VL Deep Learning for Natural Language Processing

2. Neural Networks

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AG Information Profiling and Retrieval

Summary of Previous Session

- Organization of DL4NLP lecture
  - Weekly exercises
  - Three assignments (required for exam participation; gets bonus points)

- Deep learning has revolutionized machine learning
  - No feature engineering
  - Large datasets necessary
  - Works very well for „perception“ tasks
  - DL is also a hype: it cannot solve all problems

- Machine learning learns from data (un-)supervised
  - Most methods are based on statistics
  - Can be seen as transforming input to output

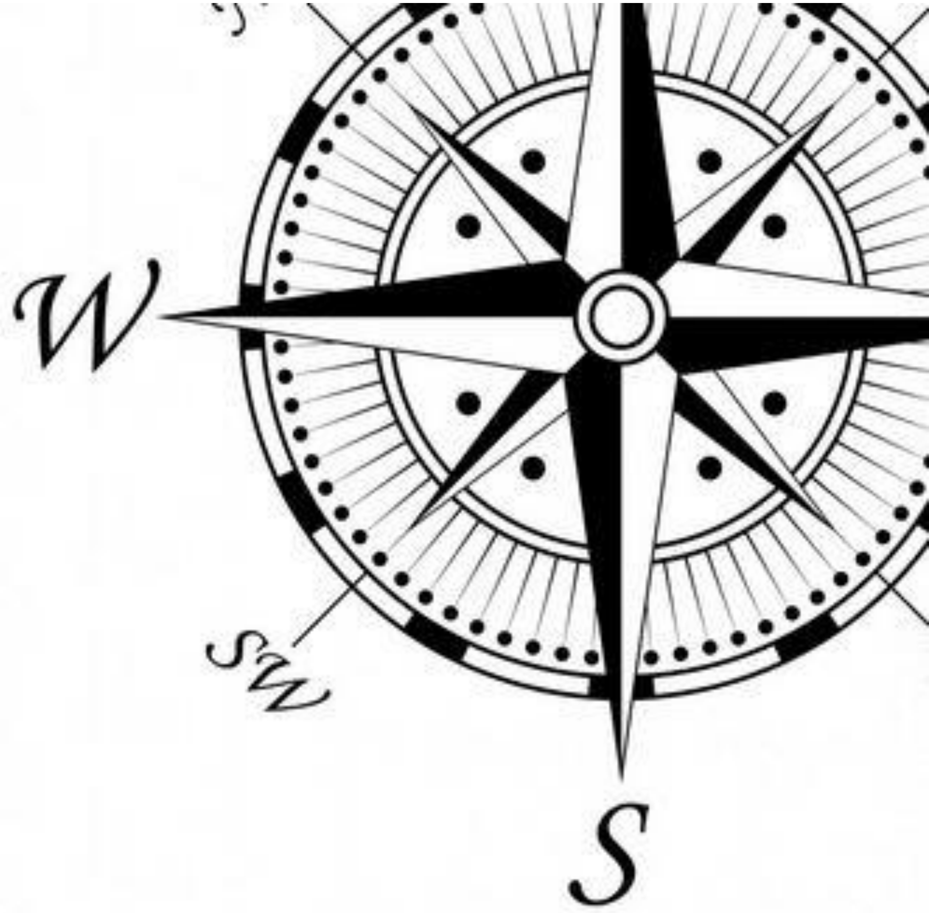
Learning Goals for this Chapter

- Know how the perceptron works
- Explain the need for multiple layers
- Understand gradient-based optimization
- Describe the components of deep neural networks
- Understand and apply the backpropagation algorithm

