中山大學
SUN YAT-SEN UNIVERSITY

Lecture 21: Training Neural Networks

Pattern Recognition and Computer Vision

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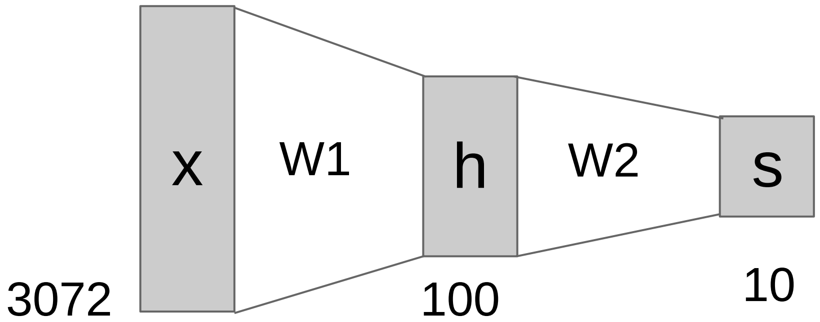
扫码签到

Where we are now...

- **Neural Networks**

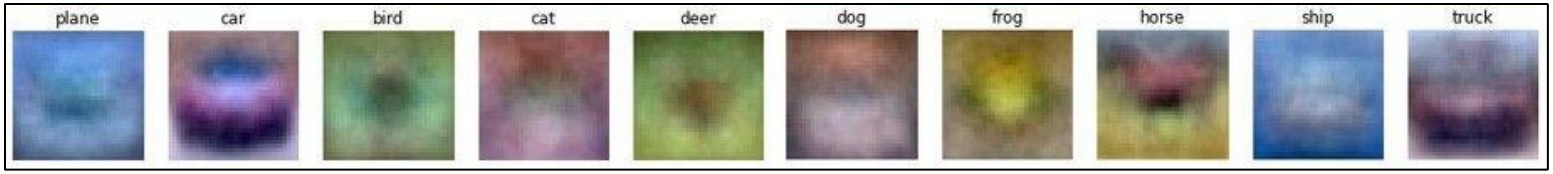
Linear score function:

2-layer Neural Network



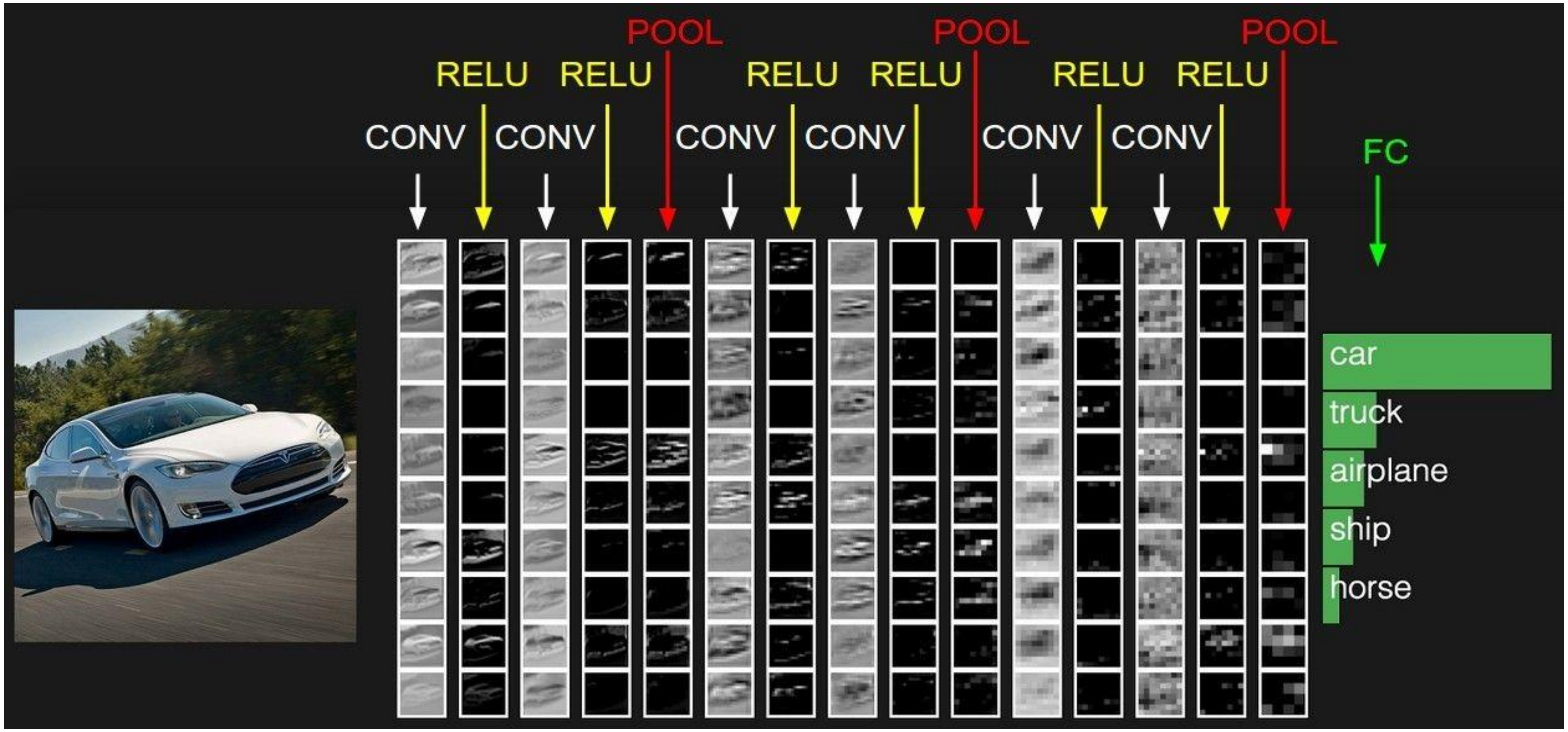
$$f = Wx$$

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



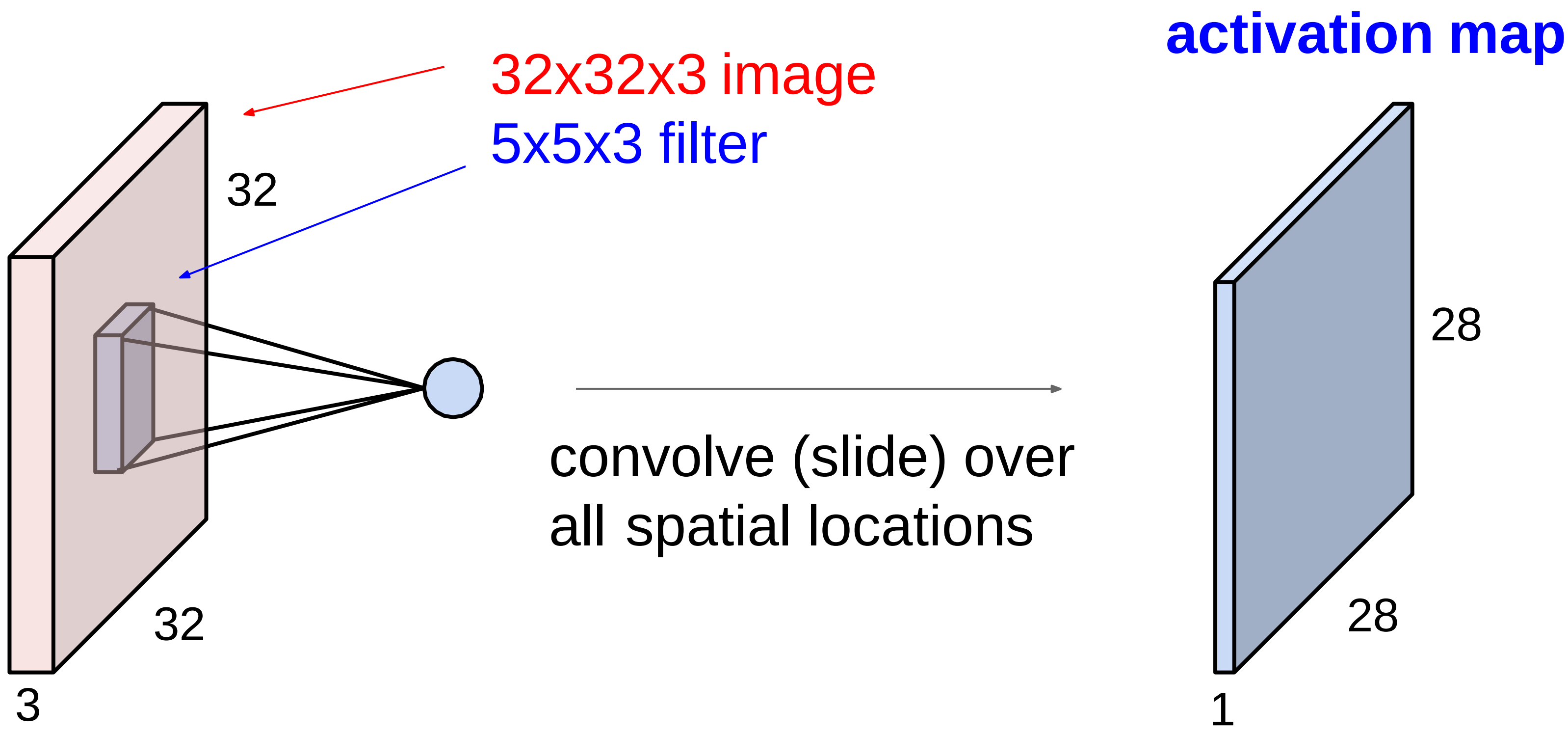
Where we are now...

- **Convolutional Neural Networks**



Where we are now...

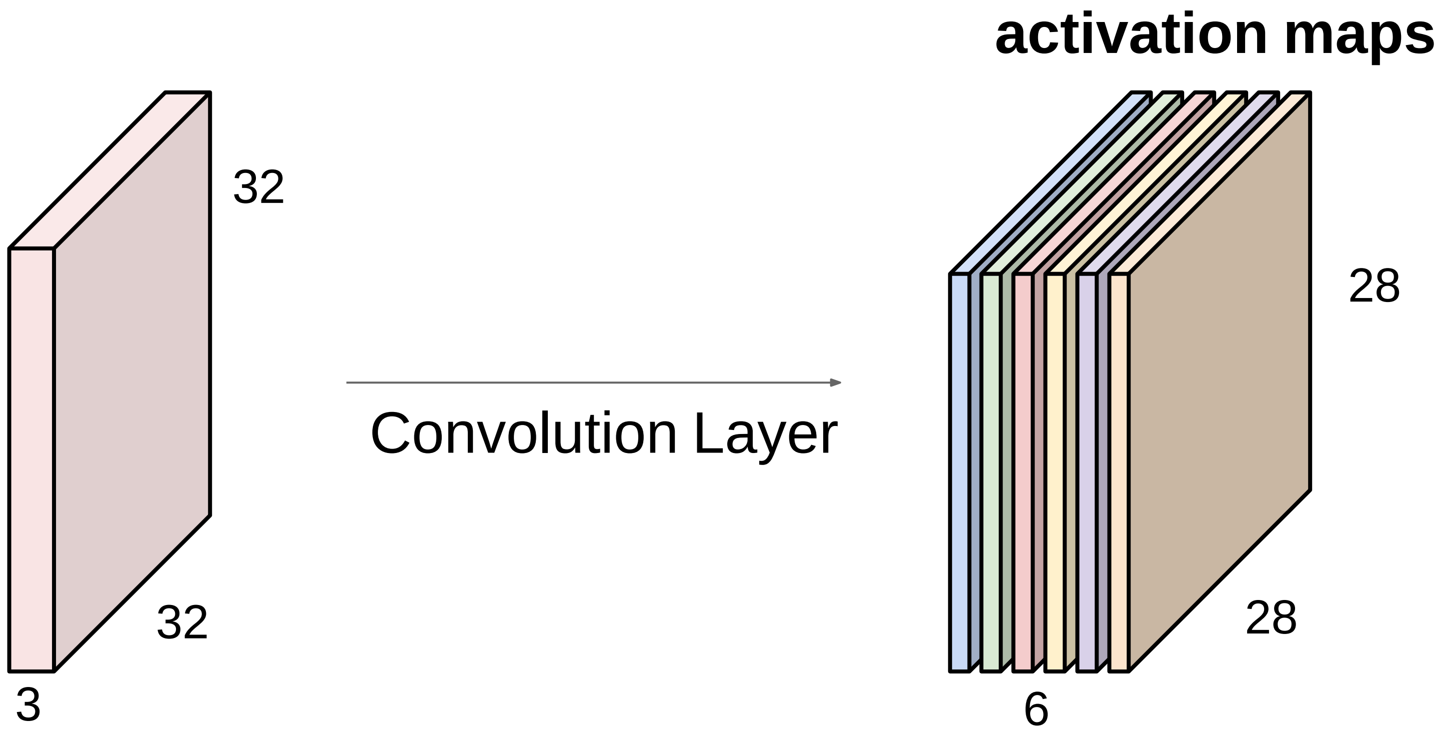
- **Convolutional Layer**



Where we are now...

- **Convolutional Layer**

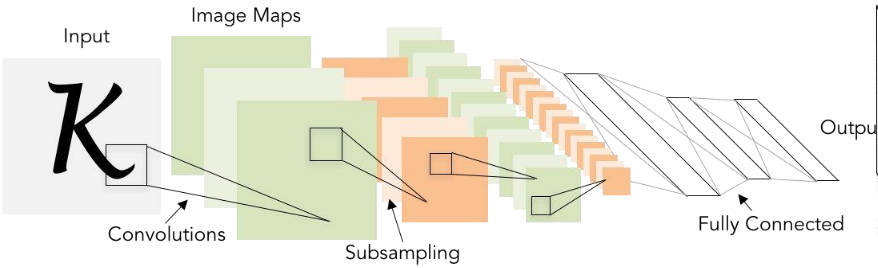
For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:

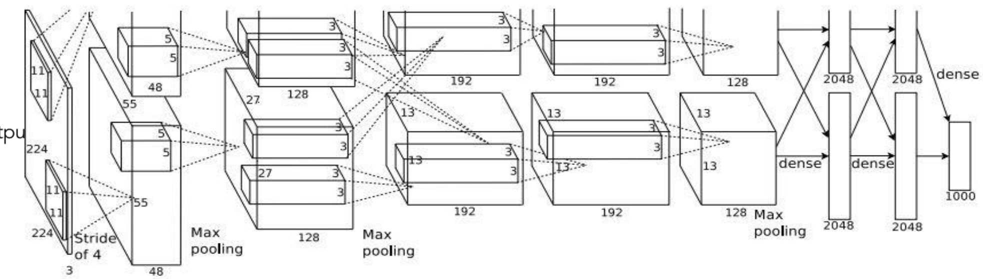


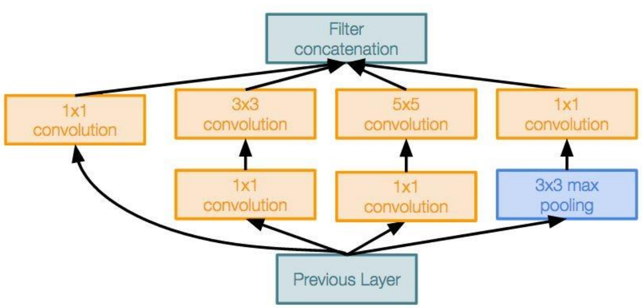
We stack these up to get a "new image" of size 28x28x6!

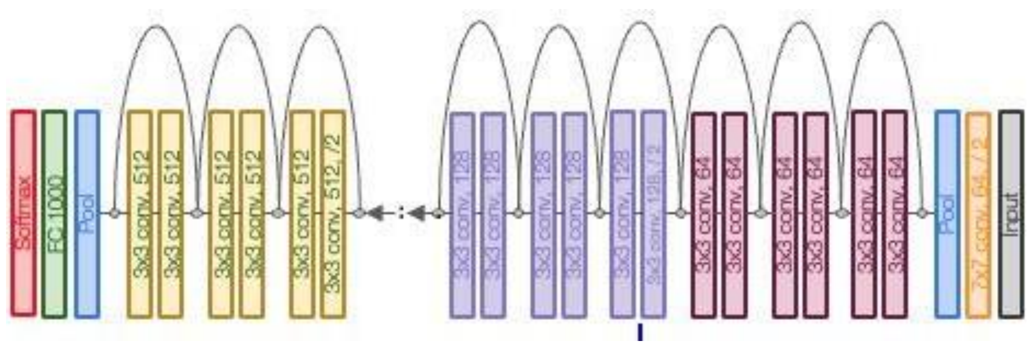
Where we are now...

- **CNN Architectures**



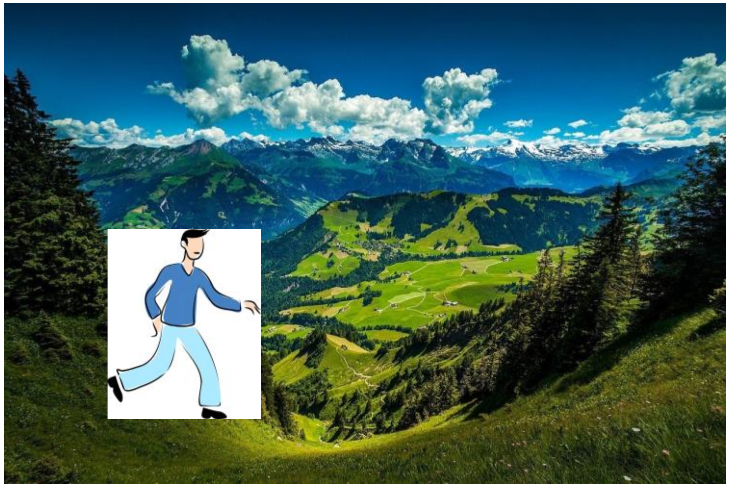






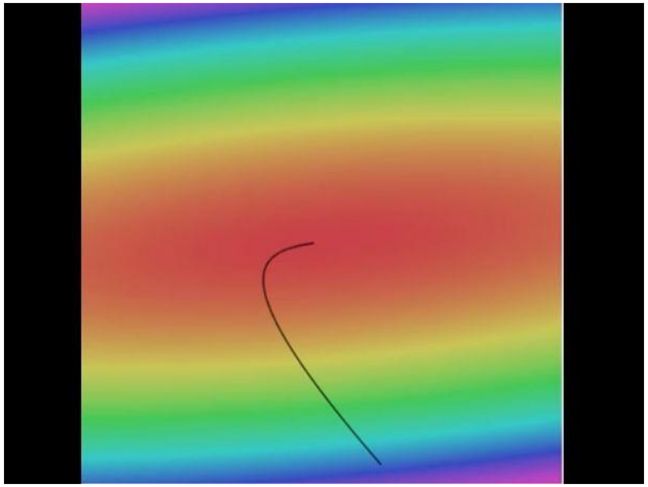
Where we are now...

