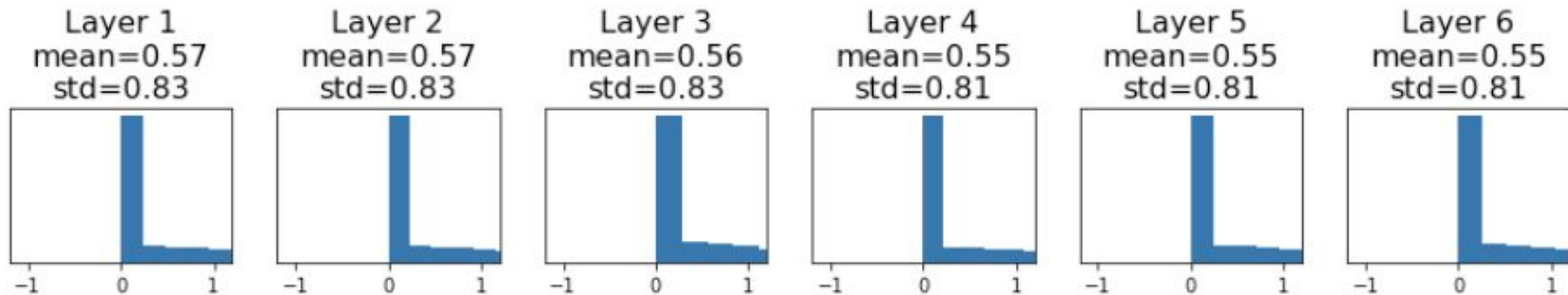
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

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

For conv layers, Din is filter_size^2 * input_channels

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

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

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 $Var(w_i) = 1/Din$

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

Weight Initialization: What about ReLU?

```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.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 =(

Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
mean=0.39	mean=0.28	mean=0.20	mean=0.14	mean=0.10	mean=0.07
std=0.58	std=0.41	std=0.30	std=0.21	std=0.15	std=0.10

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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!

Layer 1
mean=0.57
std=0.83

Layer 2
mean=0.57
std=0.83

Layer 3
mean=0.56
std=0.83

Layer 4
mean=0.55
std=0.81

Layer 5
mean=0.55
std=0.81

Layer 6
mean=0.55
std=0.81

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?[77]
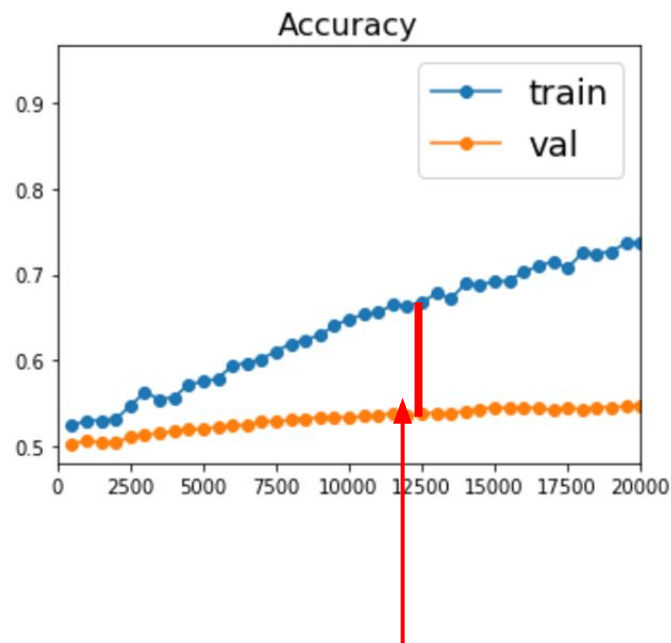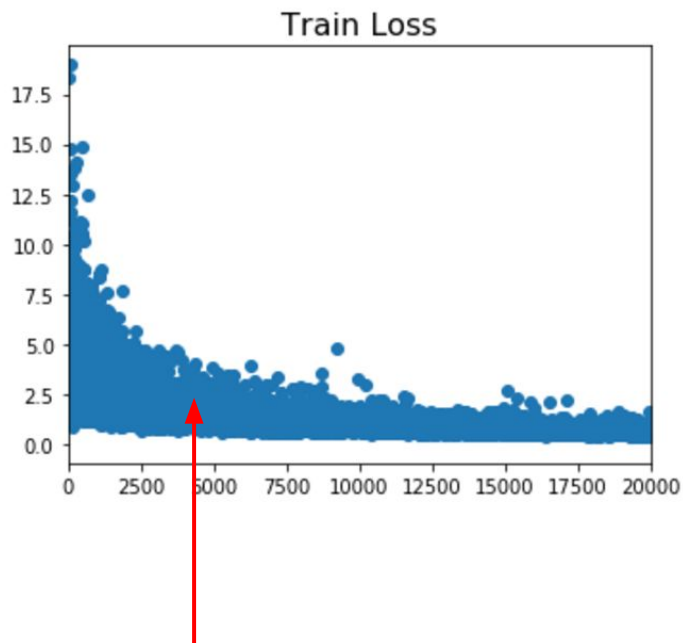
Early Stopping: Always do this
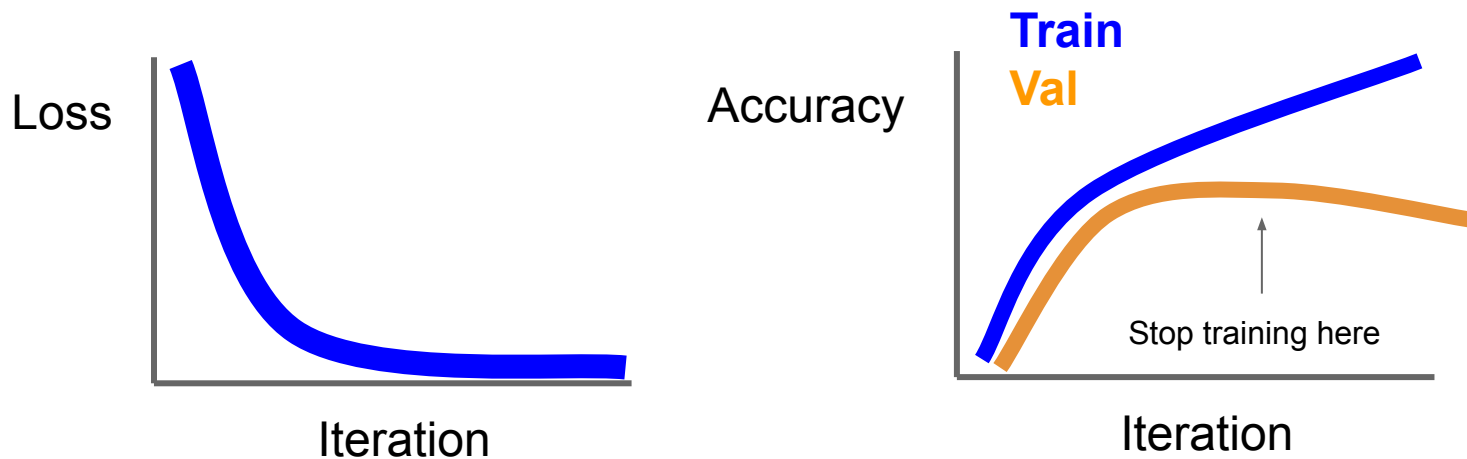
Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot
that worked best on val

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?
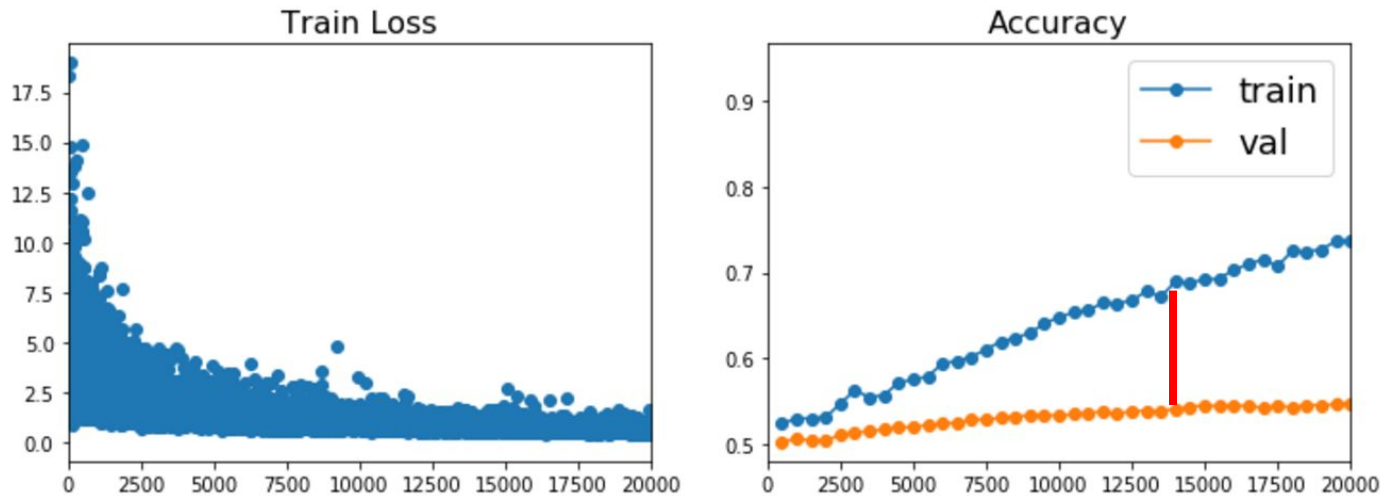
Regularization

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

Example forward pass with a 3-layer network using 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)
```

