CS6375: Machine Learning

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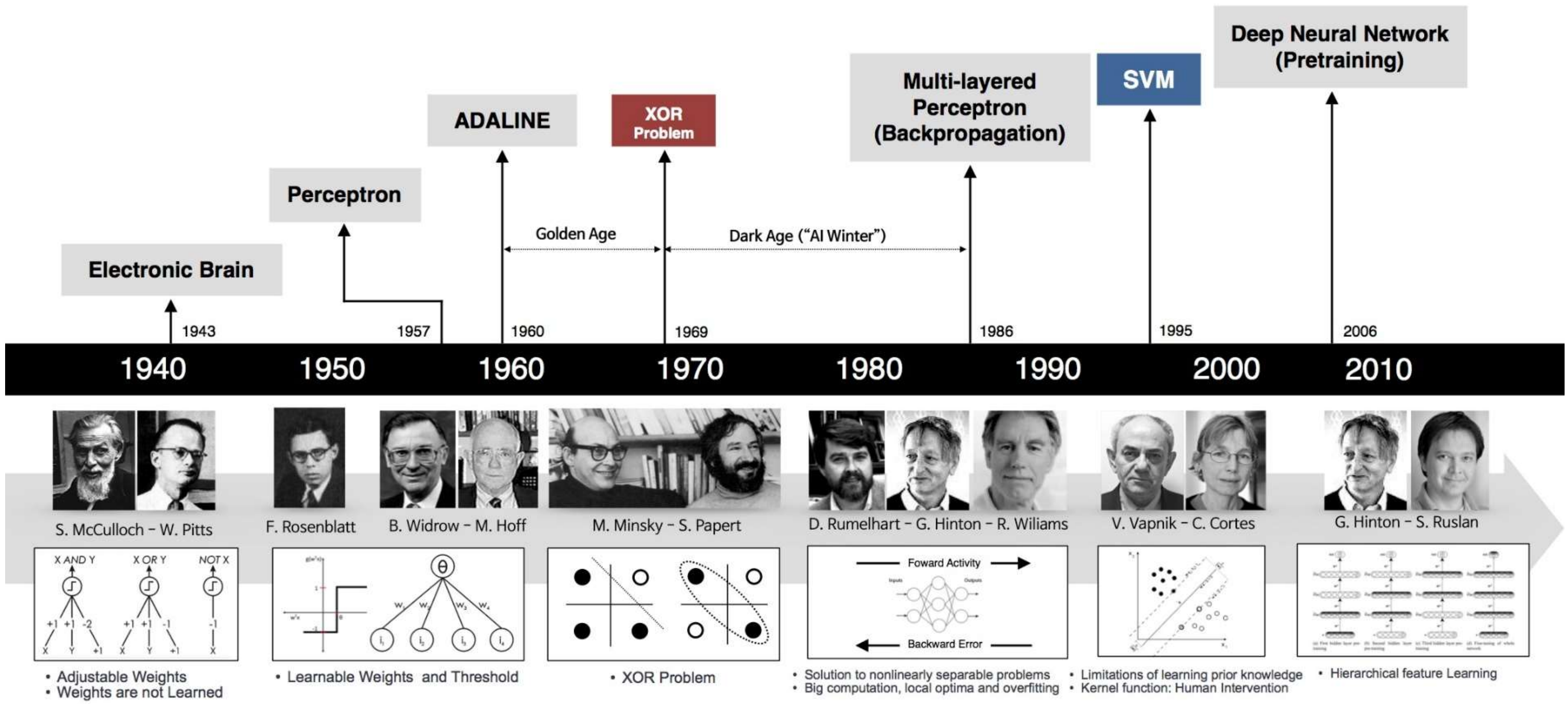
Neural Networks: A Brief History



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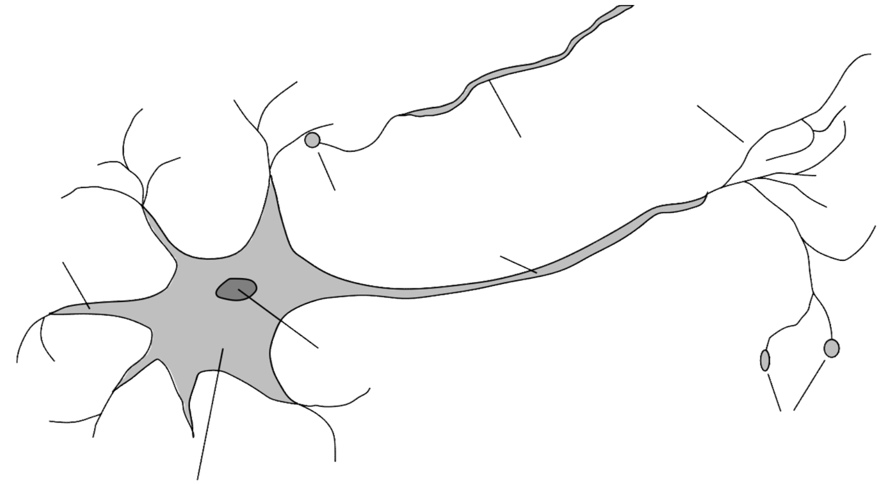
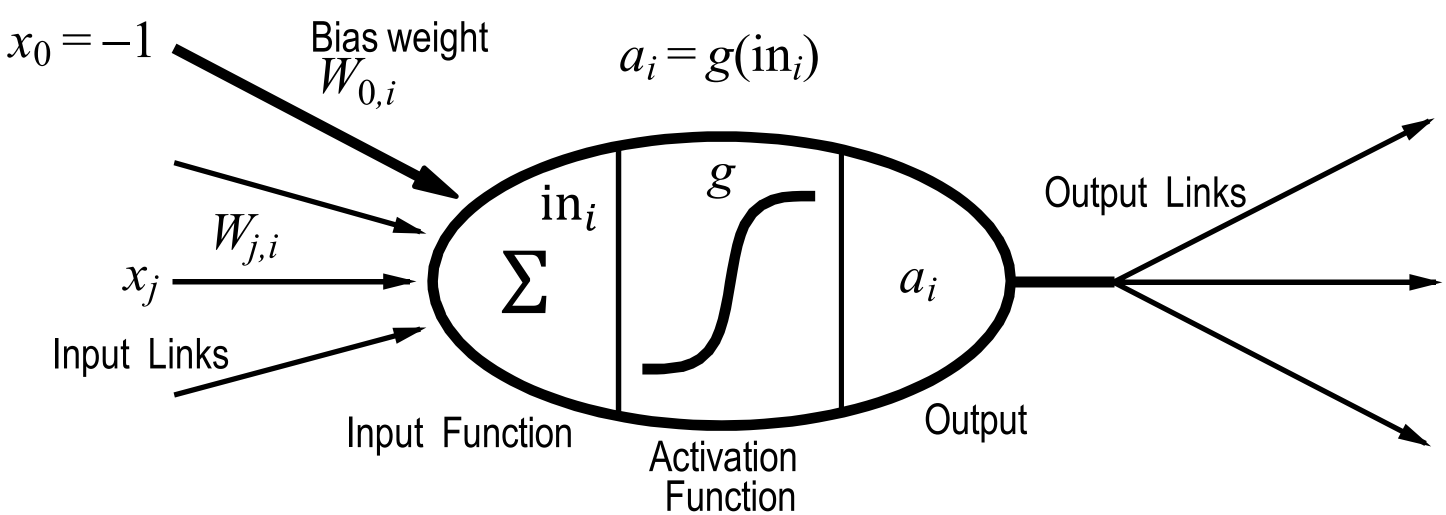
Neural Networks

