Lecture 7:

Neural Networks

Neural networks: the original linear classifier

(**Before**) Linear score function: $f = Wx$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

Neural networks: 2 layers

(**Before**) Linear score function: $f = Wx$

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

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

(In practice we will usually add a learnable bias at each layer as well)

Neural networks: also called fully connected network

(**Before**) Linear score function: $f = Wx$

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

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

"Neural Network" is a very broad term; these are more accurately called "fully-connected networks" or sometimes "multi-layer perceptrons" (MLP)

(In practice we will usually add a learnable bias at each layer as well)

Neural networks: 3 layers

(**Before**) Linear score function: $f = Wx$

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

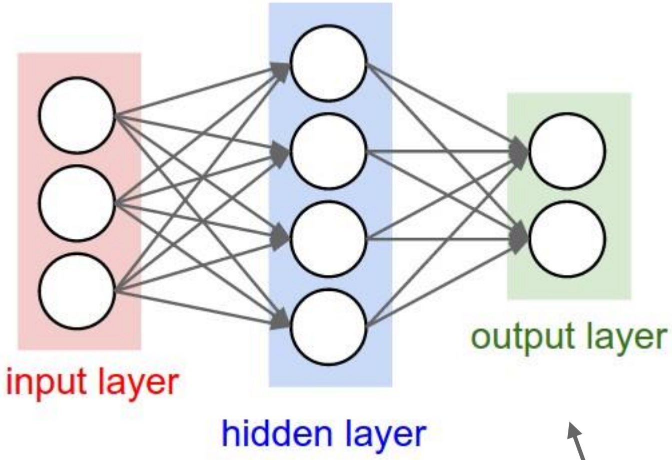
or 3-layer Neural Network

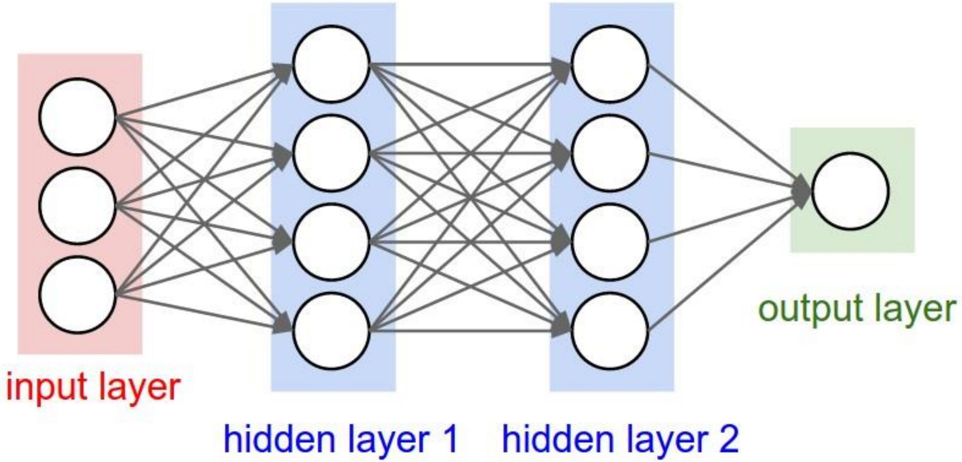
$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

(In practice we will usually add a learnable bias at each layer as well)

Neural Networks: Architectures



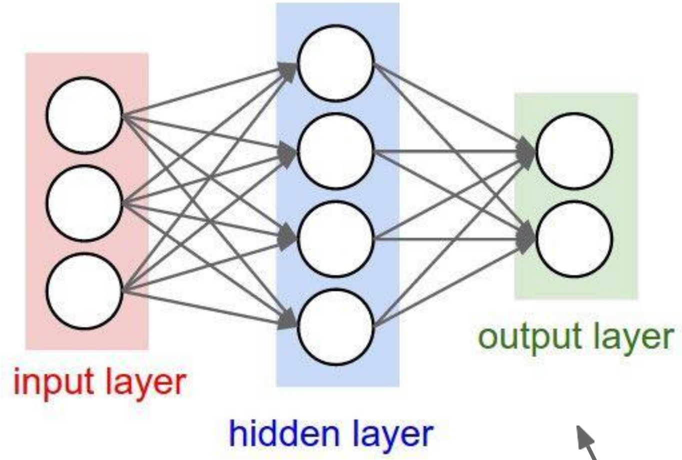


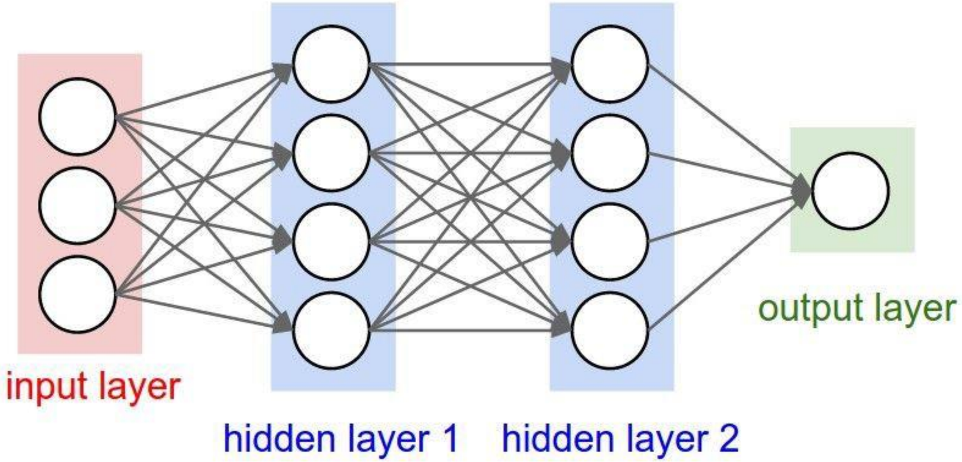
"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