- **Learning network parameters through optimization**



Landscape image is CC0 1.0 public domain

Walking man image is CC0 1.0 public domain



```
# 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

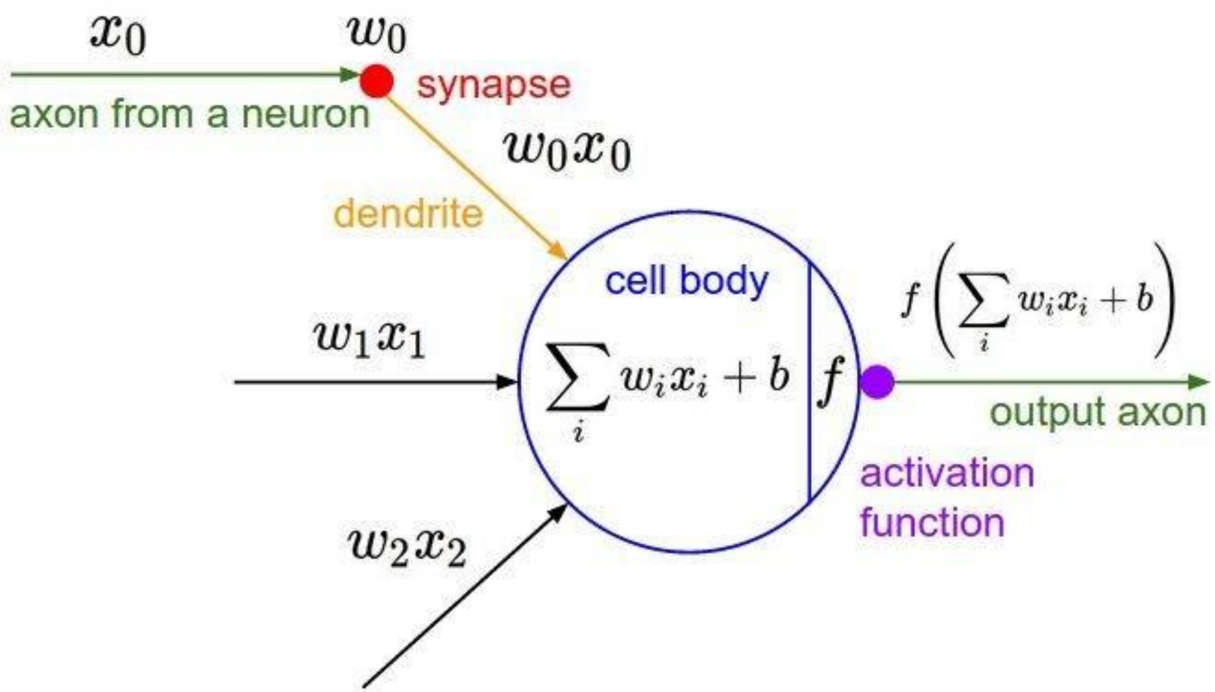
1. **One time set up**: activation functions, preprocessing, weight initialization, regularization, gradient checking

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

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

Activation Functions

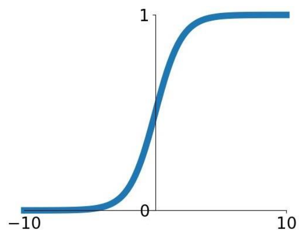
Activation Functions



Activation Functions

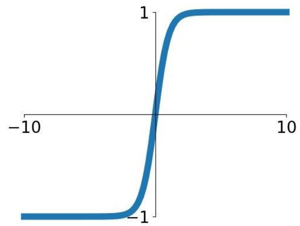
Sigmoid

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



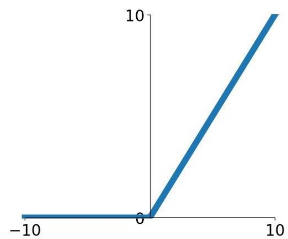
tanh

$\tanh(x)$



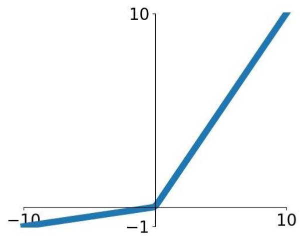
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

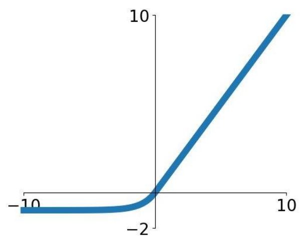


Maxout

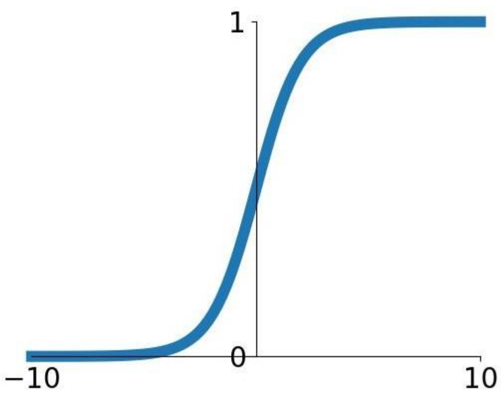
$\max(w_1^T x + b_1, w_2^T x + b_2)$

ELU

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



Activation Functions

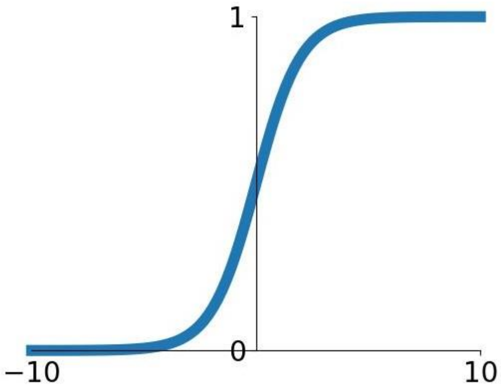


Sigmoid

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

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

Activation Functions



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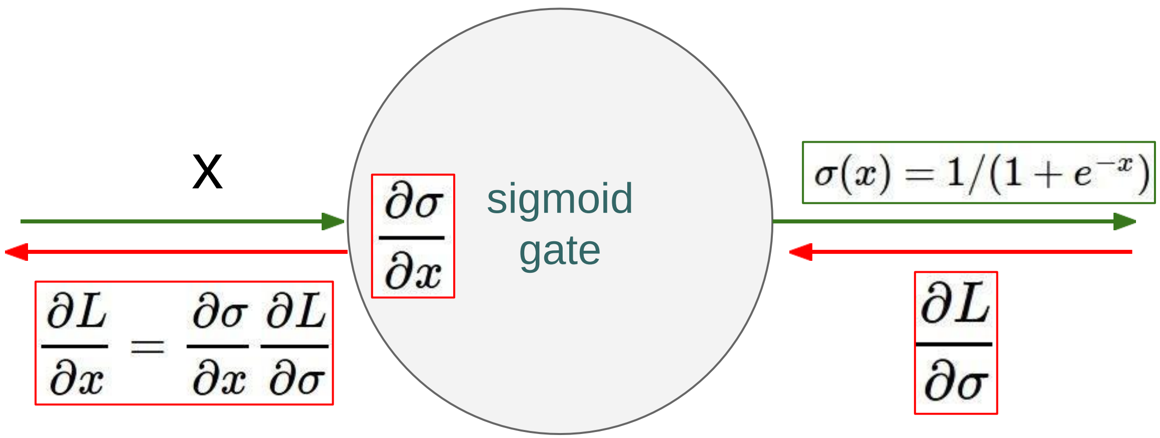
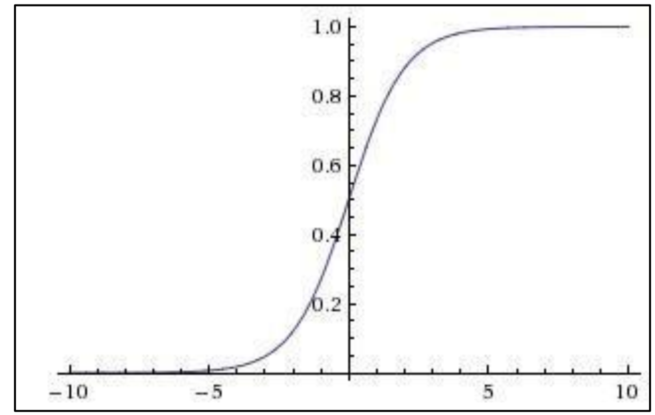
  1. Saturated neurons “kill” the gradients

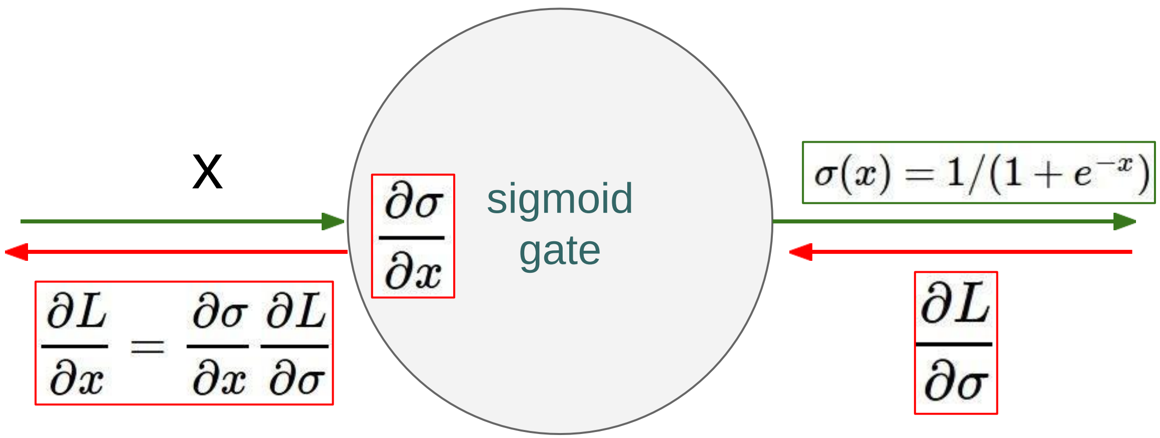
Activation Functions

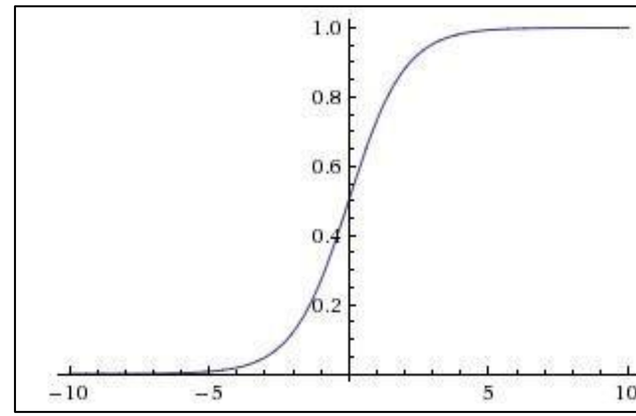




$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

Activation Functions

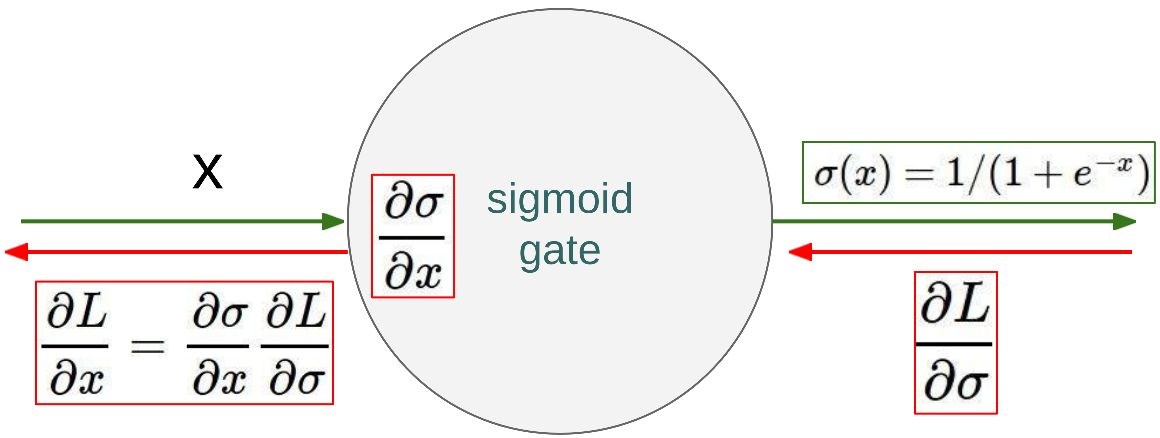


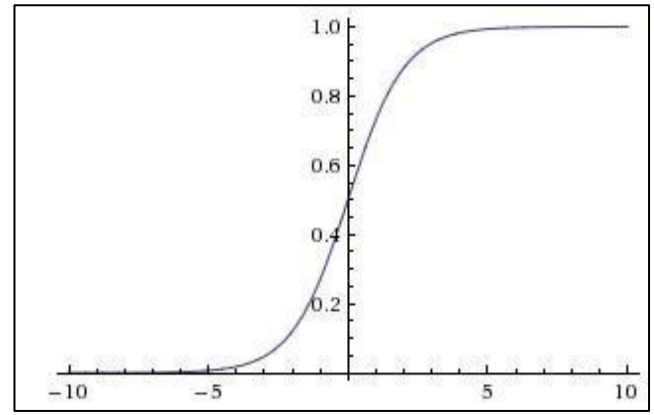


$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1-\sigma(x))$$

What happens when x = -10?

Activation Functions





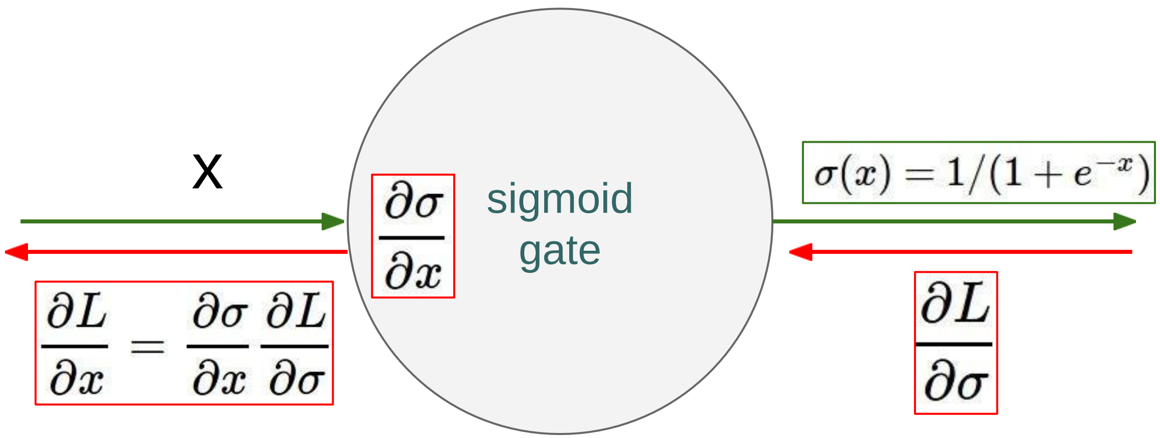
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

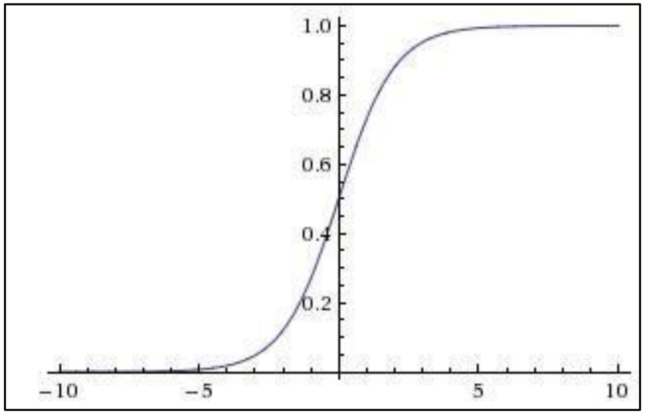
What happens when x = -10?

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

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

Activation Functions





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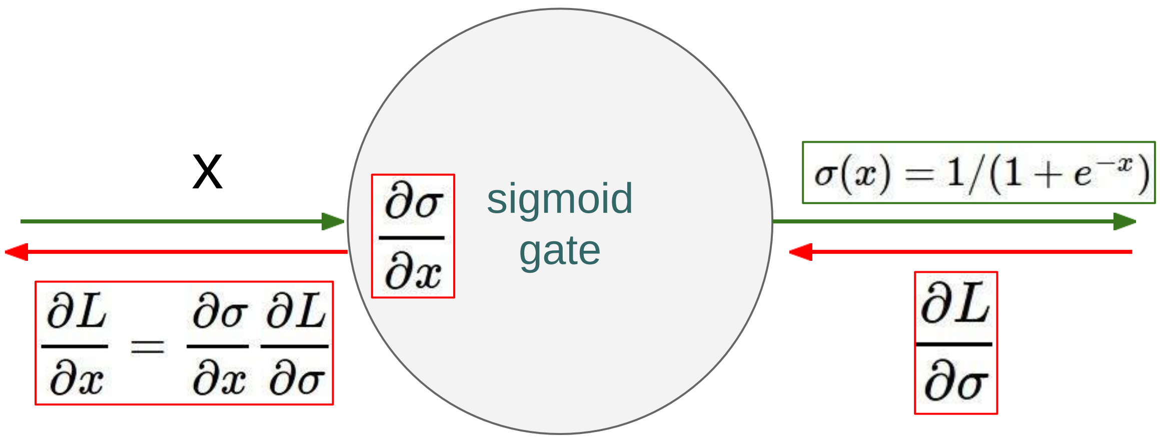
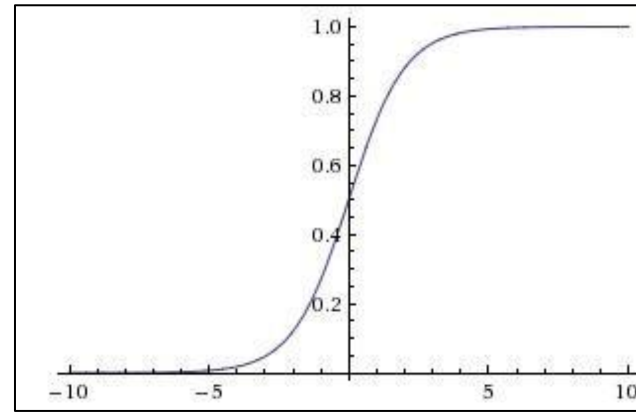
Activation Functions





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

What happens when x = -10?

What happens when x = 0?

What happens when x = 10?

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

Activation Functions

x

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

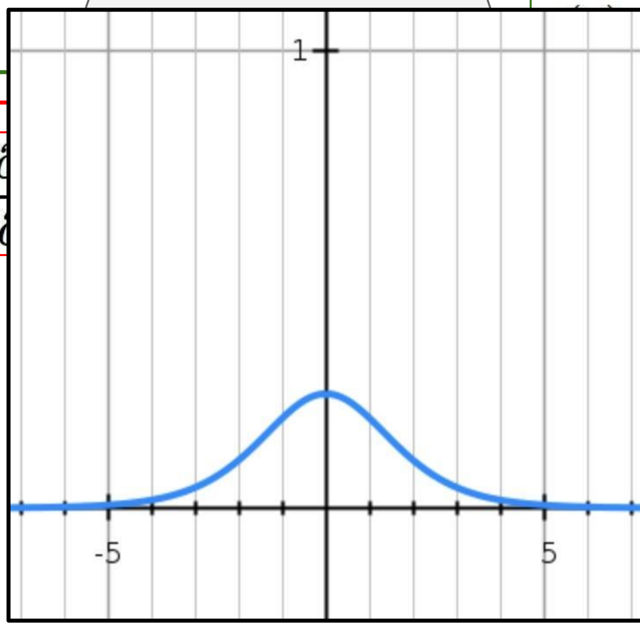
$\frac{\partial L}{\partial x} = \frac{\partial \sigma}{\partial x}$

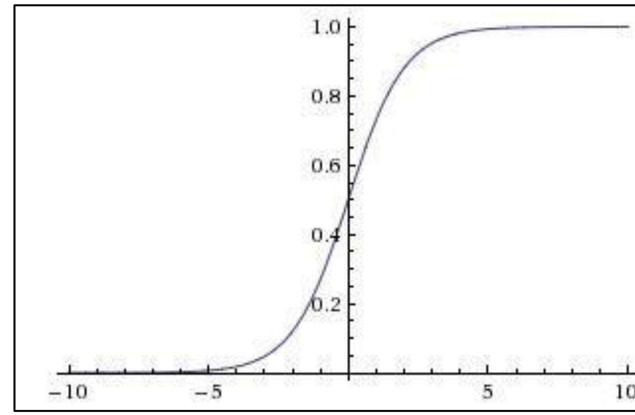
$\frac{\partial L}{\partial \sigma}$

What

What

What





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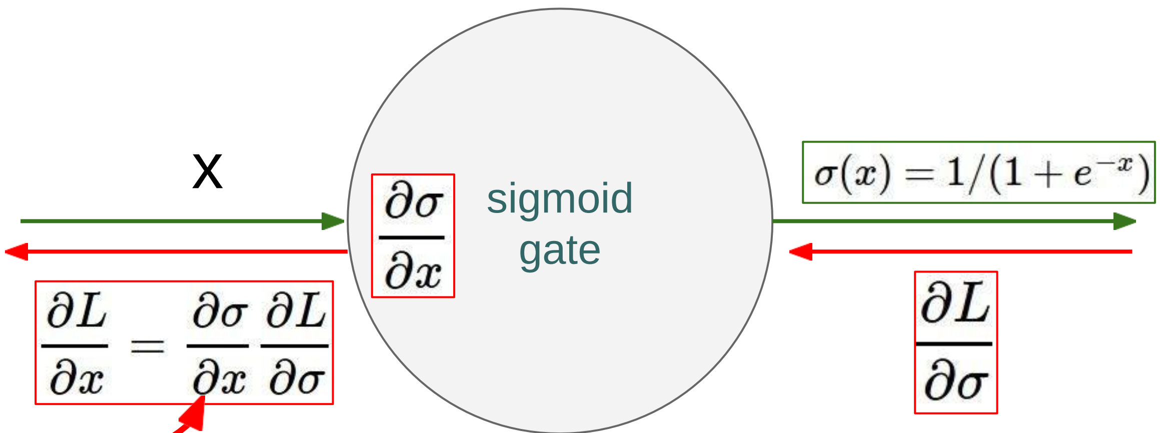
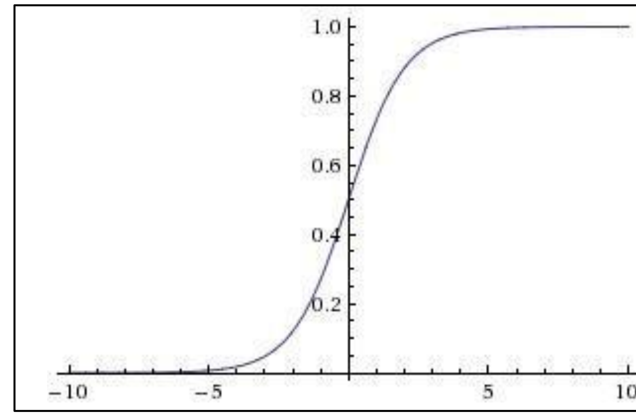
Activation Functions



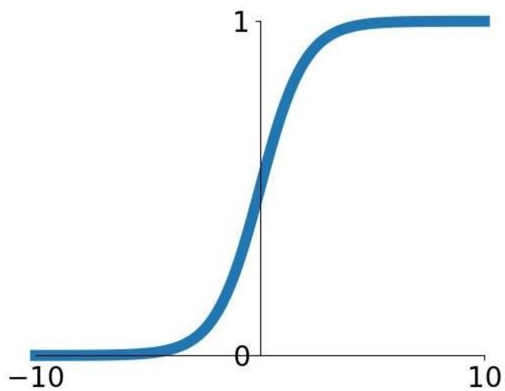


$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x))$$

Why is this a problem?

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

Activation Functions



Sigmoid

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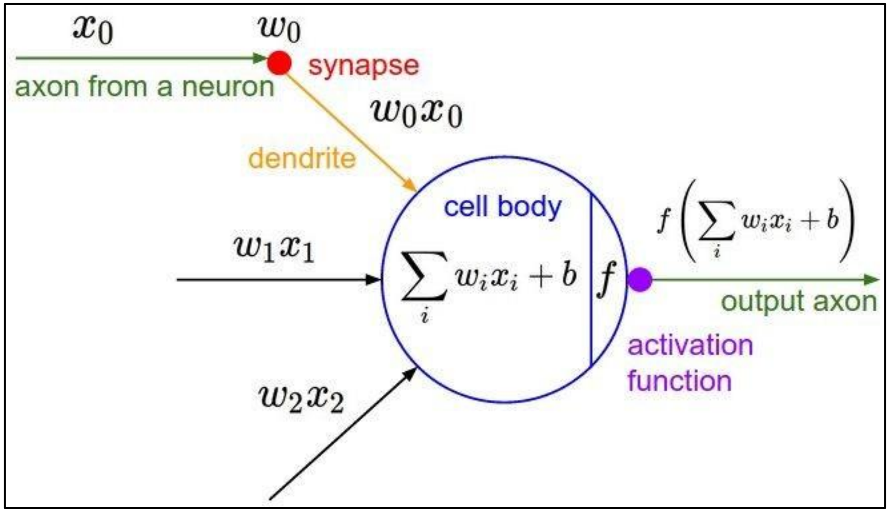
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron
- 3 problems:
  1. Saturated neurons “kill” the gradients
  2. Sigmoid outputs are not zero-centered

Activation Functions

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**?



Activation Functions

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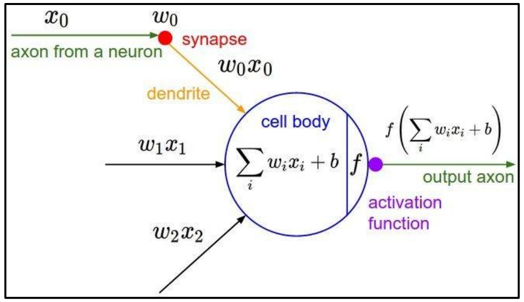

What can we say about the gradients on **w**?

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

Activation Functions

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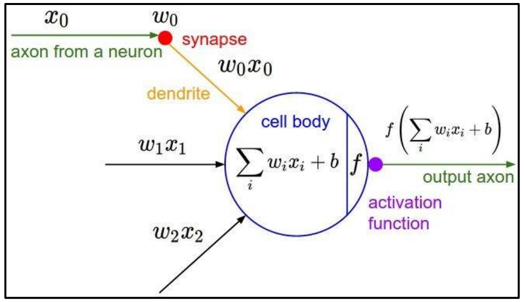