- The basis of **neural networks** was developed in the 1940s-1960s
- The idea was to build **mathematical models** that might **"compute" in the same way that neurons** in the brain do
- As a result, neural networks are **biologically inspired**, though many of the **algorithms** developed for them are **not biologically plausible**
- Perform surprisingly well for many tasks



10^{11} neurons of more than 20 types, 10^{14} synapses, 1ms–10ms cycle time; signals are noisy "spike trains" of electrical potential

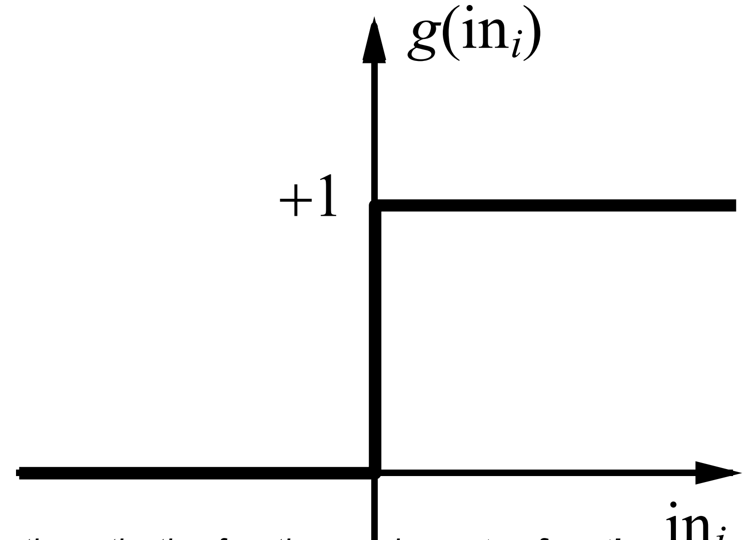
McCulloch-Pitts "unit": $a_i \leftarrow g(\mathrm{in}_i) = g\left(\sum_j W_{j,i} x_j\right)$



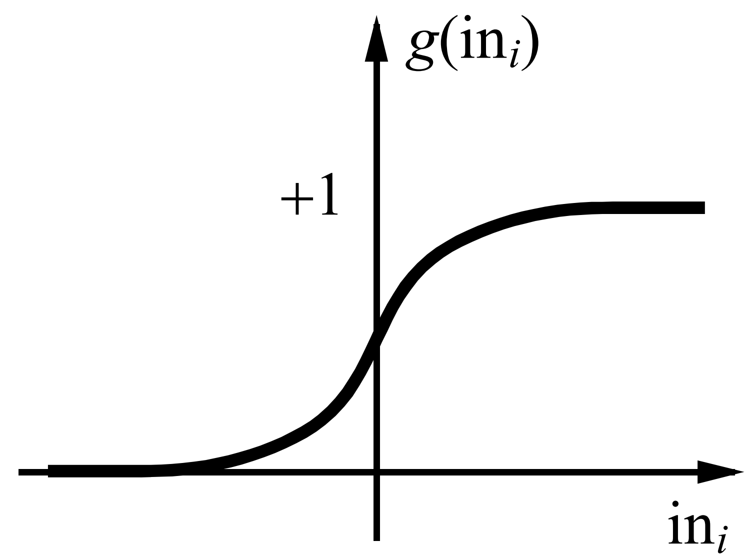
A gross oversimplification of real neurons, but its purpose is to develop an understanding of what networks of simple units can do

Neural Networks

- Neural networks consist of a **collection of artificial neurons**
- There are different types of neuron activation functions
    - the **perceptron** (one of the first studied)
    - the **sigmoid** neuron (one of the most common)
    - **rectified linear units** (deep learning)
- A neural network is a **directed graph** consisting of a collection of neurons (the **nodes**), directed **edges** (each with an associated **weight**), and a collection of **fixed binary inputs**



*the activation function can be a **step function** or **threshold function;** changing the bias weight $W_{0,i}$ moves the threshold location*



*the activation function can be a **sigmoid function**: $\frac{1}{1+e^{-x}}$; changing the bias weight $W_{0,i}$ moves the threshold location*

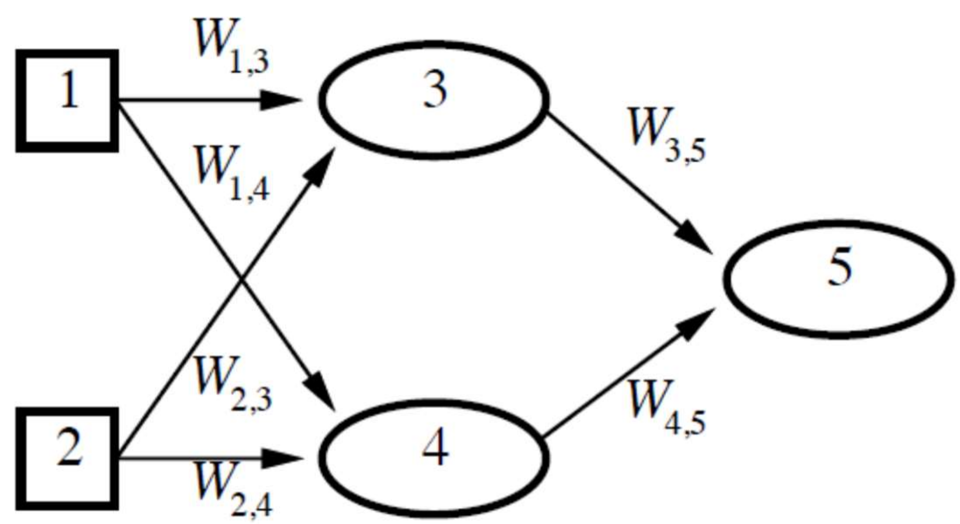
Network Architectures

Feed-forward networks implement functions, have no internal state
- single-layer perceptrons
- multi-layer perceptrons

Recurrent networks have directed cycles with delays
- have internal state (like flip-flops), can oscillate etc.

A **feed-forward network** is a parameterized family of nonlinear functions; adjusting the weights changes the function

Learning problem: learn the weights for a given architecture

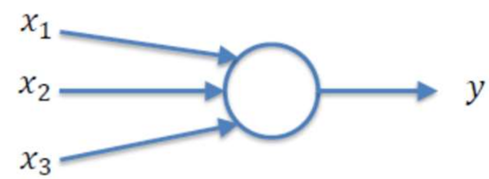


$$\begin{aligned} a_5 &= g(W_{3,5} \,.\, a_3 + W_{4,5} \,.\, a_4) \\ &= g(W_{3,5} \,.\, g(W_{1,3} \,.\, a_1 + W_{2,3} \,.\, a_2) + W_{4,5} \,.\, g(W_{1,4} \,.\, a_1 + W_{2,4} \,.\, a_2)) \end{aligned}$$

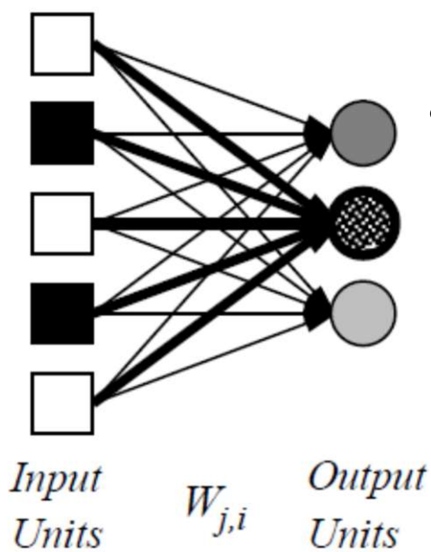
Single-Layer Perceptron

A **perceptron** is an artificial neuron that takes a collection of binary inputs and produces a binary output