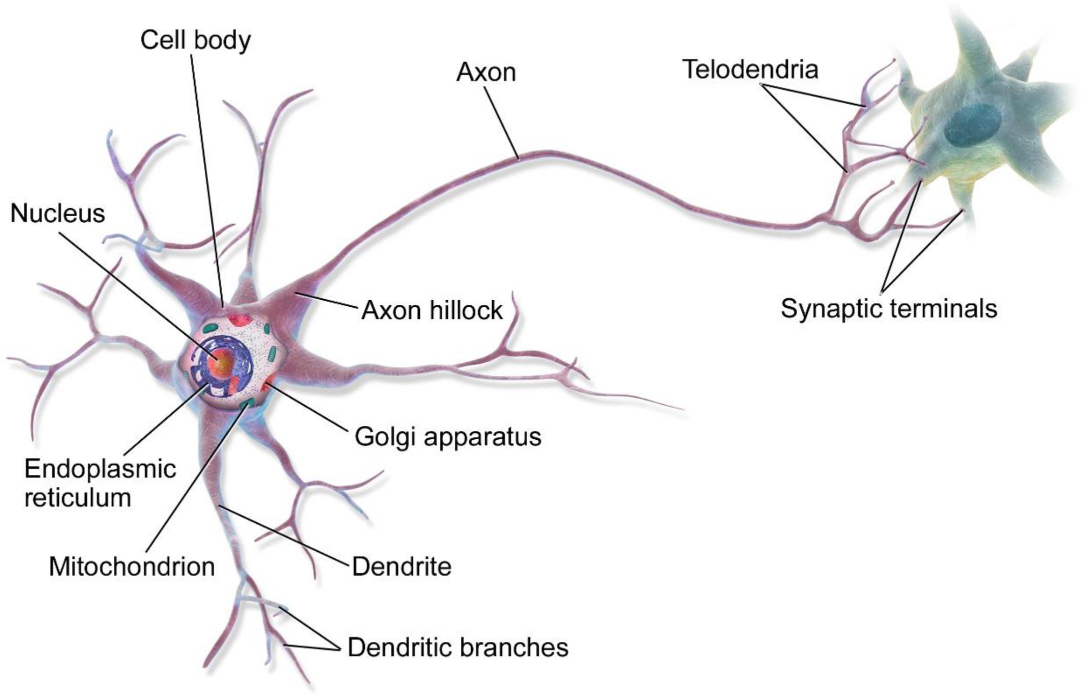
- Relevant chapters
  - P2, P3
  - S3 (2021) https://www.youtube.com/watch?v=X0Jw4kgaFlg

Topics Today

1. **Neural Network Unit**
2. The Perceptron
3. Feedforward Neural Networks
4. Gradient-Based Optimization
5. Backprop(agation Algorithm)
6. Summary



This is in your Brain



Neural Network Unit

This is not in your brain

Output value

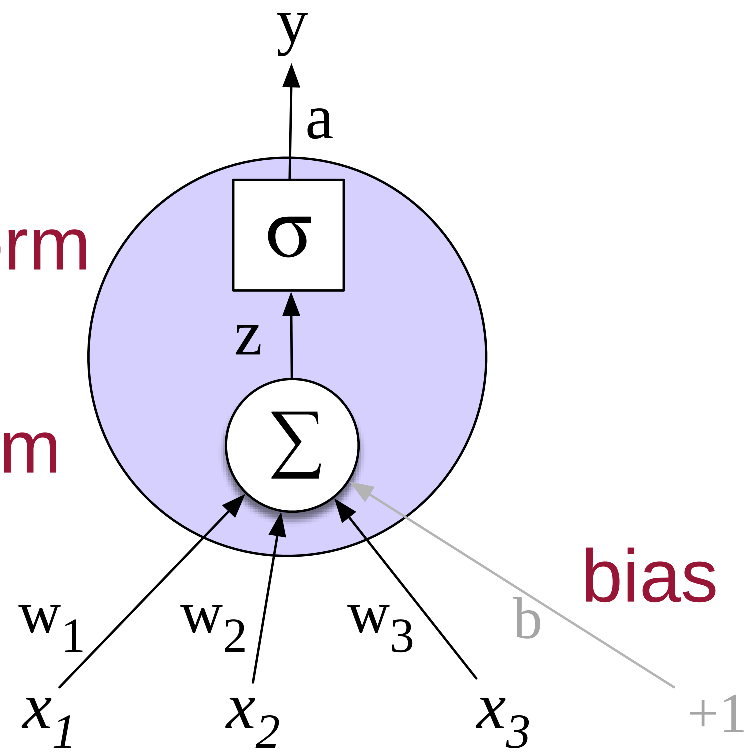
Non-linear transform

Weighted sum

Weights

Input layer

bias



Neural Unit

- Take weighted sum of inputs, plus a bias:

$$z = b + \sum_i w_i x_i$$

- Or in vector notation:

$$z = b + \boldsymbol{w} \cdot \boldsymbol{x}$$

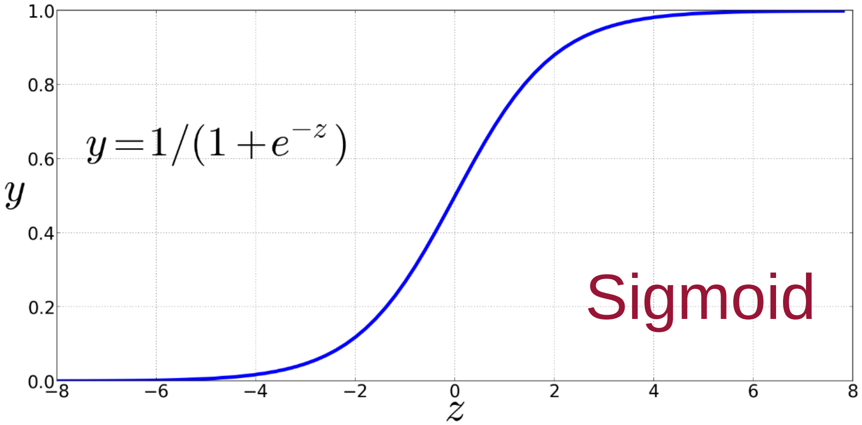
- Instead of just using z, we'll apply a nonlinear activation function f:

$$y = a = f(z)$$

Non-Linear Activation Function: Sigmoid

- E.g. sigmoid (aka logistic) function:

$$y = s(z) = \frac{1}{1 + e^{-z}}$$



Final function the neural unit is computing:

$$y = s(\boldsymbol{w} \cdot \boldsymbol{x} + b) = \frac{1}{1 + \exp(-(\boldsymbol{w} \cdot \boldsymbol{x} + b))}$$

An Example

- Suppose a unit has:

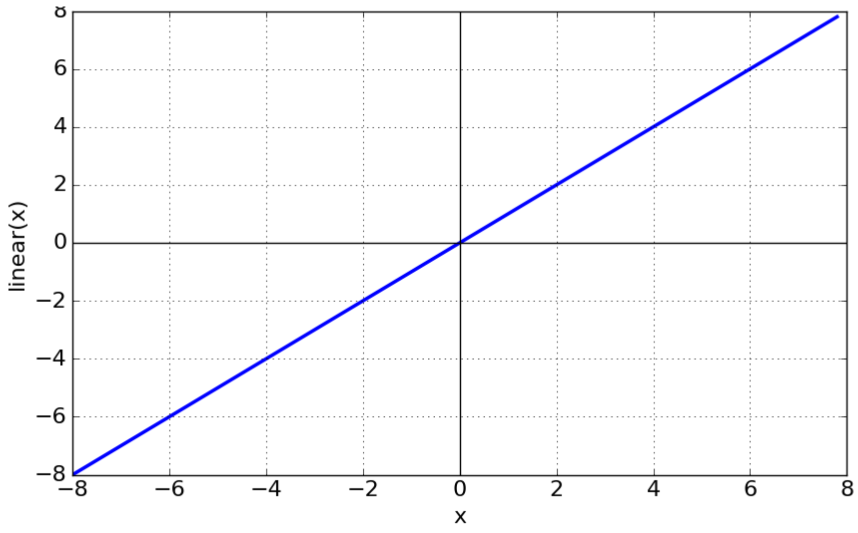
$$\boldsymbol{w} = [0.2,0.3,0.9]$$
$$b = 0.5$$