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We know that local gradient of sigmoid is always positive

Activation Functions

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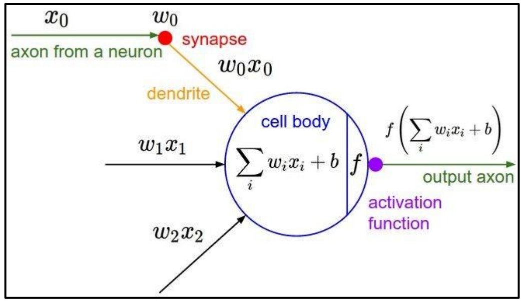

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$$\frac{\partial L}{\partial w} = \boxed{\sigma(\textstyle\sum_i w_i x_i + b)(1 - \sigma(\textstyle\sum_i w_i x_i + b))}\boxed{x} \times upstream\_gradient$$

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We are assuming x is always positive

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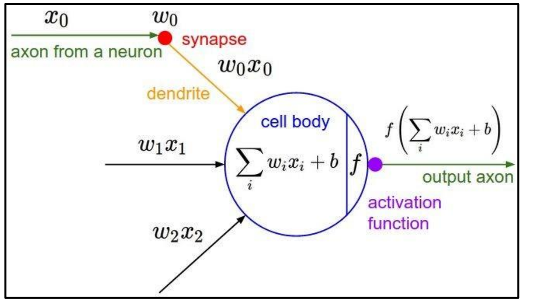

What can we say about the gradients on **w**?

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

We know that local gradient of sigmoid is always positive

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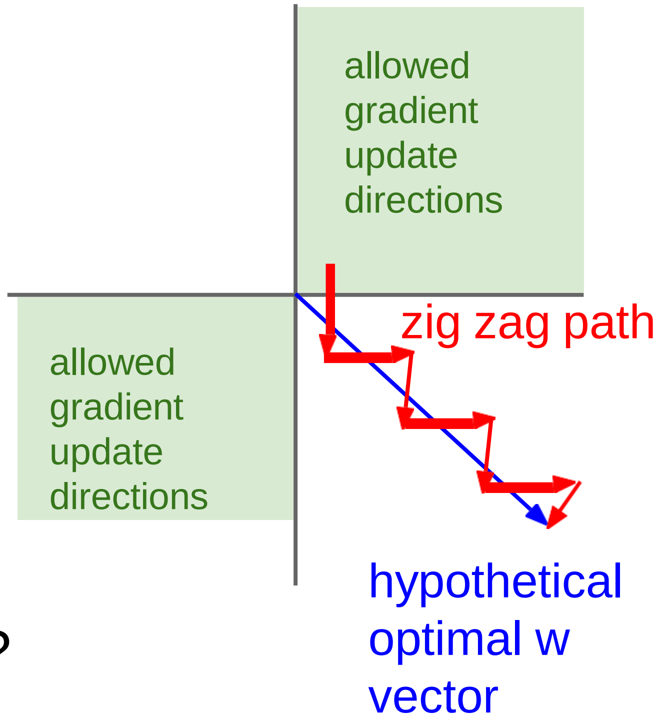
So!! Sign of gradient **for all w_i** is the same as the sign of upstream scalar gradient!

Activation Functions

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

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



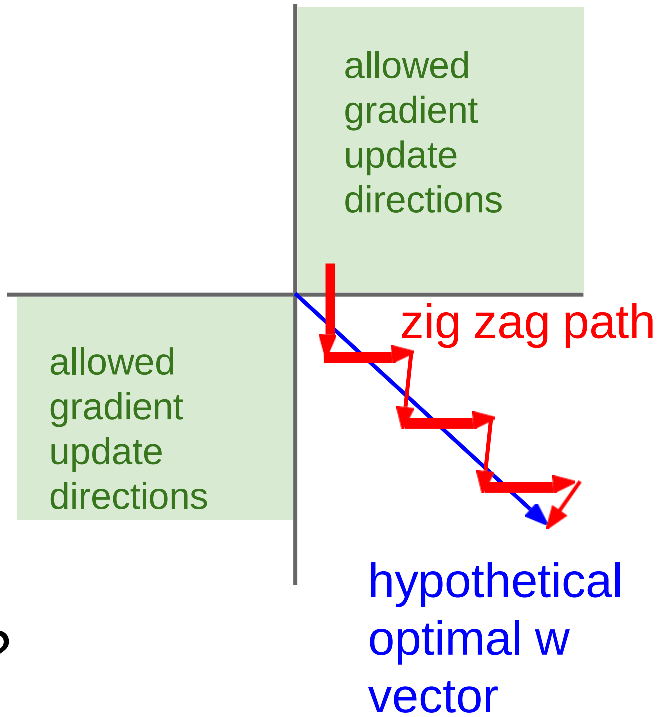
What can we say about the gradients on **w**?

Always all positive or all negative :(

Activation Functions

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

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

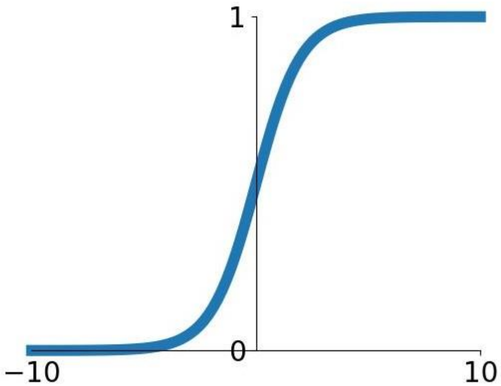


What can we say about the gradients on **w**?

Always all positive or all negative :(

(For a single element! Minibatches help)

Activation Functions



Sigmoid

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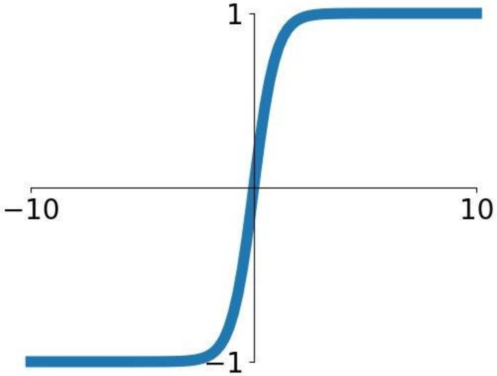
- 3 problems:
  1. Saturated neurons “kill” the gradients
  2. Sigmoid outputs are not zero-centered
  3. exp() is a bit compute expensive

Activation Functions

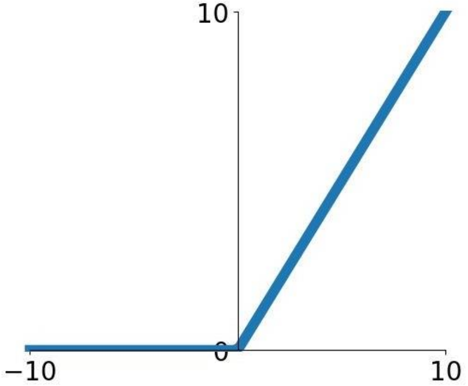


tanh(x)

[LeCun et al., 1991]

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

Activation Functions



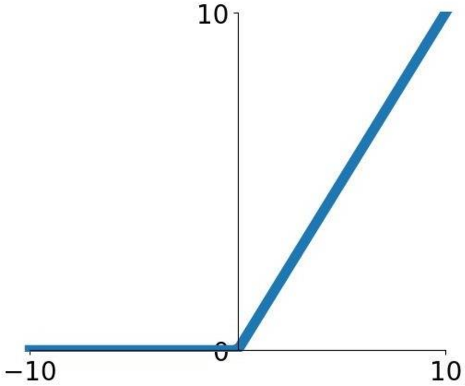
ReLU
(Rectified Linear Unit)

[Krizhevsky et al., 2012]

- 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)

Activation Functions



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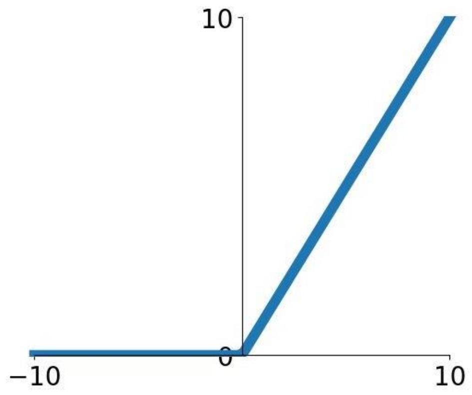
Activation Functions



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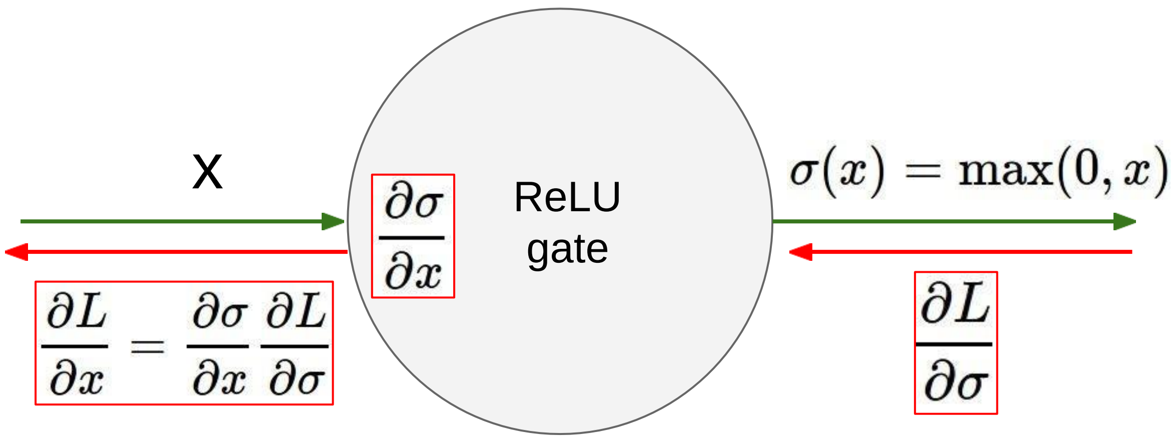
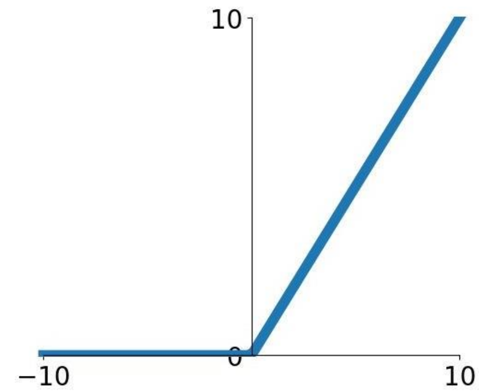
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?

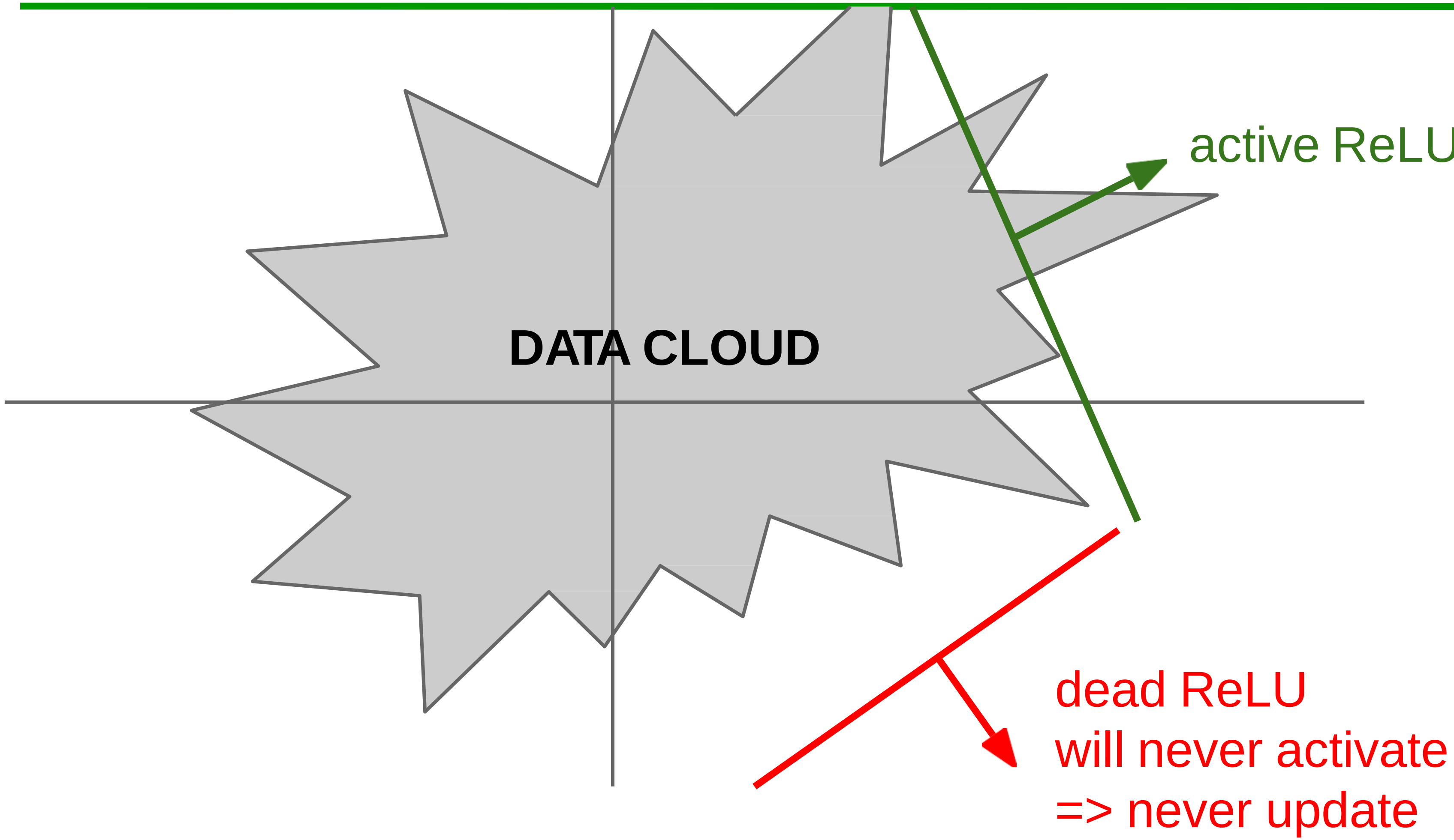
Activation Functions



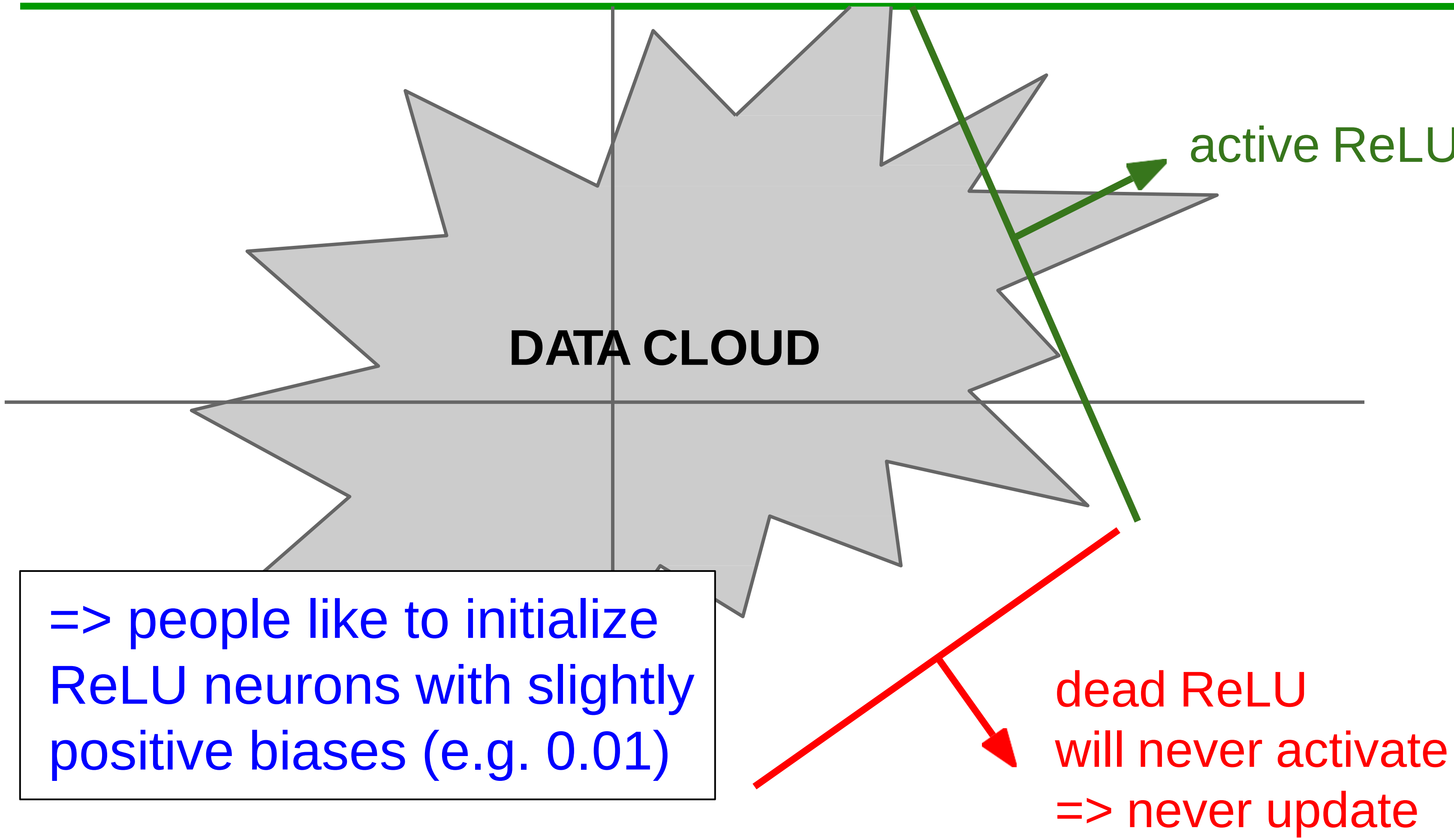


What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

Activation Functions

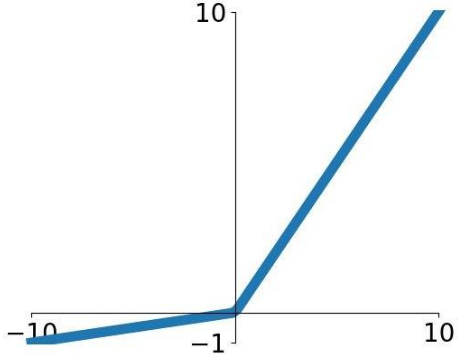


Activation Functions



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

Activation Functions



Leaky ReLU

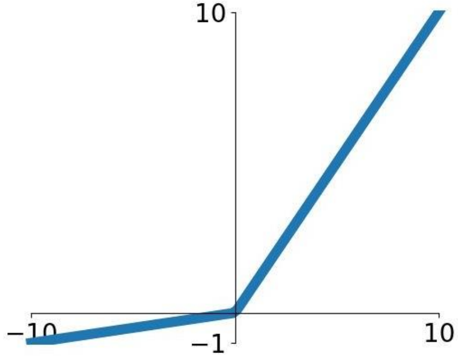
$$f(x) = \max(0.01x, x)$$

[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".**

Activation Functions



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

Leaky ReLU

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

[Mass et al., 2013]

[He et al., 2015]

Parametric Rectifier (PReLU)

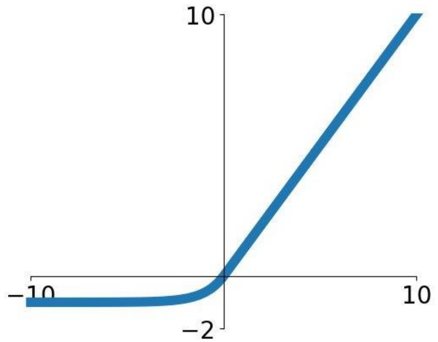
$$f(x) = \max(\alpha x, x)$$

backprop into α (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

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

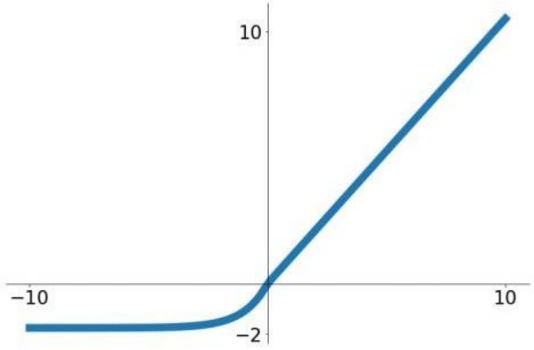
(Alpha default = 1)

- 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

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

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

Activation Functions

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 :(

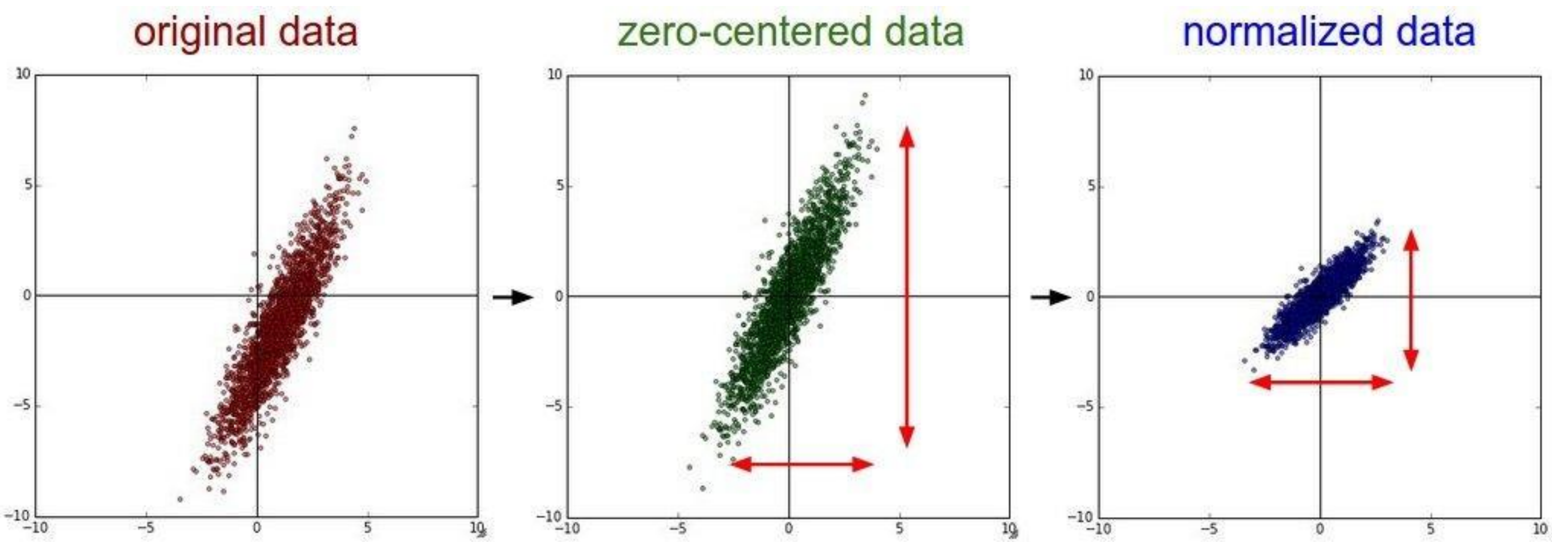
Activation Functions

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)
```