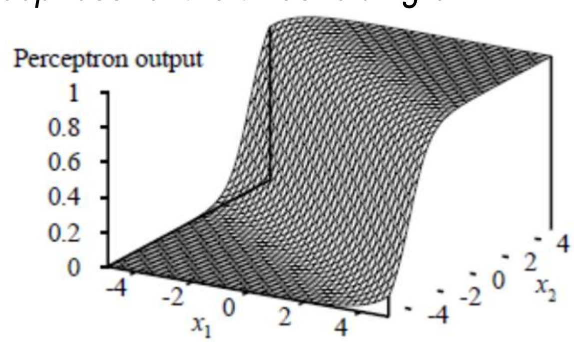
- The output of the perceptron is determined by summing up the weighted inputs and thresholding the result
- if the weighted sum is larger than the threshold, the output is one (and zero otherwise)
- the perceptron algorithm we previously studied uses the hard step function $g = \text{step}(\cdot)$



$$y = \begin{cases} 1 & w_1 x_1 + w_2 x_2 + w_3 x_3 + b > 0 \\ 0 & otherwise \end{cases}$$



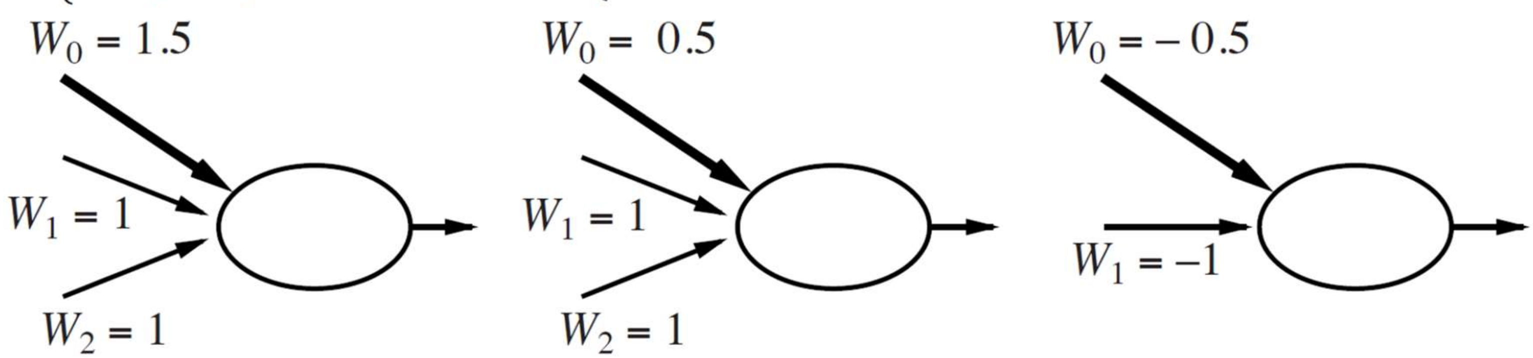
adjusting weights moves the location, orientation, and steepness of the thresholding cliff



Single-Layer Perceptron

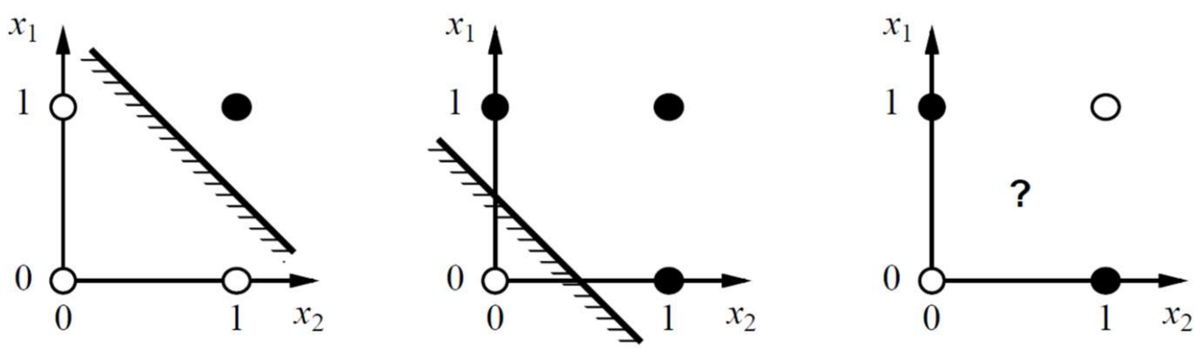
A perceptron can represent the **Boolean** functions **and**, **or** and **not** easily

$$y = \begin{cases} 1 & x_1 + x_2 > 1.5 \\ 0 & x_1 + x_2 \le 1.5 \end{cases} \qquad y = \begin{cases} 1 & x_1 + x_2 > 0 \\ 0 & x_1 + x_2 \le 0 \end{cases} \qquad y = \begin{cases} 1 & -x > -.5 \\ 0 & -x \le -.5 \end{cases}$$



AND **OR** **NOT**

and/**or** can be represented as linear functions, but **xor**?



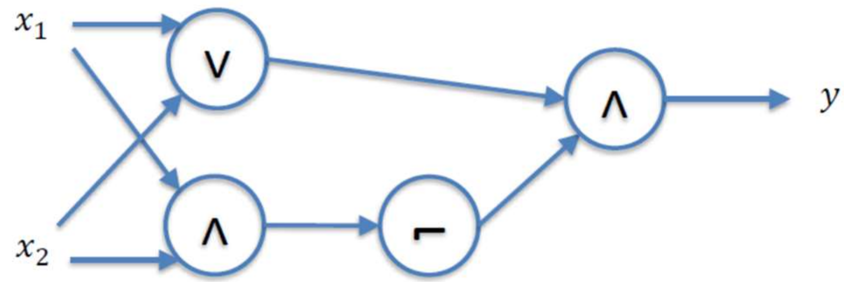
(a) x_1 **and** x_2 (b) x_1 **or** x_2 (c) x_1 **xor** x_2

Multi-Layer Perceptron

Recall that the **xor** function can be written as:

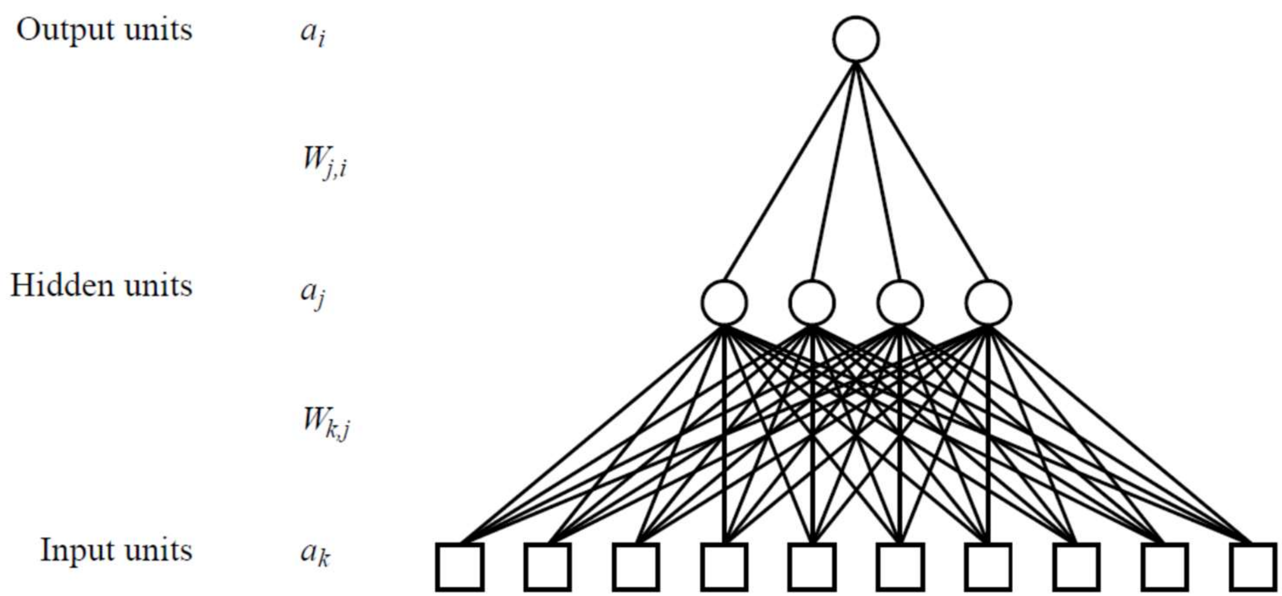
$$x_1 \oplus x_2 = (x_1 \lor x_2) \land \neg(x_1 \land x_2)$$

Can be expressed by combining **multiple perceptron units with multiple layers**!