- What happens with input **x**:

$$\boldsymbol{x} = [0.5,0.6,0.1]$$
$$y = ?$$

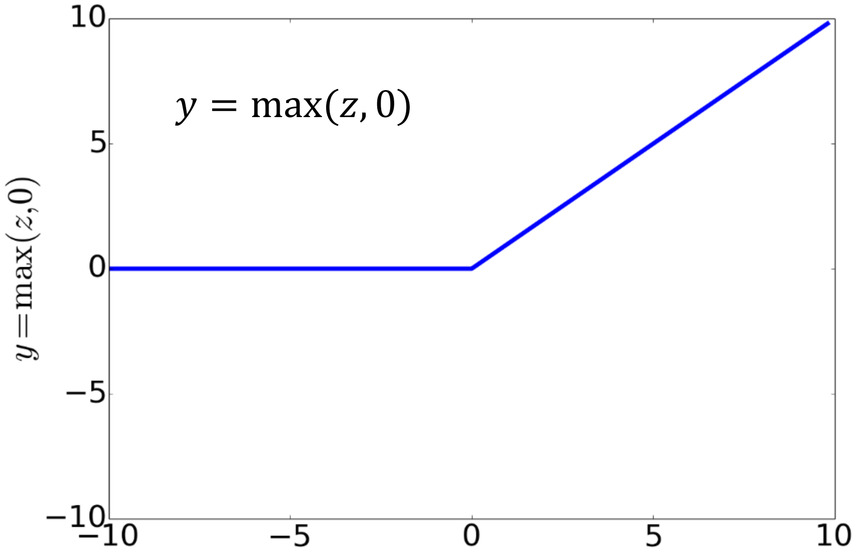
$$y = sigmoid(\boldsymbol{w}\cdot\boldsymbol{x}+b)$$
$$= \frac{1}{1+\exp(-(\boldsymbol{w}\cdot\boldsymbol{x}+b))}$$
$$= \frac{1}{1+\exp(-(0.2*0.5+0.3*0.6+0.9*0.1+0.5))}$$
$$= \frac{1}{1+\exp(-0.87)} = 0.70$$

Activation Functions Besides Sigmoid



Linear

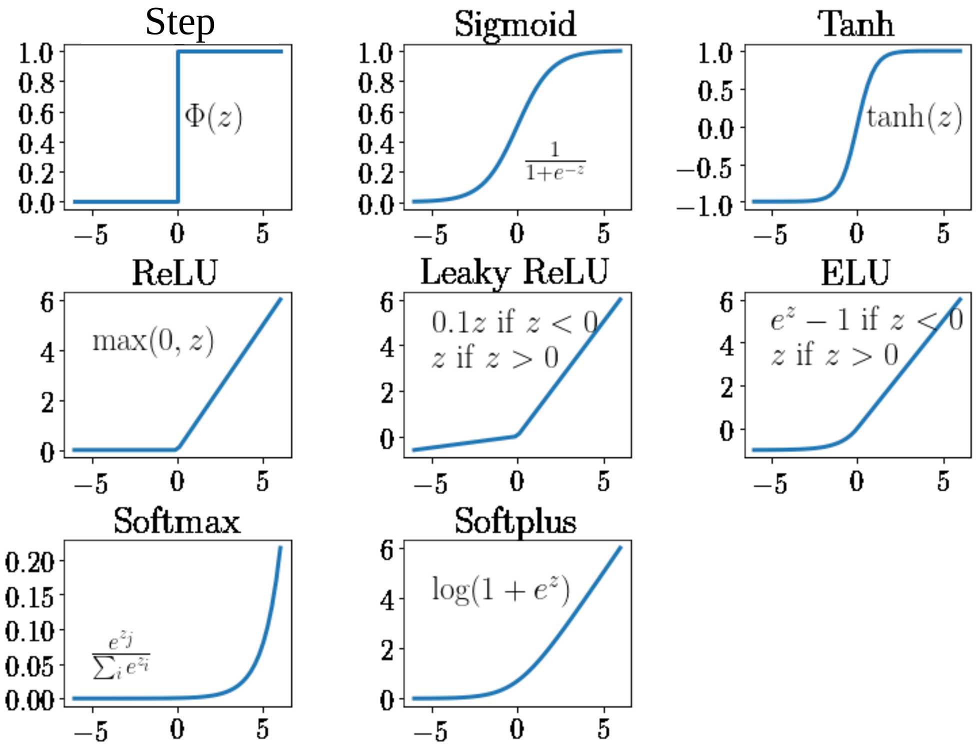
Most Common:



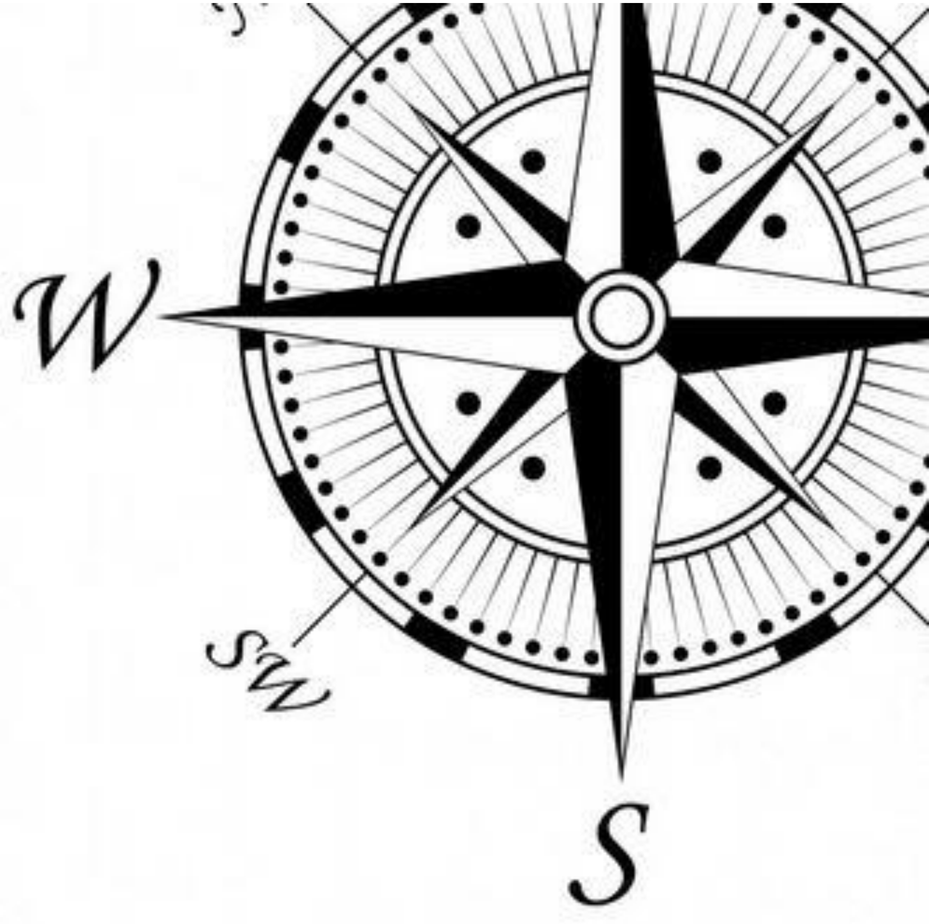
ReLU

Rectified Linear Unit

Most Common Non-Linear Activation Functions



Topics Today



1. Neural Network Unit
2. **The Perceptron**
3. Feedforward Neural Networks
4. Gradient-Based Optimization
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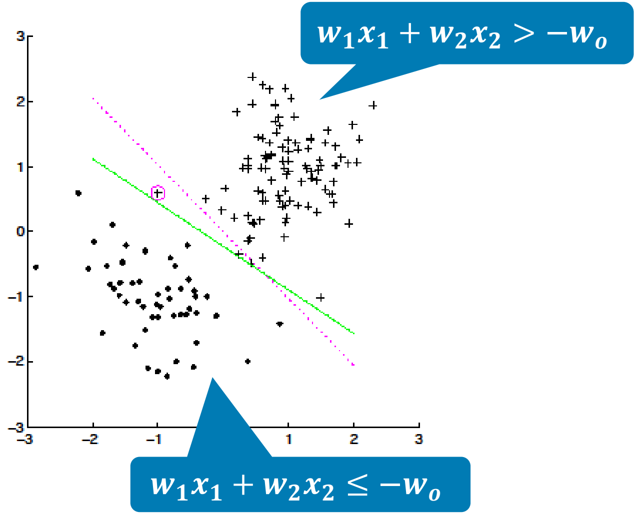
Simple Linear Classification

