# Training Neural Networks
# Practical Issues

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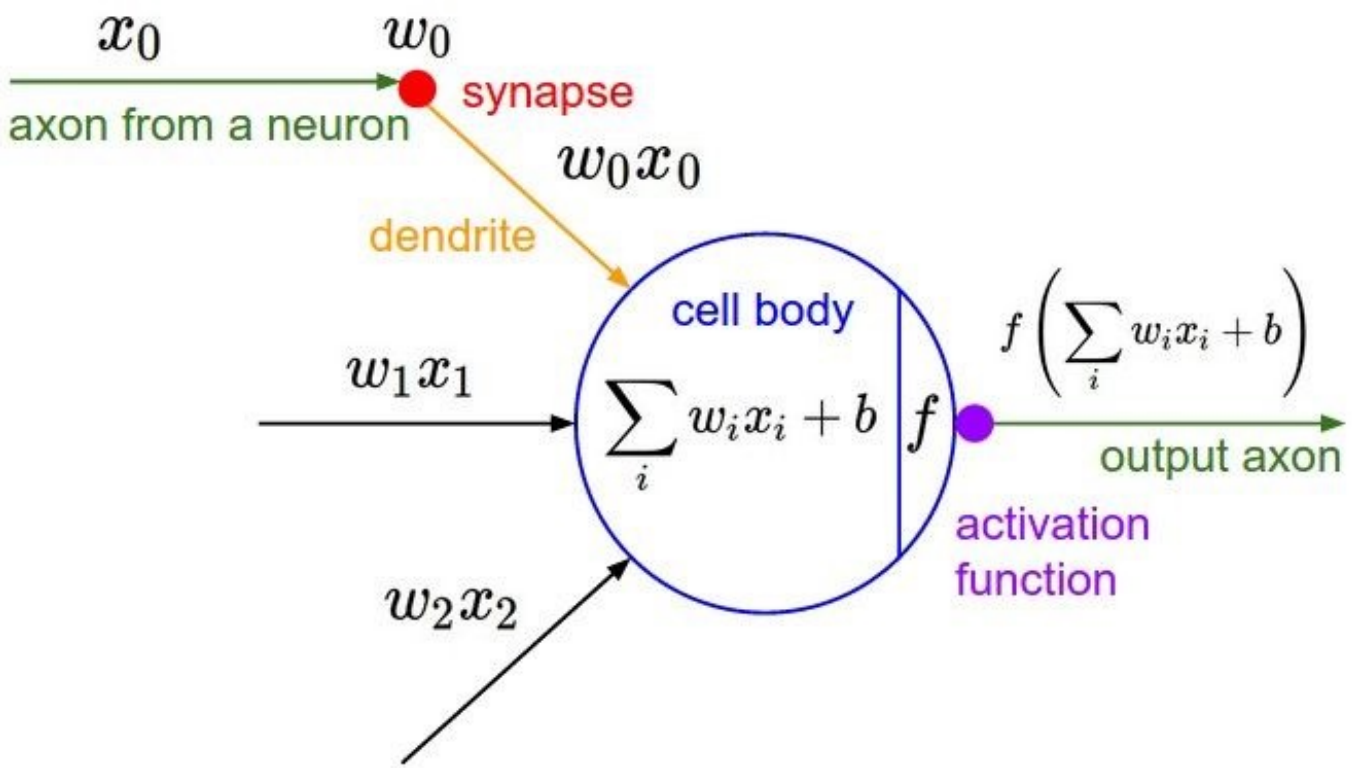
Most slides have been adapted from Fei Fei Li and colleagues lectures, cs231n

# Outline

- Activation Functions
- Data Preprocessing
- Weight Initialization
- Choosing hyperparameters

# Activation Functions

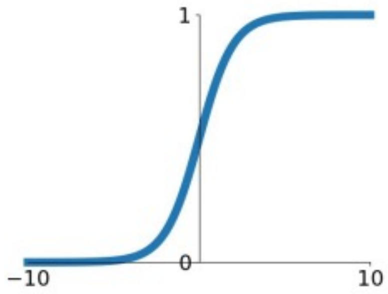
# Neuron


$x_0$
$w_0$
synapse
axon from a neuron
$w_0 x_0$
dendrite
cell body
$w_1 x_1$
$\sum_i w_i x_i + b$
$f$
$f\left(\sum_i w_i x_i + b\right)$
output axon
activation
function
$w_2 x_2$

# Activation Functions

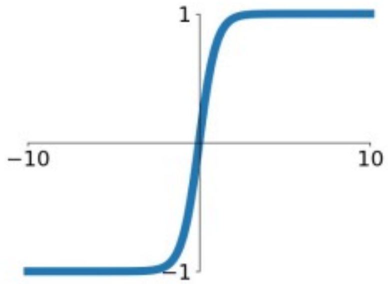
**Sigmoid**

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



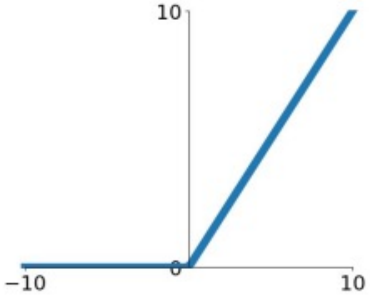

**tanh**

$\tanh(x)$



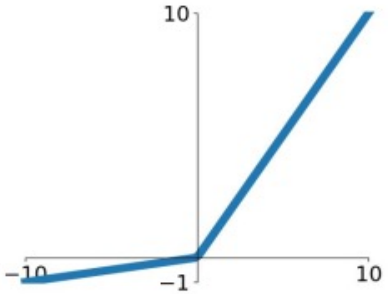

**ReLU**

$\max(0, x)$




**Leaky ReLU**

$\max(0.1x, x)$

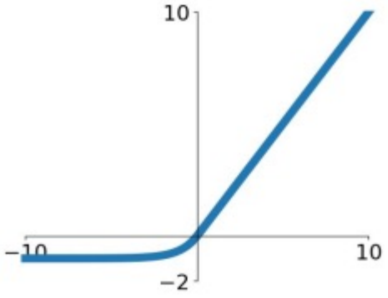



**Maxout**

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

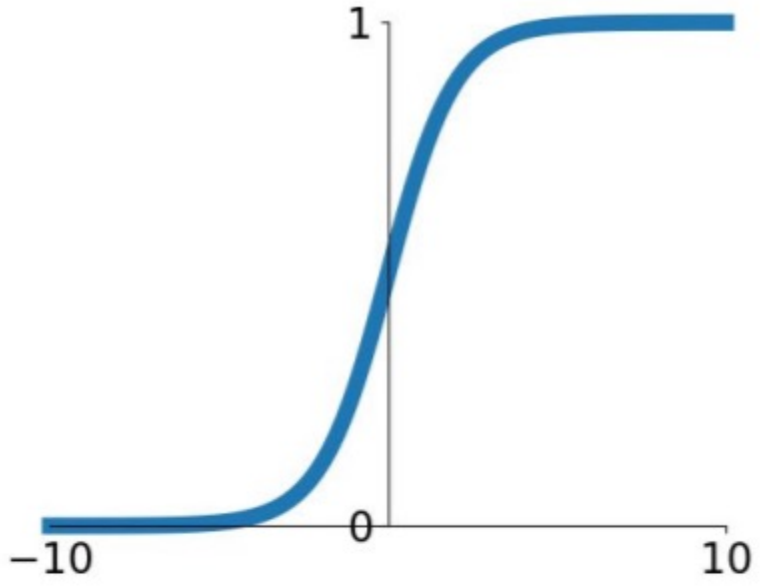
**ELU**

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



# Activation functions: sigmoid

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



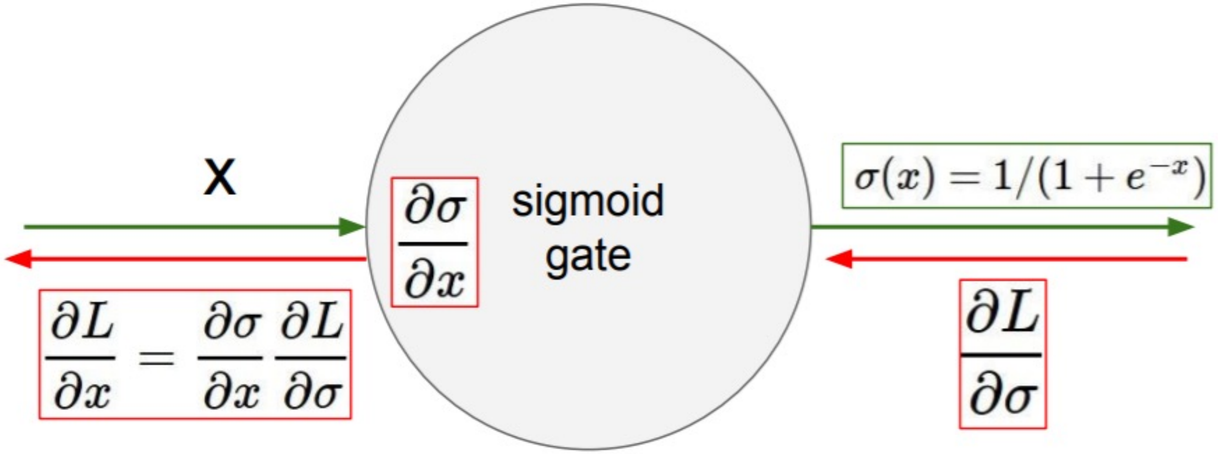

**Sigmoid**

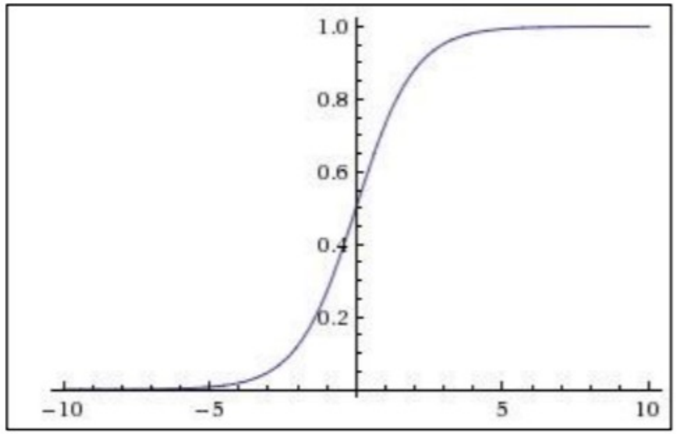
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

Problems:

1. Saturated neurons “kill” the gradients

# Activation functions: sigmoid

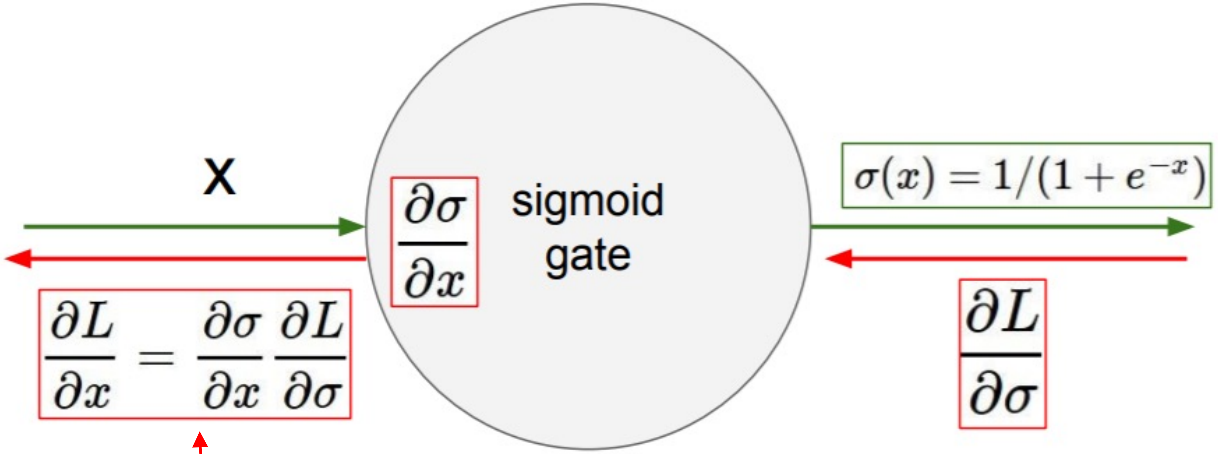


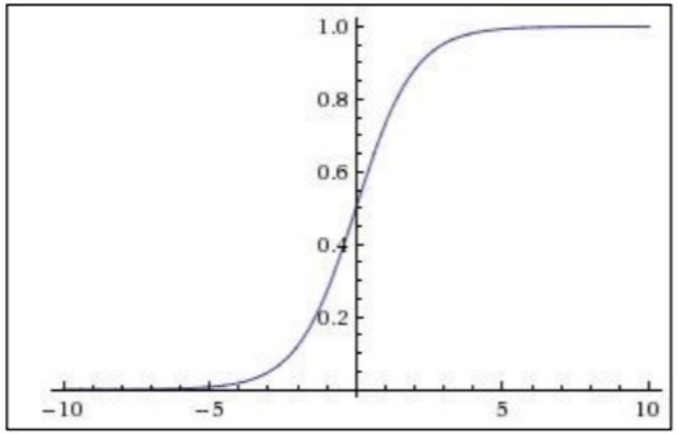



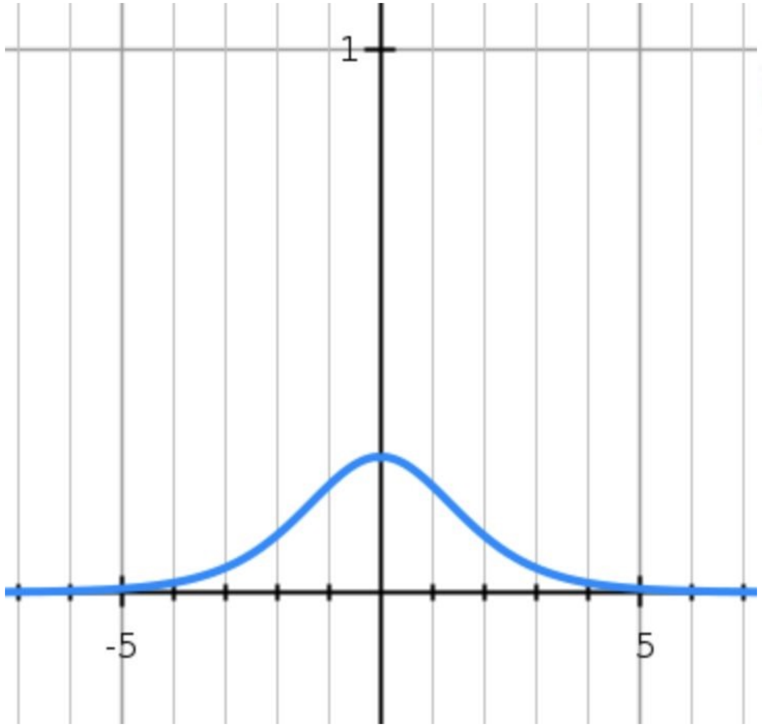

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

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

# Activation functions: sigmoid



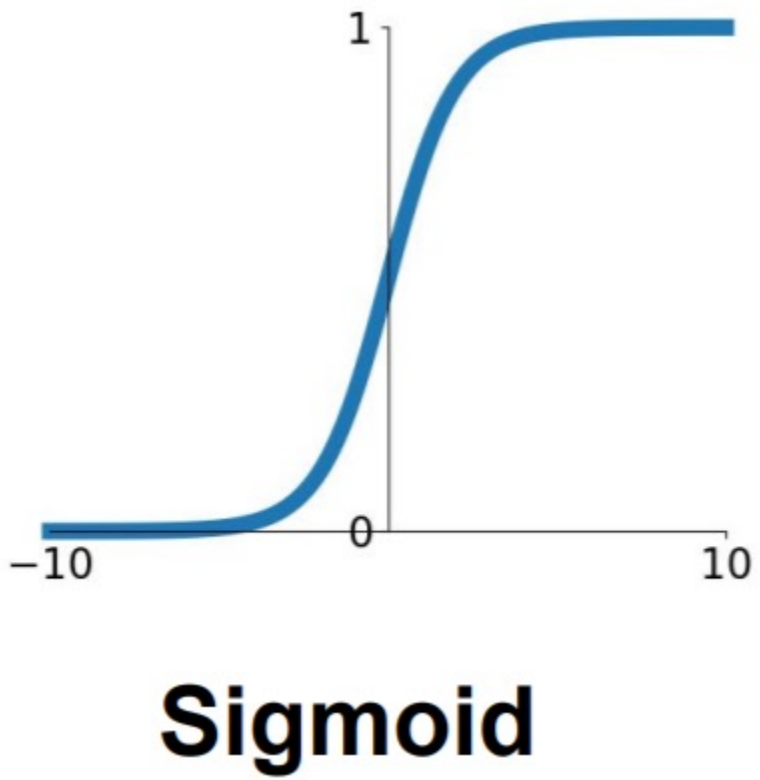

$$(1-\sigma(x))\sigma(x)$$

Why is this a problem?

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

# Activation functions: sigmoid

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




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

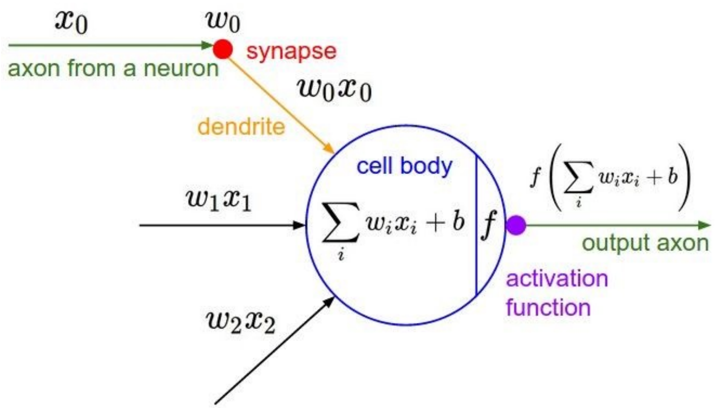
Problems:

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

# Activation functions: sigmoid

- Consider what happens when the input to a neuron (x) is always positive:

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




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

# Activation functions: sigmoid

- Consider what happens when the input to a neuron (x) 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

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

We are assuming x is always positive

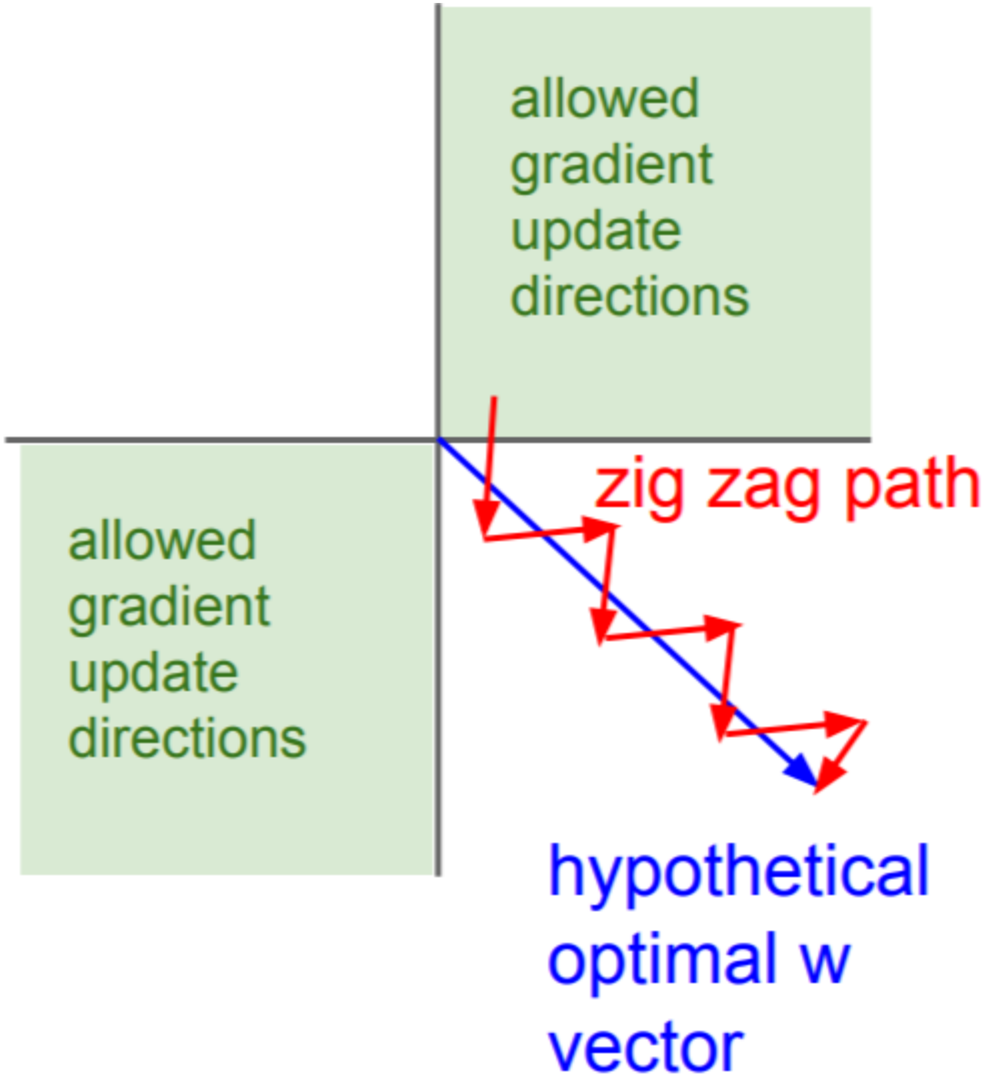
So!! Sign of gradient **for all $w_i$** is the same as the sign of upstream scalar gradient!

# Activation functions: sigmoid

- Consider what happens when the input to a neuron is always positive...
- What can we say about the gradients on w? Always all positive or all negative ☹

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

(For a single element! Minibatches help)



# Activation functions: sigmoid

- Squashes numbers to range [0,1]
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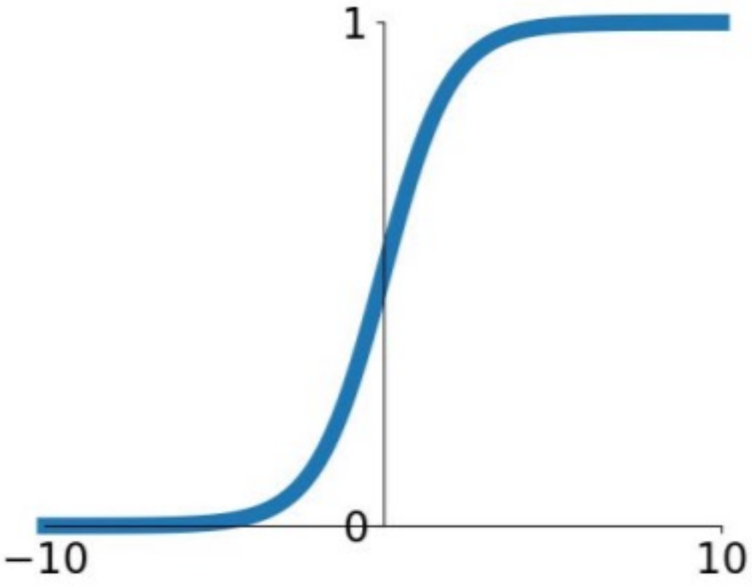



**Sigmoid**

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

3 problems:

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

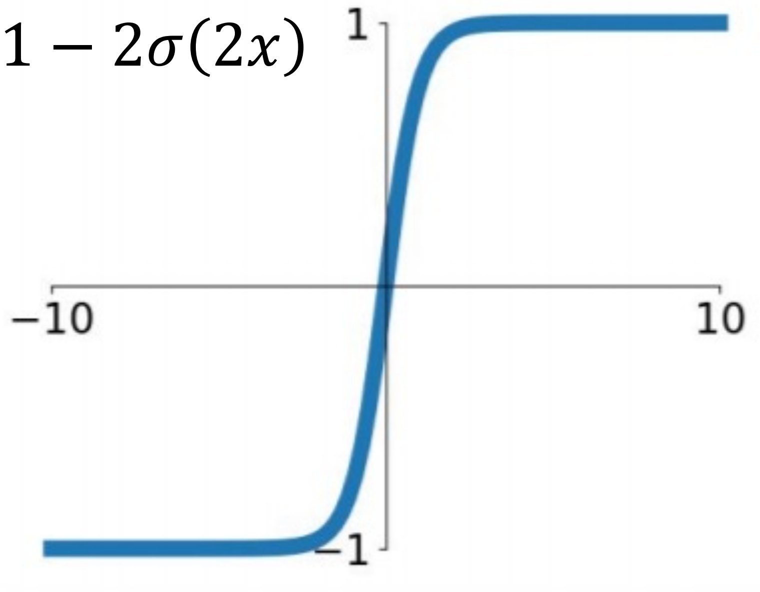
# Activation functions: tanh

[LeCun et al., 1991]