"Fully-connected" layers

Neural networks: Architectures



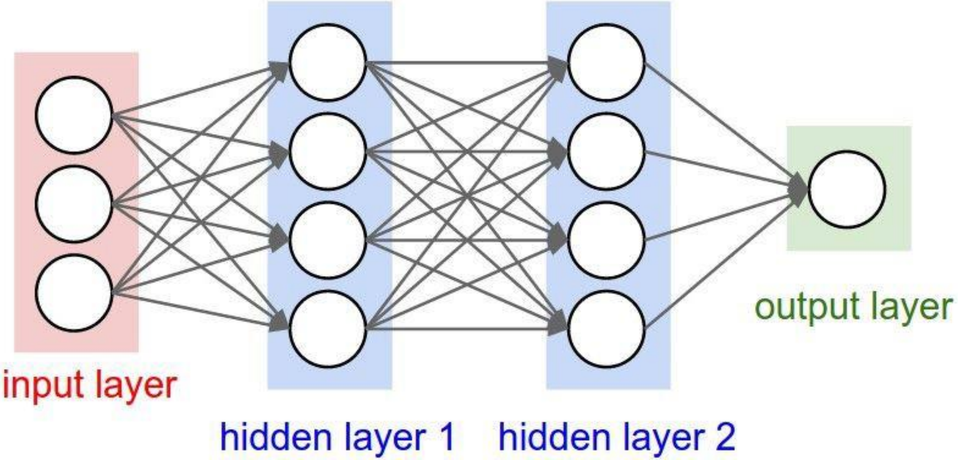


"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

"Fully-connected" layers

Example feed-forward computation of a neural network

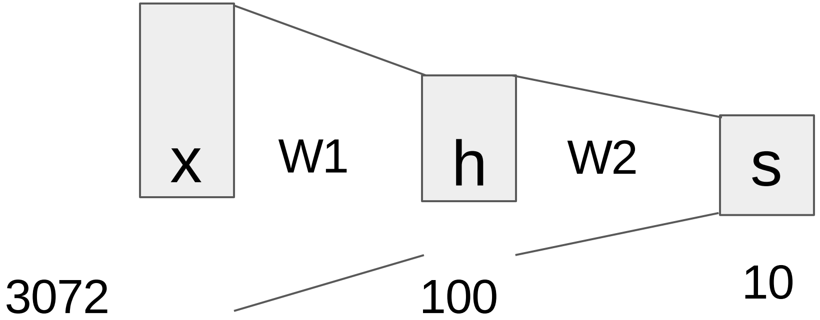



```python
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Neural networks: hierarchical computation

(**Before**) Linear score function: $f = Wx$

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

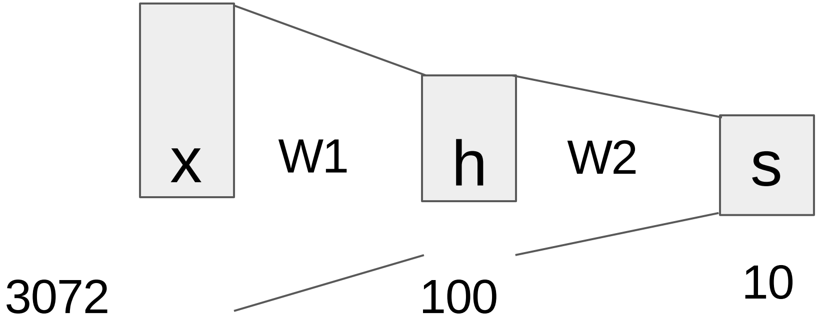


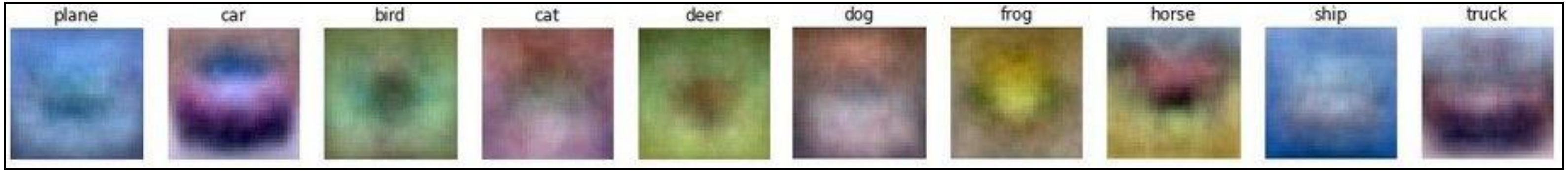
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural networks: learning 100s of templates

(**Before**) Linear score function: $f = Wx$

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

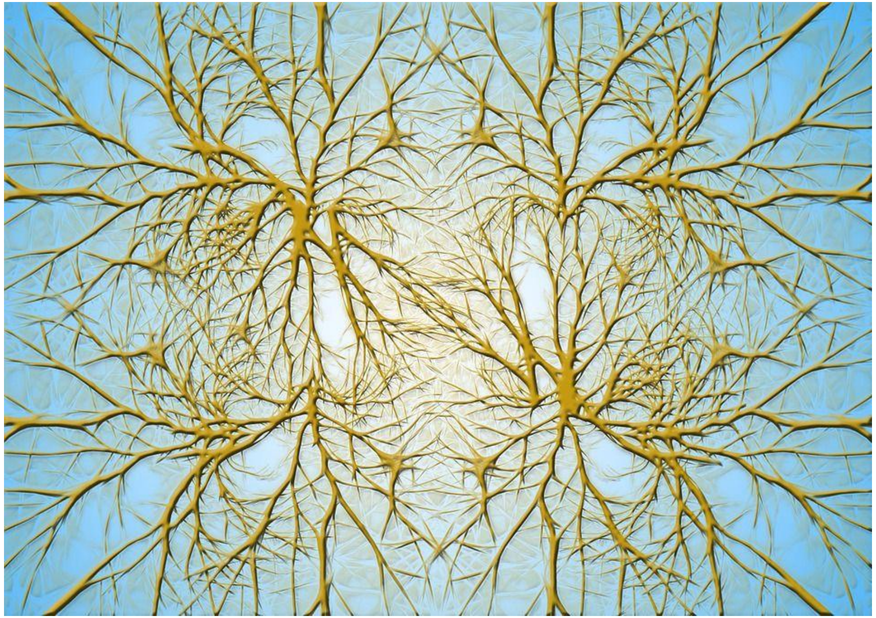




Learn 100 templates instead of 10.

Share templates between classes

Biological Neurons:
Complex connectivity patterns



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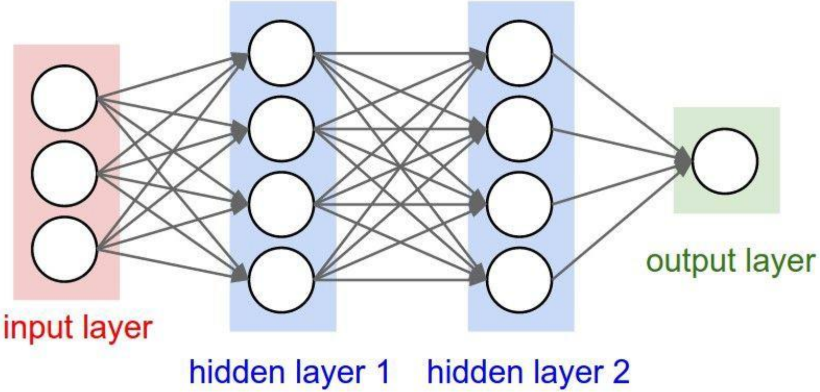
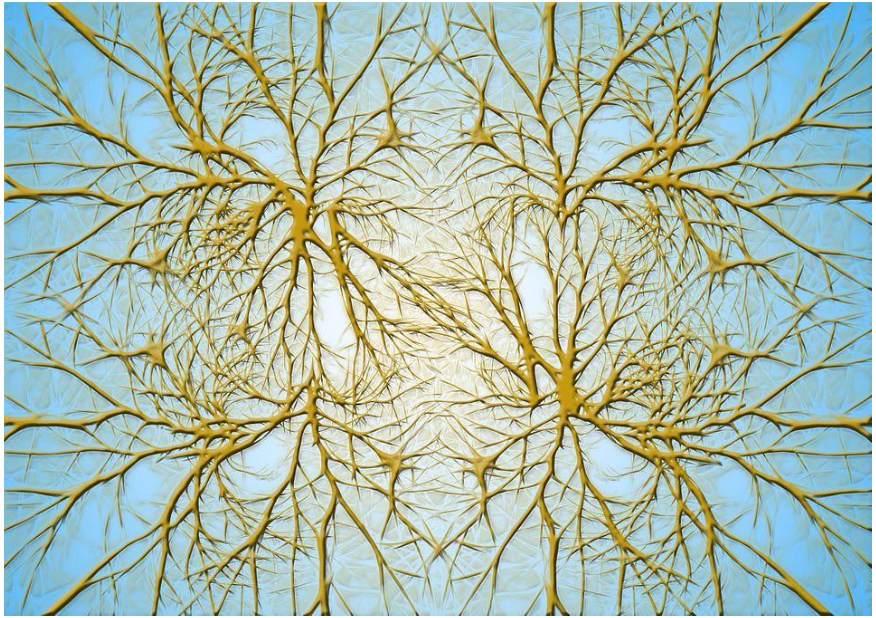
Neurons in a neural network:
Organized into regular layers for computational efficiency



Biological Neurons: Complex connectivity patterns



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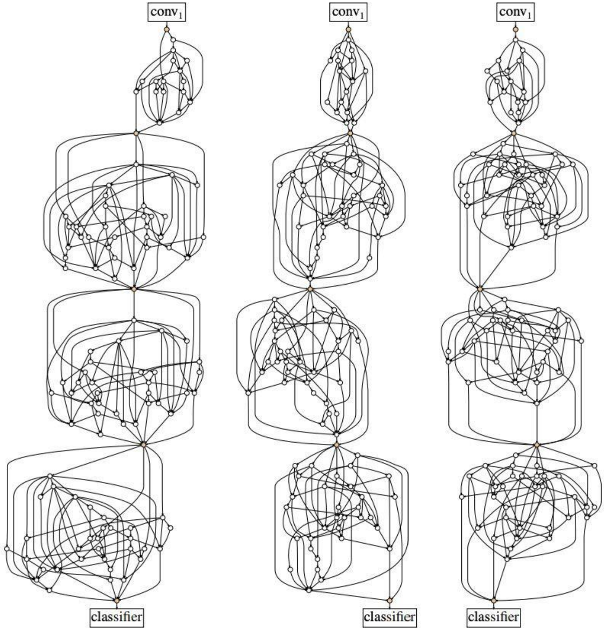
But neural networks with random connections can work too!



Xie et al, "Exploring Randomly Wired Neural Networks for Image Recognition", arXiv 2019

Training Neural Networks