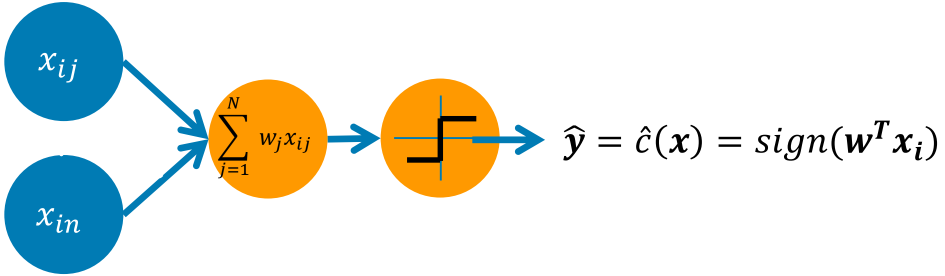
- Given a data point $\boldsymbol{x} = \binom{x_1}{x_2}$, predict to which class $\hat{y} = \{-1,1\}$ this sample belongs
- Model $M(b, w_1, w_2) = M_{\boldsymbol{\theta}}$
  - $M_{\boldsymbol{\theta}}(\boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{\theta}) = \hat{y}$
  - $\hat{y} = \begin{cases} 1 & if\ b + w_1 x_1 + w_2 x_2 > 0 \\ -1 & otherwise \end{cases}$
  - Add 1 to all $\boldsymbol{x}$ for simplification:
    - $\boldsymbol{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix}$
    - $\hat{y} = \begin{cases} 1 & if \sum_j w_j x_j > 0 \\ -1 & otherwise \end{cases}$
  - $\hat{y} = \operatorname{sign}(\boldsymbol{w}^T \boldsymbol{x})$



The Perceptron

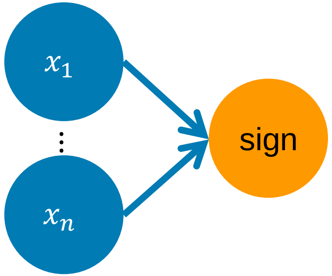
- Model:

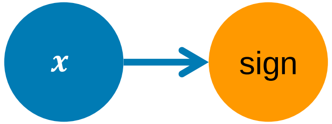
$$\hat{\boldsymbol{y}} = \text{sign}(\boldsymbol{w}^T\boldsymbol{x})$$



- Activation function of output layer:

$$sign(\boldsymbol{w}^T\boldsymbol{x})$$





Loss Function

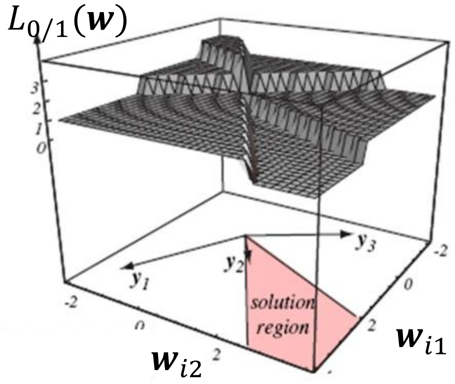
$$L_{0/1}(\hat{y}, y) = \begin{cases} 0, & \hat{y} = y \\ 1, & \hat{y} \neq y \end{cases}$$