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

$$\tanh(x) = \frac{1 - e^{-2x}}{1 + e^{-2x}}$$

$$= 1 - 2\sigma(2x)$$

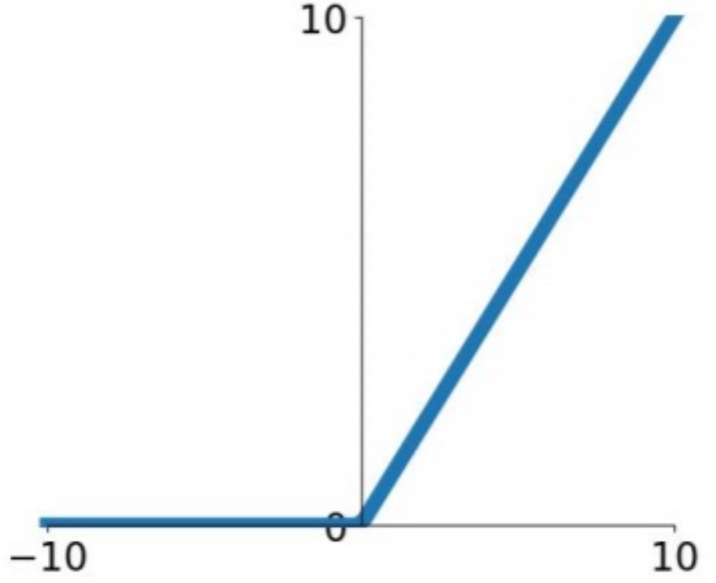



**tanh(x)**

# Activation functions: ReLU (Rectified Linear Unit)

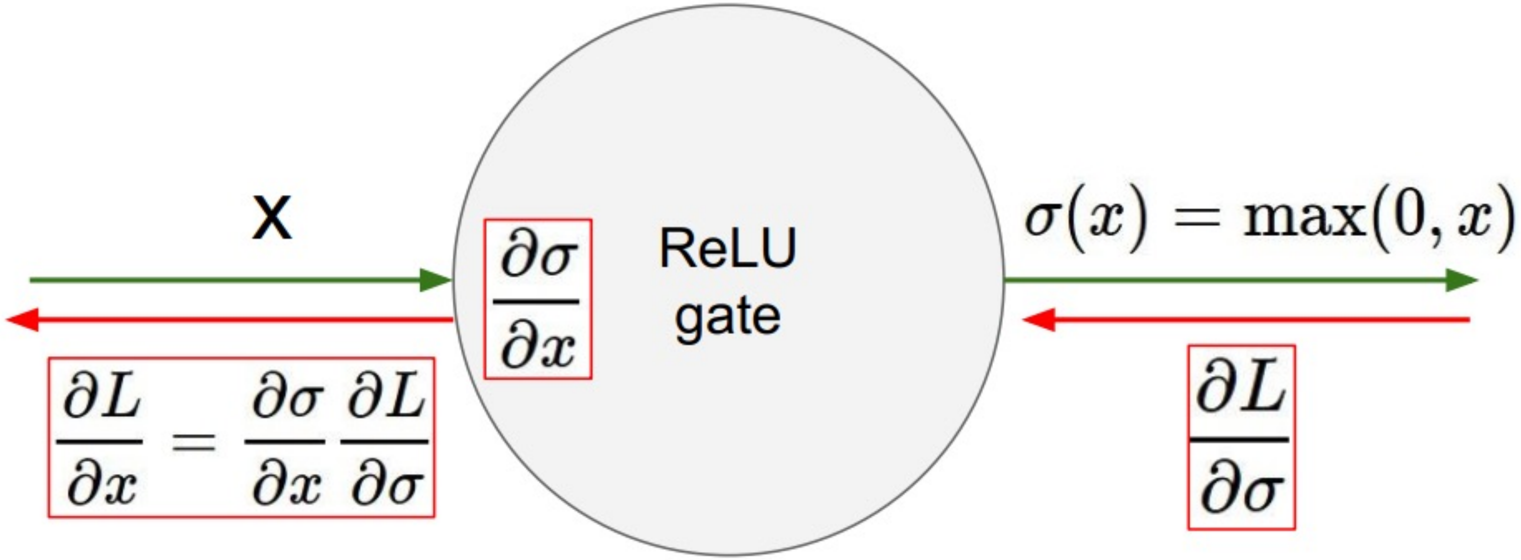
[Krizhevsky et al., 2012]

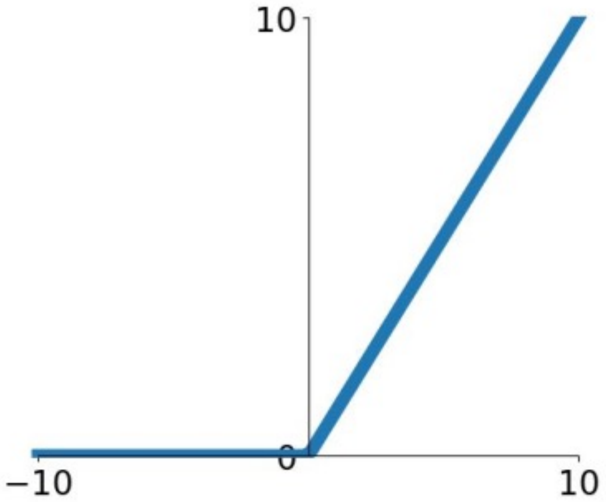
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Actually more biologically plausible than sigmoid




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

# Activation functions: ReLU



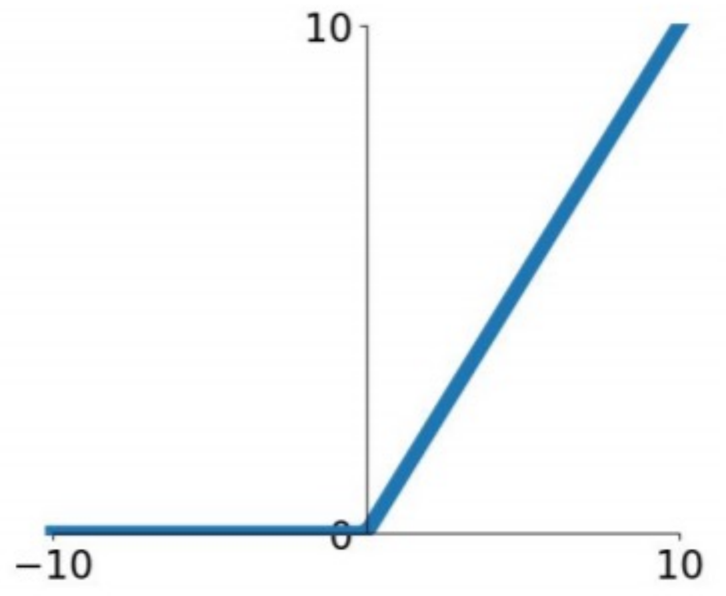

- What happens when x = -10?
- What happens when x = 0?
- What happens when x = 10?

# Activation functions: ReLU

[Krizhevsky et al., 2012]

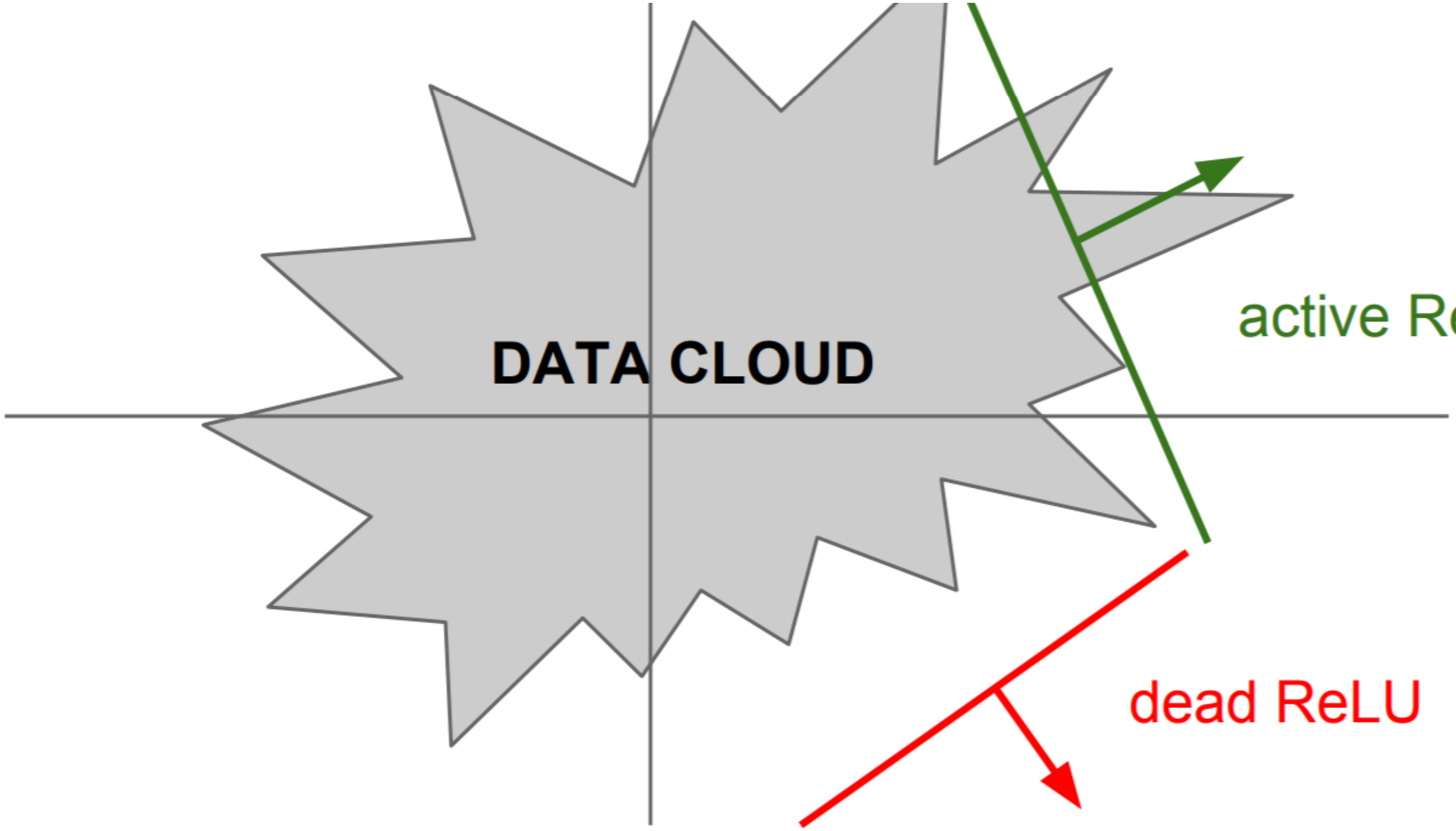
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Actually more biologically plausible than sigmoid

- Problems:
  - Not zero-centered output
  - An annoyance:
    - hint: what is the gradient when x < 0?




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

# Activation functions: ReLU



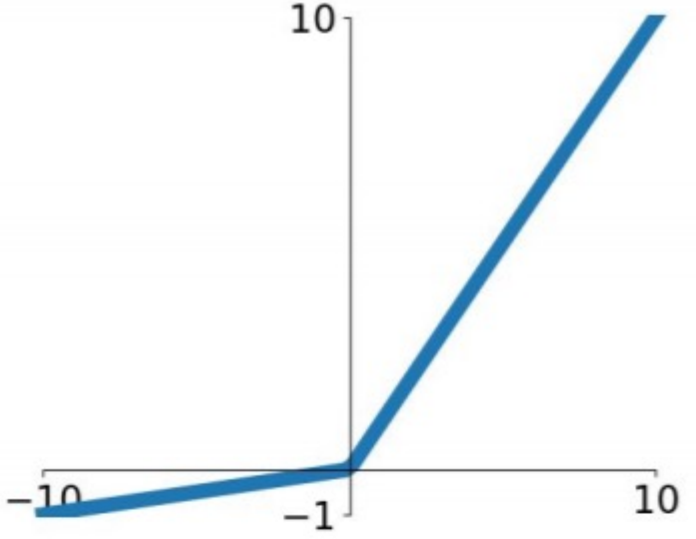

=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

It can be due initialization or high learning rate

# Activation functions: Leaky ReLU

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

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




**Parametric Rectifier (PReLU)**

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

$\alpha$ is determined during backpropagation

**Leaky ReLU**

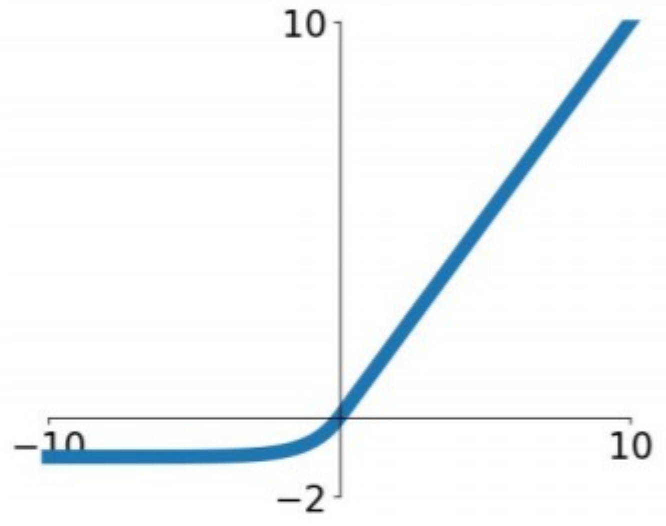
$$f(x) = \max(0.01x, x)$$

# 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

- Computation requires exp()

[Clevert et al., 2015]



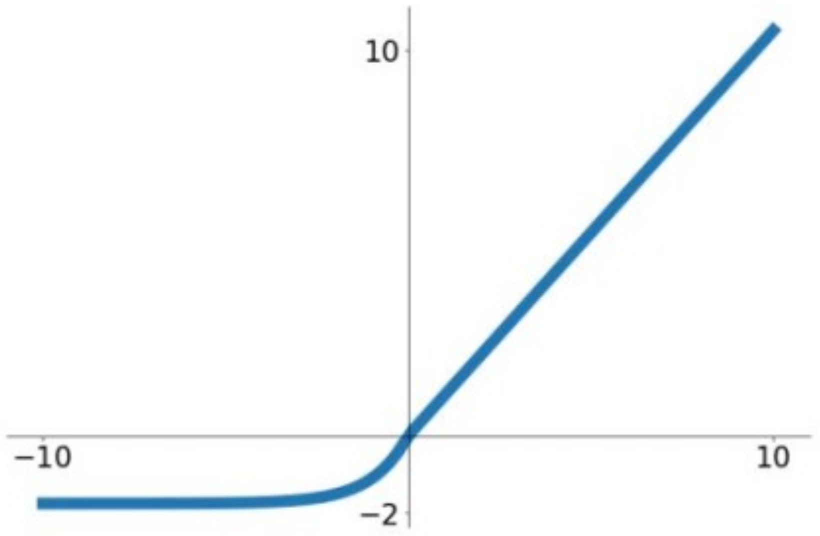

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\left(\exp(x) - 1\right) & \text{if } x \le 0 \end{cases}$$