A bit of history...

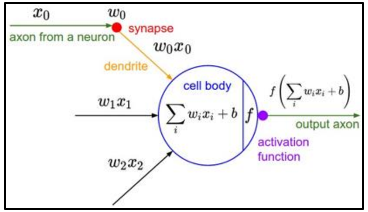
A bit of history

The **Mark I Perceptron** machine was the first implementation of the perceptron algorithm.

The machine was connected to a camera that used 20×20 cadmium sulfide photocells to produce a 400-pixel image.

recognized
letters of the alphabet

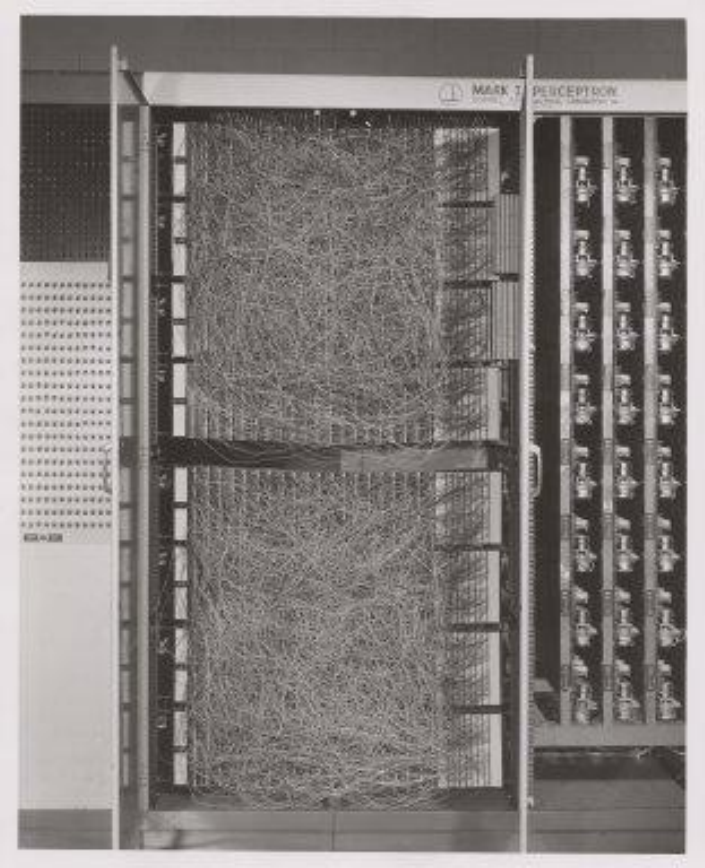
$$f(x) = \begin{cases} 1 & \text{if } w \cdot x + b > 0 \\ 0 & \text{otherwise} \end{cases}$$



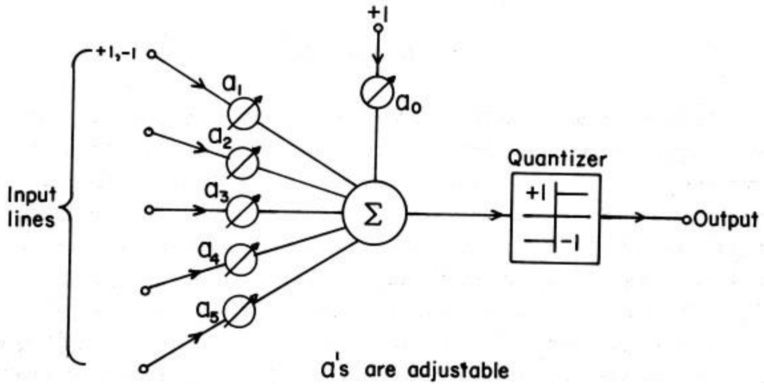
update rule:

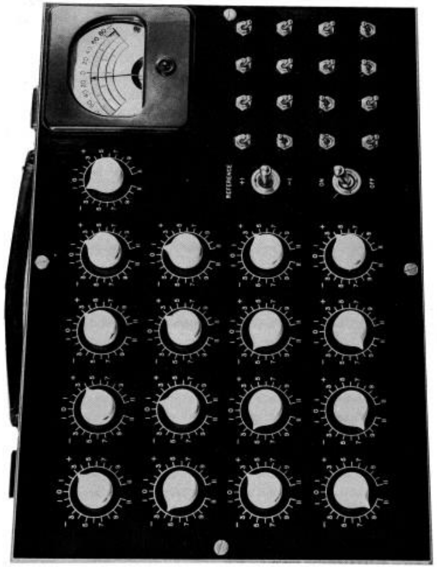
$$w_i(t+1) = w_i(t) + \alpha(d_j - y_j(t))x_{j,i},$$

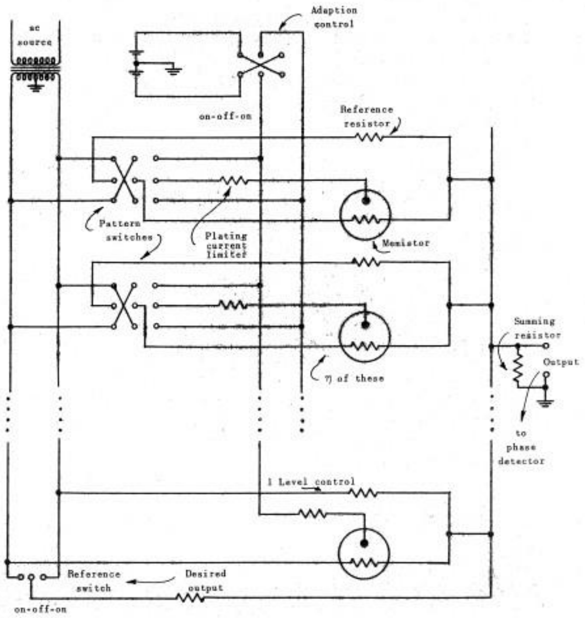
Frank Rosenblatt, ~1957: Perceptron



A bit of history

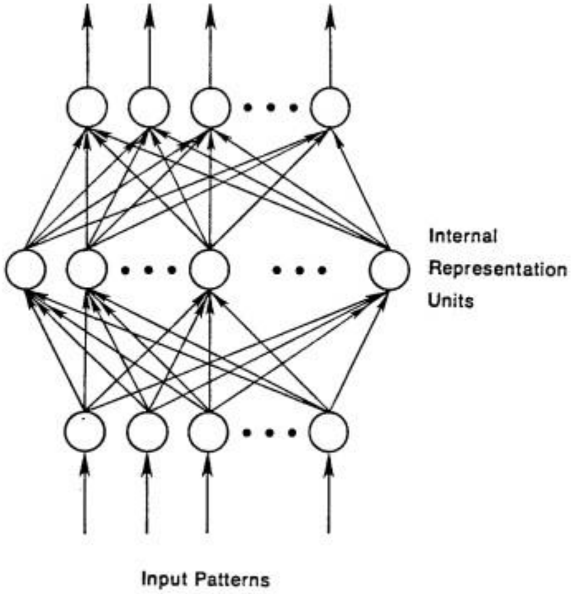






Widrow and Hoff, ~1960: Adaline/Madaline

A bit of history



To be more specific, then, let

$$E_p = \frac{1}{2}\sum_j (t_{pj} - o_{pj})^2 \qquad (2)$$

be our measure of the error on input/output pattern p and let $E = \sum E_p$ be our overall measure of the error. We wish to show that the delta rule implements a gradient descent in E when the units are linear. We will proceed by simply showing that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_{pi},$$

which is proportional to $\Delta_p w_{ji}$ as prescribed by the delta rule. When there are no hidden units it is straightforward to compute the relevant derivative. For this purpose we use the chain rule to write the derivative as the product of two parts: the derivative of the error with respect to the output of the unit times the derivative of the output with respect to the weight.