Regularization: Dropout
How can this possibly be a good idea?
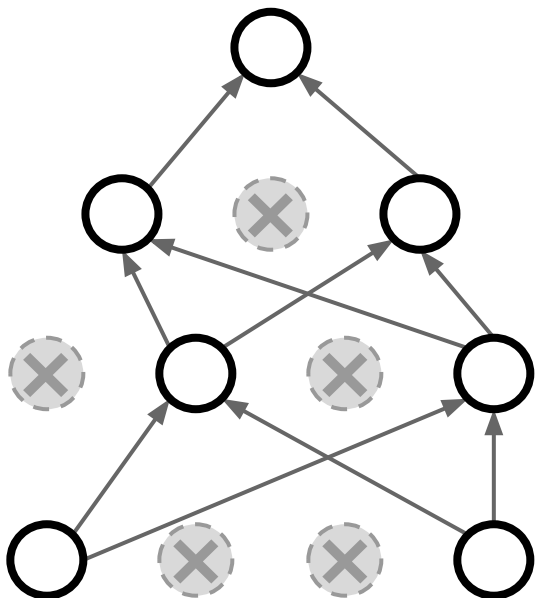
Forces the network to have a redundant representation;
Prevents co-adaptation of features

has an ear X

has a tail

is furry X

has claws

mischievous look X

cat score

Regularization: Dropout
How can this possibly be a good idea?
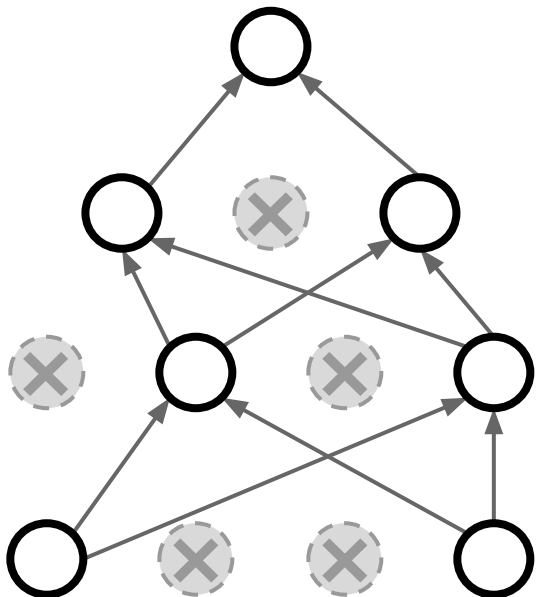
Another interpretation:

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!