(Alpha default = 1)

# 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

[Klambauer et al. ICLR 2017]




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

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

# Maxout “Neuron”

[Goodfellow et al., 2013]

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

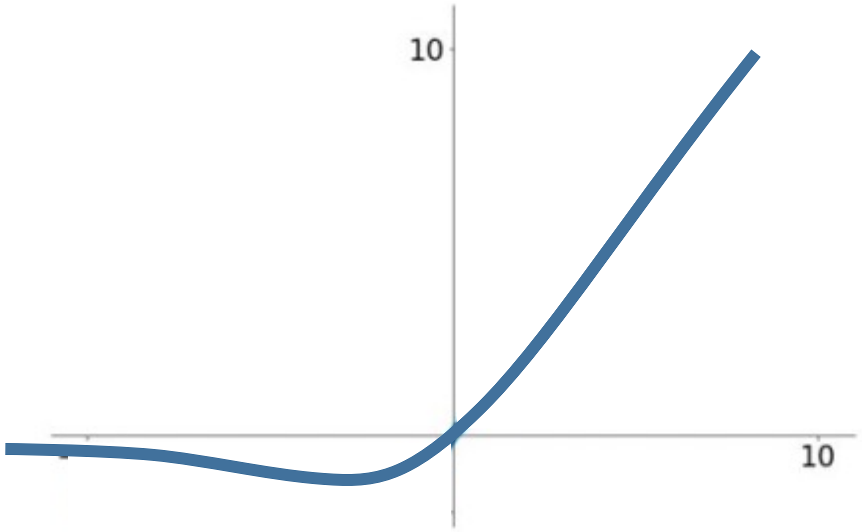
- Does not have the basic form of “dot product -> nonlinearity”
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

- Problem: doubles the number of parameters/neuron :(

# GELU

$$GELU(x) = x\phi(\alpha x) = x\int_{-\infty}^{x}\frac{1}{\sqrt{2\pi}}e^{-t^2/2}dt$$

- $\alpha$ controls the smoothness of the GELU function (generally $\alpha = 1$)
- Used in BERT, ViT, and GPT

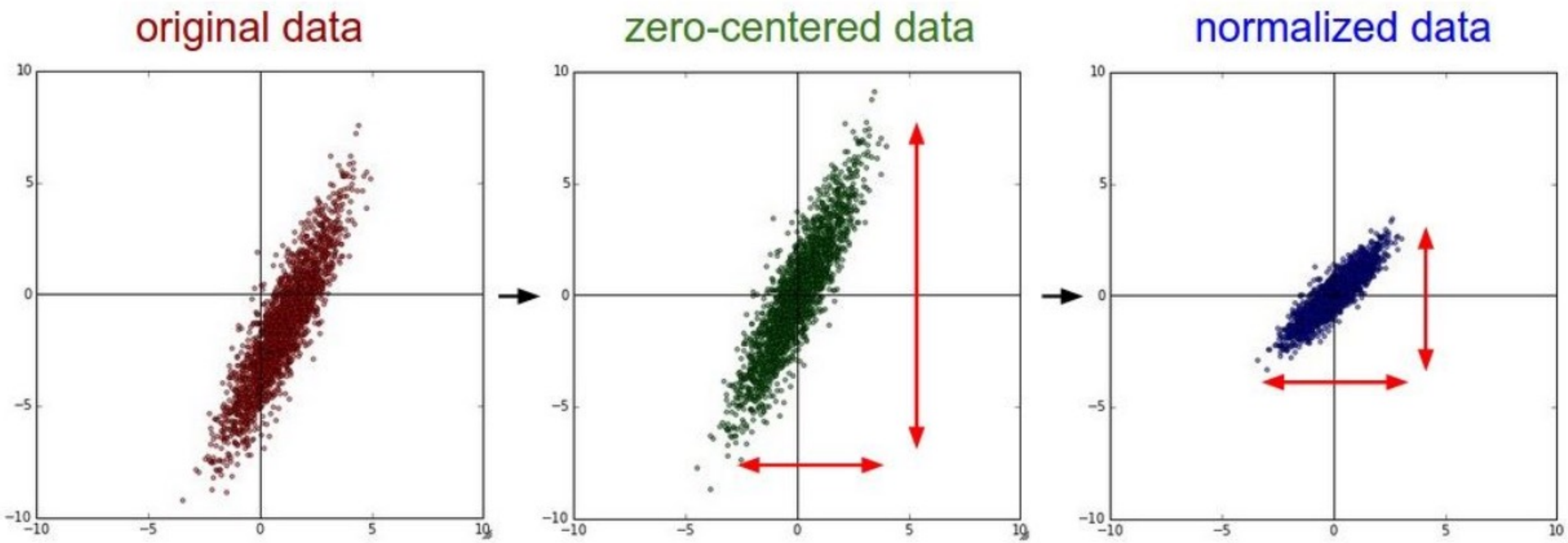


# Activation functions

- In practice:
  - Use ReLU. Be careful with your learning rates
  - Try out Leaky ReLU / Maxout / ELU / SELU / GELU
    - To squeeze out some marginal gains
  - Use sigmoid and tanh only for gating purposes

# 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)

# Normalizing the input

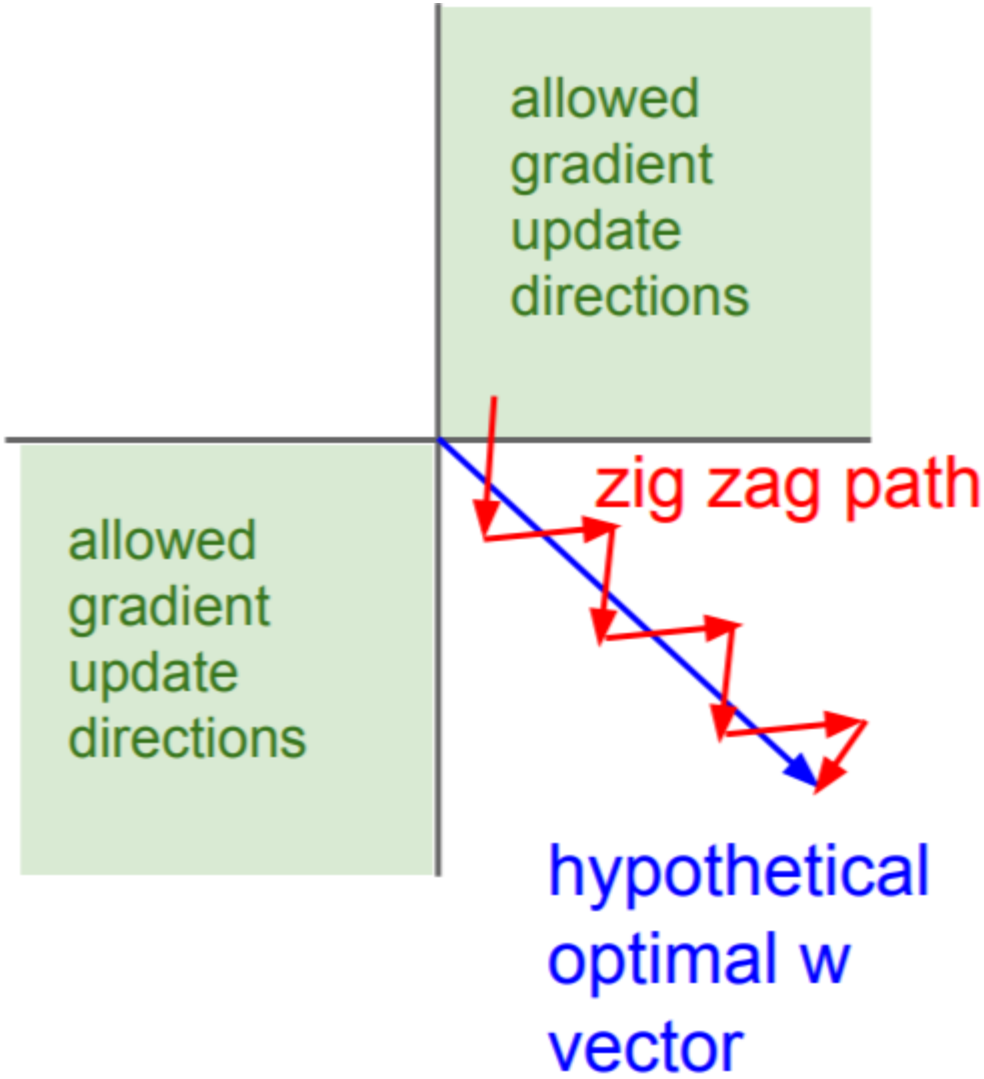
- On the training set compute mean of each input (feature)
  - $\mu_i = \frac{\sum_{n=1}^{N} x_i^{(n)}}{N}$
  - $\sigma_i^2 = \frac{\sum_{n=1}^{N} \left(x_i^{(n)} - \mu_i\right)^2}{N}$
- **Remove mean**: from each of the input mean of the corresponding input
  - $x_i \leftarrow x_i - \mu_i$
- **Normalize variance**:
  - $x_i \leftarrow \frac{x_i}{\sigma_i}$
- If we normalize the training set we use the same $\mu$ and $\sigma^2$ to normalize test data too

# Why zero-mean input?

- Reminder: sigmoid

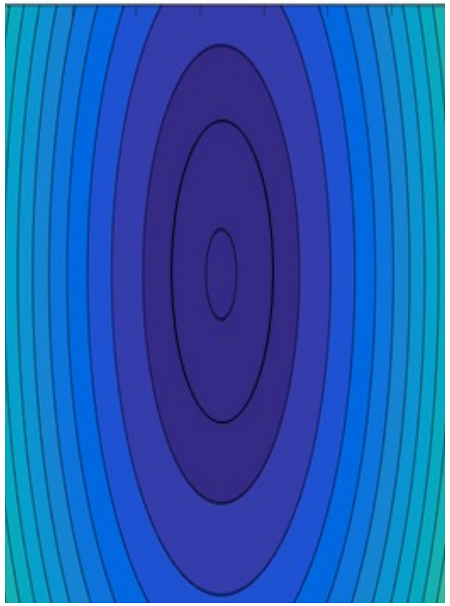
- Consider what happens when the input to a neuron is always positive...

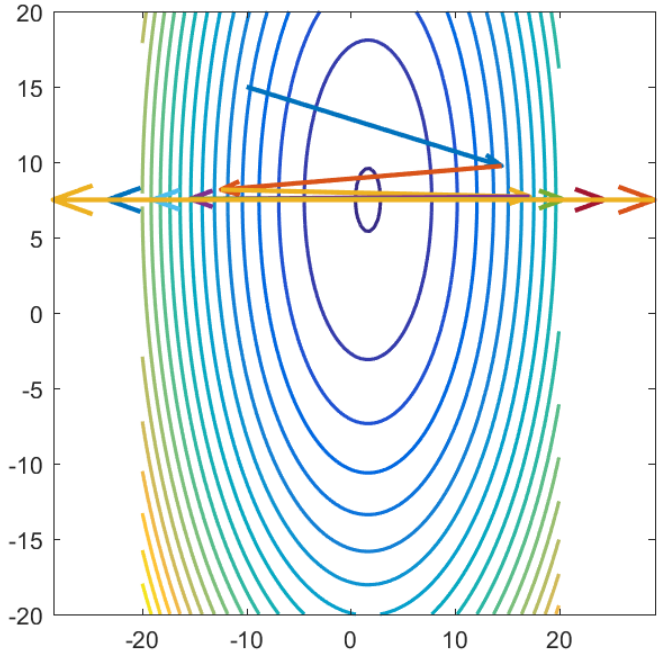
- What can we say about the gradients on w? Always all positive or all negative ☹
  - this is also why you want zero-mean data!



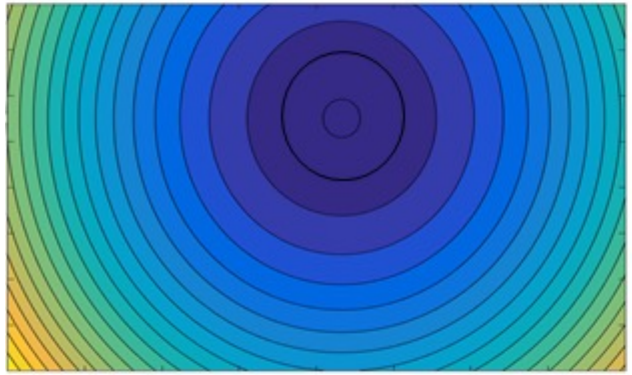
# Why normalize inputs?