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial w_{ji}}. \qquad (3)$$

The first part tells how the error changes with the output of the jth unit and the second part tells how much changing w_{ji} changes that output. Now, the derivatives are easy to compute. First, from Equation 2

$$\frac{\partial E_p}{\partial o_{pj}} = -(t_{pj} - o_{pj}) = -\delta_{pj}. \qquad (4)$$

Not surprisingly, the contribution of unit u_j to the error is simply proportional to δ_{pj}. Moreover, since we have linear units,

$$o_{pj} = \sum_i w_{ji} i_{pi}, \qquad (5)$$

from which we conclude that

$$\frac{\partial o_{pj}}{\partial w_{ji}} = i_{pi}.$$

Thus, substituting back into Equation 3, we see that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_i \qquad (6)$$

recognizable maths

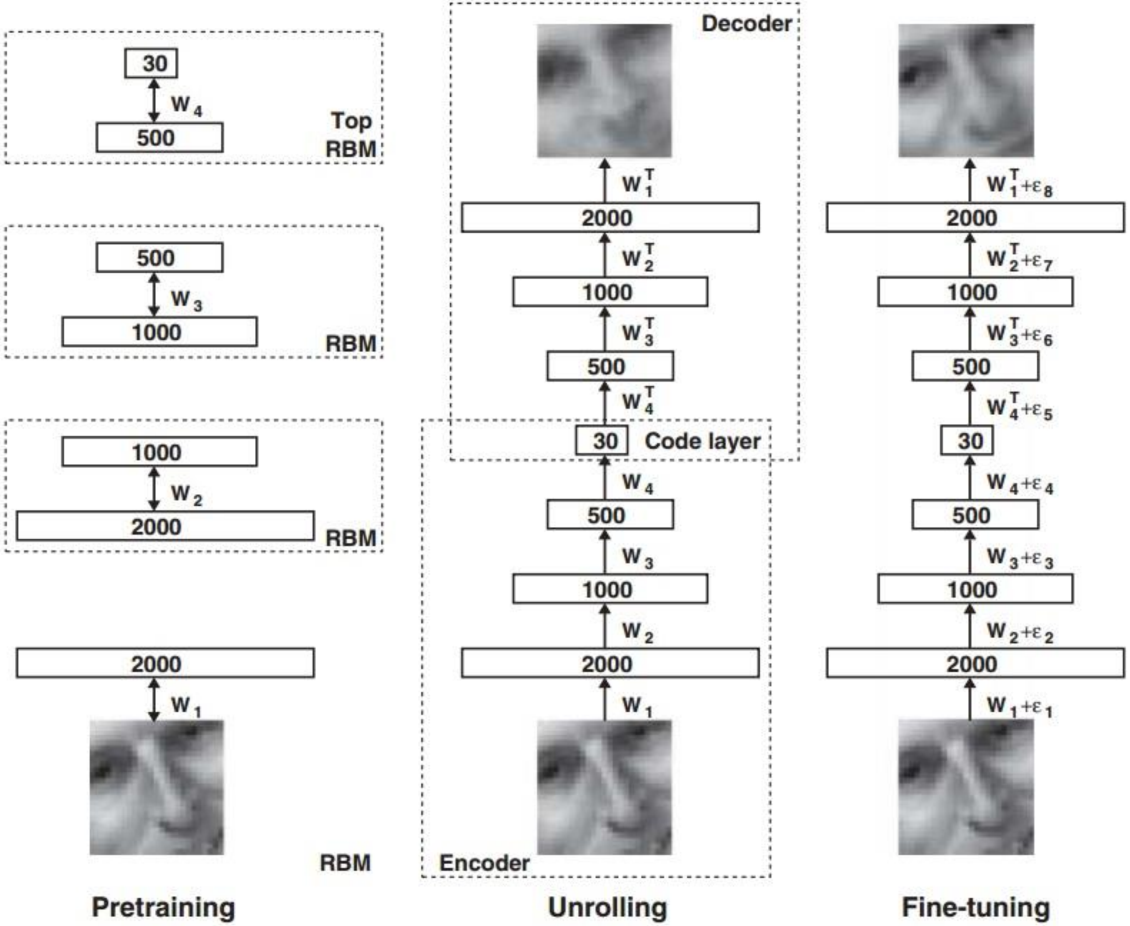
Rumelhart et al. 1986: First time back-propagation became popular

A bit of history

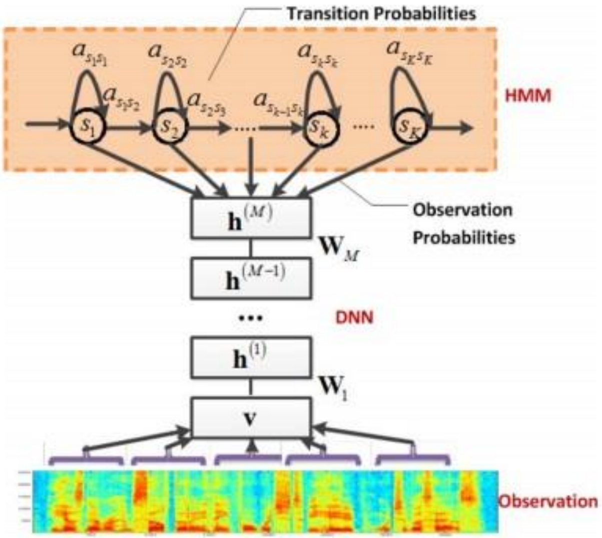
[Hinton and Salakhutdinov 2006]

Reinvigorated research in Deep Learning

NOT NEURAL NETWORKS!

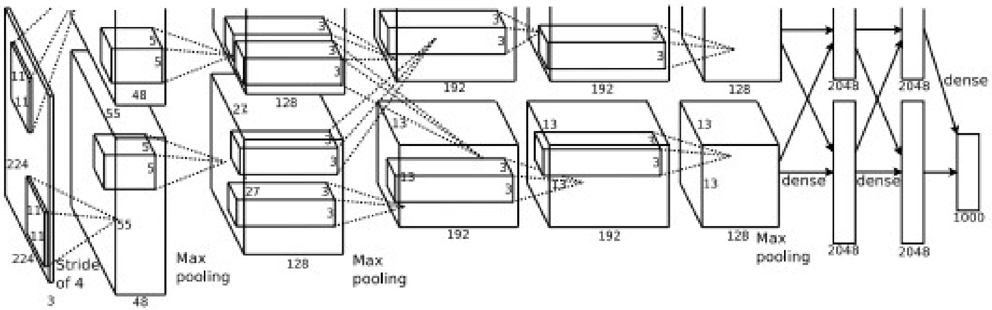


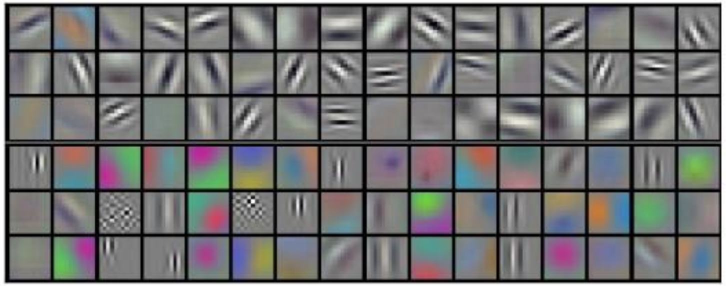
First strong results in neural nets



Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition
George Dahl, Dong Yu, Li Deng, Alex Acero, 2010

Imagenet classification with deep convolutional neural networks