Output (label)   Input (image)

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

Random mask

Want to "average out" the randomness at test-time

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

But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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

Consider a single neuron.

a

w_1 w_2

x   y

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: $E\big[a\big] = w_1 x + w_2 y$

w_1 w_2

a

x   y

Dropout: Test time

Want to approximate the integral
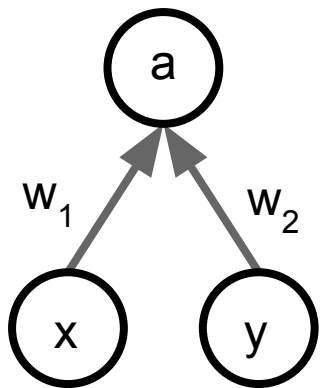
$$y = f(x) = E_z\big[f(x, z)\big] = \int p(z)f(x, z)dz$$

Consider a single neuron.

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

During training we have:

$$E\big[a\big] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y)$$
$$+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y)$$
$$= \frac{1}{2}(w_1 x + w_2 y)$$

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: $E\big[a\big] = w_1 x + w_2 y$

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$$E[a] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y)$$
$$+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y)$$
$$= \frac{1}{2}(w_1 x + w_2 y)$$
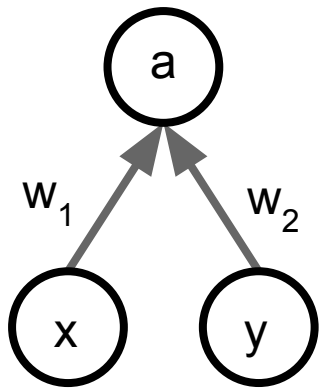
At test time, **multiply** by dropout probability

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Dropout: Test time

```python
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

```python
""" 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

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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)

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

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Regularization: Data Augmentation

Load image and label

"cat"

CNN

Compute loss

Regularization: Data Augmentation

Load image
and label

"cat"

Compute
loss

CNN

Transform image
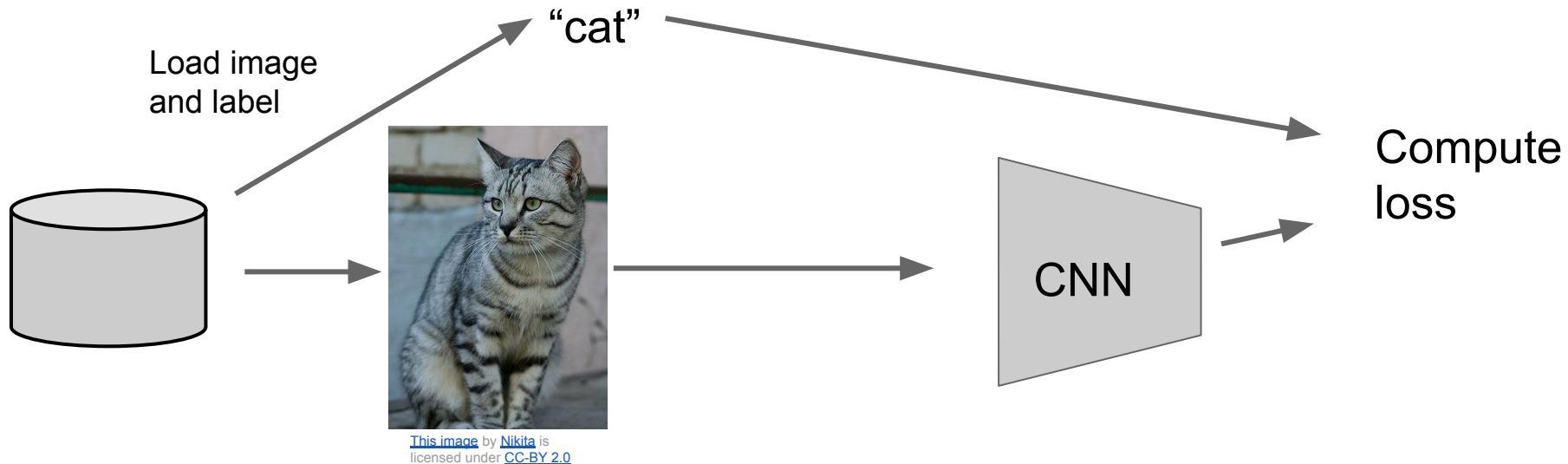
Data Augmentation
Horizontal Flips

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
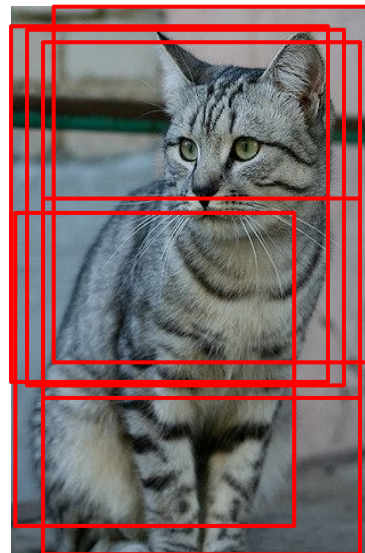
Data Augmentation
Random crops and scales

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

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
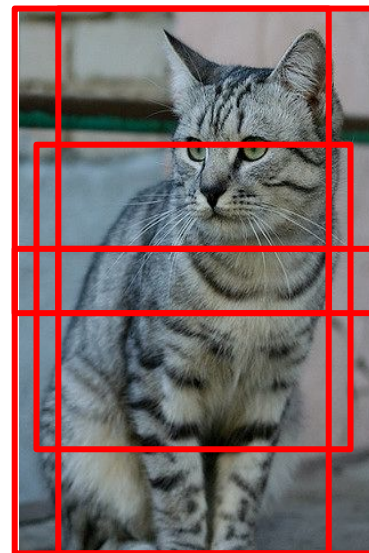
Data Augmentation
Color Jitter

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)
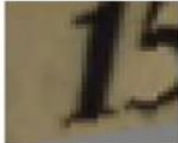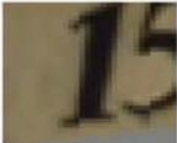
Data Augmentation
Get creative for your problem!