Gluing a bunch of perceptrons together gives us a **neural network**

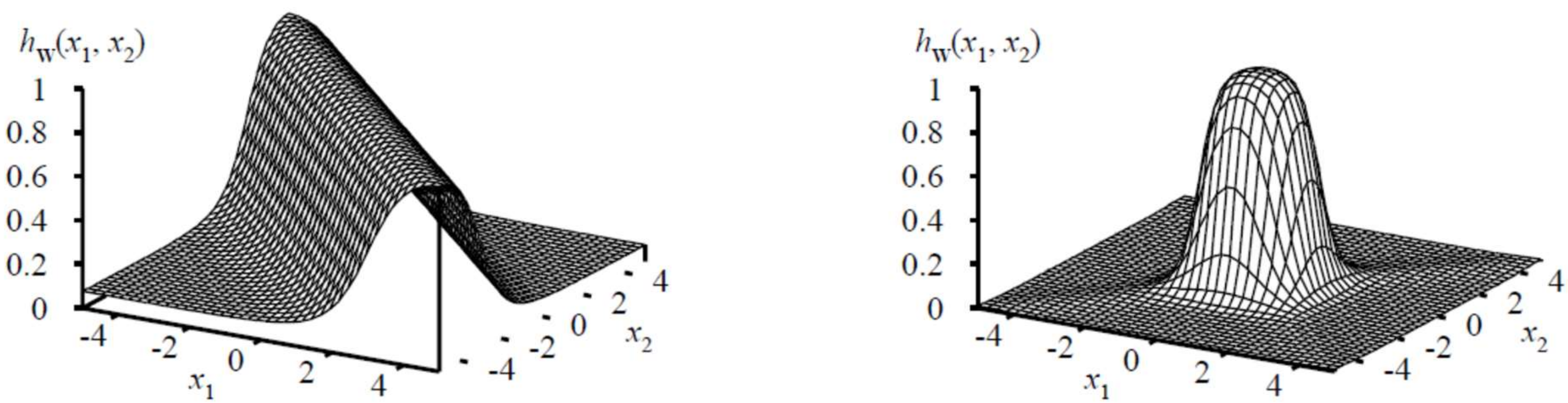
- in general, neural nets have a collection of inputs and a collection of outputs; can be binary, continuous (need appropriate loss functions)
- layers are usually **fully connected**
- numbers of **hidden units** typically chosen by hand



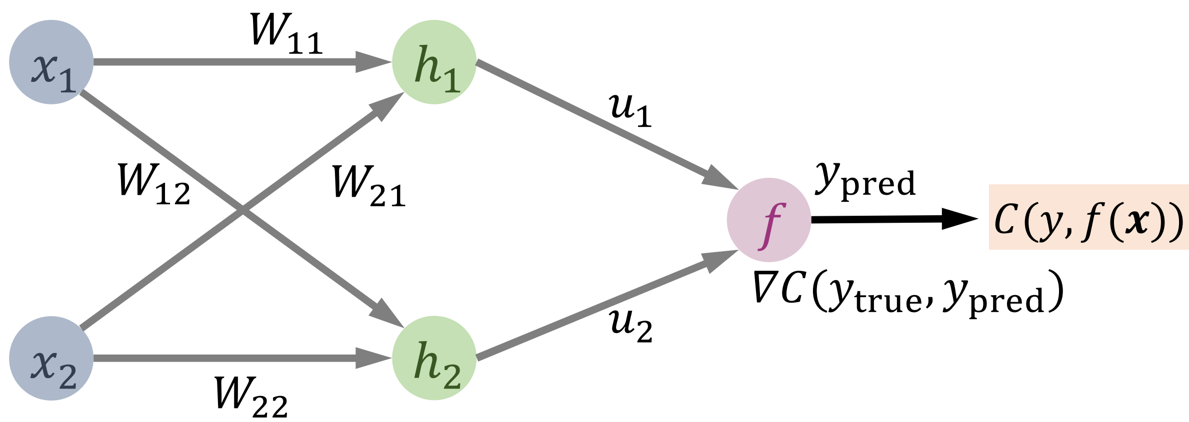
Multi-Layer Perceptron

Multi-layer perceptrons can encode **all continuous functions with 2 layers**, **all functions with 3 layers**

- combine two opposite-facing threshold functions to make a **ridge**
- combine two perpendicular ridges to make a **bump**
- add bumps of various sizes and locations to fit any **surface**
- proof requires **exponentially many hidden units**



Backpropagation: Forward Pass



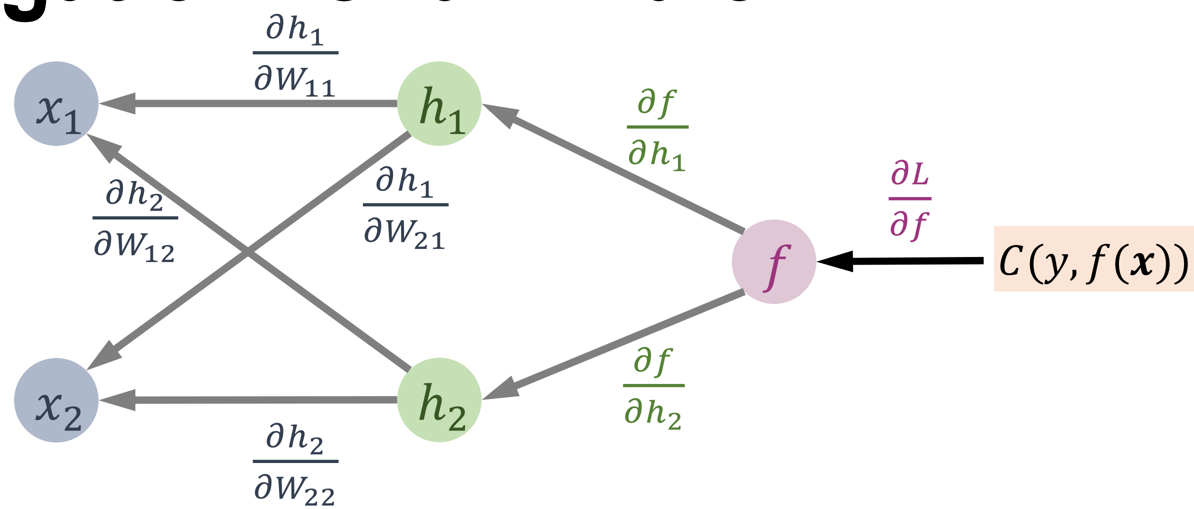
For **each example**, with the **current network parameters**, compute the prediction by **forward-propagating** the inputs through the network