Alex Krizhevsky, Ilya Sutskever, Geoffrey E Hinton, 2012

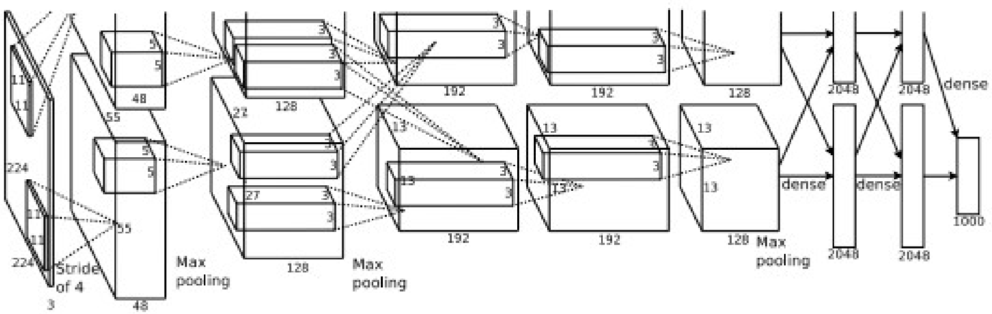


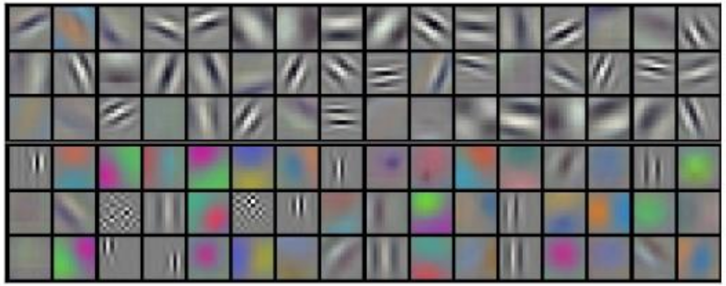


First strong results

Dropout training and ReLU’s...

Imagenet classification with deep convolutional neural networks
Alex Krizhevsky, Ilya Sutskever, Geoffrey E Hinton, 2012





Overview

1. **One time setup**
   activation functions, preprocessing, weight initialization, regularization, gradient checking
1. **Training dynamics**
   babysitting the learning process, parameter updates, hyperparameter optimization
1. **Evaluation**
   model ensembles

Activation Functions

Activation Function: **Non-linearities**

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \boxed{\max(0,} W_1 x)$

The function $\max(0, z)$ is called the **activation function.**

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

Activation Function: **Non-linearities**

(**Before**) Linear score function: $f = Wx$

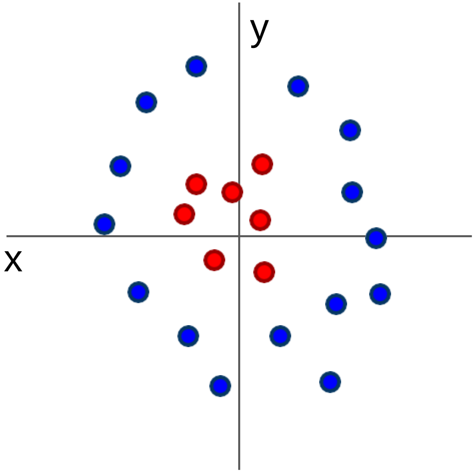
(**Now**) 2-layer Neural Network $f = W_2 \boxed{\max(0,} W_1 x)$

The function $\max(0, z)$ is called the **activation function.**
Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x \qquad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

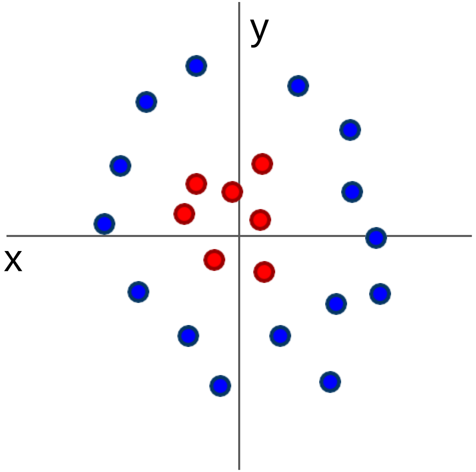
A: We end up with a linear classifier again!

Why do we want non-linearity?



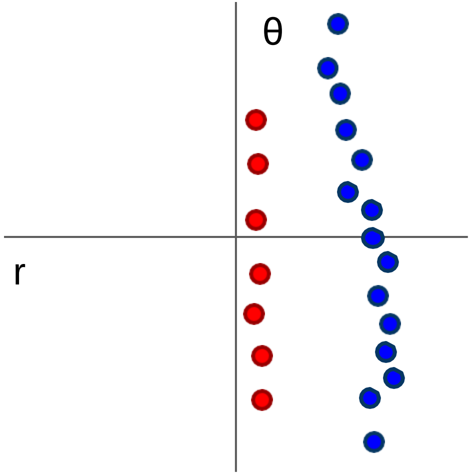
Cannot separate red and blue points with linear classifier