Examples of data augmentations:
- translation
- rotation
- stretching
- shearing,
- lens distortions, … (go crazy)

Automatic Data Augmentation

	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)
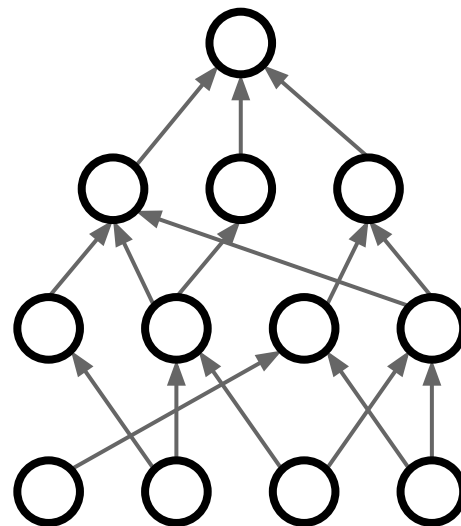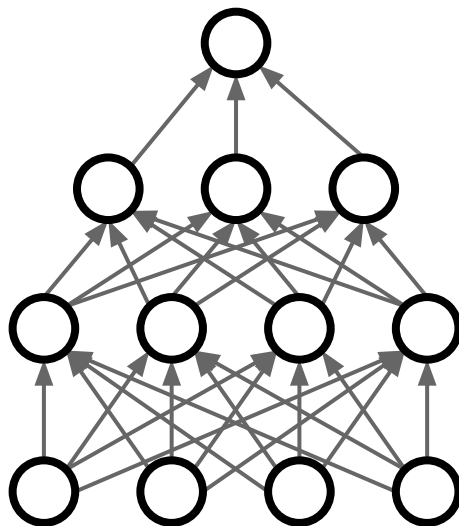**Testing**: Use all the connections

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
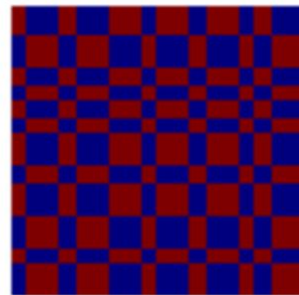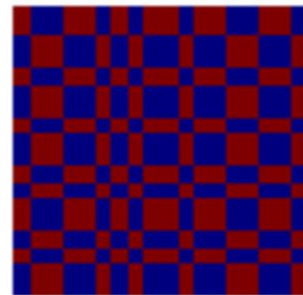**Testing**: Average predictions from several regions

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling

Graham, "Fractional Max Pooling", arXiv 2014
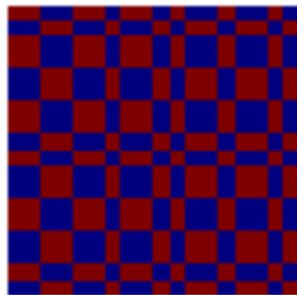
Regularization: Stochastic Depth

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
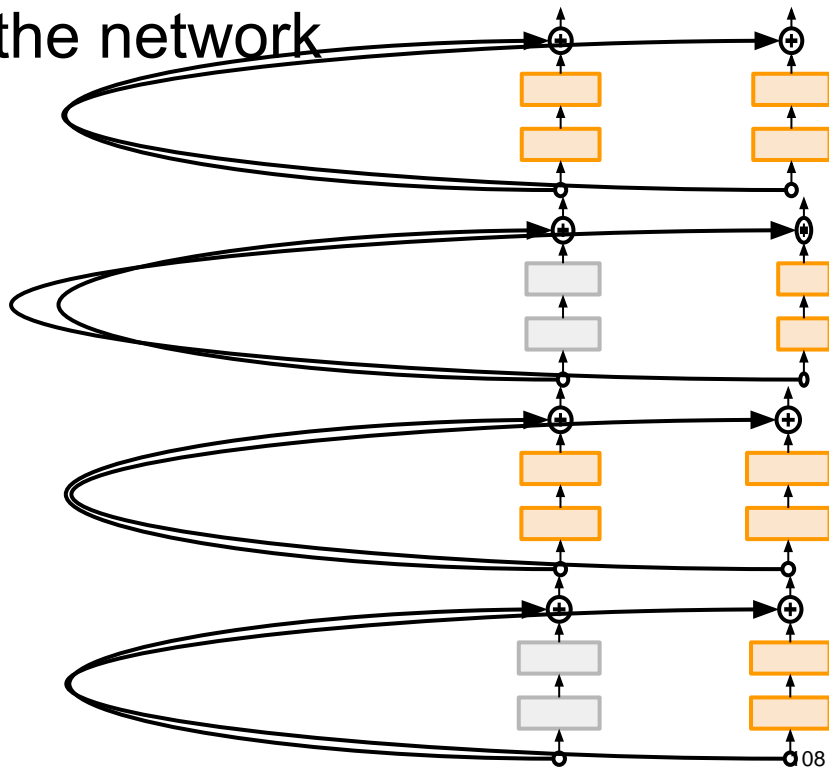
Training: Set random image regions to zero

Testing: Use full image

Examples:
Dropout
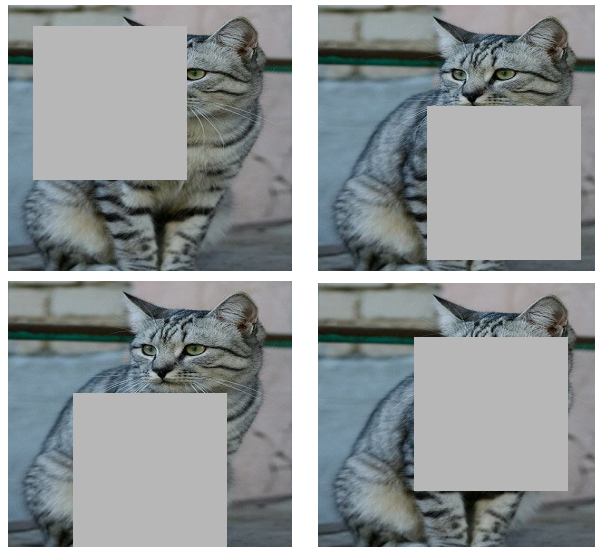Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Crop