- hidden layer values depend on the input layer: e.g., $h_1 = \sigma(W_{11}x_1 + W_{21}x_2) = \sigma(\boldsymbol{w}_1^T\boldsymbol{x})$
- output layer values depend on the hidden layer: $f = u_1 h_1 + u_2 h_2$
- activation function is sigmoid, $\sigma(z) = \frac{1}{1+e^{-x}}$

Use the **squared loss (cost)** to evaluate the prediction

$$C\left(y_{\text{true}}, y_{\text{pred}}\right) = \frac{1}{2}(y - f(\boldsymbol{x}))^2 = \frac{1}{2}(y - \boldsymbol{u}^T\sigma(W\boldsymbol{x}))^2$$

Backpropagation: Chain Rule

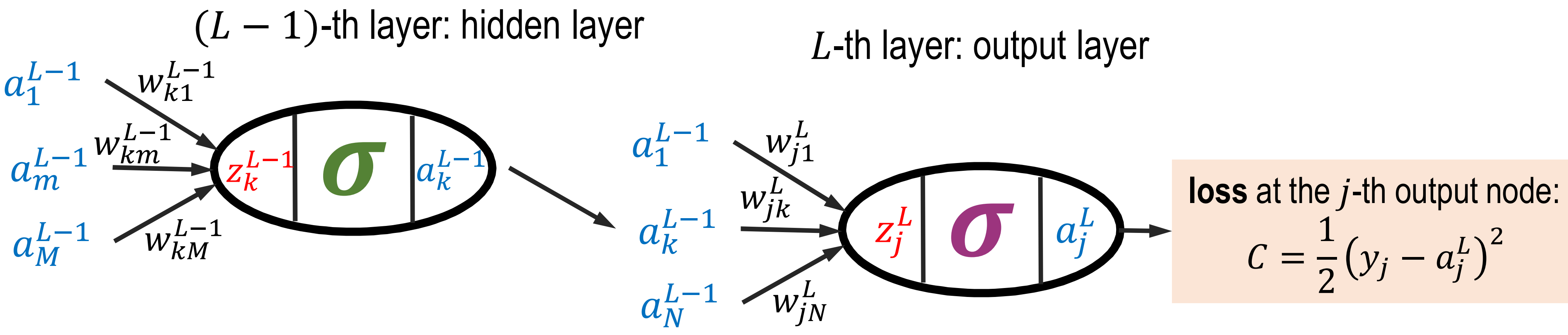


- **sigmoid functions** have a nice property, $\frac{\partial}{\partial z}\sigma(z) = \sigma(z)(1-\sigma(z))$
- we can **chain derivatives** to compute gradients e.g.,

$$\frac{\partial C}{\partial W_{11}} = \frac{\partial C}{\partial f} \cdot \frac{\partial f}{\partial h_1} \cdot \frac{\partial h_1}{\partial W_{11}}$$

$$= -(y - f(\boldsymbol{x})) \cdot \sigma(\boldsymbol{w}_1^T \boldsymbol{x})(1 - \sigma(\boldsymbol{w}_1^T \boldsymbol{x})) \cdot x_1$$

Backpropagation: Multiple Layers



z_j^L: **input** to the j-th neuron in the L-th layer

$$z_j^L = \sum_k w_{jk}^L a_k^{L-1}$$

a_j^L: **output** of the j-th neuron in the L-th layer

$$a_j^L = \boldsymbol{\sigma}(z_j^L)$$

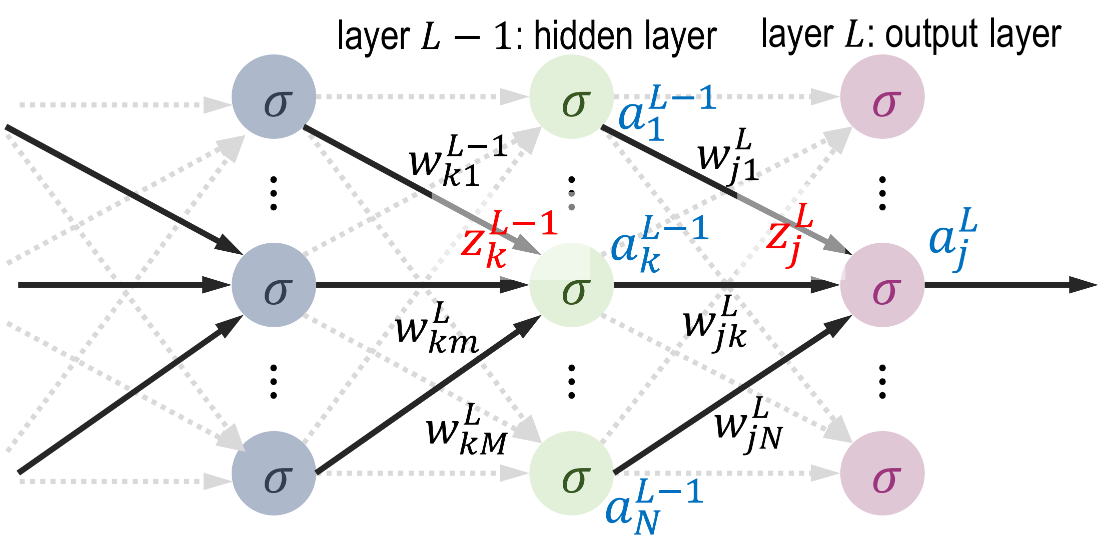
z_k^{L-1}: **input** to the k-th neuron in the $(L-1)$-th layer

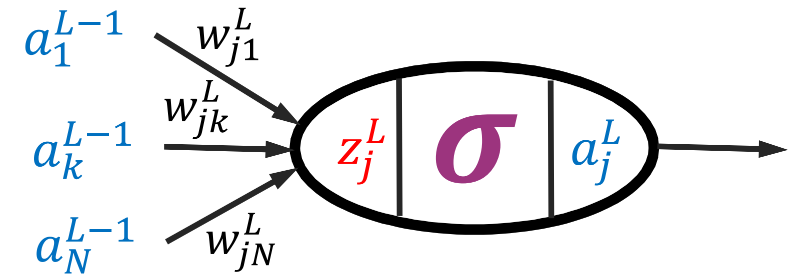
$$z_k^{L-1} = \sum_m w_{km}^{L-1} a_m^{L-2}$$