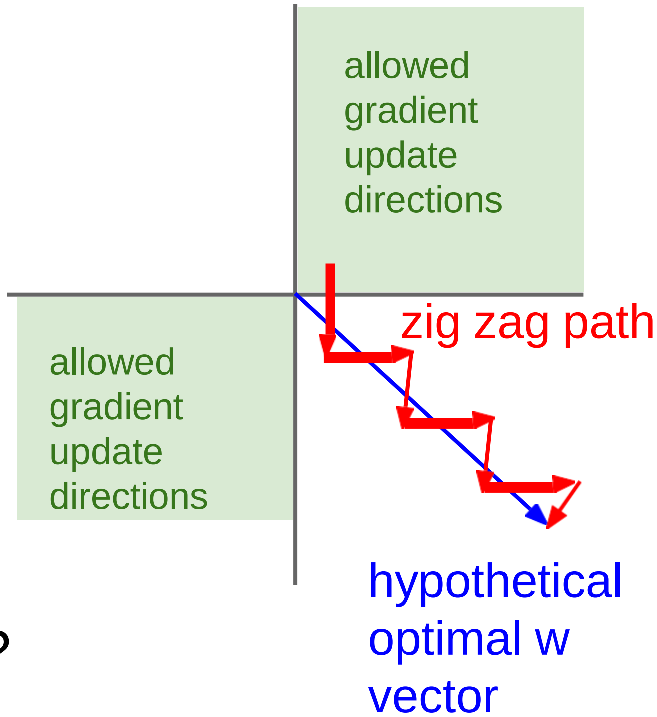
```
X /= np.std(X, axis = 0)
```

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

Activation Functions

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

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

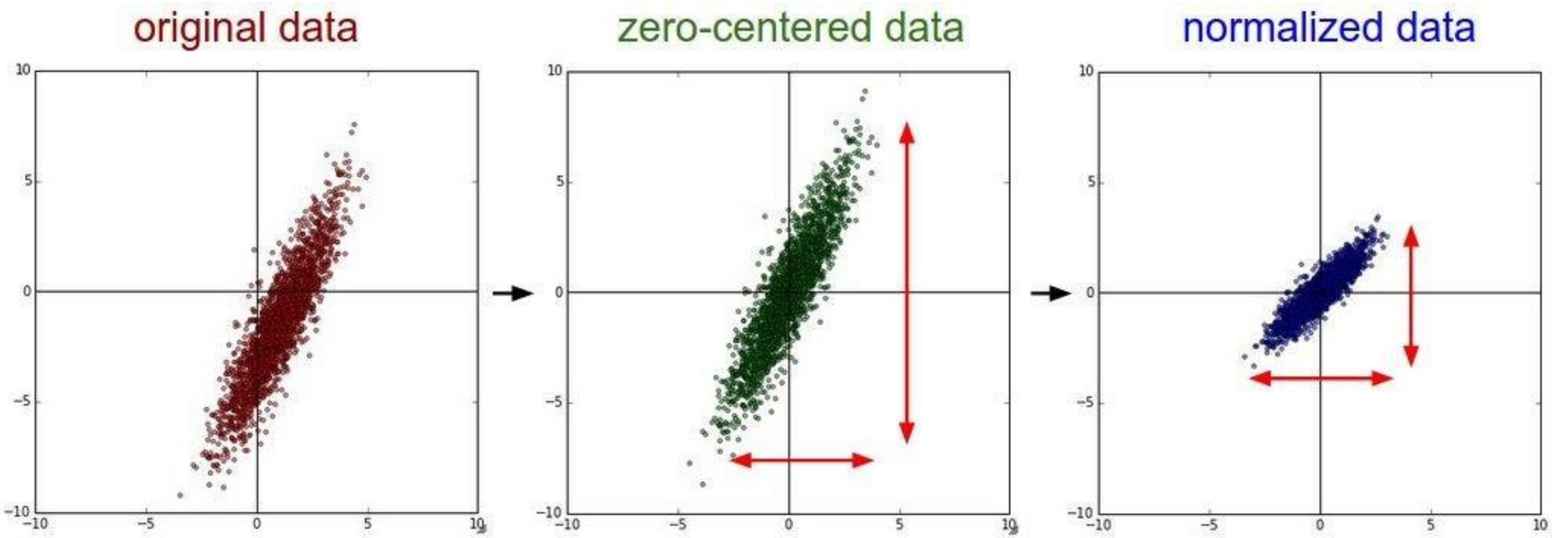


What can we say about the gradients on **w**?

Always all positive or all negative :(

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

Data Preprocessing



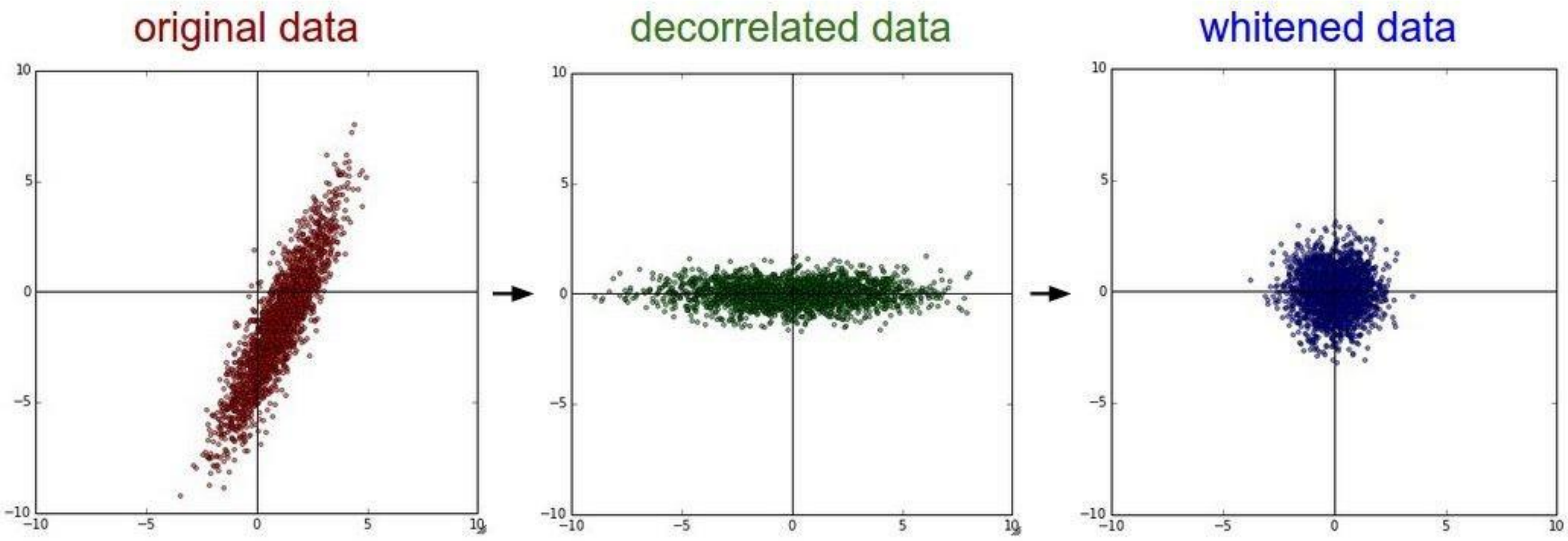

```
X -= np.mean(X, axis = 0)
```

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

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

Data Preprocessing

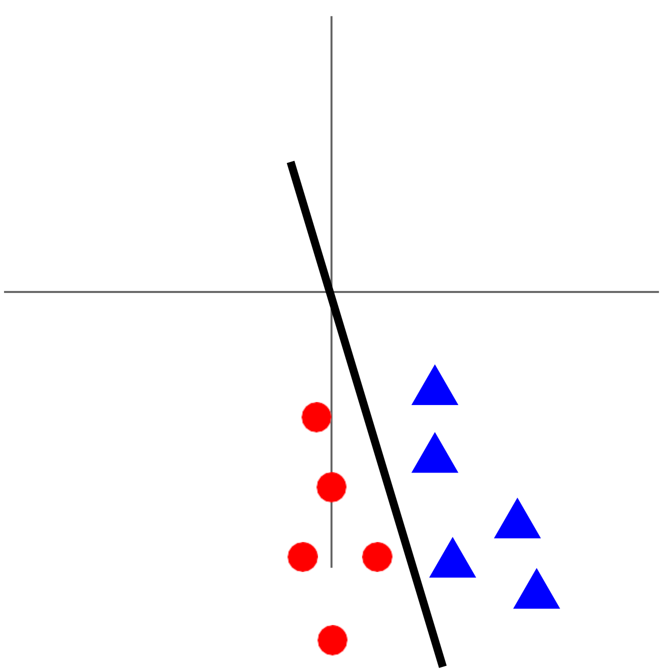
In practice, you may also see **PCA** and **Whitening** of the data

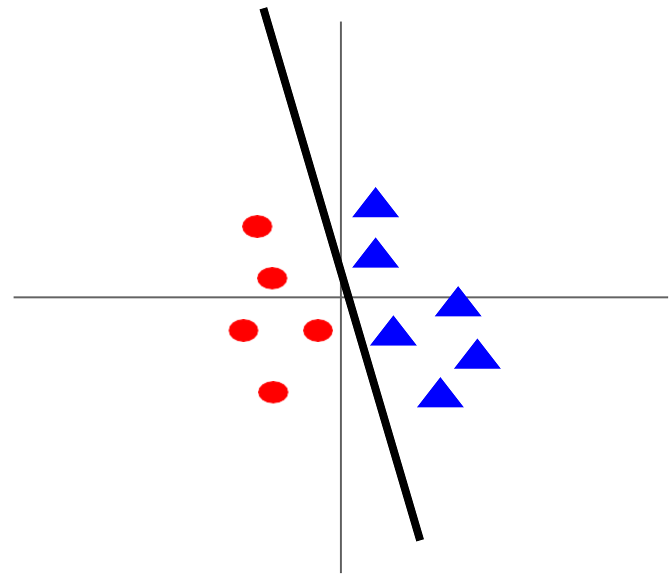


(data has diagonal covariance matrix)

(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

Data Preprocessing

TLDR: In practice for Images: center only

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

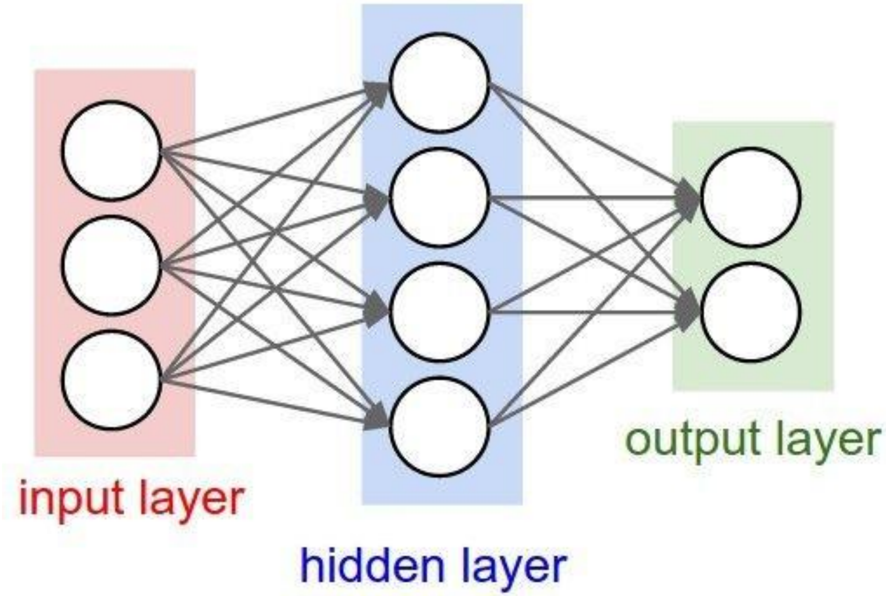
- Subtract the mean image (e.g. AlexNet)
- (mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet)
- (mean along each channel = 3 numbers)
- Subtract per-channel mean and
  Divide by per-channel std (e.g. ResNet)
  (mean along each channel = 3 numbers)

Not common to do PCA or whitening

Weight Initialization

Weight Initialization

- Q: what happens when W=constant init is used?