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
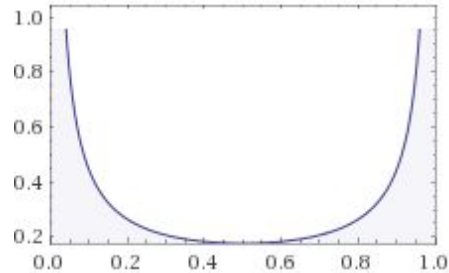Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Crop
Mixup

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

CNN

Target label:
cat: 0.4
dog: 0.6

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

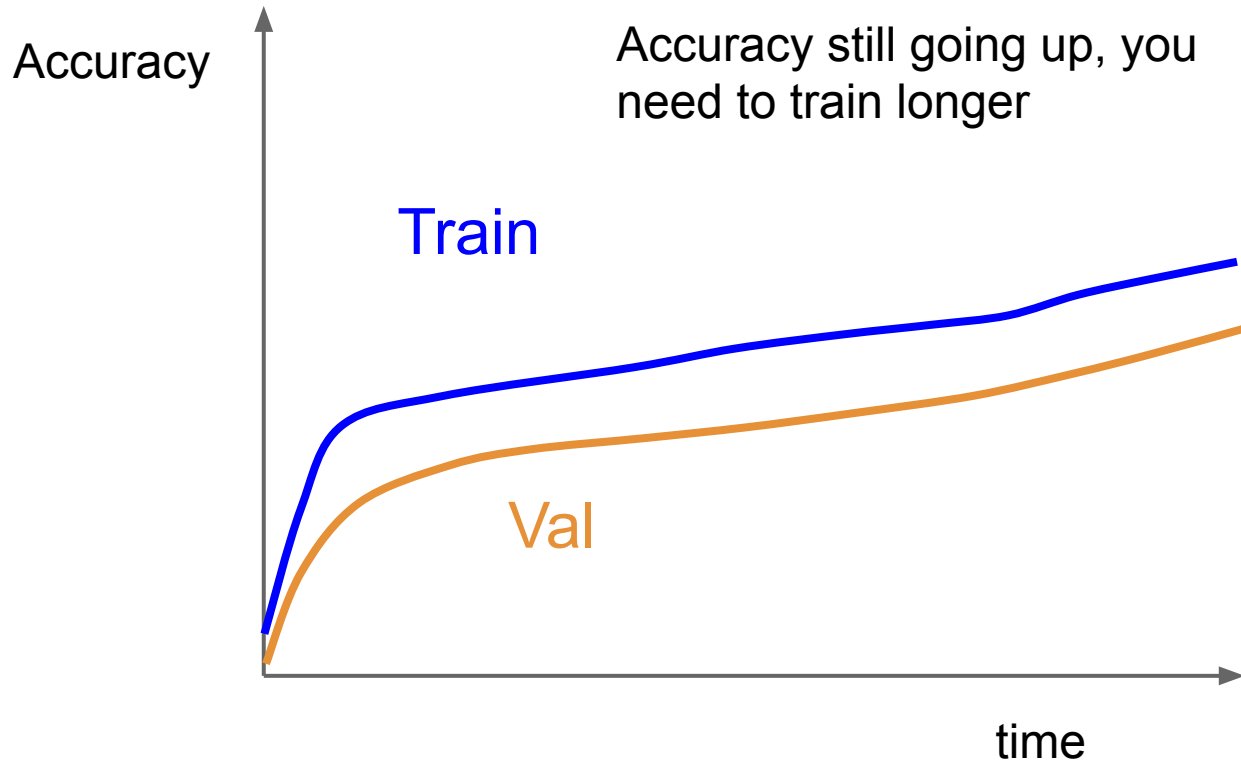# Choosing Hyperparameters

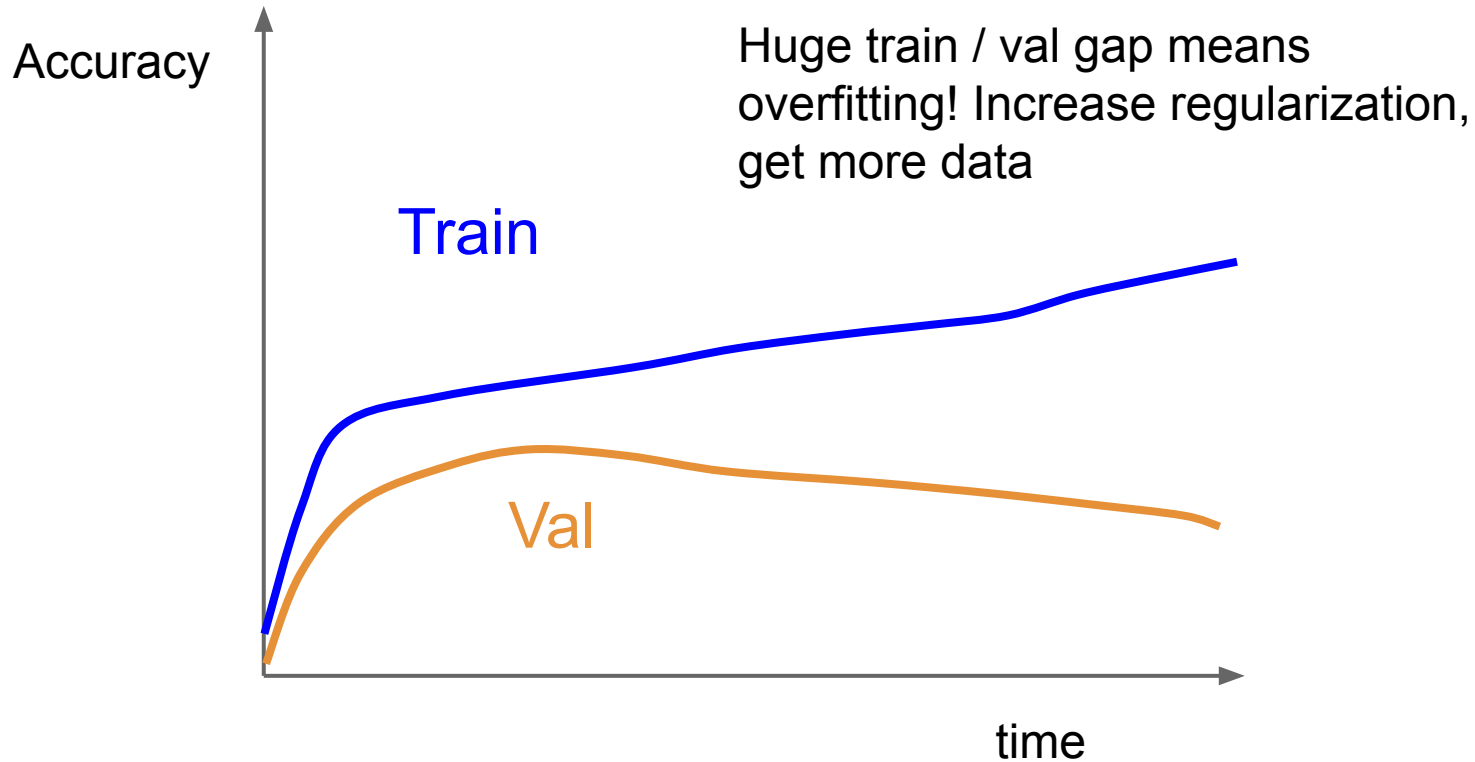**Step 1**: Check initial loss
Step 2: Overfit a small sample
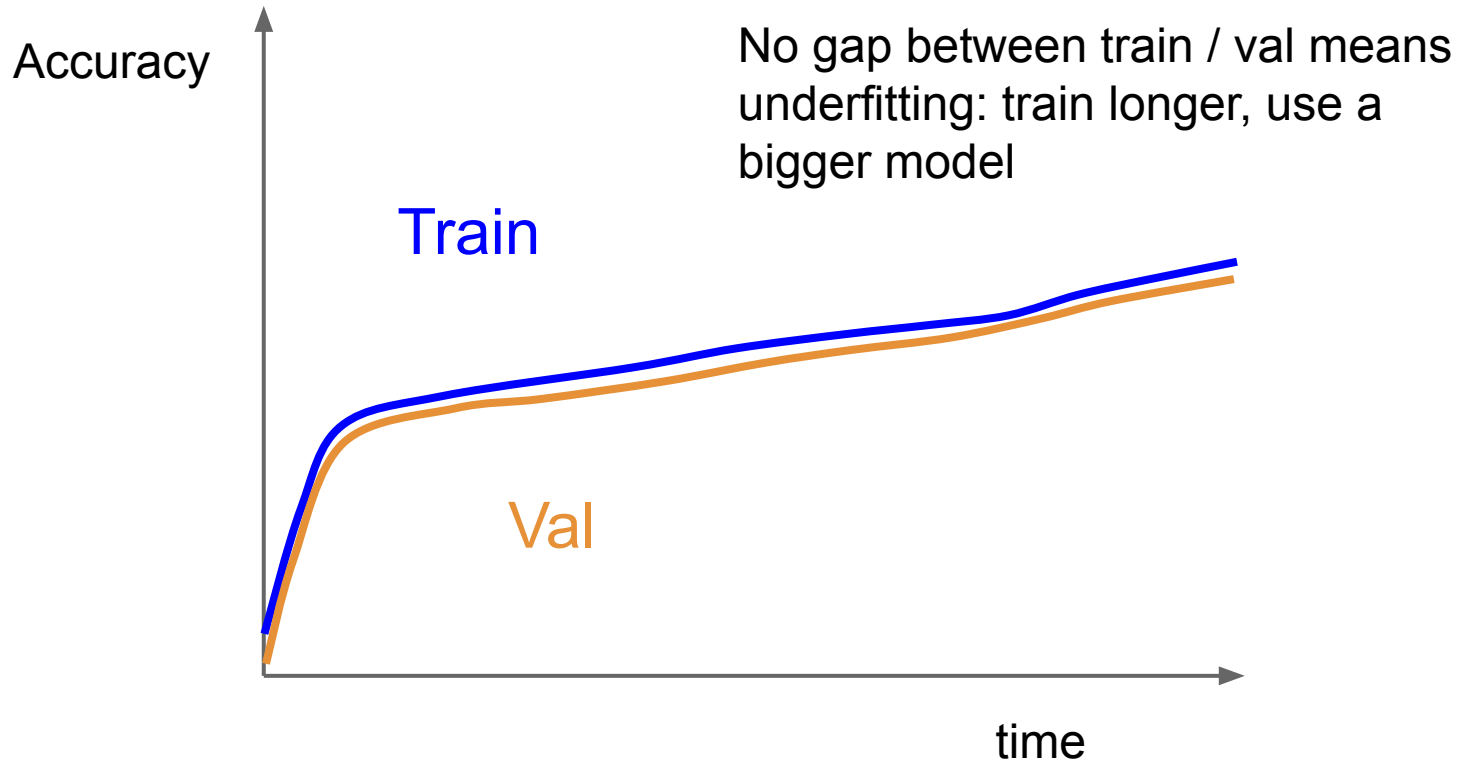**Step 3**: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at loss and accuracy curves