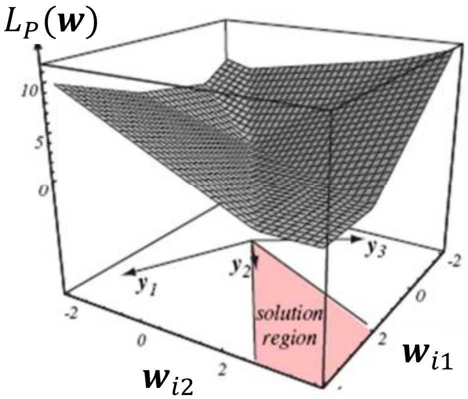
$$L_{0/1}(\boldsymbol{w}) = \frac{1}{N}\sum_{i=1}^{N}[y_j == sign(\boldsymbol{w}^T \boldsymbol{x}_i)]$$

$$L_p(\boldsymbol{w}) = \frac{1}{N}\sum_{i=1}^{N}\max(0, -y_i \boldsymbol{w}^T \boldsymbol{x}_i)$$

$$L_p(\boldsymbol{w}) = \sum_{\substack{i=missclassified \\ Samples}} -y_i \boldsymbol{w}^T \boldsymbol{x}_i$$

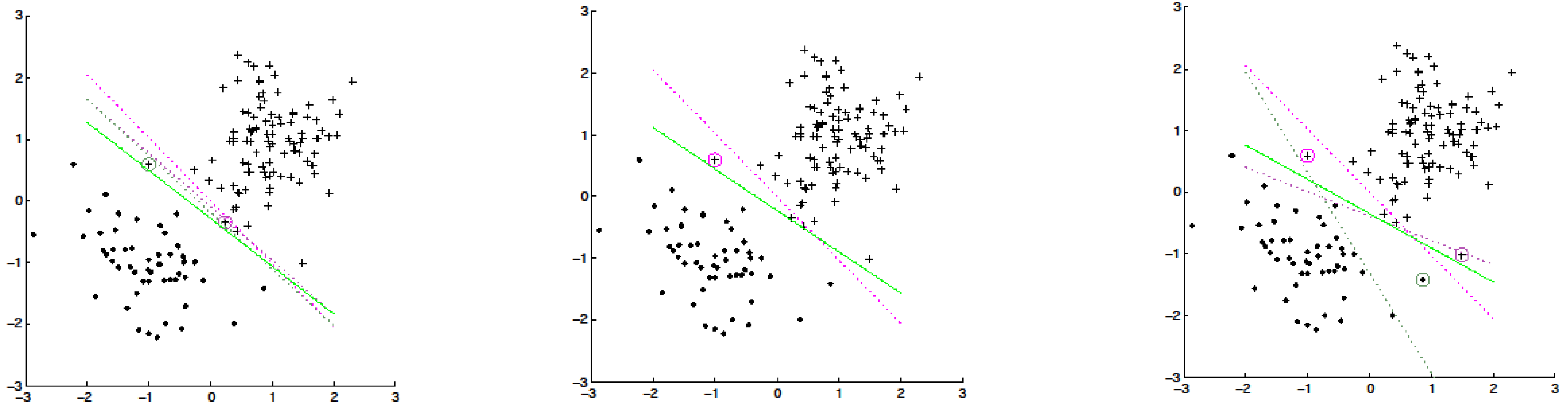
- Optimization
  - Gradient-based $\longrightarrow \boldsymbol{w} = \boldsymbol{w} + \eta y_i \boldsymbol{x}_i$
  - For missclassified sample x_i
  - $\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}_j} = -y_i x_{ij} \qquad \nabla L(\boldsymbol{w}) = -y_i \boldsymbol{x}_i$





http://ttsuchi.github.io/2015/08/26/perceptron.html

Learning Rate for the Perceptron

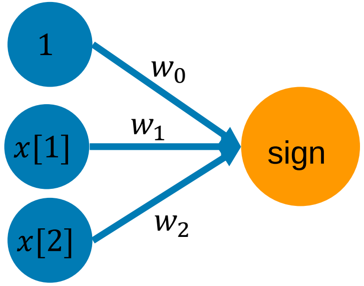


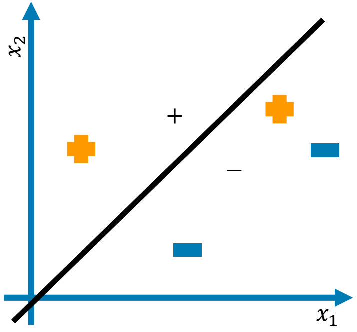
- $\boldsymbol{w} = \boldsymbol{w} + \eta y_i \boldsymbol{x}_i$
- Different learning rates
  - $\eta = 0.2, \eta = 0.5, \eta = 1.0$