Weight Initialization

- First idea: **Small random numbers**

(gaussian with zero mean and 1e-2 standard deviation)

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

Weight Initialization

- 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

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

Weight Initialization: Activation statistics

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
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```
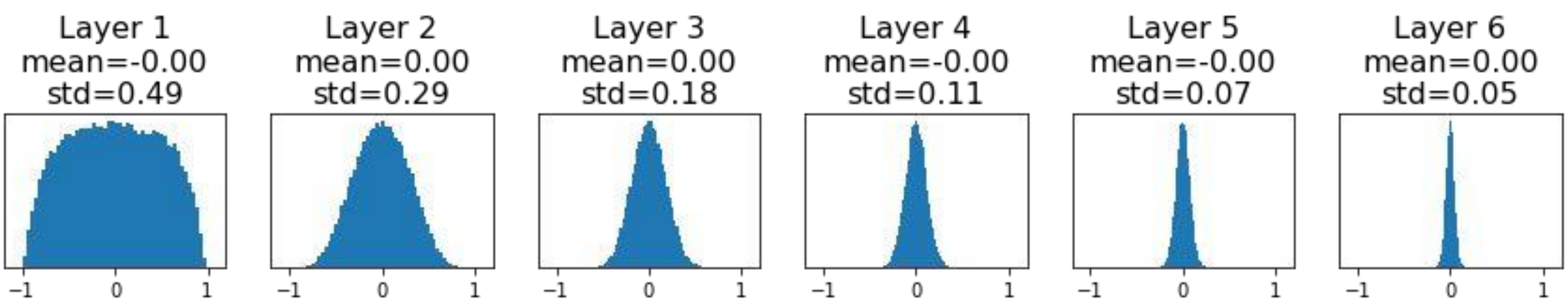

Forward pass for a 6-layer net with hidden size 4096

All activations tend to zero for deeper network layers

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



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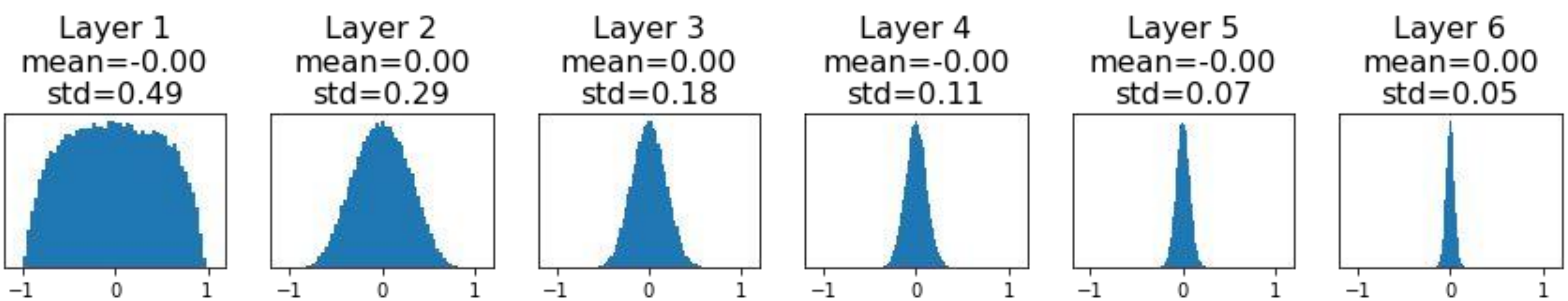
```

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 =(



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```

Increase std of initial weights from 0.01 to 0.05

What will happen to the activations for the last layer?

Weight Initialization

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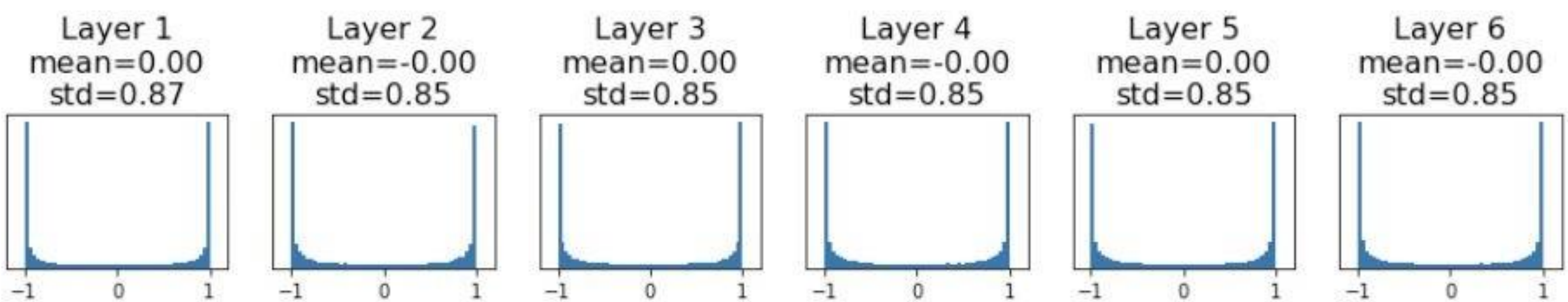
Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?



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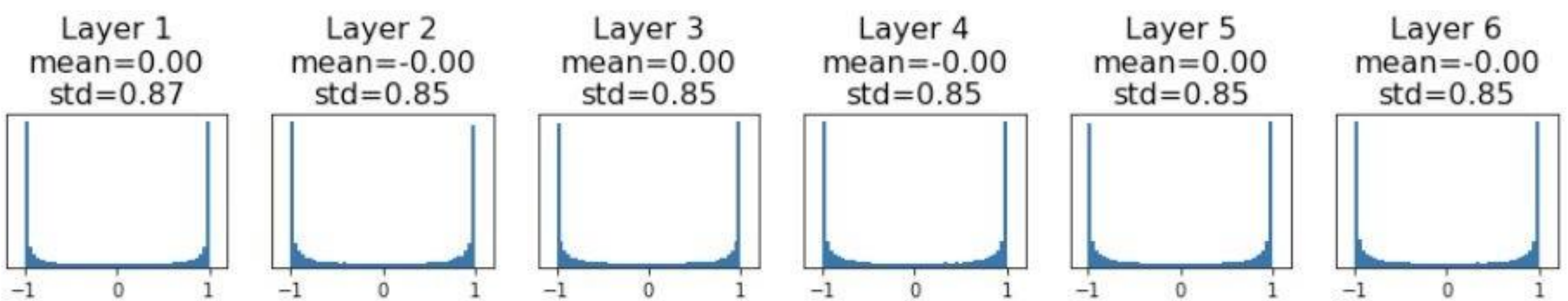
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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 =(



Weight Initialization

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

Weight Initialization: “Xavier” Initialization

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    hs.append(x)
```

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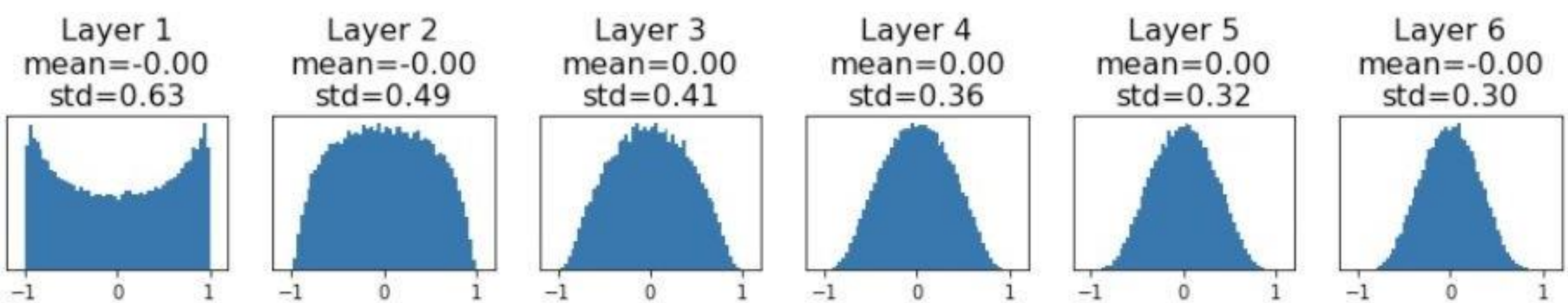
“Just right”: Activations are nicely scaled for all layers!



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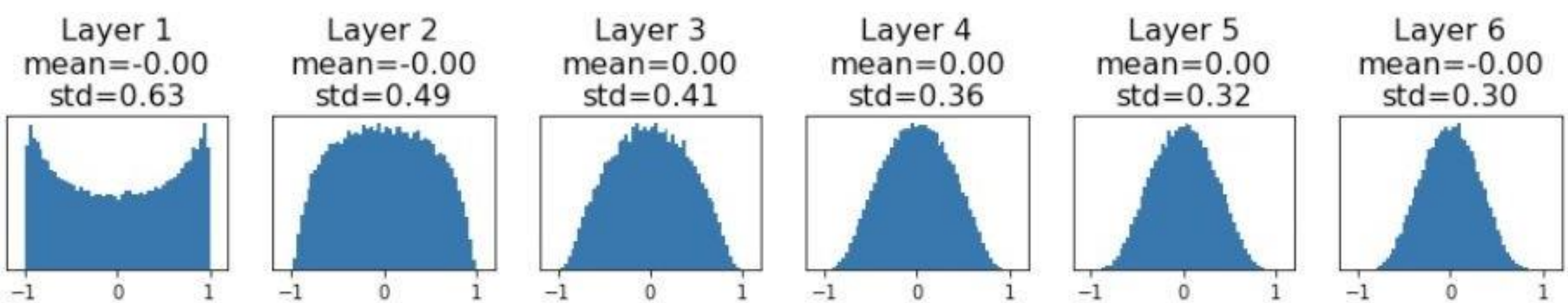

For conv layers, Din is filter_size^2 * input_channels

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For conv layers, Din is filter_size^2 * input_channels

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

Weight Initialization

Weight Initialization: "Xavier" Initialization

```
dims = [4096] * 7
hs = []
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    hs.append(x)
```

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std = 1/sqrt(Din)

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For conv layers, Din is filter_size^2 * input_channels

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

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

Weight Initialization

Weight Initialization: “Xavier” Initialization

```
dims = [4096] * 7
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for Din, Dout in zip(dims[:-1], dims[1:]):
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    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

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

We want: Var(y) = Var(xi)

Weight Initialization

Weight Initialization: “Xavier” Initialization

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
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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: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

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

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

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

Weight Initialization

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

We want: Var(y) = Var(xi)

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$

$= Din\ Var(x_iw_i)$

[Assume all x_i, w_i are iid]

Weight Initialization

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

We want: Var(y) = Var(xi)

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

[Assume all x_i, w_i are zero mean]

Weight Initialization

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

We want: Var(y) = Var(xi)

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

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

Weight Initialization

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

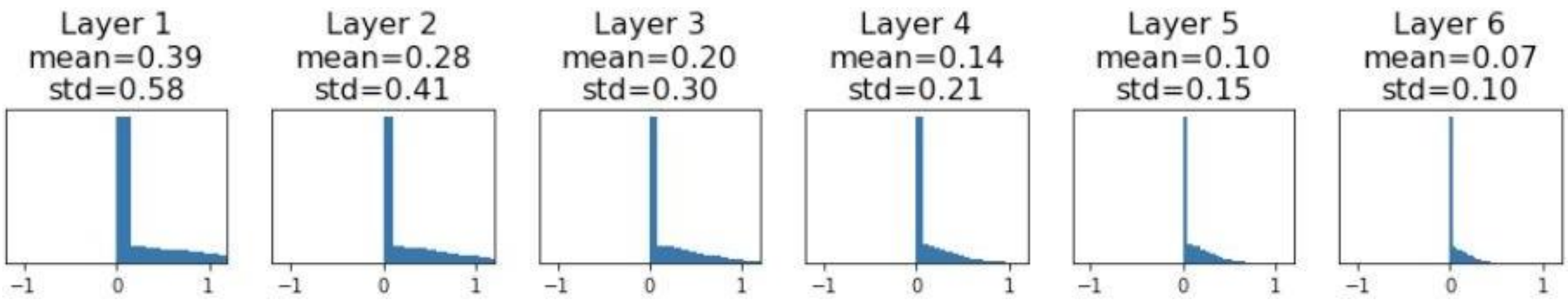
Weight Initialization: What about ReLU?

```
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 =(



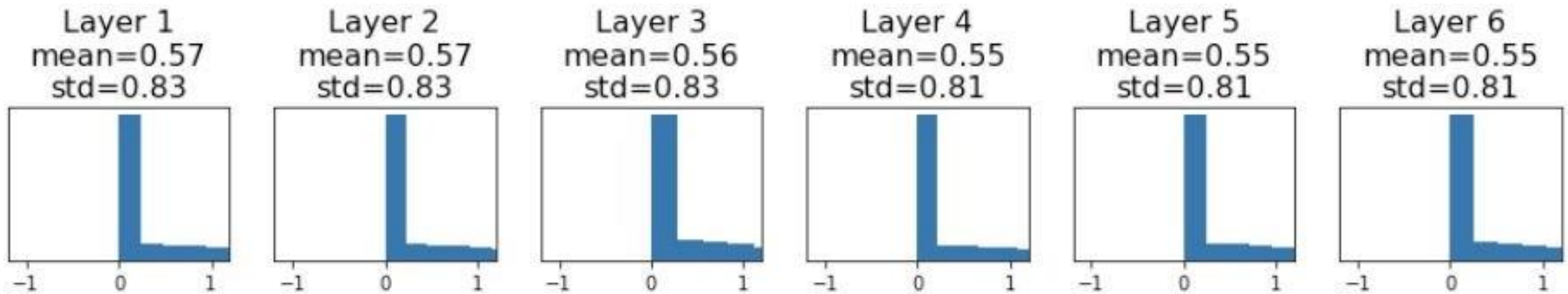
Weight Initialization

Weight Initialization: Kaiming / MSRA Initialization

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

ReLU correction: 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

Weight Initialization

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

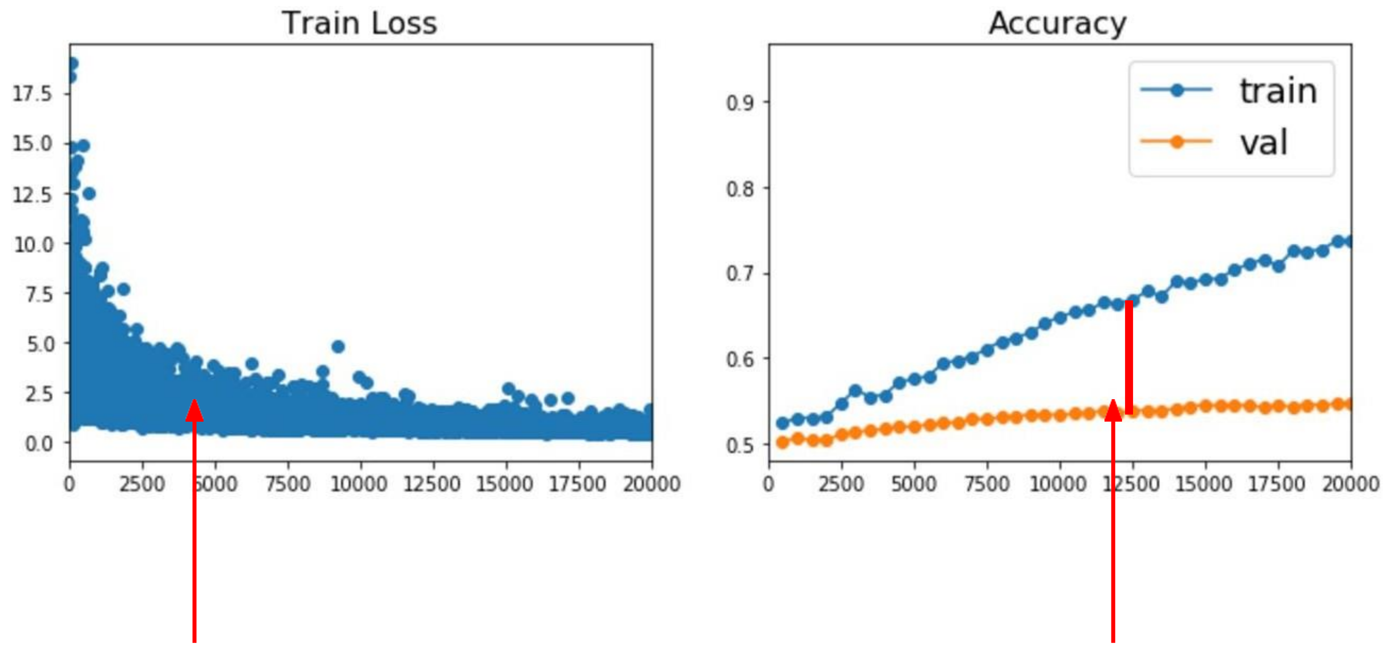
Fixup Initialization: Residual Learning Without Normalization, Zhang et al, 2019