a_k^{L-1}: **output** of the k-th neuron in the $(L-1)$-th layer

$$a_k^{L-1} = \boldsymbol{\sigma}(z_k^{L-1})$$

Backpropagation: Output Layer





z_j^L: **input** to the j-th neuron in the L-th layer

$$z_j^L = \sum_k w_{jk}^L a_k^{L-1}$$

a_j^L: **output** of the j-th neuron in the L-th layer

$$a_j^L = \sigma(z_j^L)$$

z_k^{L-1}: **input** to the k-th neuron in the $(L-1)$-th layer

$$z_k^{L-1} = \sum_m w_{km}^{L-1} a_m^{L-2}$$

a_k^{L-1}: **output** of the k-th neuron in the $(L-1)$-th layer

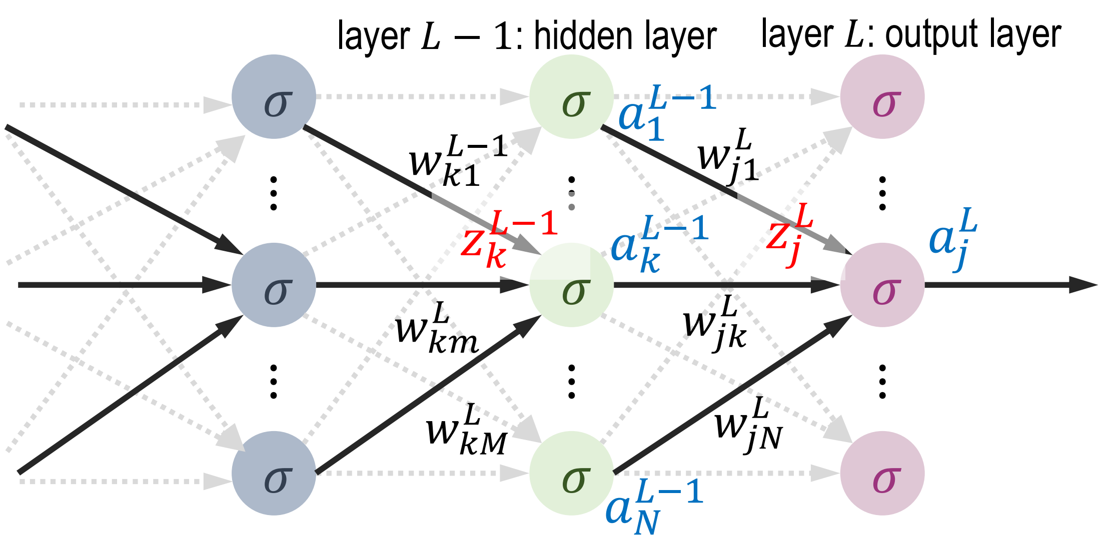
$$a_k^{L-1} = \sigma(z_k^{L-1})$$

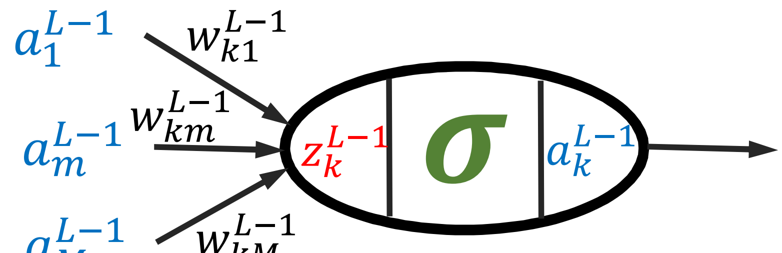
loss at the j-th output node:

$$C = \frac{1}{2}\left(y_j - a_j^L\right)^2$$

$$\begin{aligned}\frac{\partial C}{dz_j^L} &= -\left(y_j - a_j^L\right)\frac{\partial a_j^L}{\partial z_j^L} \\ &= -\left(y_j - a_j^L\right)\frac{\partial \sigma\left(z_j^L\right)}{\partial z_j^L} \\ &= -\left(y_j - a_j^L\right)\sigma\left(z_j^L\right)\left(1 - \sigma\left(z_j^L\right)\right) \\ &= \delta_j^L\end{aligned}$$

Backpropagation: Hidden Layers





z_j^L: **input** to the j-th neuron in the L-th layer

$$z_j^L = \sum_k w_{jk}^L a_k^{L-1}$$

a_j^L: **output** of the j-th neuron in the L-th layer

$$a_j^L = \sigma(z_j^L)$$

z_k^{L-1}: **input** to the k-th neuron in the $(L-1)$-th layer

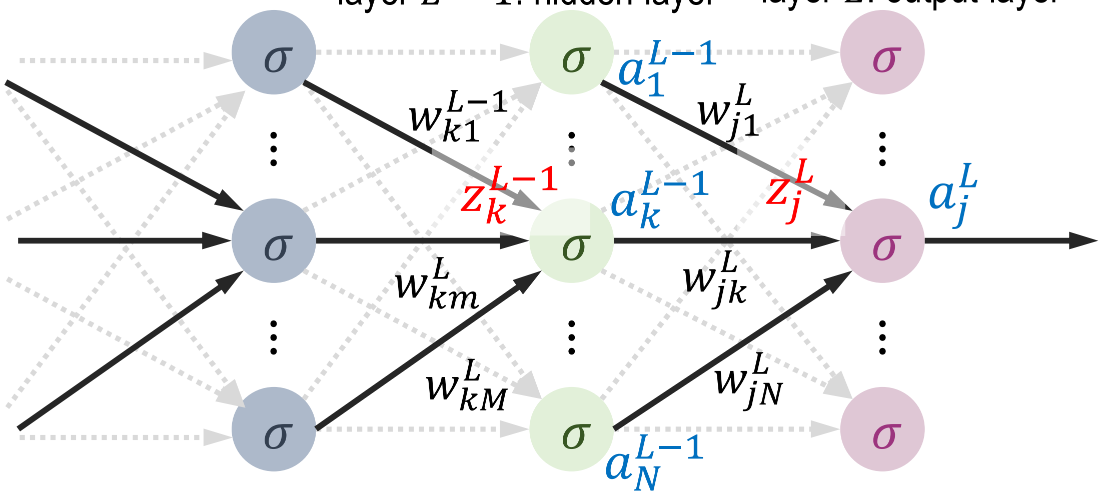
$$z_k^{L-1} = \sum_m w_{km}^{L-1} a_m^{L-2}$$

a_k^{L-1}: **output** of the k-th neuron in the $(L-1)$-th layer

$$a_k^{L-1} = \sigma(z_k^{L-1})$$

$$\begin{aligned}
\frac{\partial C}{dz_k^{L-1}} &= \sum_j (a_j^L - y_j)\frac{\partial a_j^L}{\partial z_k^{L-1}} \\
&= \sum_j (a_j^L - y_j)\frac{\partial \sigma(z_j^L)}{\partial z_k^{L-1}} \\
&= \sum_j (a_j^L - y_j)\,\sigma(z_j^L)\left(1-\sigma(z_j^L)\right)\frac{\partial z_j^L}{\partial z_k^{L-1}} \\
&= \sum_j (a_j^L - y_j)\,\sigma(z_j^L)\left(1-\sigma(z_j^L)\right)\frac{\partial \sum_{k'} w_{jk'}^L a_{k'}^{L-1} + b_j^L}{\partial z_k^{L-1}} \\
&= \sum_j (a_j^L - y_j)\,\sigma(z_j^L)\left(1-\sigma(z_j^L)\right)\sigma(z_k^{L-1})\left(1-\sigma(z_k^{L-1})\right) w_{jk}^L \\
&= \left((\delta^L)^T w_{*k}^L\right)\left(1-\sigma(z_k^{L-1})\right)\sigma(z_k^{L-1})
\end{aligned}$$

Backpropagation: Parameter Gradients



We can compute these derivatives one layer at a time

$$\frac{\partial C}{dz_k^{L-1}} = \delta^{L-1} = \left((\delta^L)^T w^L\right)\left(1-\sigma(z^{L-1})\right)\sigma(z^{L-1})$$

$$\delta^l = \left((\delta^{l+1})^T w^{l+1}\right)\left(1-\sigma(z^l)\right)\sigma(z^l)$$