Accuracy

Accuracy still going up, you need to train longer

Train

Val

time

Accuracy

Train

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

Val

time

Accuracy

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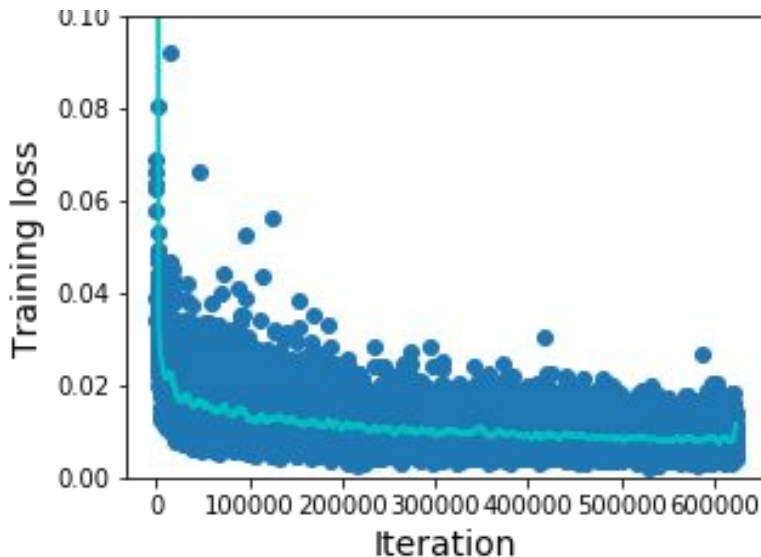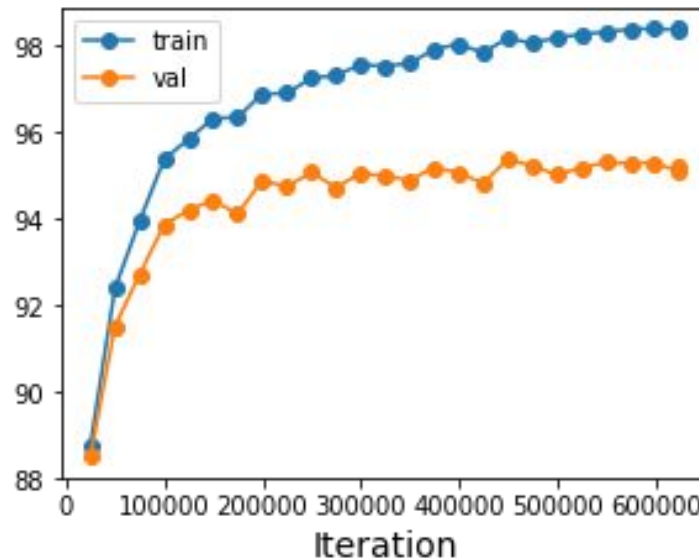
Train