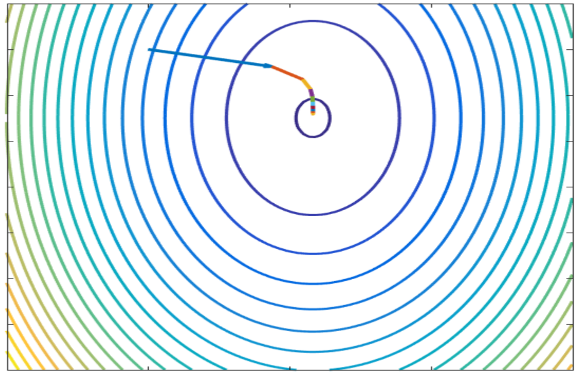
Very different range of input features





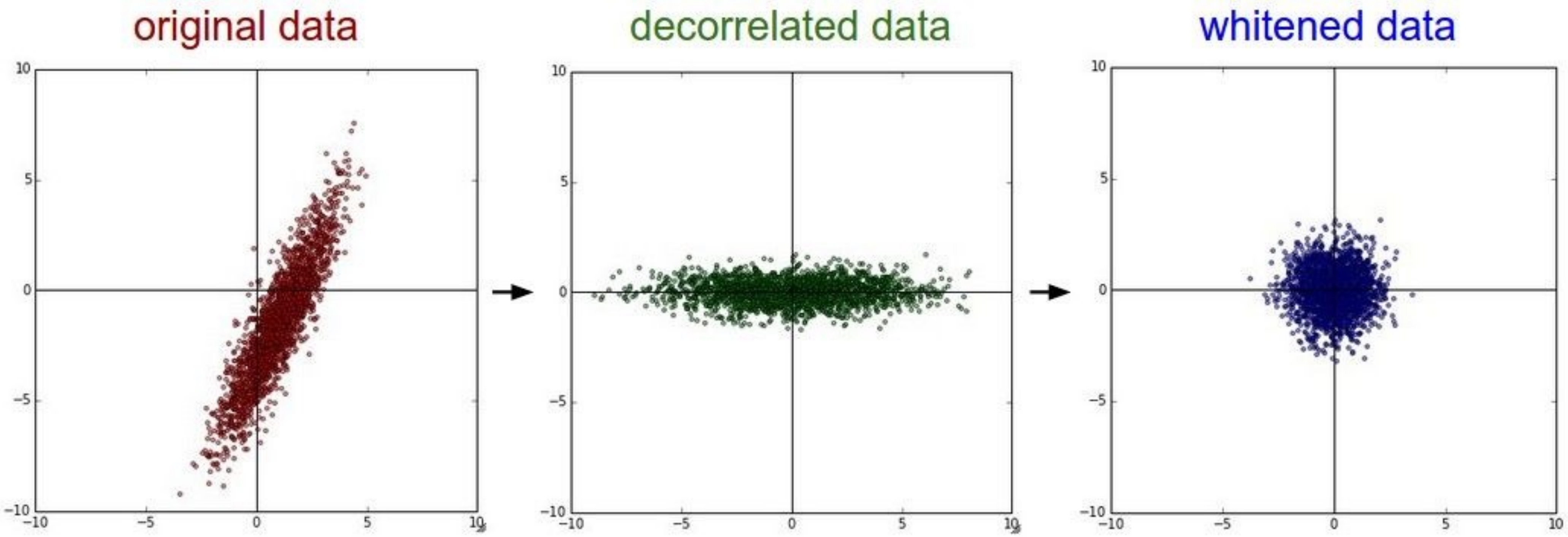

Normalized input: Speedup training





# Data Preprocessing

Not common to normalize variance, to do PCA or whitening

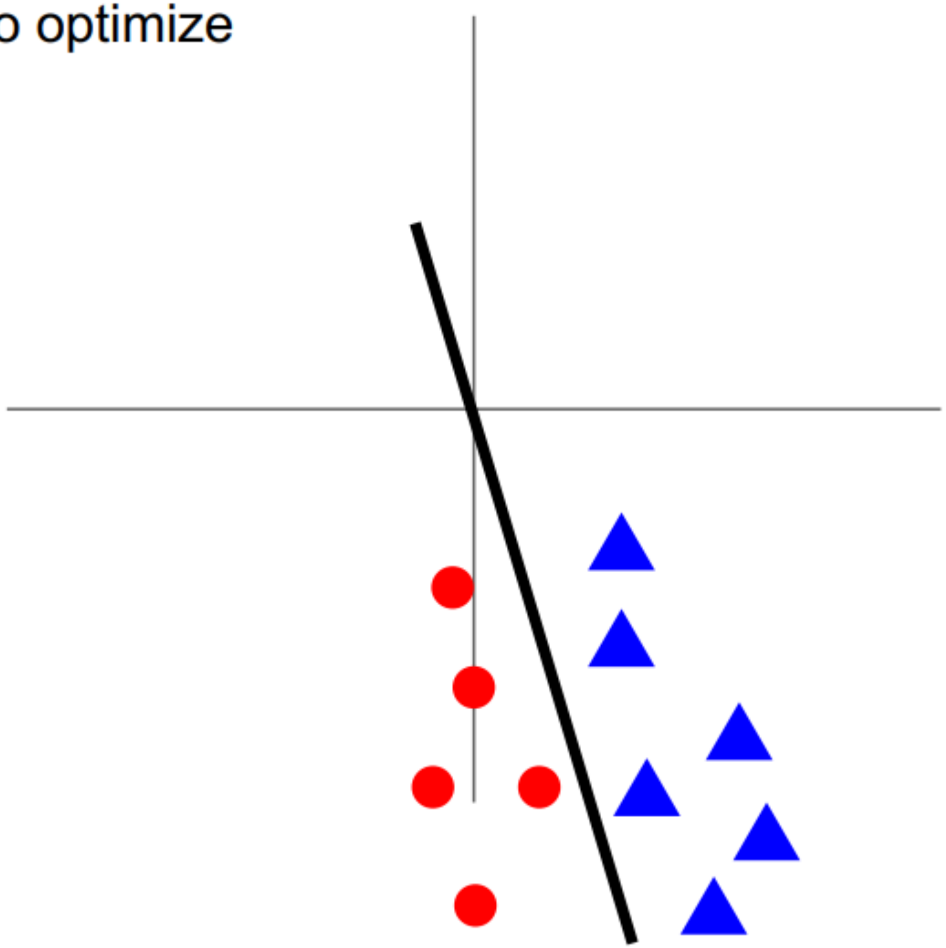



(data has diagonal covariance matrix)

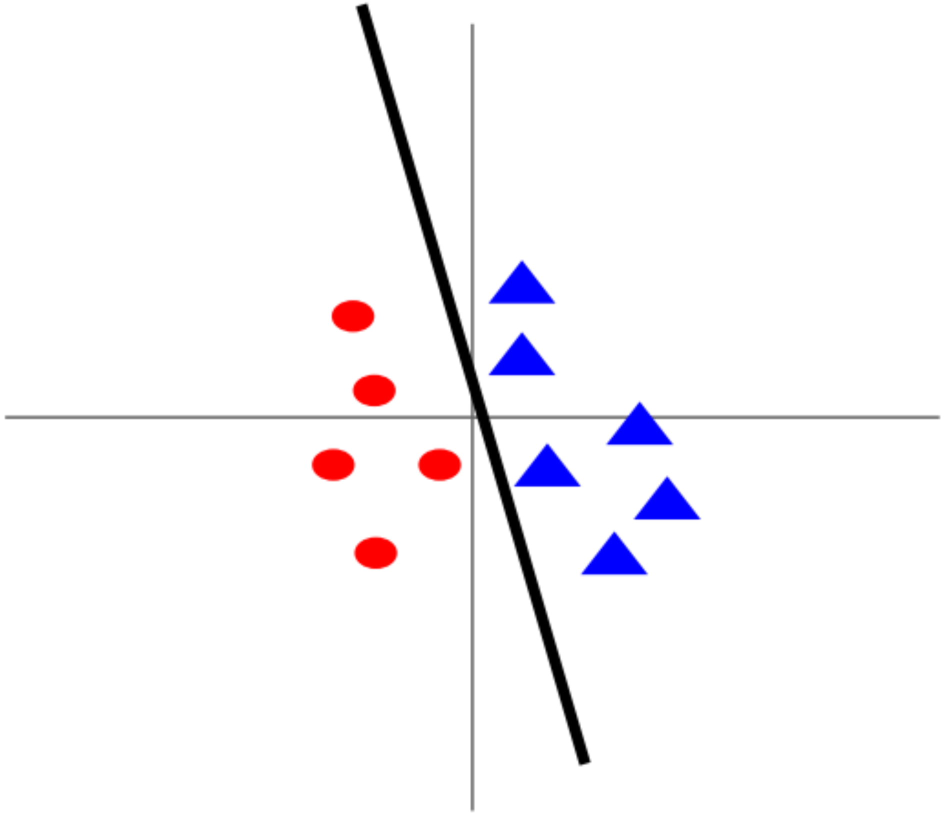
(covariance matrix is the identity matrix)

# 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

- Example: 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)

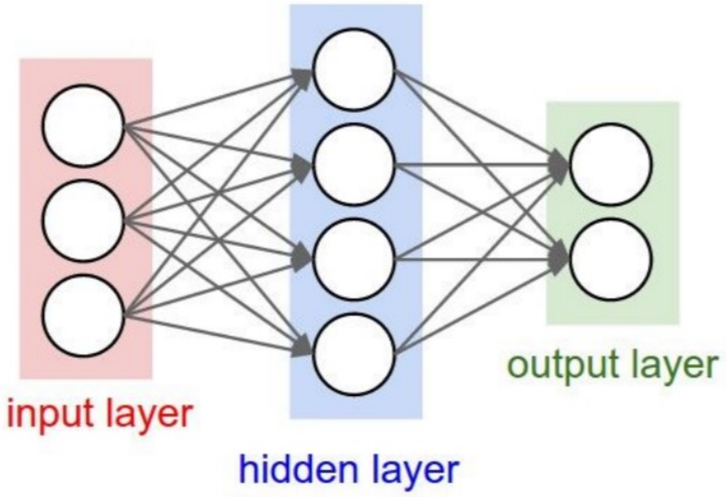
# Weight Initialization

# Weight initialization

- How to choose the starting point for the iterative process of optimization

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

- Key point: neurons with identical connections that are identically initialized will never diverge
  - All neurons of a layer do the same thing



# 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: Activation statistics

```python
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)
```

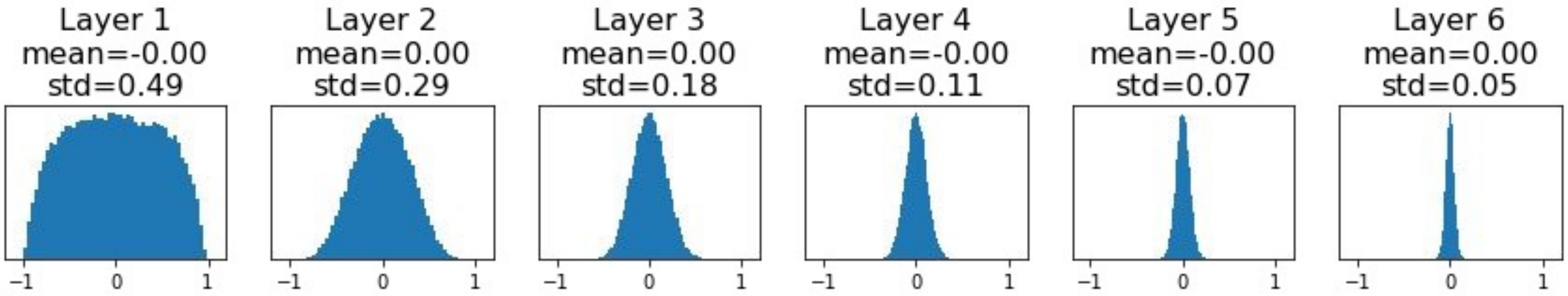
Forward pass for a 6-layer net with hidden size 4096

What will happen to the activations for the last layer?

All activations tend to zero for deeper network layers

What do the gradients dL/dW look like?