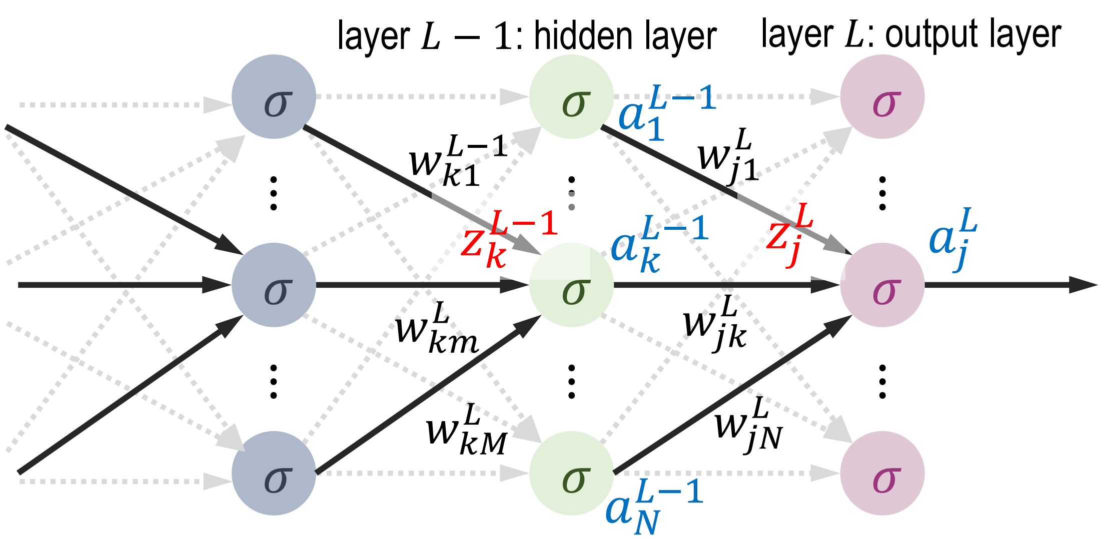
Can use stochastic gradient descent to update gradients one example at a time!

$$\frac{\partial C}{\partial b_j^l} = \frac{\partial C}{\partial z_j^l}\cdot\frac{\partial z_j^l}{\partial b_j^l} = \delta_j^l$$

bias term is implicit in each node

$$\frac{\partial C}{\partial w_{jk}^l} = \frac{\partial C}{\partial z_j^l}\cdot\frac{\partial z_j^l}{\partial w_{jk}^l} = \delta_j^l a_k^{l-1}$$

Backpropagation



- Backpropagation converges to a **local minimum** (loss is not convex in the weights and biases)
- Like EM, can just run it several times with **different initializations**
- Training can take a **very long time**
    - even with stochastic gradient descent
- **Prediction after learning is fast**
- Sometimes include a **momentum** term α in the gradient update

$$w(t) = w(t-1) - \gamma \cdot \nabla_w C(t-1) + \alpha(-\gamma \cdot \nabla_w C(t-2))$$

- Compute the inputs/outputs for each layer by starting at the input layer and applying the sigmoid functions
- Compute δ^L for the output layer

$$\delta^L = -(y_j - a_j^L)\, \sigma(z_j^L)\left(1 - \sigma(z_j^L)\right)$$

- Starting from $l = L-1$ and working backwards, compute

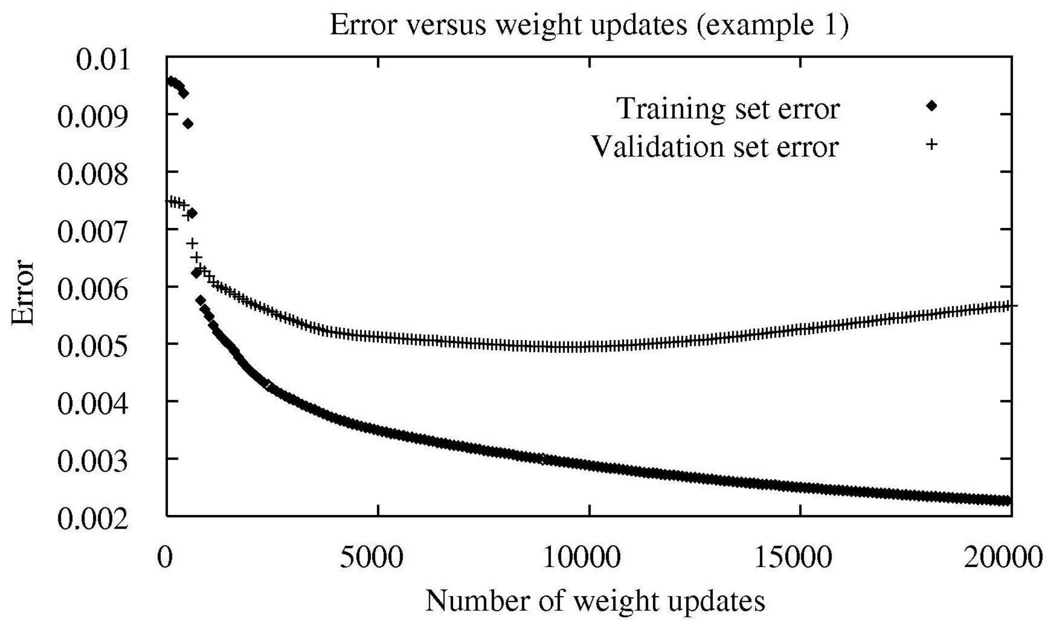
$$\delta^l = \left((\delta^{l+1})^T w^{l+1}\right) \sigma(z^l)\left(1 - \sigma(z^l)\right)$$