Val

time

Look at learning curves!
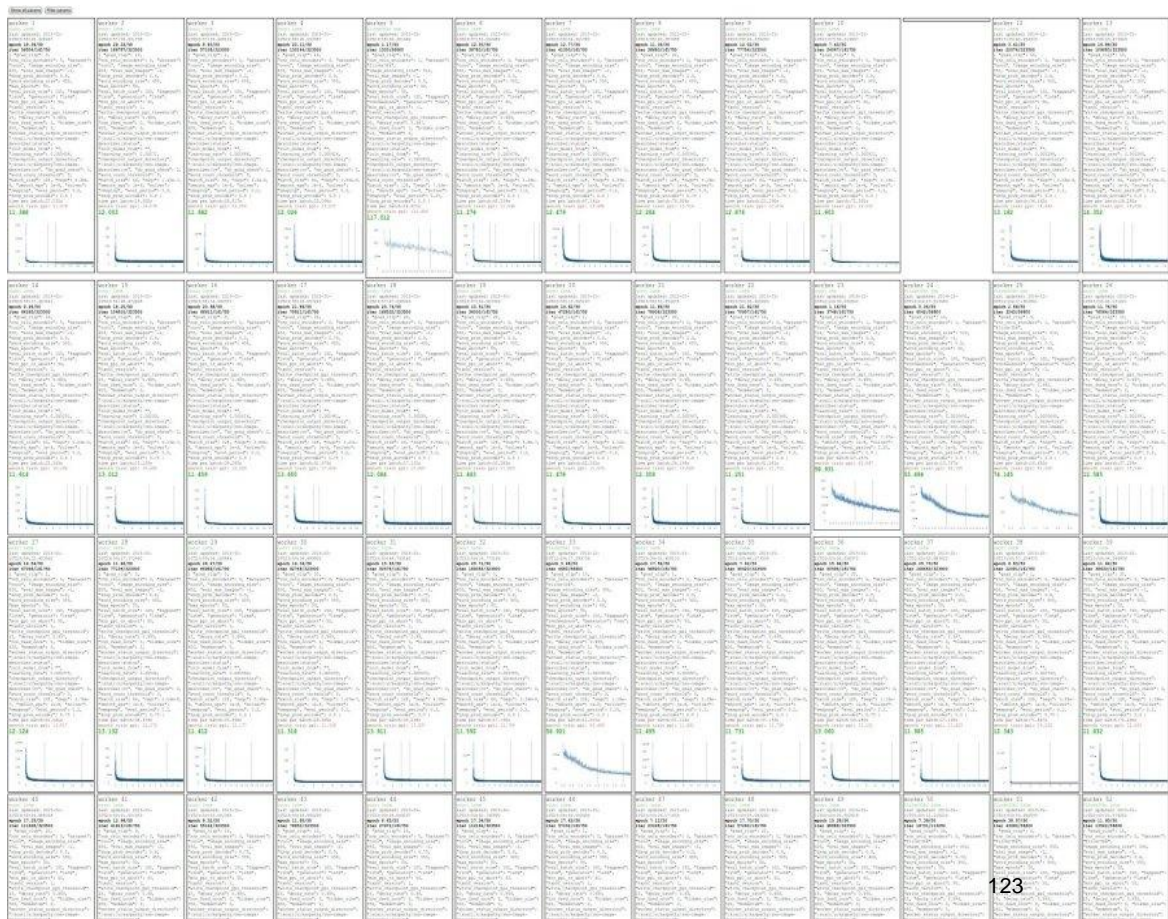
Training Loss

Train / Val Accuracy

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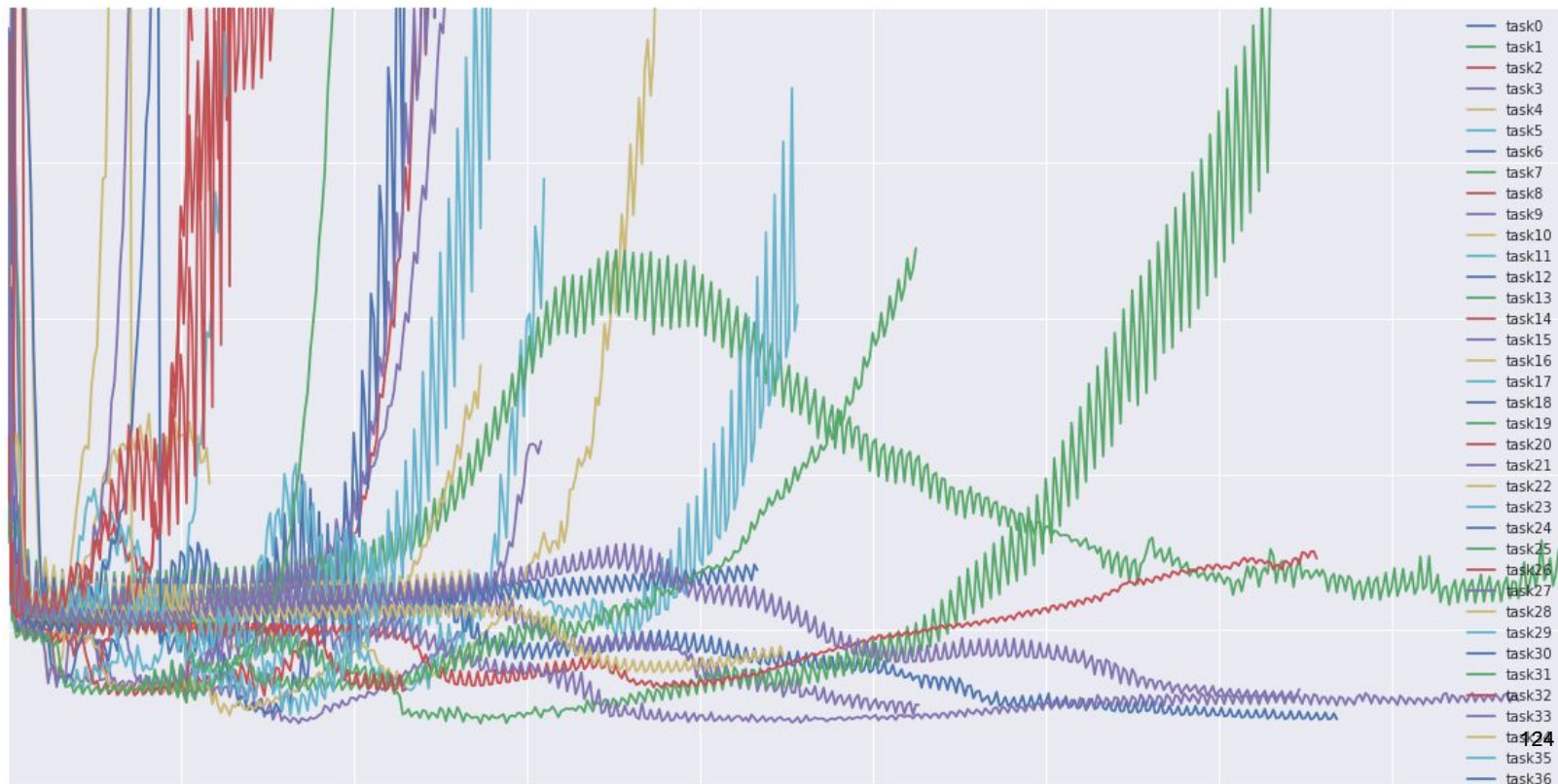average to see trends better

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

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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
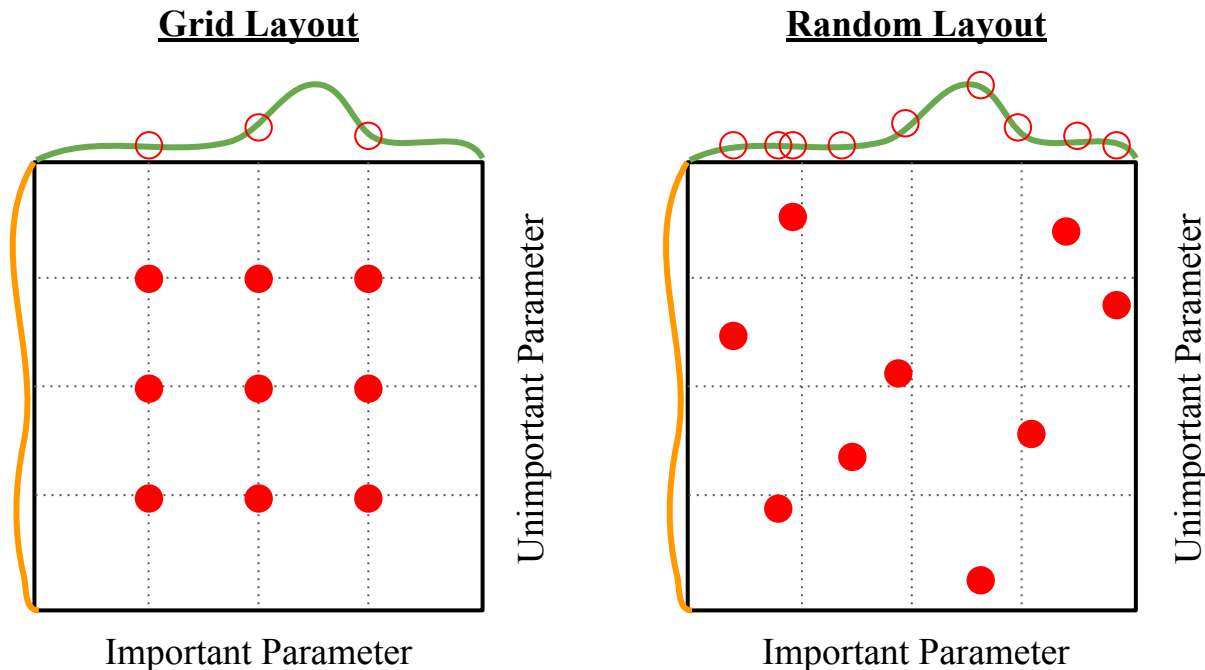**Step 4**: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at loss and accuracy curves
Step 7: GOTO step 5

Random Search vs. Grid Search

Grid Layout

Random Layout

Unimportant Parameter

Important Parameter

Unimportant Parameter

Important Parameter

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!)