All zero, no learning =(



# Weight Initialization: Activation statistics

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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)
```

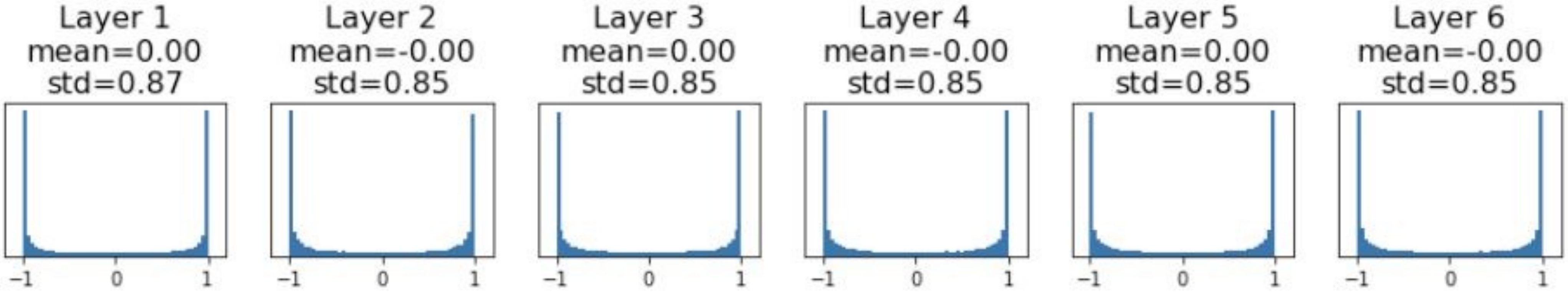
Increase std of initial weights from 0.01 to 0.05

What will happen to the activations for the last layer?

All activations saturate

What do the gradients look like?

Local gradients all zero, no learning =(



# Weight Initialization: "Xavier" Initialization

Initialization: Gaussian with zero mean and $1/\sqrt{\text{fan\_in}}$ standard deviation

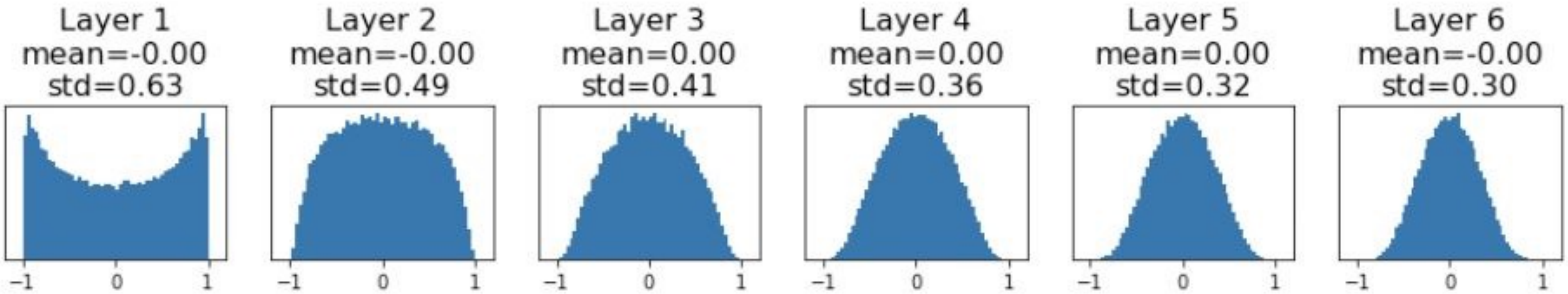
fan_in for fully connected layers = number of neurons in the previous layer

[Glorot et al., 2010]

```
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!




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

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

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

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

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

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

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

---

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

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

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

# Weight Initialization: “Xavier” Initialization

```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!

---

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

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

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

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

# Weight Initialization: “Xavier” Initialization

```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 $\text{filter\_size}^2 * \text{input\_channels}$

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

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

[Assume all $x_i$, $w_i$ are iid]

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

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

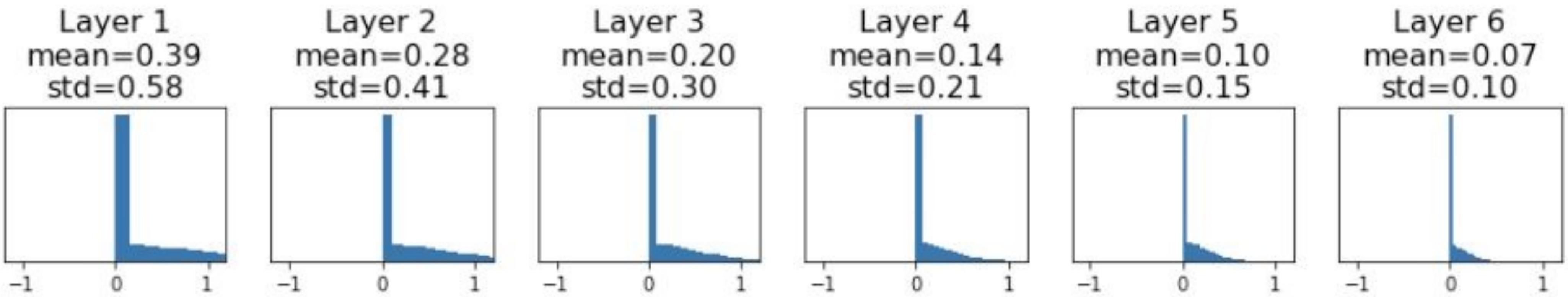
# Weight Initialization: What about ReLU?

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

Change from tanh to ReLU

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning =(



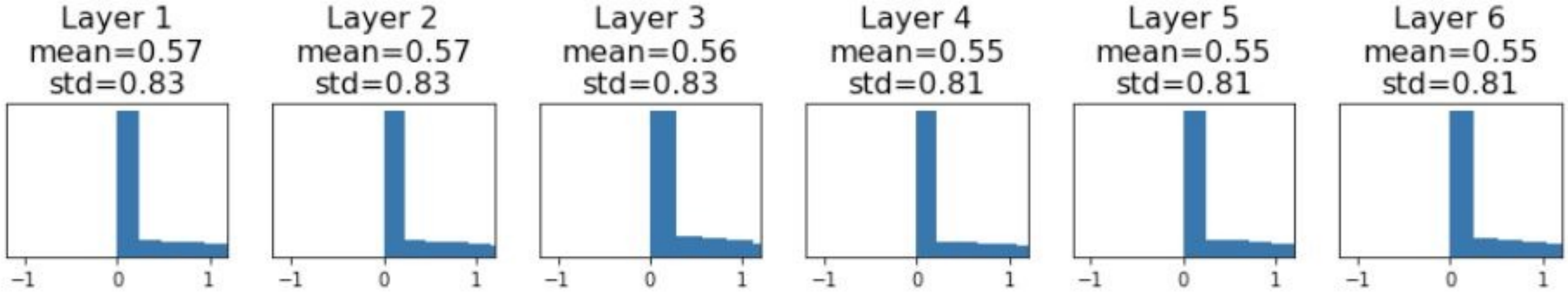
# Weight Initialization: Kaiming / MSRA Initialization

Initialization: gaussian with zero mean and $1/\sqrt{\text{fan}_{\text{in}}/2}$ standard deviation

ReLU correction: std = sqrt(2 / Din)

```
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)
```

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




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

# Proper initialization is an active area of research…

- ***Understanding the difficulty of training deep feedforward neural networks*** by Glorot and Bengio, 2010
- ***Exact solutions to the nonlinear dynamics of learning in deep linear neural networks*** by Saxe et al, 2013
- ***Random walk initialization for training very deep feedforward networks*** by Sussillo and Abbott, 2014
- ***Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification*** by He et al., 2015
- ***Data-dependent Initializations of Convolutional Neural Networks*** by Krähenbühl et al., 2015
- ***All you need is a good init***, Mishkin and Matas, 2015
- ***Fixup Initialization: Residual Learning Without Normalization***, Zhang et al, 2019
- ***The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks***, Frankle and Carbin, 2019

# 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 mini-batches); fiddle with architecture, learning rate, weight initialization

```
Finished epoch 195 / 200: cost 0.002694, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 196 / 200: cost 0.002674, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 197 / 200: cost 0.002655, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 198 / 200: cost 0.002635, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 199 / 200: cost 0.002617, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 200 / 200: cost 0.002597, train: 1.000000, val 1.000000, lr 1.000000e-03
finished optimization. best validation accuracy: 1.000000
```

Take the first 20 examples from CIFAR-10
turn off regularization
use simple vanilla SGD

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

# Hyperparameter search

- Larger Neural Networks typically require a long time to train
  - so performing hyperparameter search can take many days/weeks

- A single validation set of respectable size substantially simplifies the code base, without the need for cross-validation with multiple folds

# Validation strategy

- **coarse -> fine** validation in stages
  - Zoom in to smaller region of hyperparameters and sample very densely in them

- **First stage**: only a few epochs to get rough idea of what params work

- **Second stage**: longer running time, finer search … (repeat as necessary)

# 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

# For example: run coarse search for 5 epochs

```python
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-5, 5)
      lr = 10**uniform(-3, -6)

      trainer = ClassifierTrainer()
      model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
      trainer = ClassifierTrainer()
      best_model_local, stats = trainer.train(X_train, y_train, X_val, y_val,
                                   model, two_layer_net,
                                   num_epochs=5, reg=reg,
                                   update='momentum', learning_rate_decay=0.9,
                                   sample_batches = True, batch_size = 100,
                                   learning_rate=lr, verbose=False)
```

note it's best to optimize in log space!

```
val_acc: 0.412000, lr: 1.405206e-04, reg: 4.793564e-01, (1 / 100)
val_acc: 0.214000, lr: 7.231888e-06, reg: 2.321281e-04, (2 / 100)
val_acc: 0.208000, lr: 2.119571e-06, reg: 8.011857e+01, (3 / 100)
val_acc: 0.196000, lr: 1.551131e-05, reg: 4.374936e-05, (4 / 100)
val_acc: 0.079000, lr: 1.753300e-05, reg: 1.200424e+03, (5 / 100)
val_acc: 0.223000, lr: 4.215128e-05, reg: 4.196174e+01, (6 / 100)
val_acc: 0.441000, lr: 1.750259e-04, reg: 2.110807e-04, (7 / 100)
val_acc: 0.241000, lr: 6.749231e-05, reg: 4.226413e+01, (8 / 100)
val_acc: 0.482000, lr: 4.296863e-04, reg: 6.642555e-01, (9 / 100)
val_acc: 0.079000, lr: 5.401602e-06, reg: 1.599828e+04, (10 / 100)
val_acc: 0.154000, lr: 1.618508e-06, reg: 4.925252e-01, (11 / 100)
```

nice

# Now run finer search

```
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-5, 5)
      lr = 10**uniform(-3, -6)
```

adjust range

```
max_count = 100
for count in xrange(max_count):
      reg = 10**uniform(-4, 0)
      lr = 10**uniform(-3, -4)
```

```
val_acc: 0.527000, lr: 5.340517e-04, reg: 4.097824e-01, (0 / 100)
val_acc: 0.492000, lr: 2.279484e-04, reg: 9.991345e-04, (1 / 100)
val_acc: 0.512000, lr: 8.680827e-04, reg: 1.349727e-02, (2 / 100)
val_acc: 0.461000, lr: 1.028377e-04, reg: 1.220193e-02, (3 / 100)
val_acc: 0.460000, lr: 1.113730e-04, reg: 5.244309e-02, (4 / 100)
val_acc: 0.498000, lr: 9.477776e-04, reg: 2.001293e-03, (5 / 100)
val_acc: 0.469000, lr: 1.484369e-04, reg: 4.328313e-01, (6 / 100)
val_acc: 0.522000, lr: 5.586261e-04, reg: 2.312685e-04, (7 / 100)
val_acc: 0.530000, lr: 5.808183e-04, reg: 8.259964e-02, (8 / 100)
val_acc: 0.489000, lr: 1.979168e-04, reg: 1.010889e-04, (9 / 100)
val_acc: 0.490000, lr: 2.036031e-04, reg: 2.406271e-03, (10 / 100)
val_acc: 0.475000, lr: 2.021162e-04, reg: 2.287807e-01, (11 / 100)
val_acc: 0.460000, lr: 1.135527e-04, reg: 3.905040e-02, (12 / 100)
val_acc: 0.515000, lr: 6.947668e-04, reg: 1.562808e-02, (13 / 100)
val_acc: 0.531000, lr: 9.471549e-04, reg: 1.433895e-03, (14 / 100)
val_acc: 0.509000, lr: 3.140888e-04, reg: 2.857518e-01, (15 / 100)
val_acc: 0.514000, lr: 6.438349e-04, reg: 3.033781e-01, (16 / 100)
val_acc: 0.502000, lr: 3.921784e-04, reg: 2.707126e-04, (17 / 100)
val_acc: 0.509000, lr: 9.752279e-04, reg: 2.850865e-03, (18 / 100)
val_acc: 0.500000, lr: 2.412048e-04, reg: 4.997821e-04, (19 / 100)
val_acc: 0.466000, lr: 1.319314e-04, reg: 1.189915e-02, (20 / 100)
val_acc: 0.516000, lr: 8.039527e-04, reg: 1.528291e-02, (21 / 100)
```

But this best cross-validation result is worrying. Why?