Why do we want non-linearity?



Cannot separate red and blue points with linear classifier

$f(x, y) = (r(x, y), \theta(x, y))$

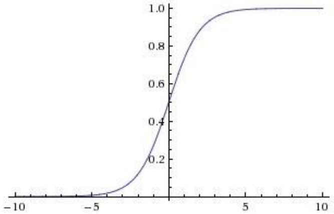


After applying feature transform, points can be separated by linear classifier

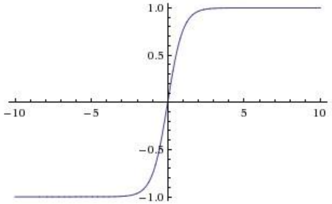
Activation Functions

Sigmoid

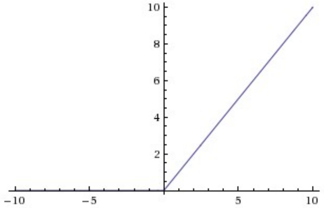
$$\sigma(x) = 1/(1 + e^{-x})$$



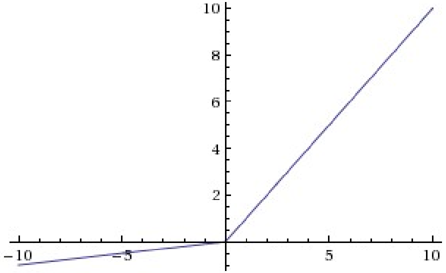
tanh tanh(x)



ReLU max(0,x)



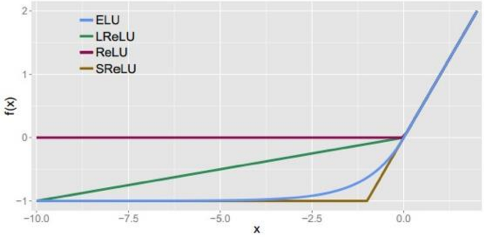
Leaky ReLU
max(0.1x, x)



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

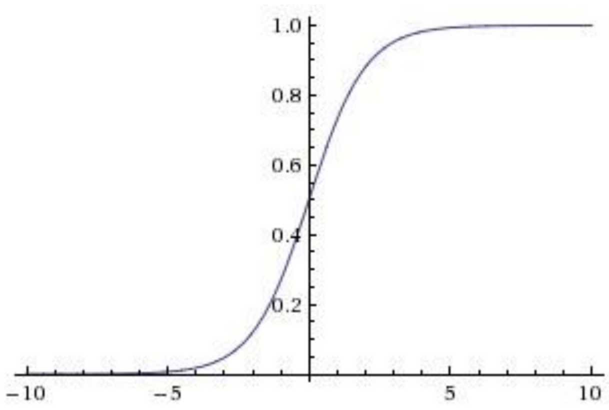
ELU

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



Activation Functions

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

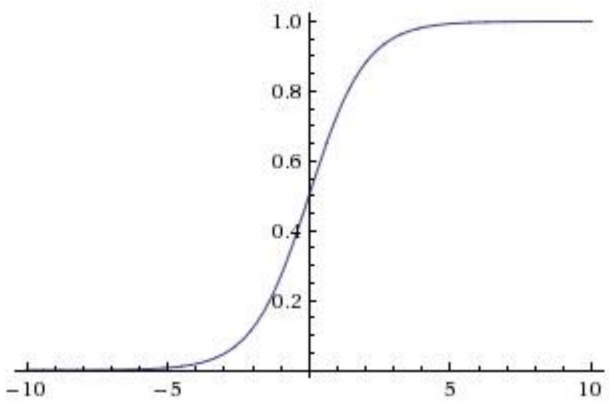


Sigmoid

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

Activation Functions

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



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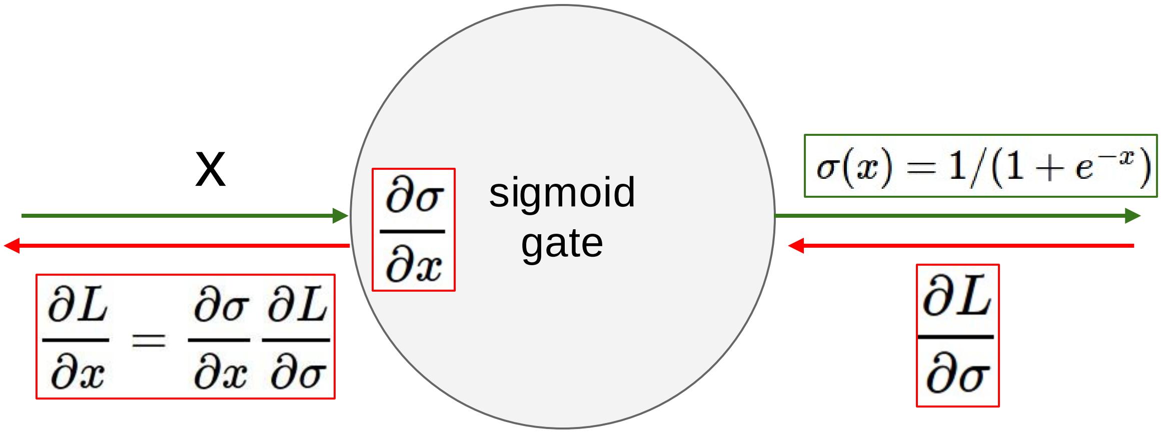
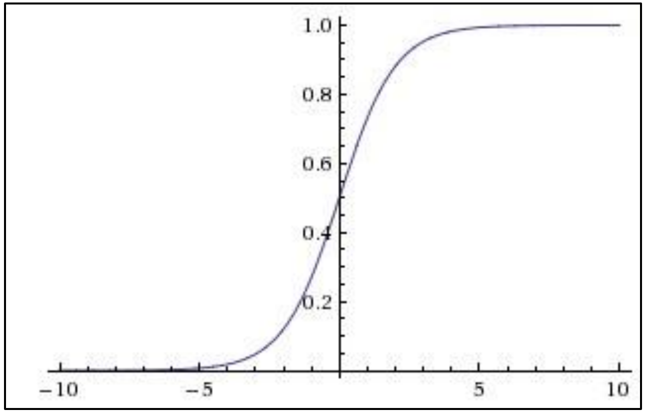
3 problems:

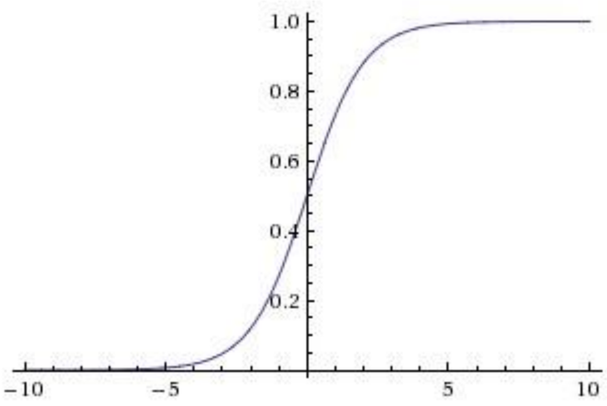
1. Saturated neurons “kill” the gradients





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

Activation Functions



Sigmoid

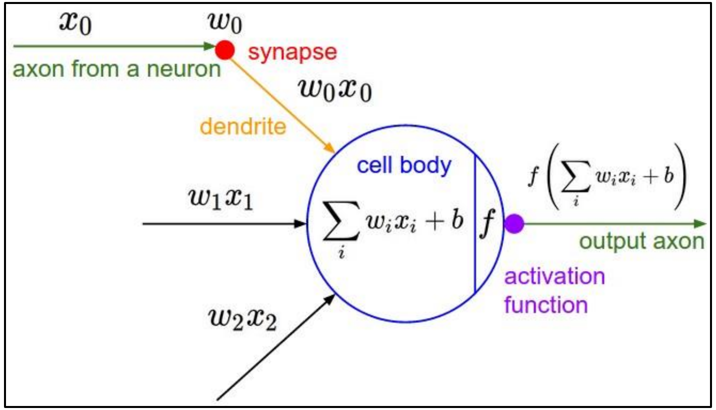
$$\sigma(x) = 1/(1 + e^{-x})$$

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

3 problems:

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