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

Training vs. Testing Error

Training vs. Testing Error

Beyond Training Error

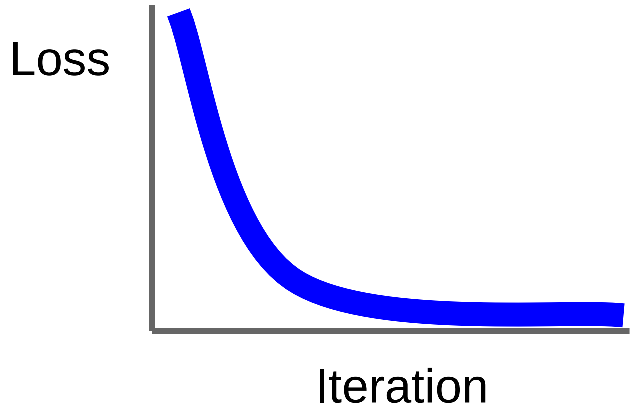


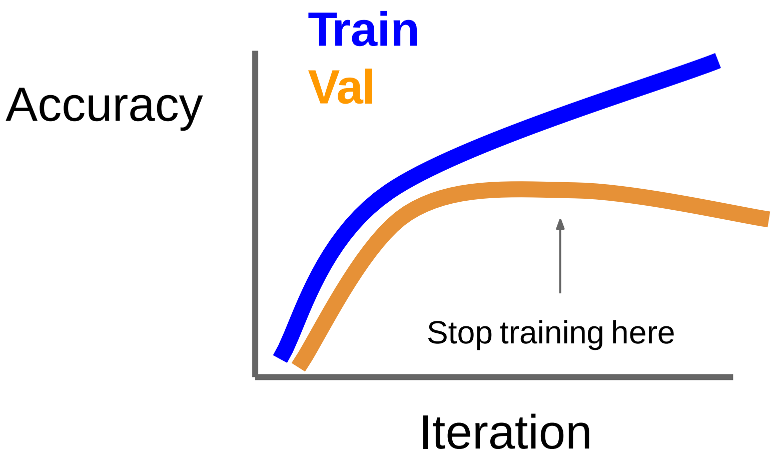
Better optimization algorithms help reduce training loss

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

Training vs. Testing Error

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

Training vs. Testing Error

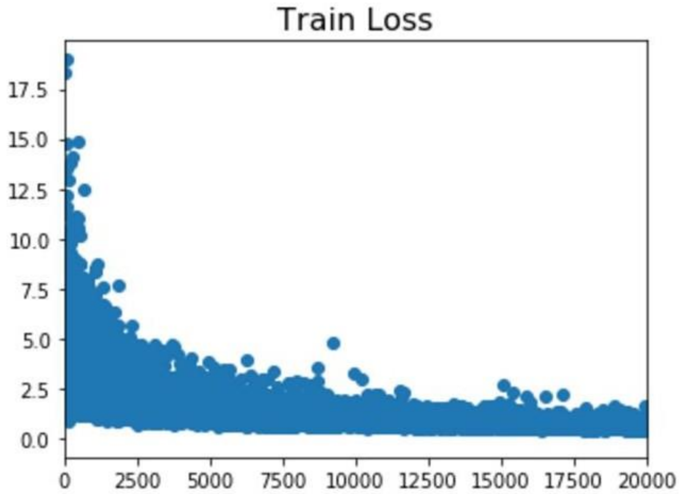
Model Ensembles

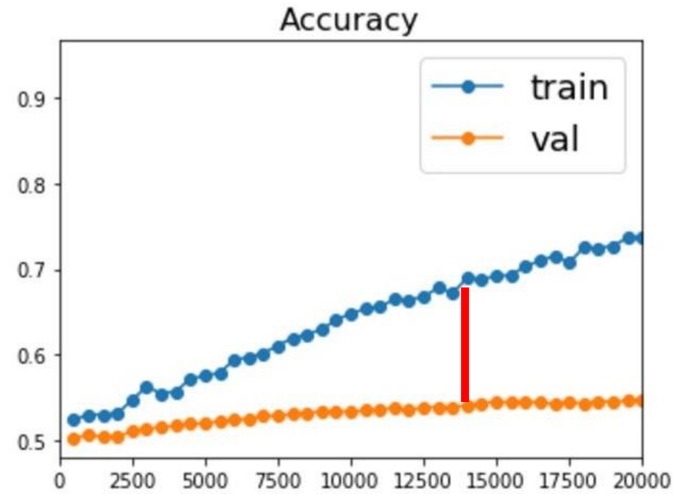
1. Train multiple independent models
2. At test time average their results
   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

Training vs. Testing Error

How to improve single-model performance?





Regularization

Training vs. Testing Error

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)

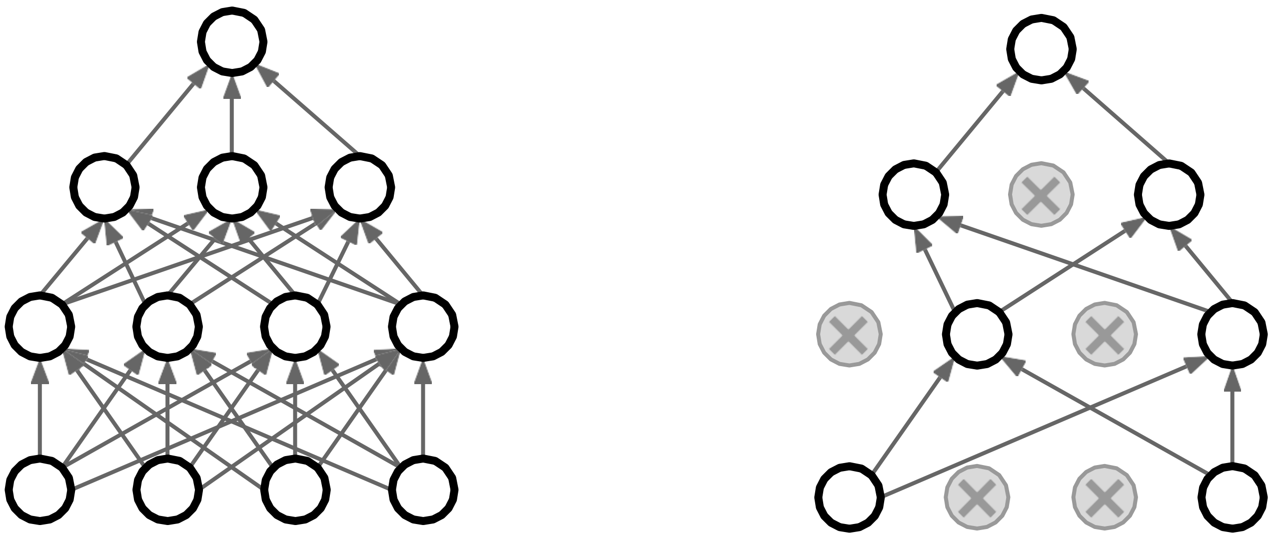
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Training vs. Testing Error

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

Training vs. Testing Error

Regularization: Dropout

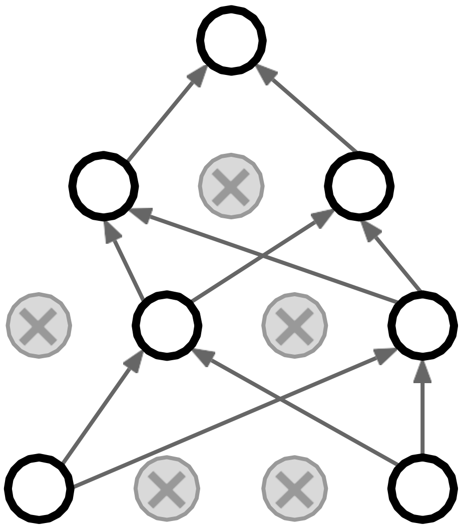
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

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

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

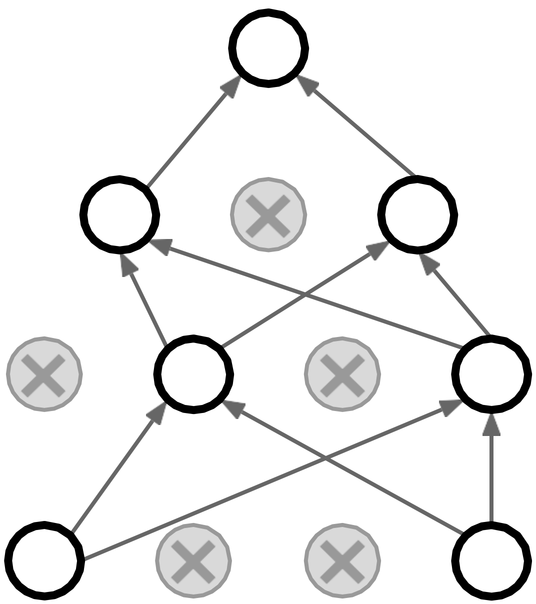
Example forward pass with a 3-layer network using dropout



Training vs. Testing Error

Regularization: Dropout

How can this possibly be a good idea?

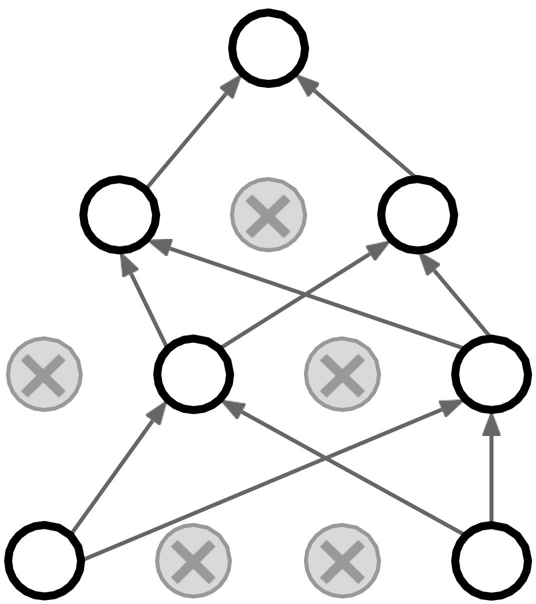


Forces the network to have a redundant representation; Prevents co-adaptation of features

Training vs. Testing Error

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...

Training vs. Testing Error

Dropout: Test time

Dropout makes our output random!

Output (label) Input (image) Random mask

$$\boxed{y} = f_W(\boxed{x}, \boxed{z})$$

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 …

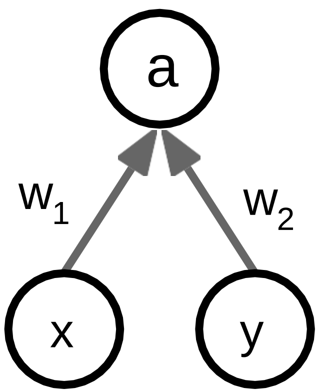
Training vs. Testing Error

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.

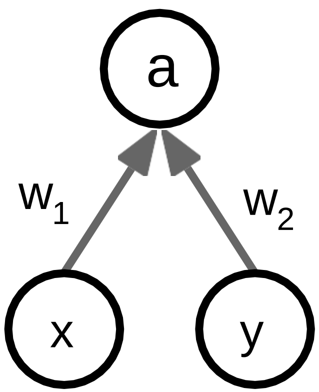


Training vs. Testing Error

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.

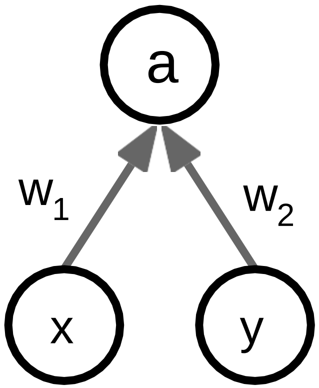
At test time we have: $E\big[a\big] = w_1 x + w_2 y$

Training vs. Testing Error

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

During training we have:

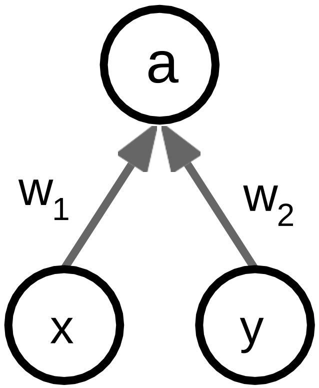
$$\begin{aligned} E\left[a\right] =& \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y) \\ &+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y) \\ =& \frac{1}{2}(w_1 x + w_2 y) \end{aligned}$$

Training vs. Testing Error

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.

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

Training vs. Testing Error

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>

Training vs. Testing Error

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

Training vs. Testing Error

More common: “Inverted dropout”

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

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

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

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

test time is unchanged!

Training vs. Testing Error

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Training vs. Testing Error

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

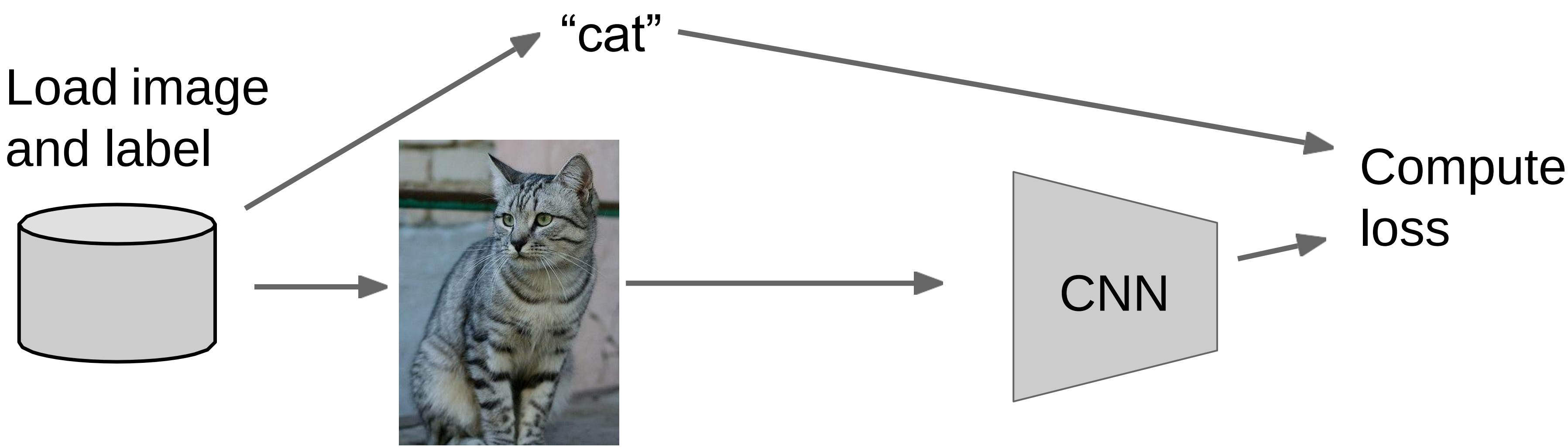
Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

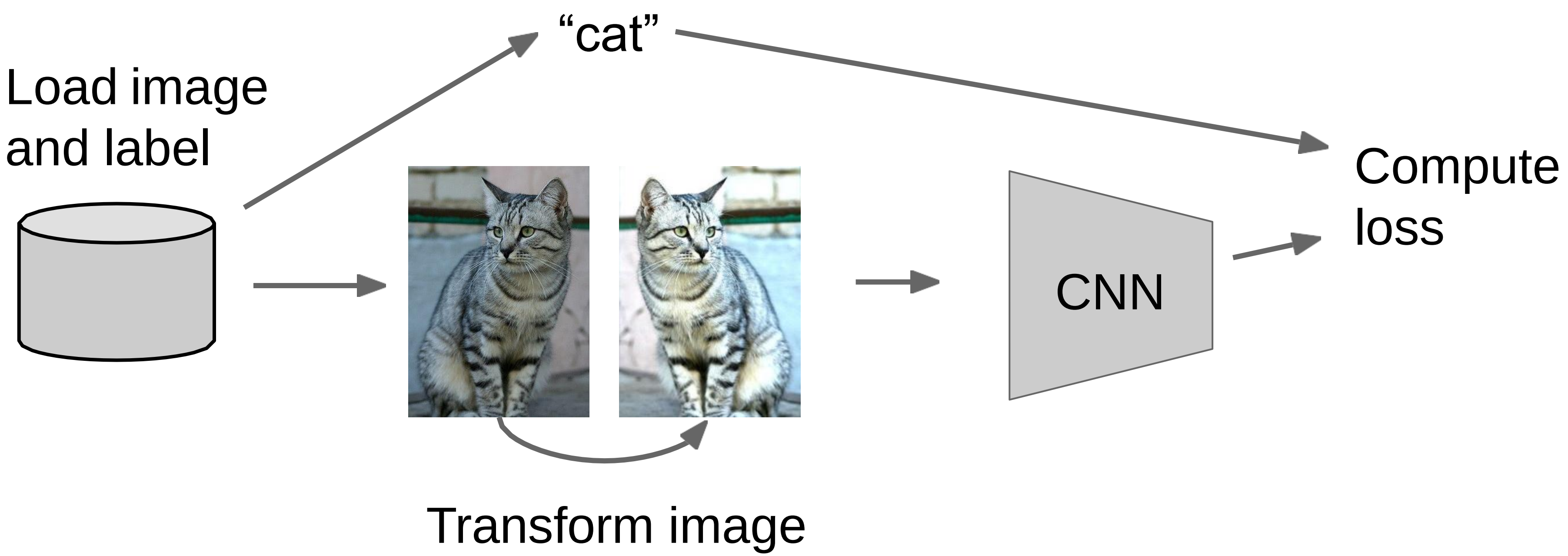
Training vs. Testing Error

Regularization: Data Augmentation



Training vs. Testing Error

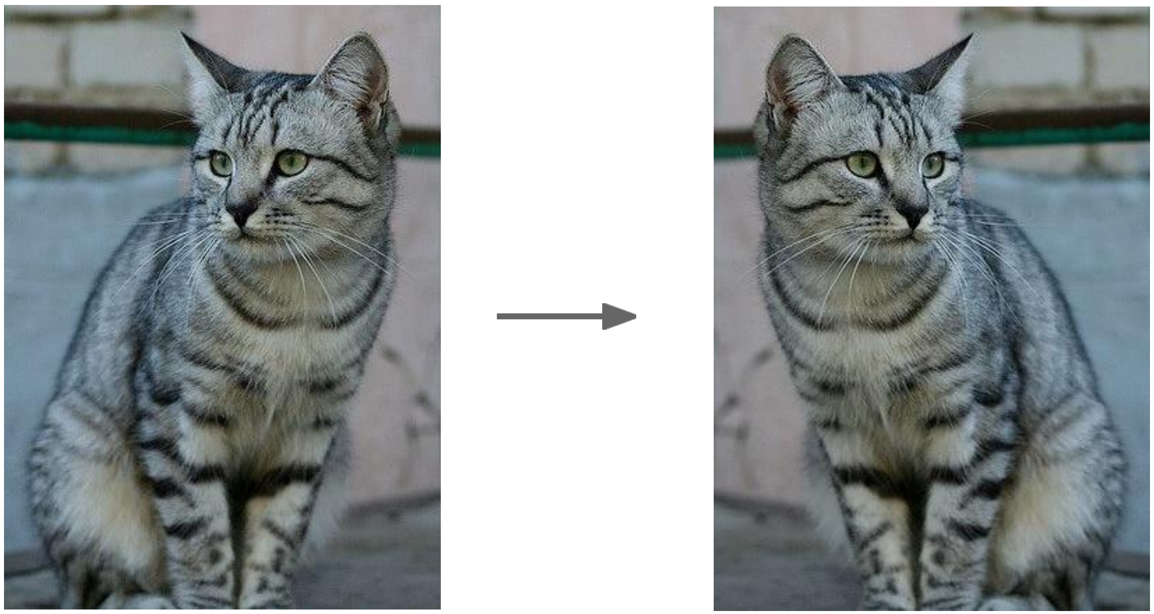
Regularization: Data Augmentation



Training vs. Testing Error

Data Augmentation

Horizontal Flips



Training vs. Testing Error

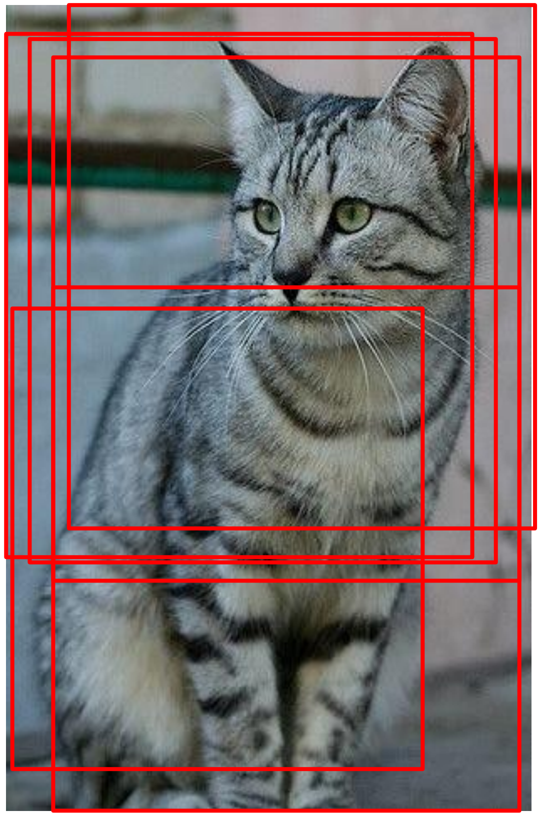
Data Augmentation

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



Training vs. Testing Error

Data Augmentation
Random crops and scales

Training: sample random crops / scales

ResNet:

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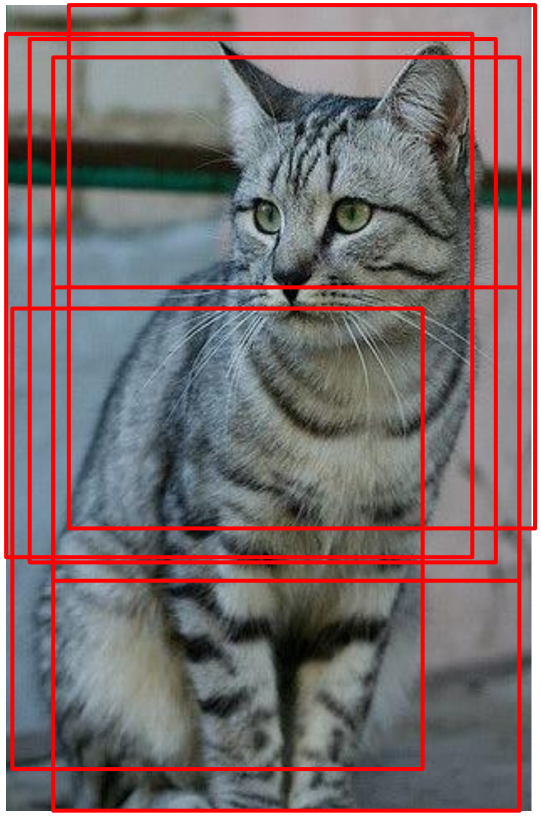


Testing: average a fixed set of crops

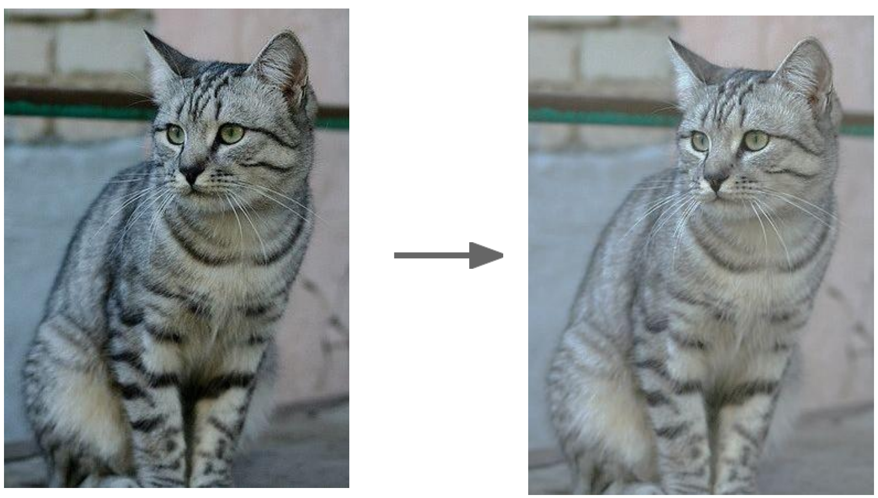
ResNet:

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

Training vs. Testing Error

Data Augmentation
Color Jitter

Simple: Randomize contrast and brightness



Training vs. Testing Error

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)

Training vs. Testing Error

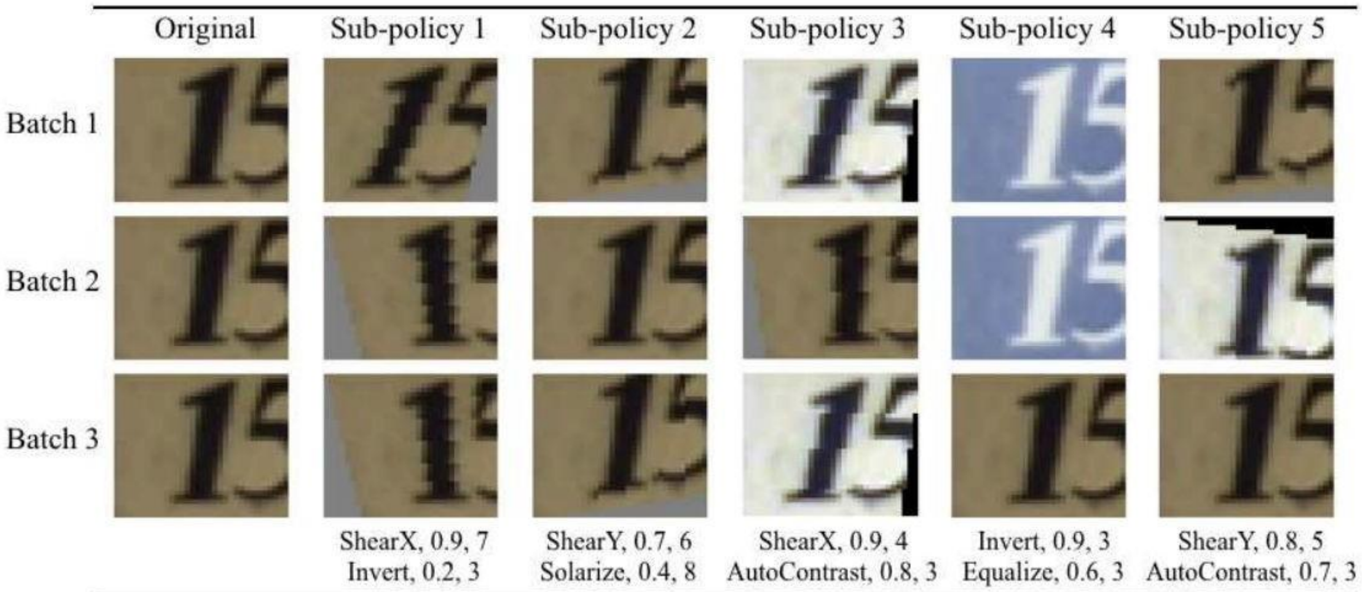
Data Augmentation

- **Get creative for your problem!**

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

Training vs. Testing Error

Automatic Data Augmentation



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

Training vs. Testing Error

Regularization: A common pattern

Training: Add random noise
Testing: Marginalize over the noise

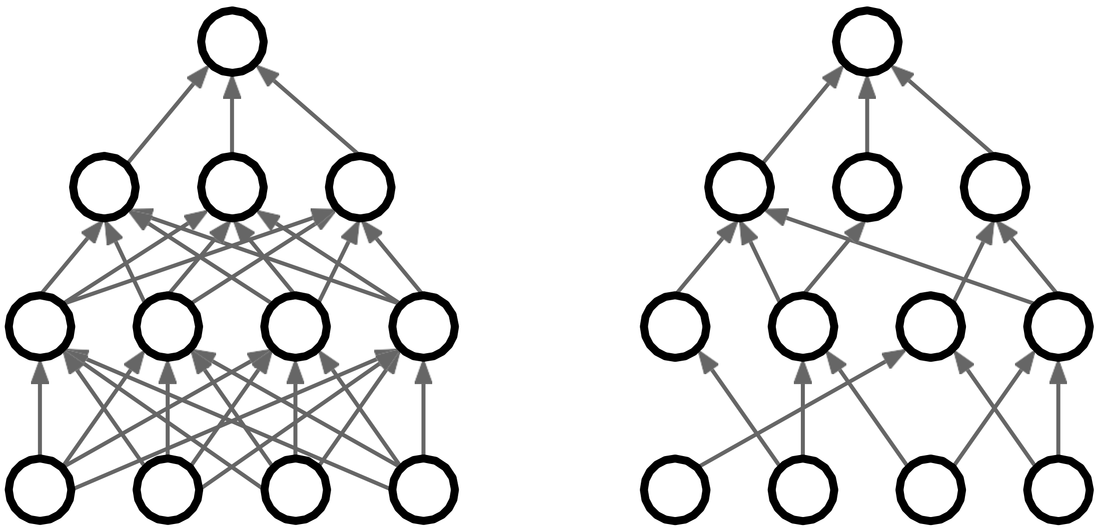
Examples:
Dropout
Batch Normalization
Data Augmentation

Training vs. Testing Error

Regularization: A common pattern

Training: Drop connections between neurons (set weights to 0)
Testing: Use all the connections

Examples:
- Dropout
- Batch Normalization
- Data Augmentation
- Drop Connect



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

Training vs. Testing Error

Regularization: A common pattern

Training: Use randomized pooling regions

Testing: Average predictions from several regions

Examples:

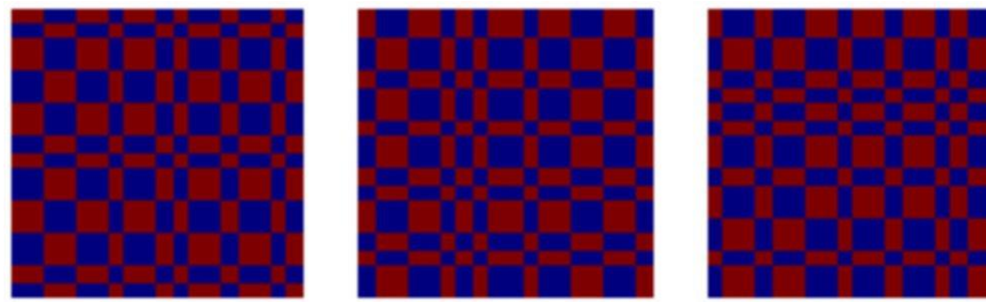
Dropout

Batch Normalization

Data Augmentation

Drop Connect

Fractional Max Pooling



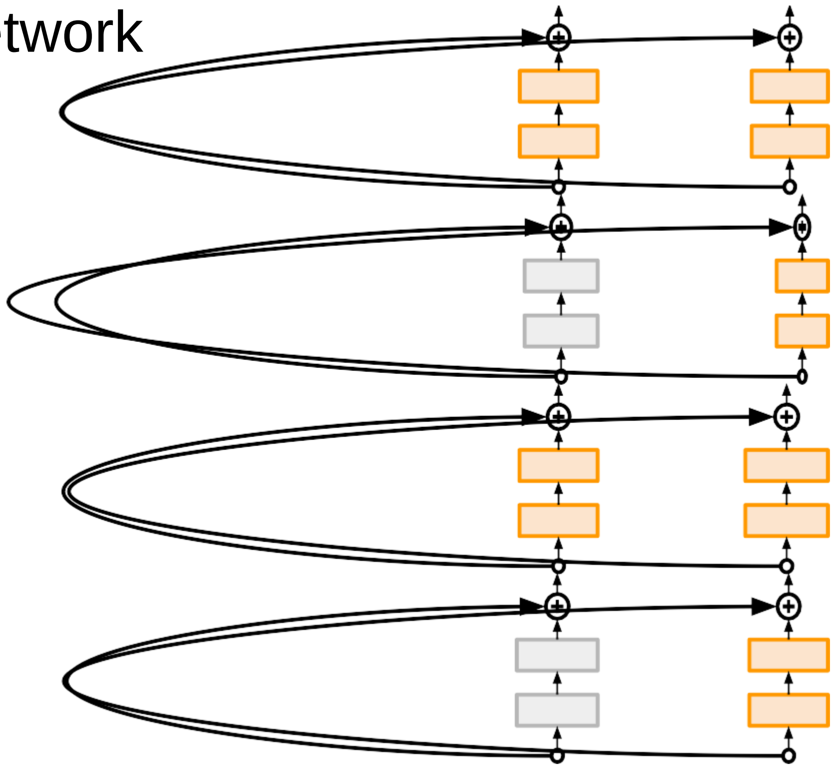
Graham, “Fractional Max Pooling”, arXiv 2014

Training vs. Testing Error

Regularization: A common pattern

Training: Skip some layers in the network

Testing: Use all the layer



Examples:

Dropout

Batch Normalization

Data Augmentation

Drop Connect

Fractional Max Pooling

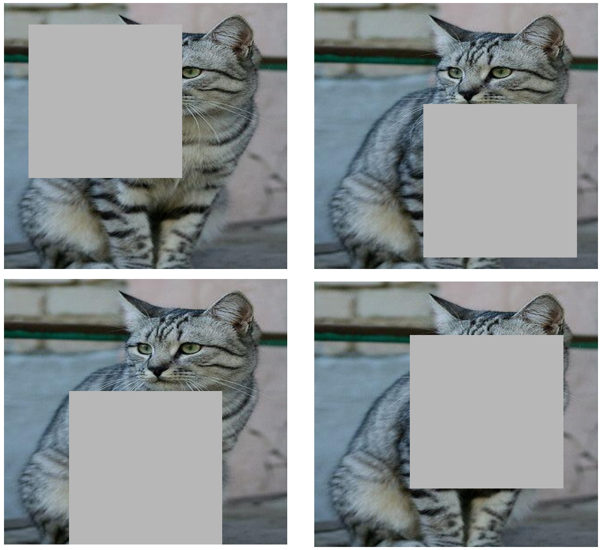
Stochastic Depth

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

Training vs. Testing Error

Regularization: A common pattern

Training: Set random image regions to 0
Testing: Use full image



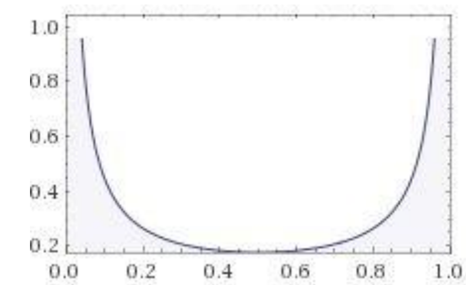
Examples:
- Dropout
- Batch Normalization
- Data Augmentation
- Drop Connect
- Fractional Max Pooling
- Stochastic Depth
- Cutout / Random Crop

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

Training vs. Testing Error

Regularization: A common pattern

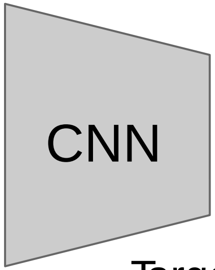


Training: Train on random blends of images

Testing: Use original images

Examples:

- Dropout
- Batch Normalization
- Data Augmentation
- Drop Connect
- 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

Training vs. Testing Error

Regularization: In practice

Training: Train on random blends of images
Testing: Use original images

Examples:
Dropout
Batch Normalization
Data Augmentation
Drop Connect
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

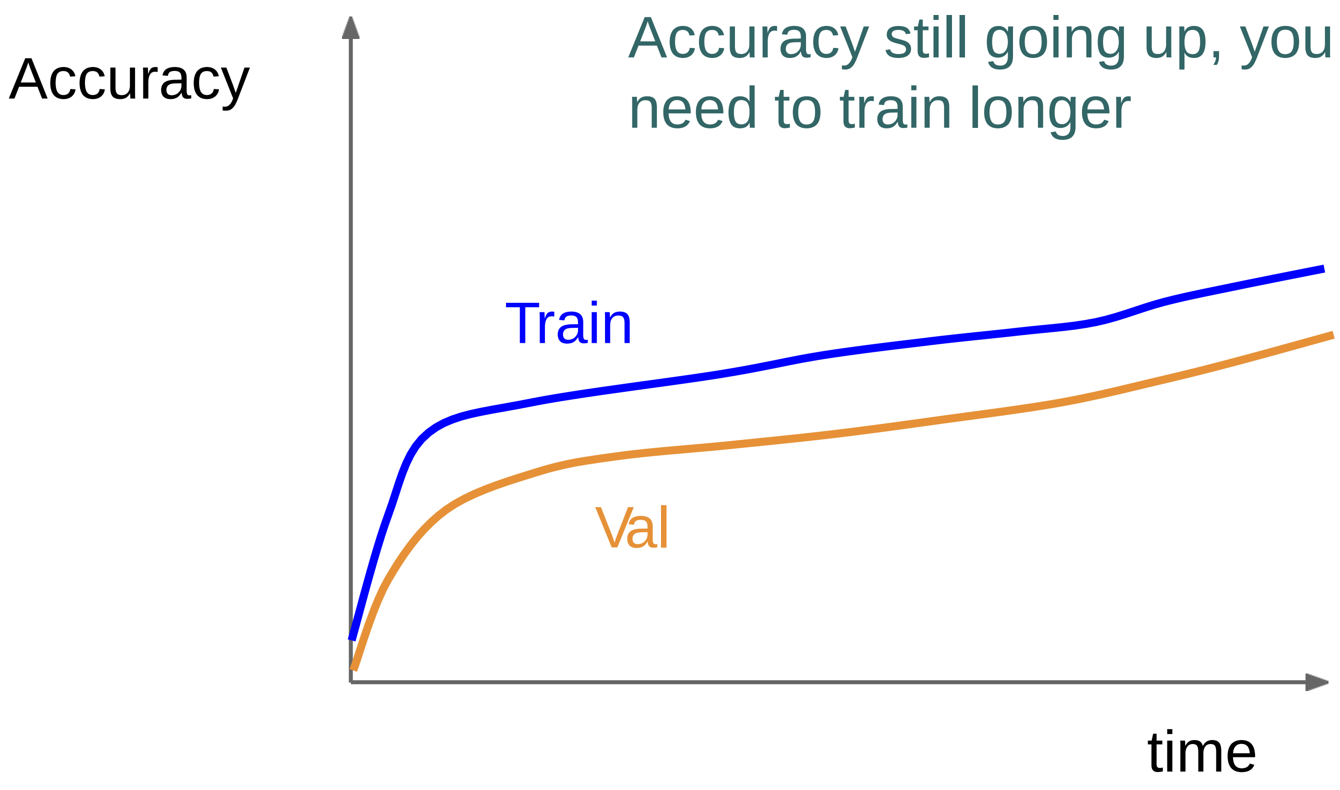
Step 3: Find LR that makes loss go down

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

Step 5: Refine grid, train longer

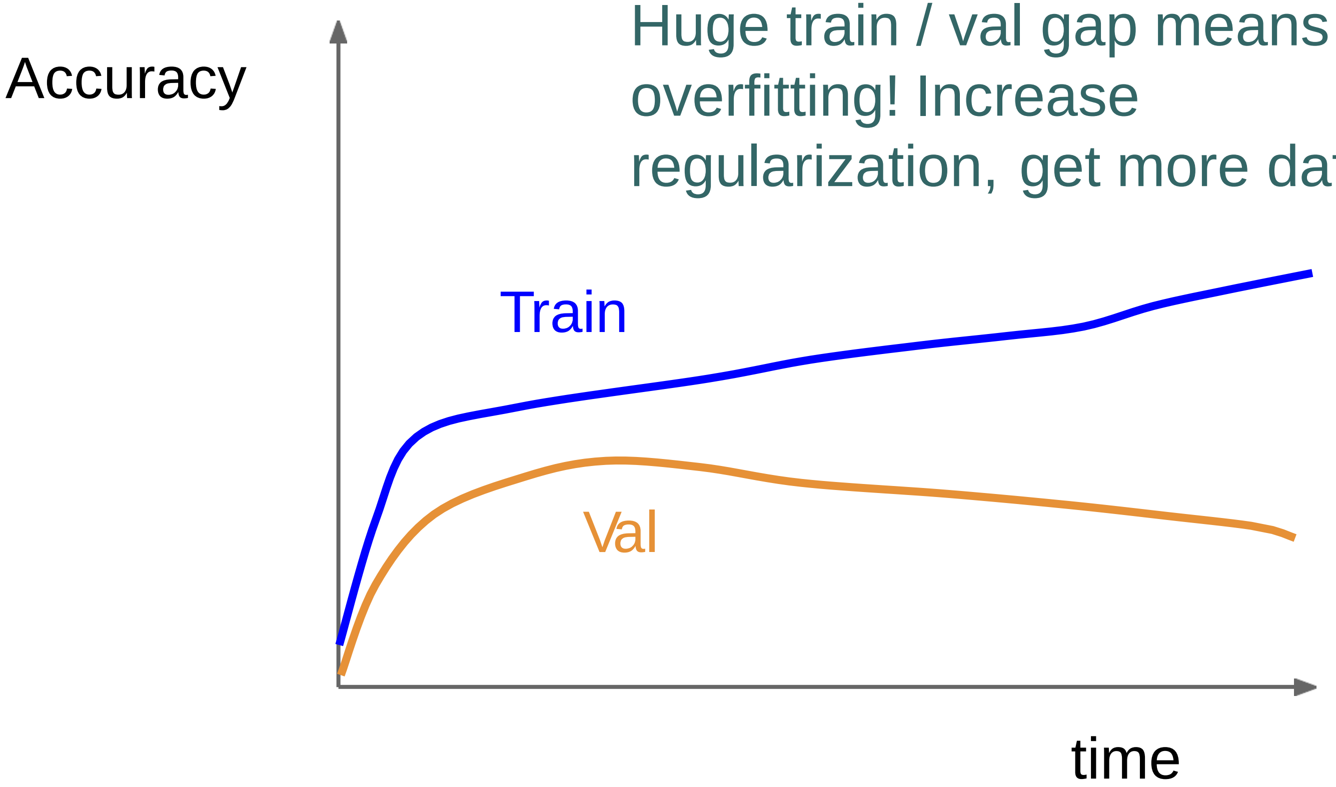
Step 6: Look at loss and accuracy curves