**Careful with best values on border**

# Random search vs. grid search

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

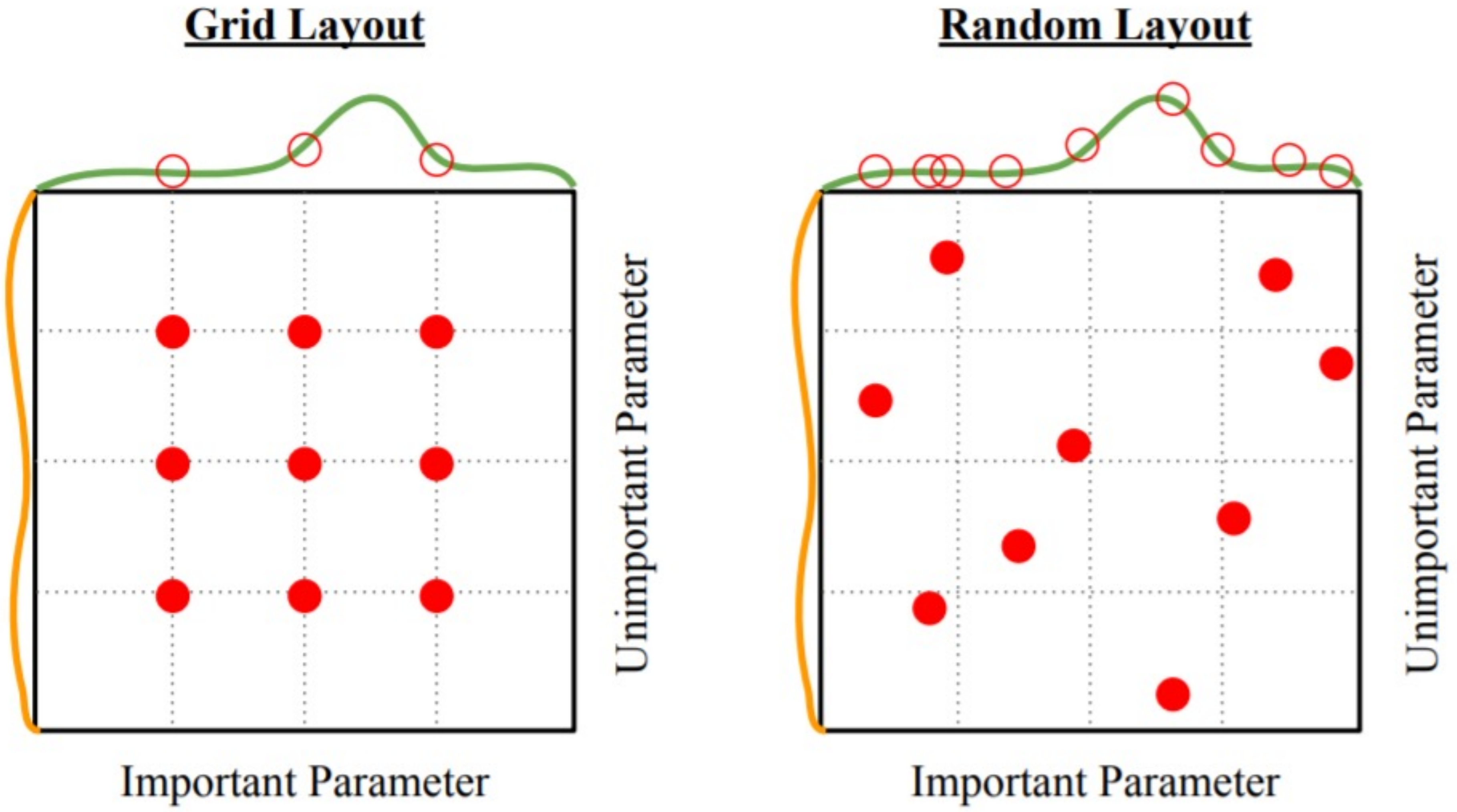


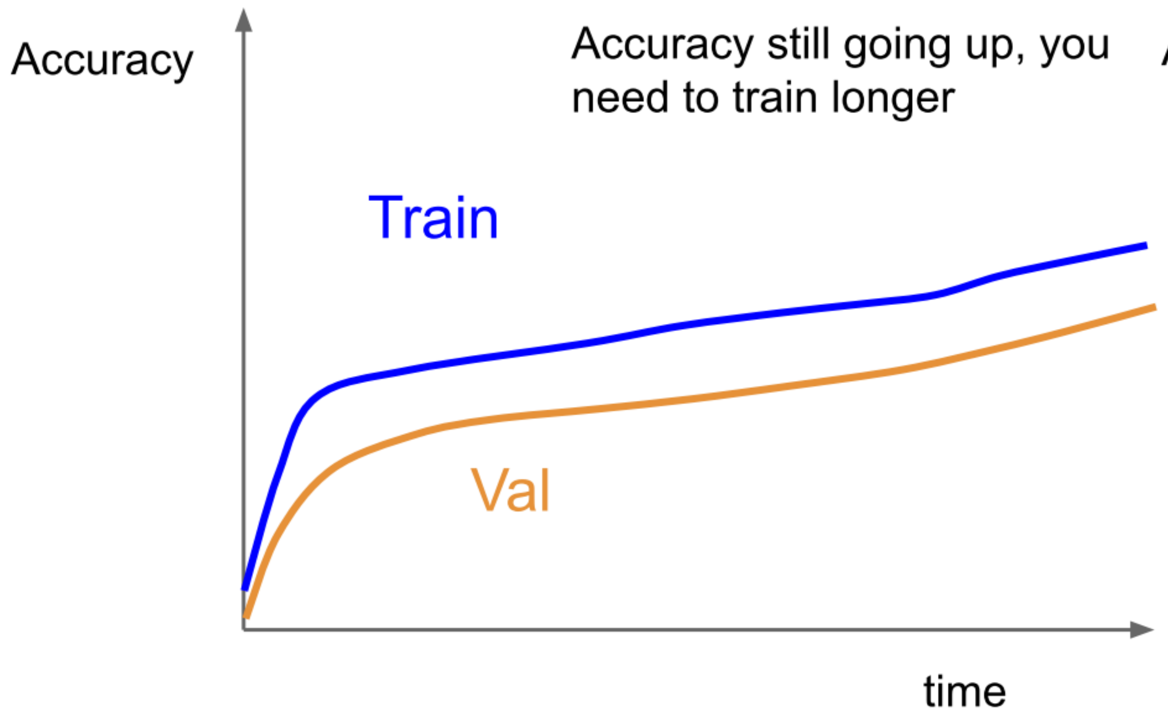

Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

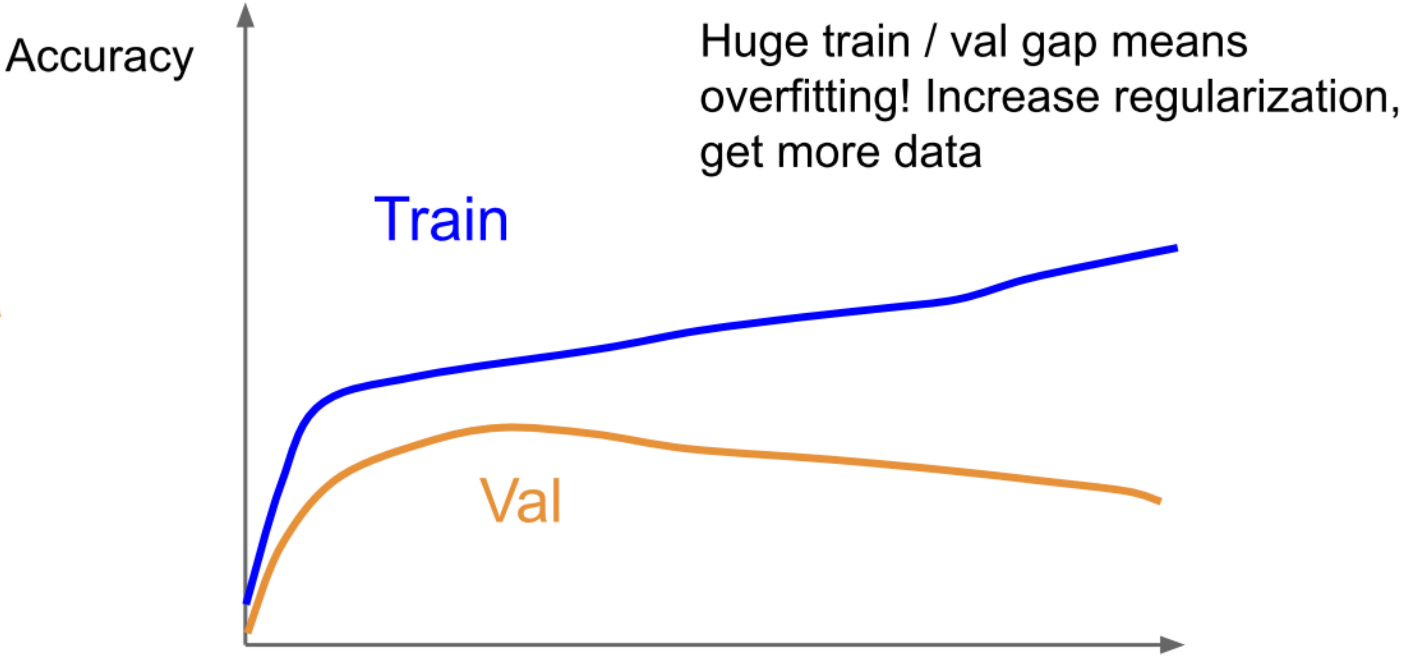
# Random search

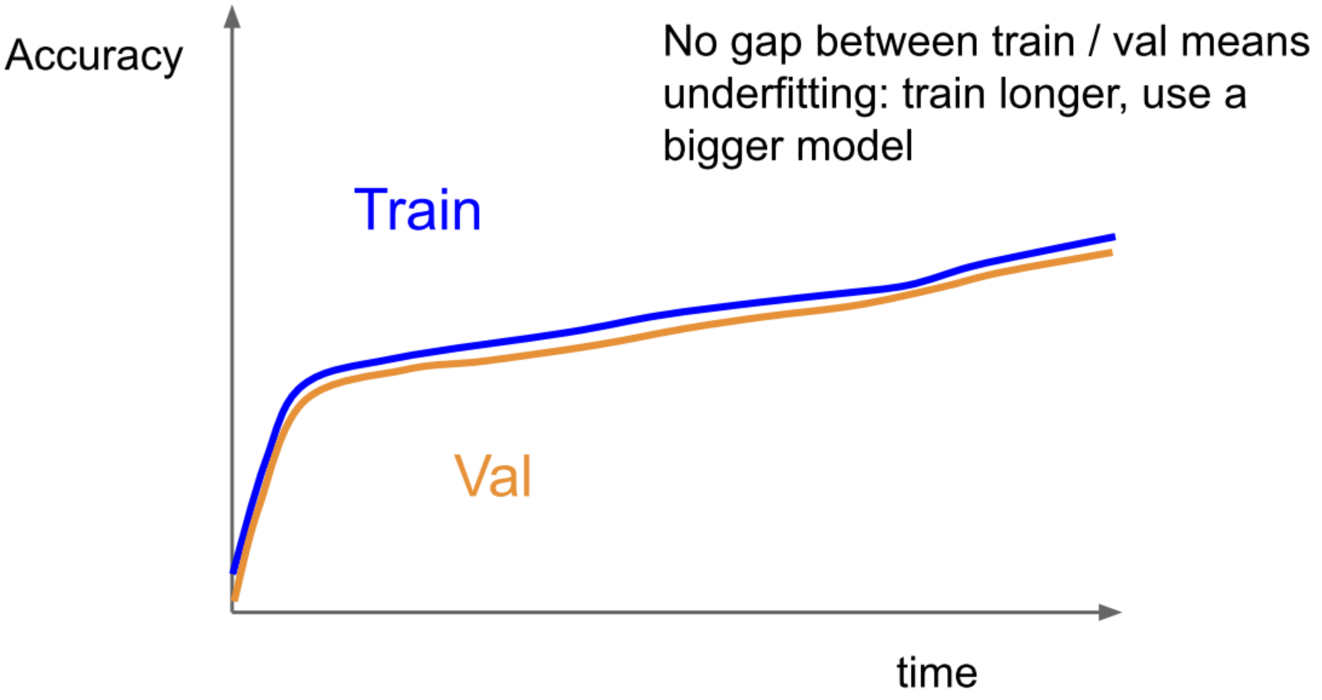
- Random search is more effective and richly exploring when:
  - The performance may not be such sensitive to the value of all hyperparameters (some parameters are actually much more important)
    - We don’t know it in advance
    - More distinct values of the more important hyperparameter are tried.
    - Especially when the number of hyperparameters becomes larger