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 gradients with respect to **w**?

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

$$\frac{\partial f}{\partial w}$$

Let $$y = \sum_i w_i x_i.$$

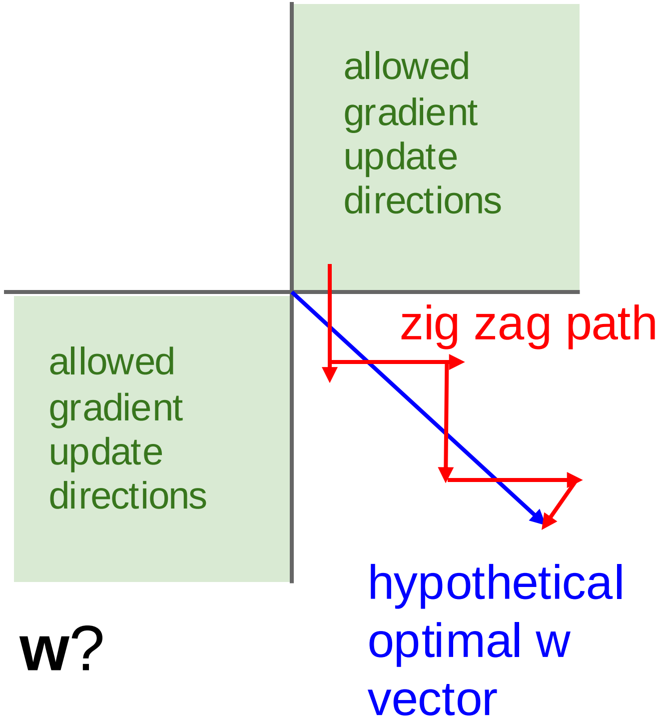
$$\frac{\partial f}{\partial w} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial w}.$$

Then $$\frac{\partial y}{\partial w} = x.$$

So $$\frac{\partial f}{\partial w} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial w} = \frac{\partial f}{\partial y}x$$

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

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



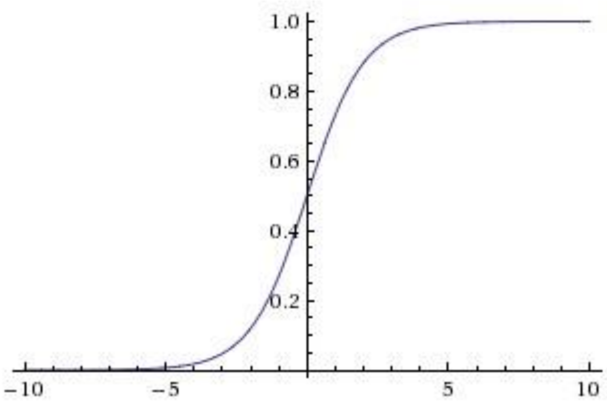
What can we say about the gradients on **w**?

Always all positive or all negative :(

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

Activation Functions

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



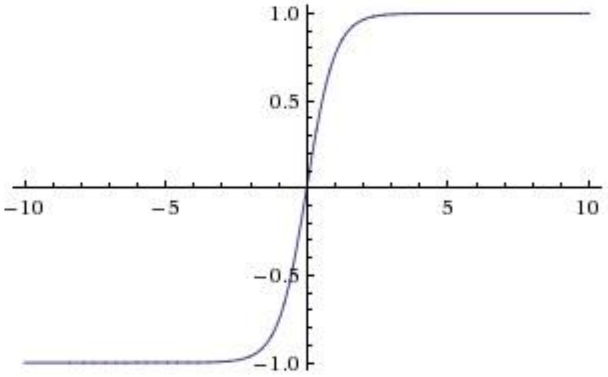
Sigmoid

- 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

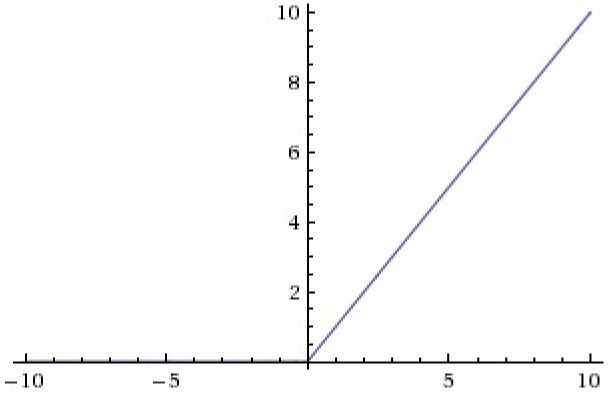


tanh(x)

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

[LeCun et al., 1991]

Activation Functions



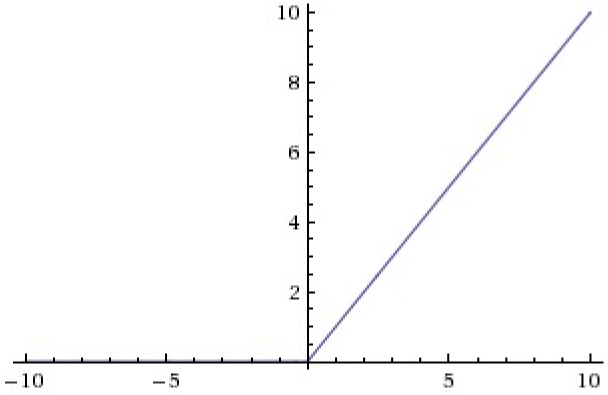
ReLU
(Rectified Linear Unit)

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

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

[Krizhevsky et al., 2012]

Activation Functions



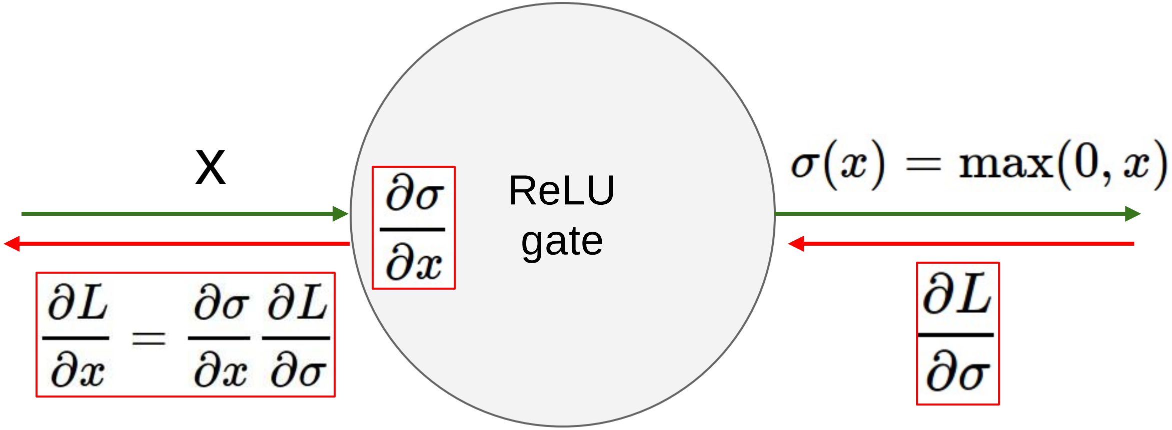
ReLU
(Rectified Linear Unit)