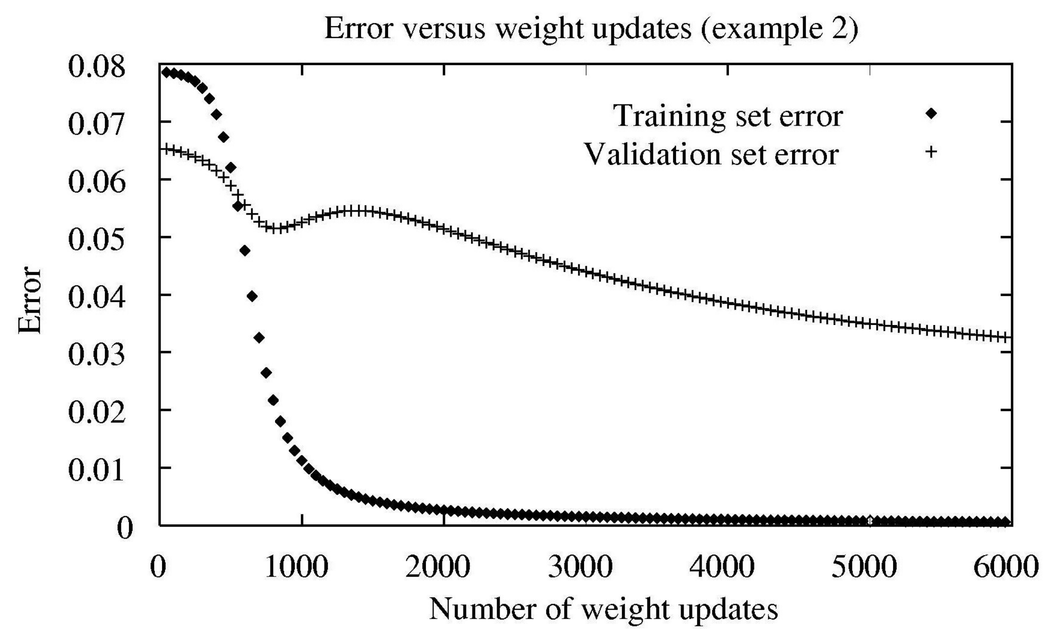
- Perform gradient descent

$$b_j^l = b_j^l - \gamma \cdot \delta_j^l$$

$$w_{jk}^l = w_{jk}^l - \gamma \cdot \delta_j^l a_k^{l-1}$$

Overfitting





Neural Networks in Practice

Many ways to improve weight learning in NNs

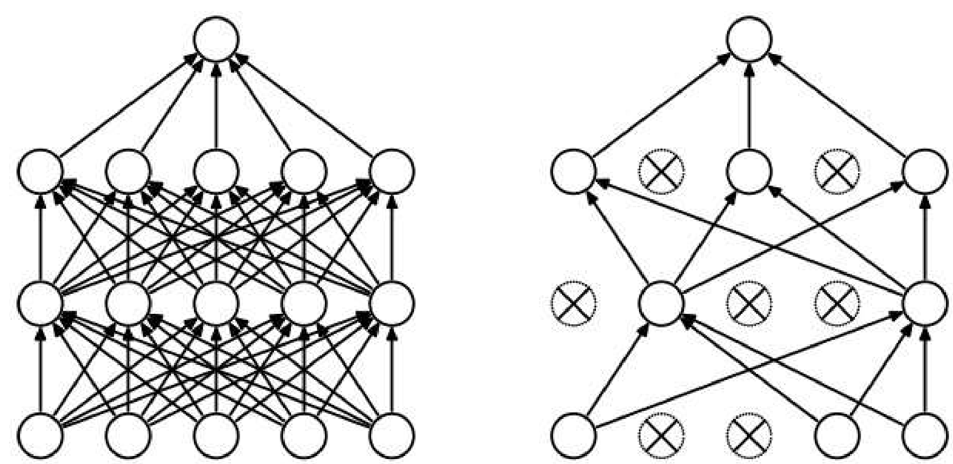
- Use **regularized squared loss (cost)** prediction (can still use backpropagation in this setting)

$$C\left(y_{\text{true}}, y_{\text{pred}}\right) = \frac{1}{2}\left(y - f(\boldsymbol{x}; \boldsymbol{w}, b)\right)^2 + \frac{\lambda}{2}\|w\|_2^2$$

  - L_1 regularization can also be useful
  - $\lambda > 0$ should be chosen with a **validation set**
- Try other loss functions, e.g., the **cross entropy**
  - $C\left(y_{\text{true}}, y_{\text{pred}}\right) - y \log f(\boldsymbol{x}) - (1 - y) \log\left(1 - f(x)\right)$
- **Initialize weights** of the network more cleverly
  - Random initializations are likely to be far from optimal
- Learning procedure can have **numerical difficulties** if there are a **large number of layers**
  - **Early stopping**: stop the learning early in the hopes that this prevents overfitting

Drop out: A **heuristic** **bagging-style approach** applied to neural networks to **counteract overfitting**

- **Randomly remove** a certain percentage of **neurons from the network** and then train only on the remaining neurons
- networks **recombined using an approximate averaging**
- keeping around too many networks and doing proper bagging can be costly in practice



(a) Standard Neural Net　　(b) After applying dropout.

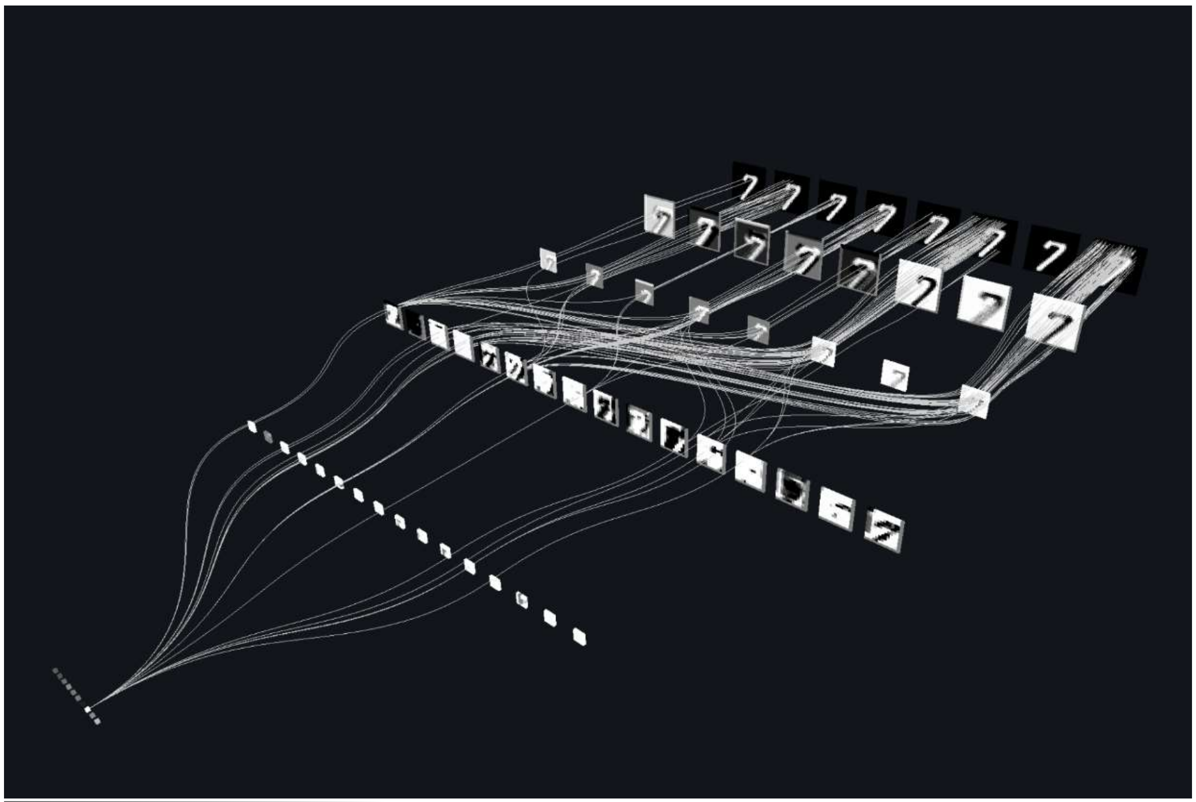
Parameter Tying

Parameter tying: Assume some of the weights in the model are the same to reduce the **dimensionality** of the learning problem;

- Also a way to learn “simpler” models
- Can lead to significant compression in neural networks (i.e., >90%)

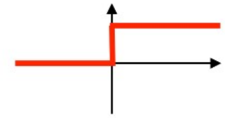
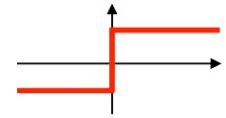
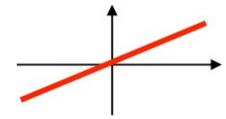
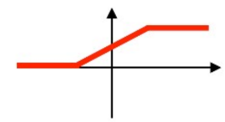
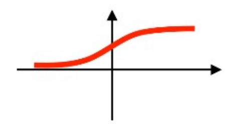
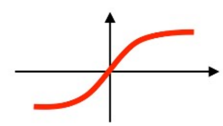
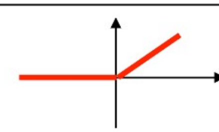
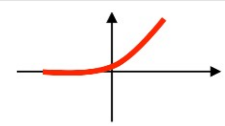
Convolutional neural networks

- Instead of the output of every neuron at layer ℓ being used as an input to every neuron at layer $\ell + 1$, edges between layers are chosen more locally
- Many tied weights and biases
  - convolution nets apply the same process to many different local chunks of neurons
- Often combined with pooling layers
  - layers that replacing small regions of neurons with their aggregated output
- Used extensively for image classification tasks



Topological Visualization of a Convolutional Neural Network by Terence Broad http://terencebroad.com/nnvis.html

Activation Functions

Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 0.5, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	Multi-layer Neural Networks	
Rectifier, ReLU (Rectified Linear Unit)	$\phi(z) = max(0, z)$	Multi-layer Neural Networks	
Rectifier, softplus	$\phi(z) = \ln(1 + e^z)$	Multi-layer Neural Networks	

Example: Self Driving Cars