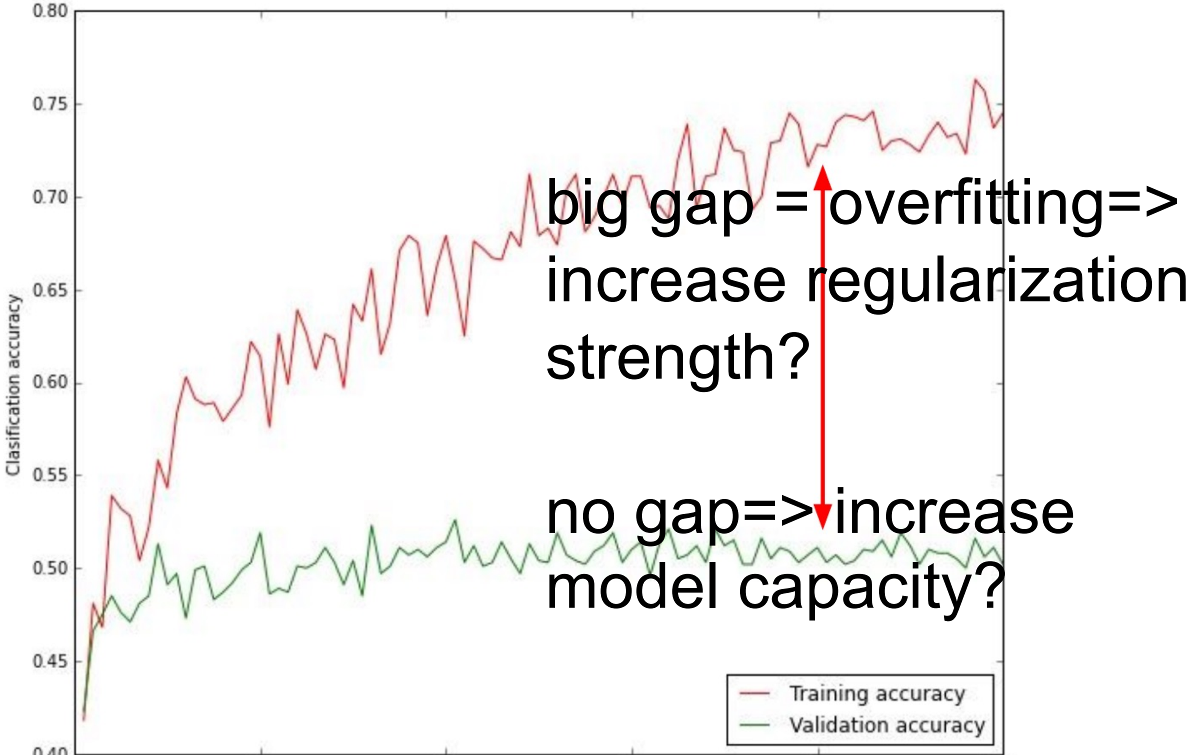
# Choosing Hyperparameters

- 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

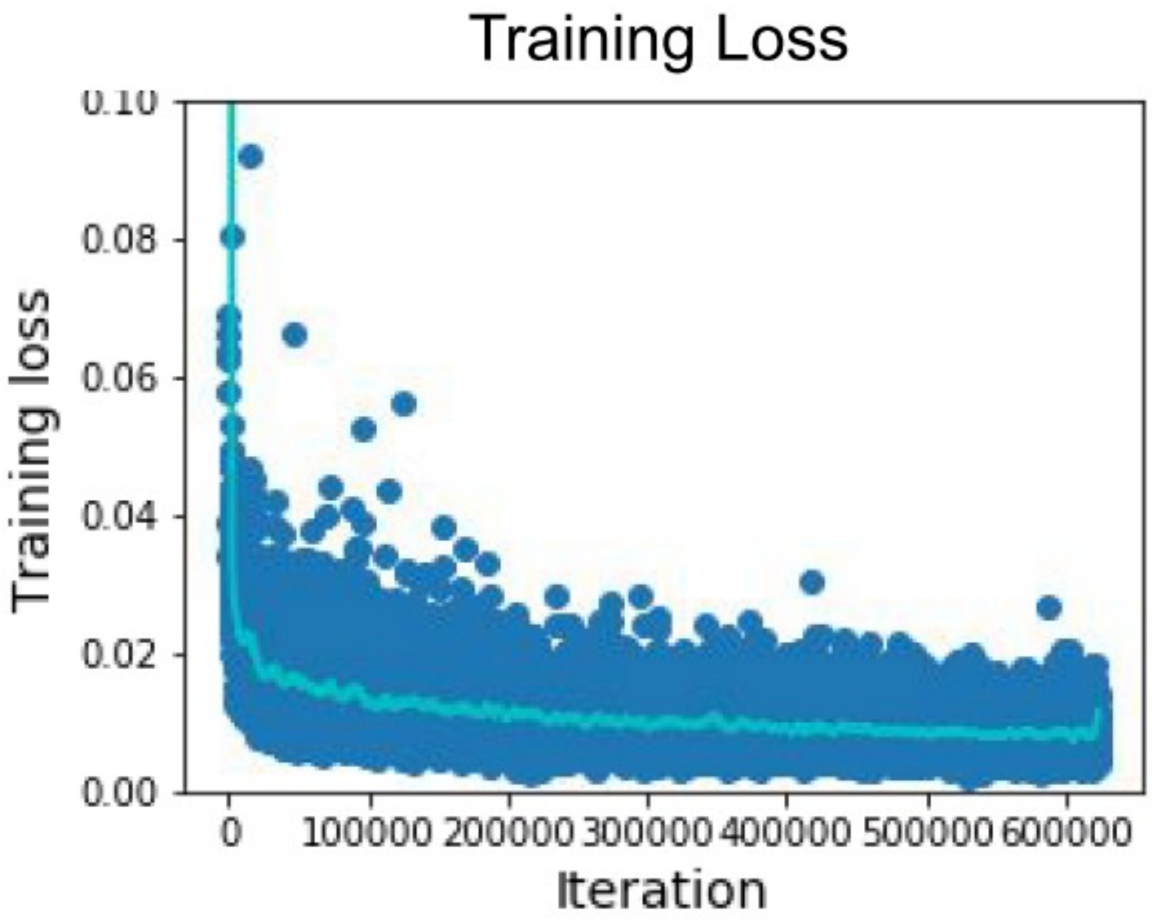

Accuracy
Accuracy still going up, you need to train longer
Train
Val
time

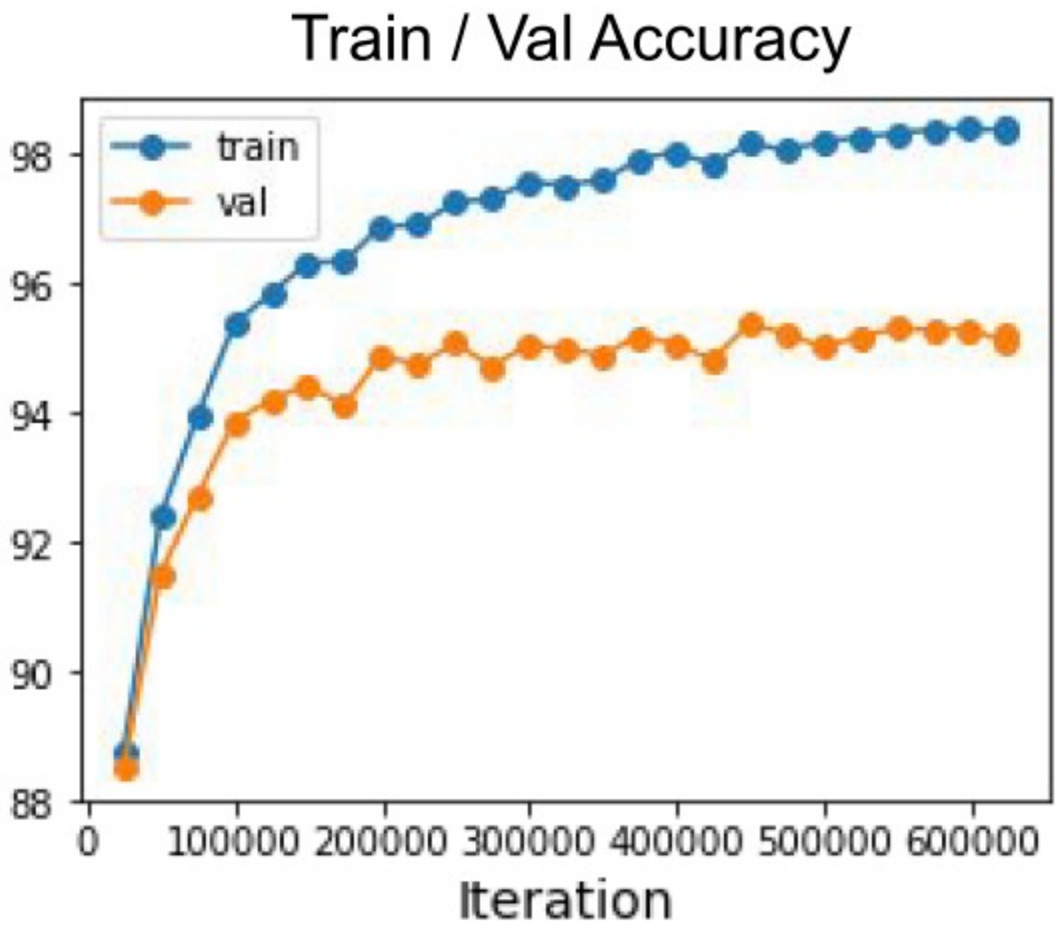

Accuracy
Huge train / val gap means overfitting! Increase regularization, get more data
Train
Val


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


0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
Clasification accuracy
big gap = overfitting=> increase regularization strength?
no gap=> increase model capacity?
Training accuracy
Validation accuracy

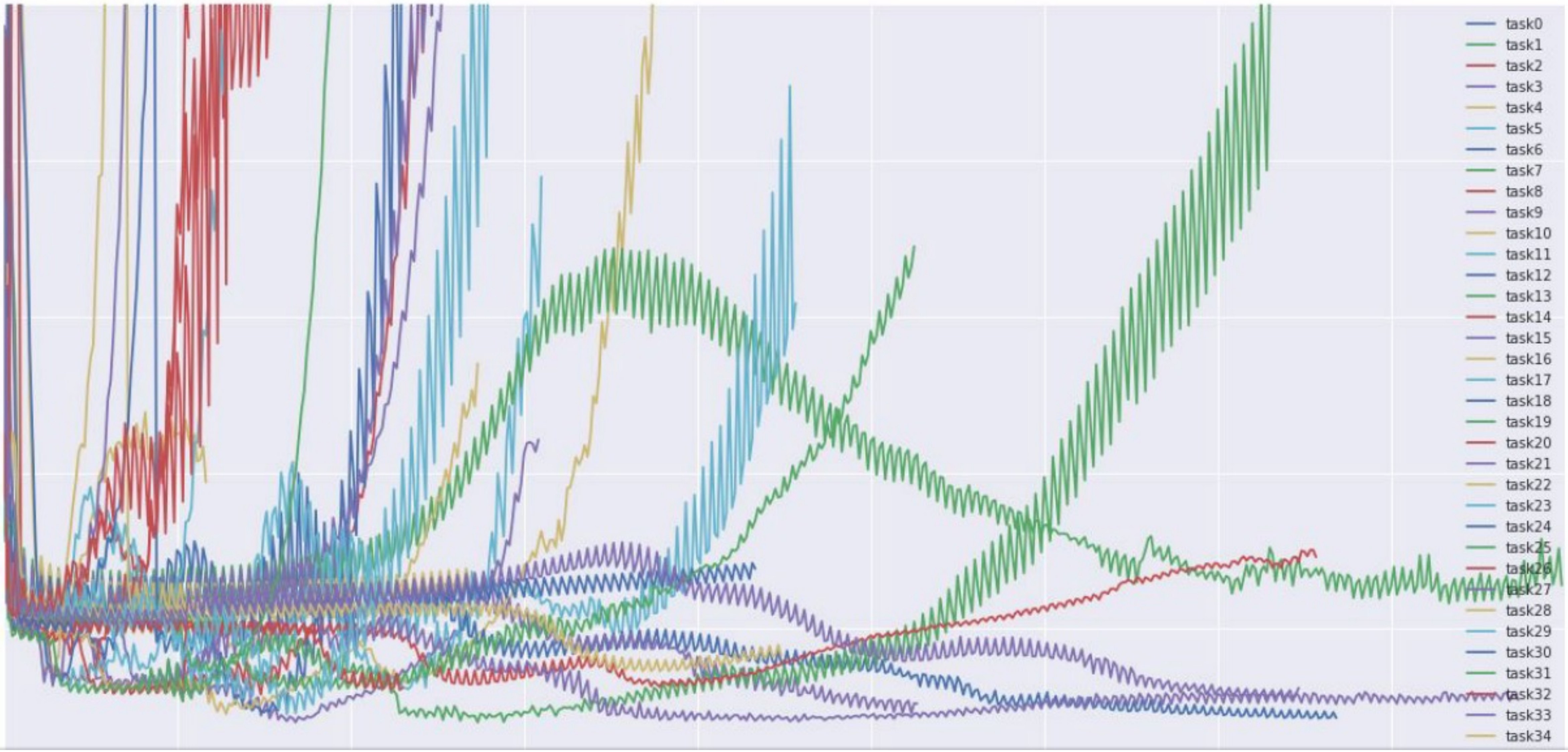
# Look at learning curves




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

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



# 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

# Hyperparameter selection

- Finding a good set of hyperparameters to provide better convergence
  - initial learning rate $\alpha$
  - regularization strength (L2 penalty, dropout strength)
  - # of hidden units and # of layers
  - mini-batch size
  - decay schedule (such as the decay constant), update type
  - parameters of optimization algorithms (momentum, adam, … )
    - These are usually fixed to $\beta_1 = 0.9$, $\beta_2 = 0.999$, and $\epsilon = 10^{-8}$ or $10^{-7}$

# Babysitting one model vs. training models in parallel

- When we do not have sufficient computational resources to train a lot of models
  - Watching performance of one model during the time and tune its parameters by nudging them up and down
- Train many different models in parallel (with different hyperparameetrs) and just pick the one that works best
- Babysitting one model called Panda while training many models in parallel called Cavier approach for selecting hyperparameters

# Summary

- Activation Functions (use ReLU)
- Data Preprocessing (subtract mean and some times scale according to standard deviation)
- Weight Initialization (use Xavier init)
- Hyper-parameter Optimization (random sample hyperparams, in log space when appropriate)
- Babysitting the learning process

# Setting up a problem

- Obtain training data
  - Use appropriate representation for inputs and outputs
- Choose the appropriate loss function
  - Choose regularization
- Choose network architecture
  - More neurons need more data
  - Deep is better, but harder to train
- Choose heuristics (batch norm, dropout, etc.)
- Choose optimization algorithm
  - E.g. Adam
- Perform a grid search for hyper parameters (learning rate, regularization parameter, …) on held-out data
- Train
  - Evaluate periodically on validation data, for early stopping if required

# Resource

- Please see the following notes:
  - http://cs231n.github.io/neural-networks-2/
  - http://cs231n.github.io/neural-networks-3/