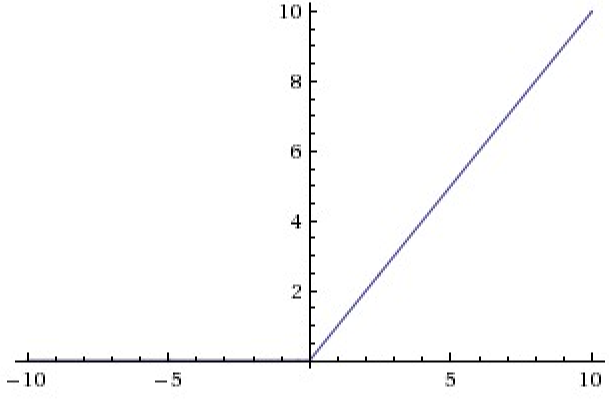
- Computes **f(x) = max(0,x)**

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

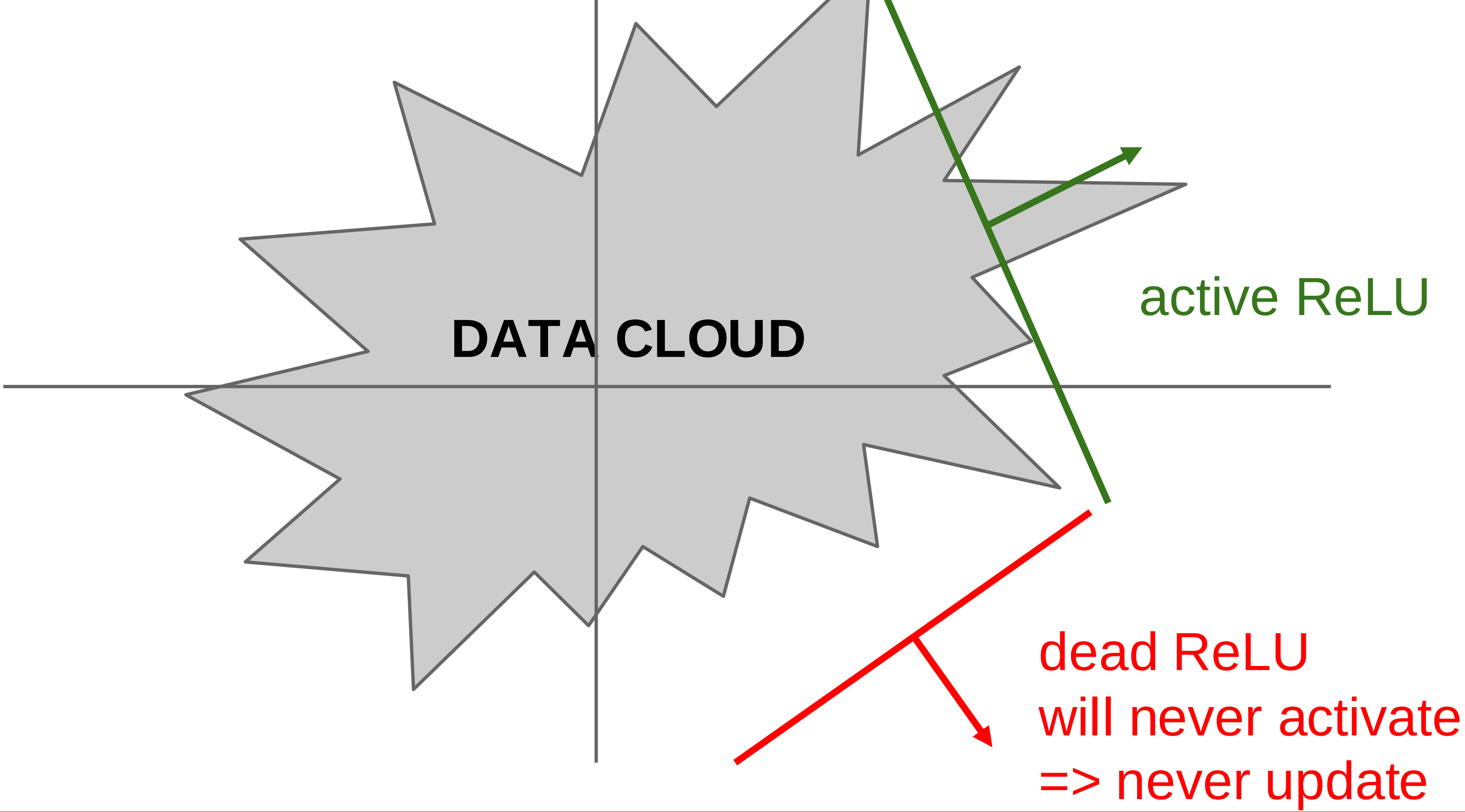
- Not zero-centered output
- An annoyance:

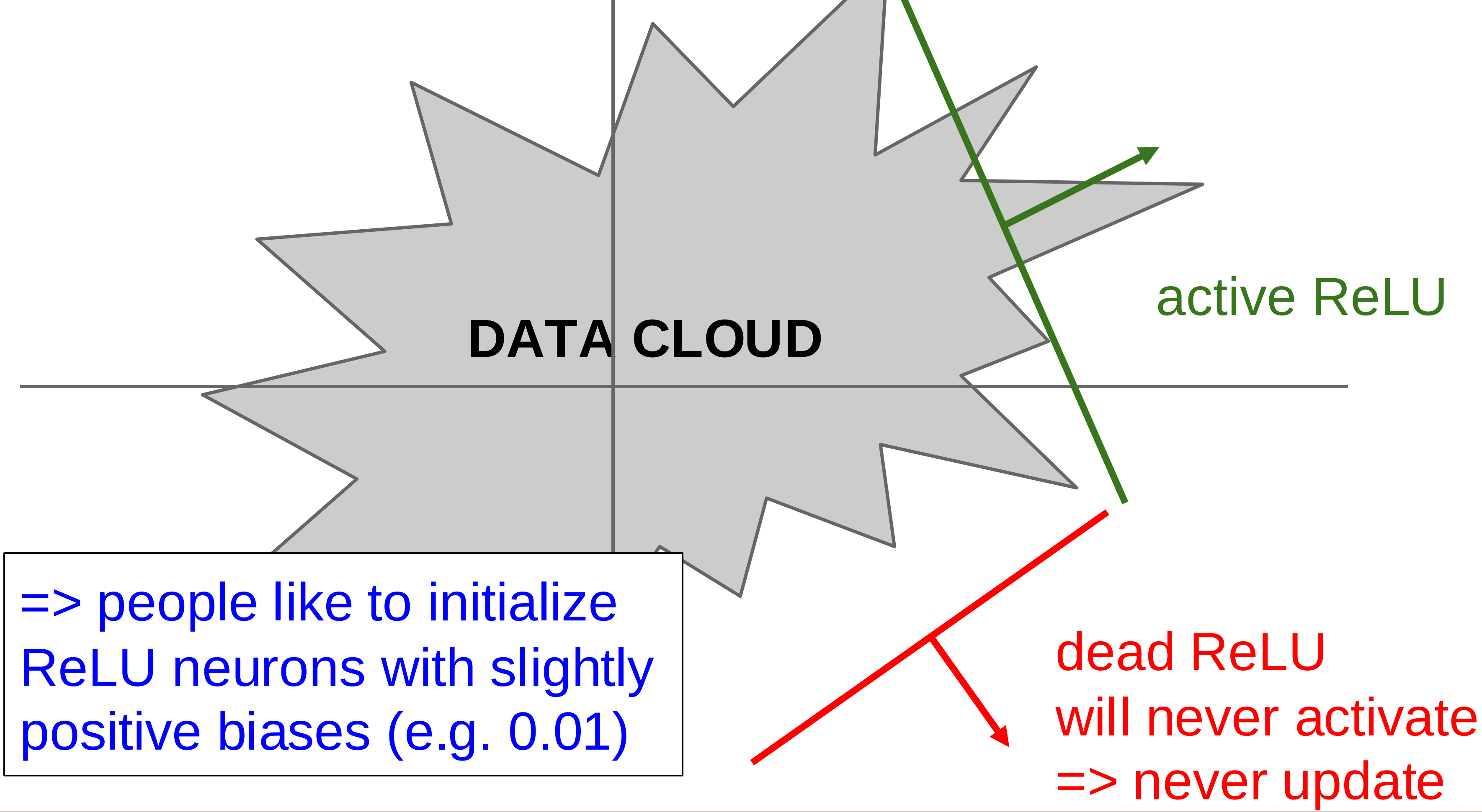
hint: what is the gradient when $x < 0$?





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

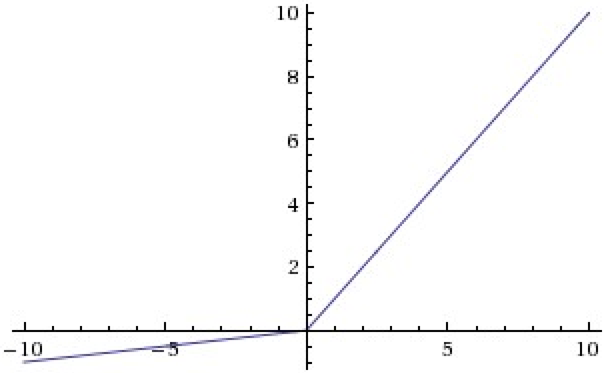

DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update



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

Activation Functions

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

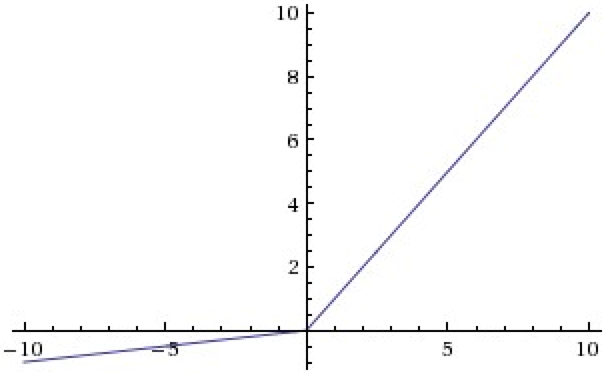


- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

Leaky ReLU

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

Activation Functions



Leaky ReLU

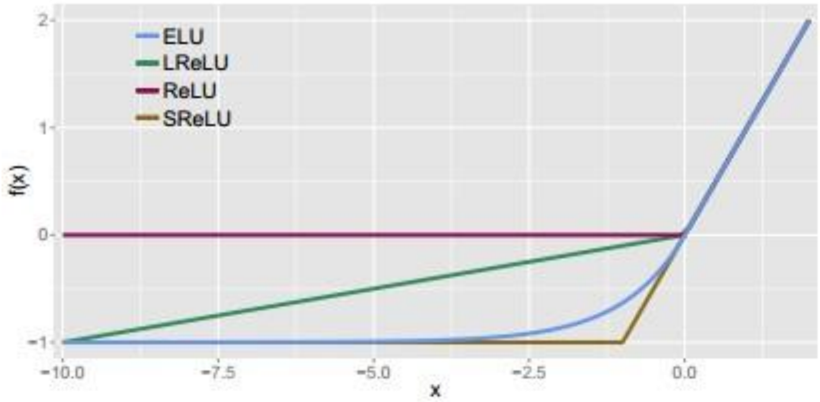
$$f(x) = \max(0.01x, x)$$

- Make up your own parametric rectifier! (Project idea!!!)
  - How about shifting the hinge?
  - How about shifting the slope?
  - How about changing the shape of the right side?
  - How about a diversity of ReLU's. What are pros and cons?

Activation Functions

[Clevert et al., 2015]

Exponential Linear Units (ELU)



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

- Most benefits of ReLU
- Does not die
- Closer to zero mean outputs

- Computation requires exp()

Maxout "Neuron"

[Goodfellow et al., 2013]

- 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
- Try out tanh but don’t expect much
- Don’t use sigmoid