Choosing Hyperparameters

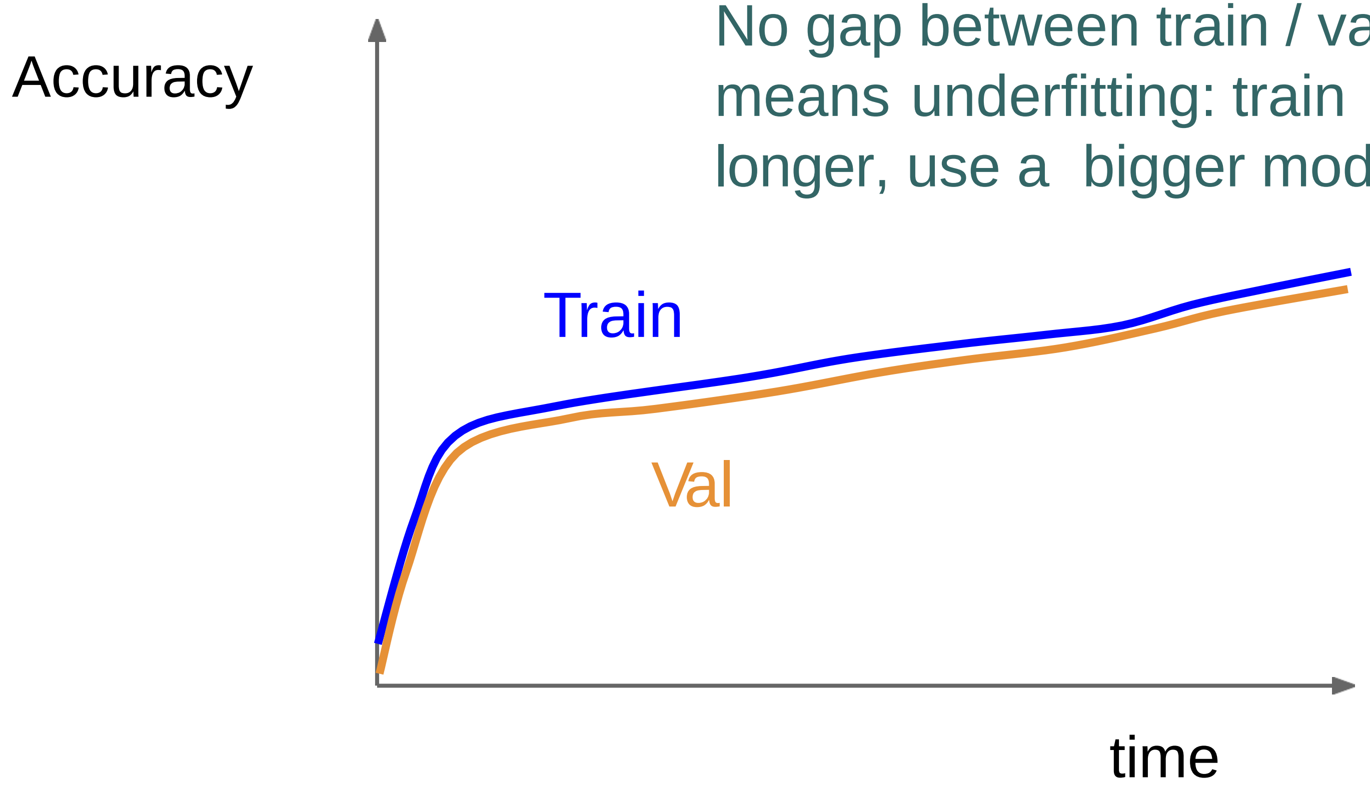


Choosing Hyperparameters

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



Choosing Hyperparameters

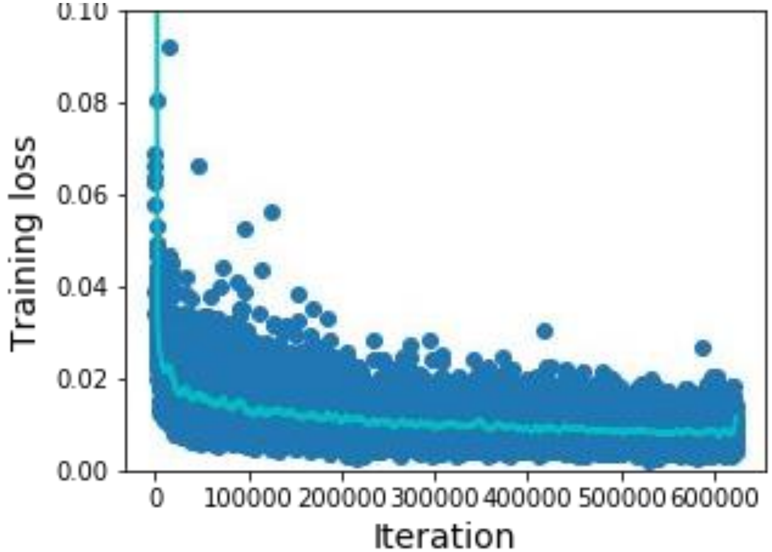


No gap between train / val means underfitting: train longer, use a bigger model

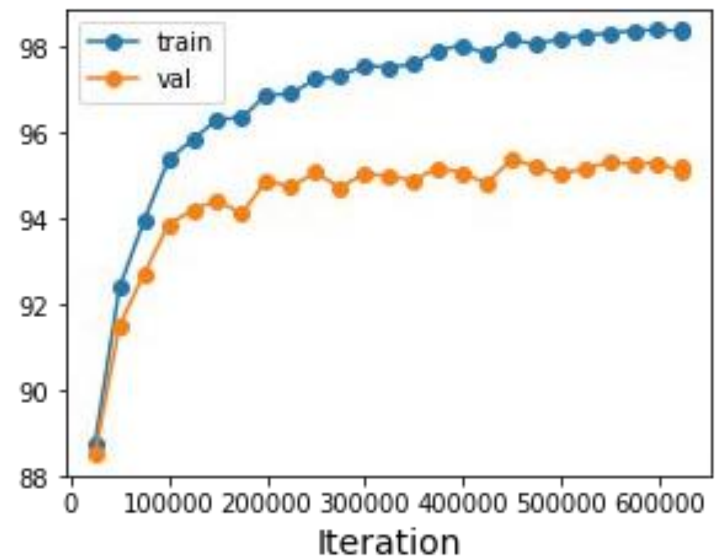
Choosing Hyperparameters

Look at learning curves!

Training Loss



Train / Val Accuracy

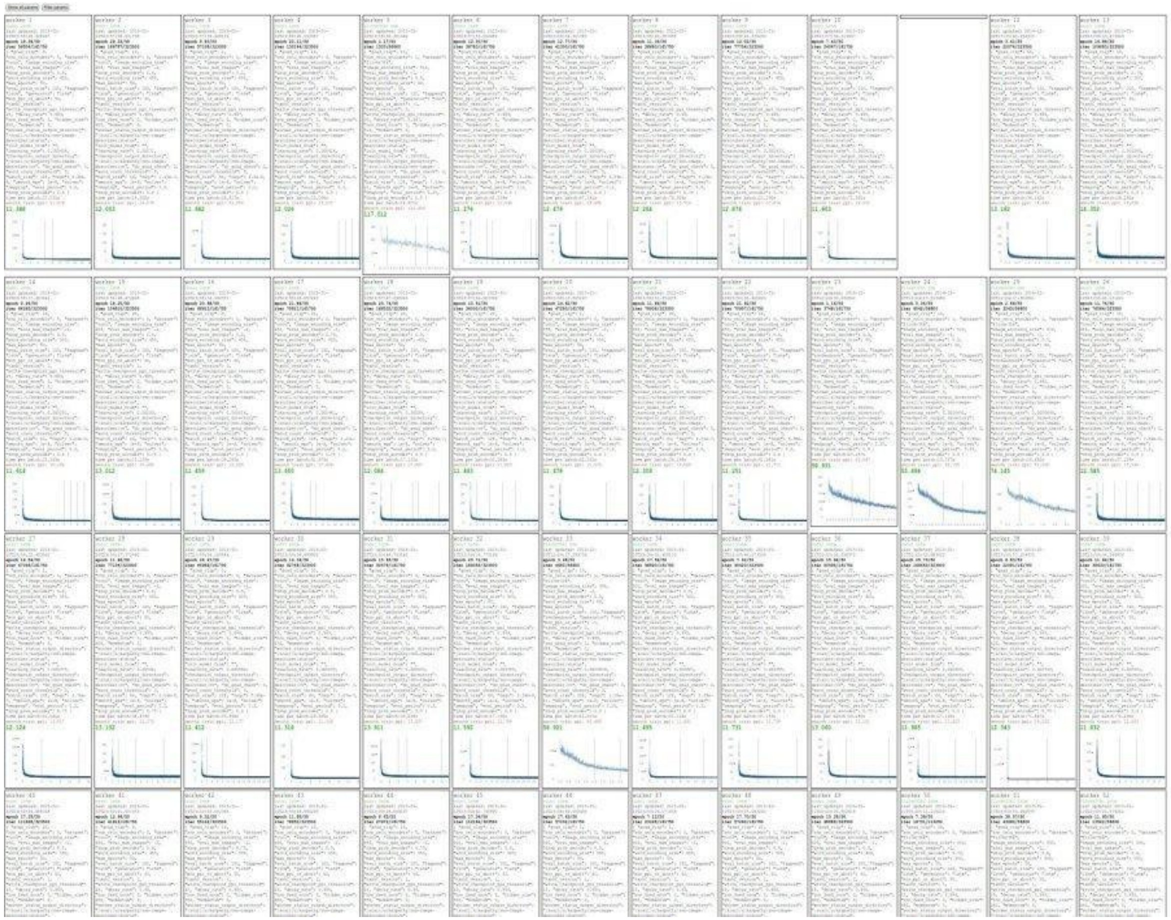


Losses may be noisy, use a scatter plot and also plot moving average to see trends better

Choosing Hyperparameters

Cross-validation

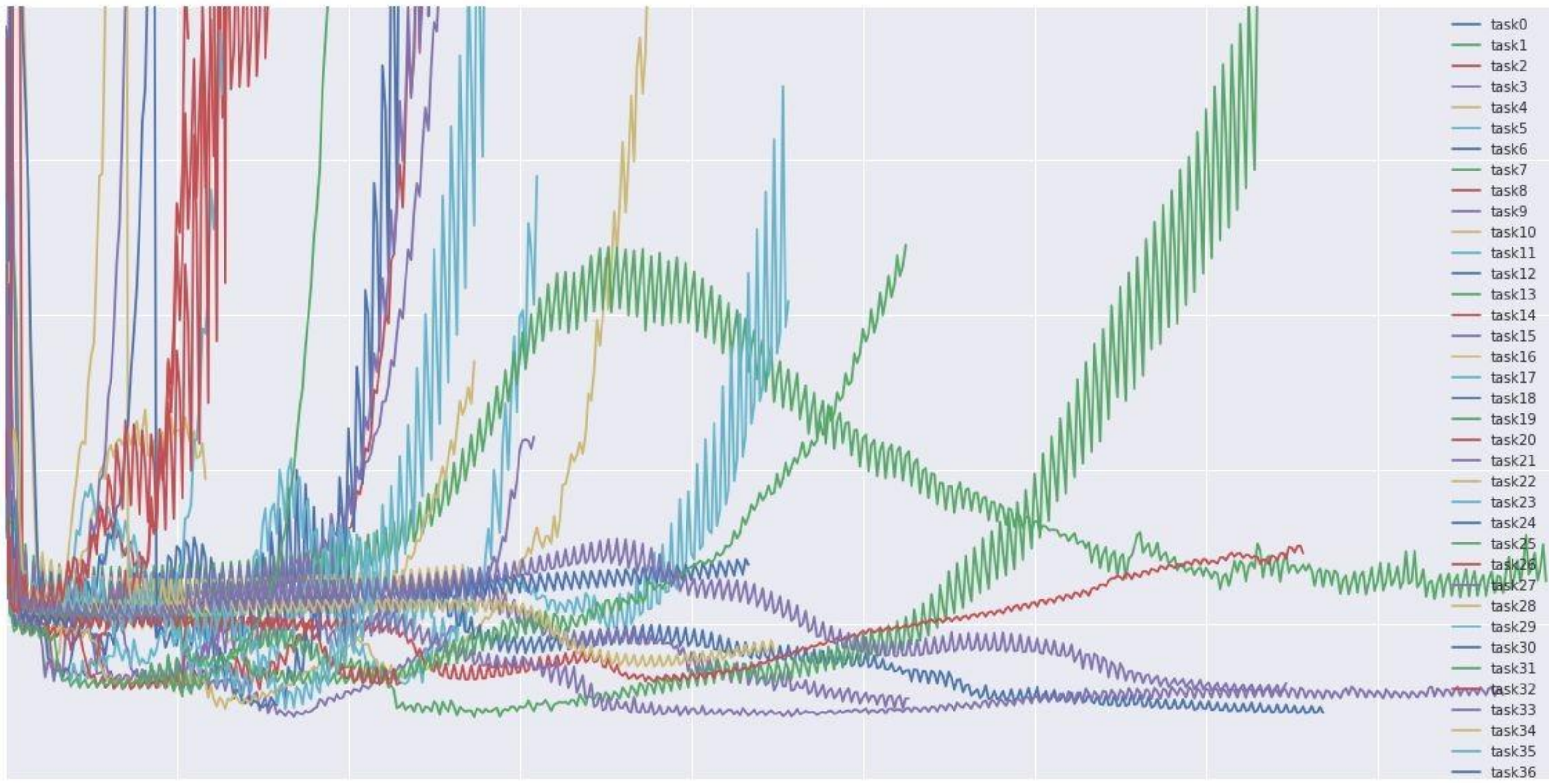
We develop "command centers" to visualize all our models training with different hyperparameters



check out weights and biases

Choosing Hyperparameters

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



Choosing Hyperparameters

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

Choosing Hyperparameters

Random Search vs. Grid Search

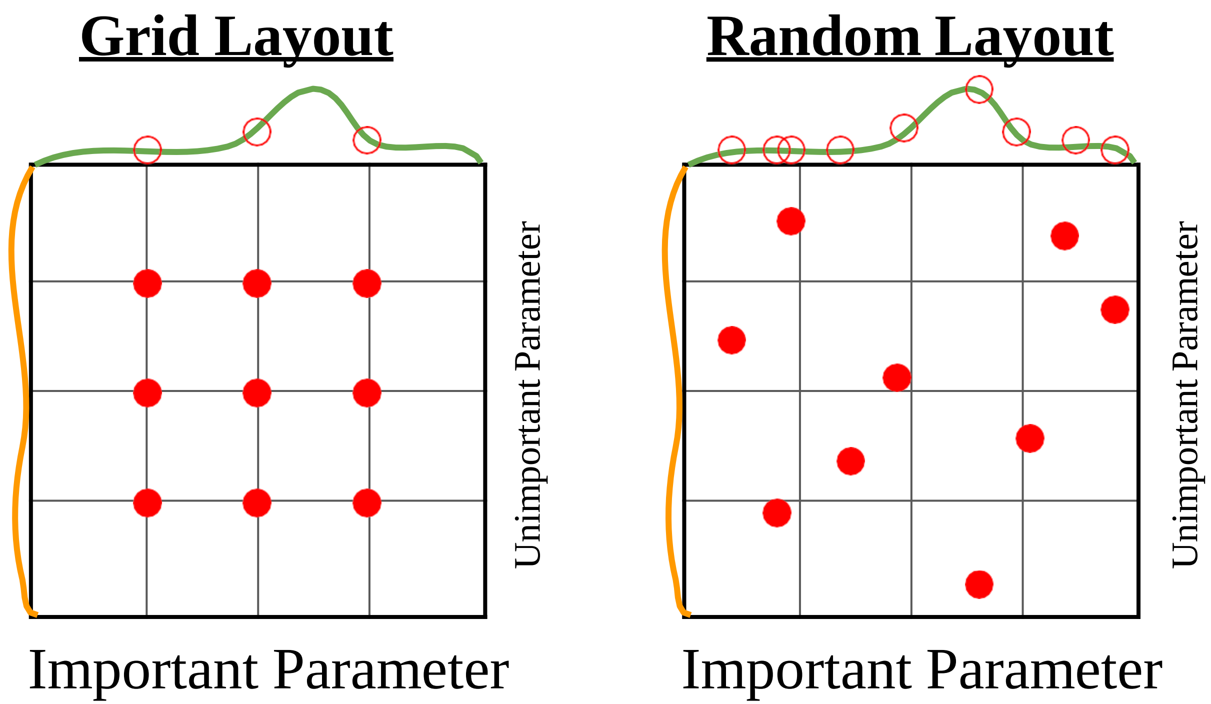


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

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

Summary

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

Summary

- **We looked in detail at:** TLDRs

- 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

Pattern Recognition and Computer Vision

Guanbin Li,
School of Computer Science and Engineering, Sun Yat-Sen University

Most of our slides have been borrowed from the courses of Stanford CS131 and CS231N, Thanks!