Perceptron Training I

- Postive samples
  - $\boldsymbol{x}_0 = \begin{bmatrix}1\\3\end{bmatrix}$ $\boldsymbol{x}_1 = \begin{bmatrix}5\\4\end{bmatrix}$
- Negative samples
  - $\boldsymbol{x}_2 = \begin{bmatrix}6\\3\end{bmatrix}$ $\boldsymbol{x}_3 = \begin{bmatrix}3\\1\end{bmatrix}$
- Initial weights
  - $w_0 = 0; w_1 = -1; w_2 = 1$
- Extended data points
  - $\boldsymbol{x}_0 = \begin{bmatrix}1\\1\\3\end{bmatrix}$ $\boldsymbol{x}_1 = \begin{bmatrix}1\\5\\4\end{bmatrix}$ $\boldsymbol{x}_2 = \begin{bmatrix}1\\6\\3\end{bmatrix}$ $\boldsymbol{x}_3 = \begin{bmatrix}1\\3\\1\end{bmatrix}$

$$\boldsymbol{y} = \begin{bmatrix}1\\1\\-1\\-1\end{bmatrix} \quad \boldsymbol{w} = \begin{bmatrix}0\\-1\\1\end{bmatrix}$$

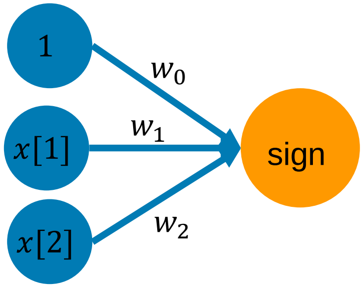




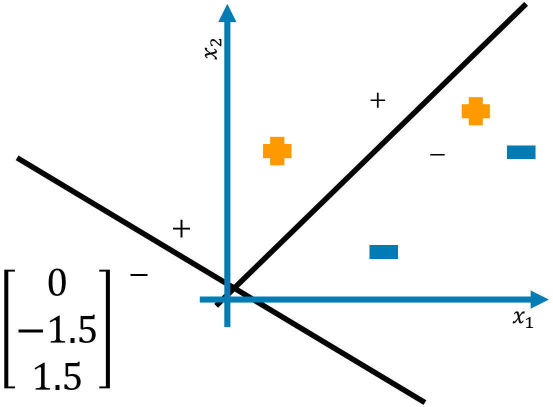
- Loss function
  - $L = \max(0, -y_i \boldsymbol{w}^T \boldsymbol{x}_i)$

$$\nabla \boldsymbol{L} = \begin{cases} 0 & if\ y_i \boldsymbol{w}^T \boldsymbol{x}_i > 0 \\ -y_i \boldsymbol{x}_i & otherwise \end{cases}$$

Perceptron Training II



- $\boldsymbol{x}_0 = \begin{bmatrix}1\\1\\3\end{bmatrix}$ $\boldsymbol{x}_1 = \begin{bmatrix}1\\5\\4\end{bmatrix}$ $\boldsymbol{x}_2 = \begin{bmatrix}1\\6\\3\end{bmatrix}$ $\boldsymbol{x}_3 = \begin{bmatrix}1\\3\\1\end{bmatrix}$ $\boldsymbol{y} = \begin{bmatrix}1\\1\\-1\\-1\end{bmatrix}$ $\boldsymbol{w} = \begin{bmatrix}0\\-1\\1\end{bmatrix}$
- $L_i = \max(0, -y_i \boldsymbol{w}^T \boldsymbol{x}_i)$ $\quad \nabla \mathrm{L_i} = \begin{cases} 0 & if\ y_i \boldsymbol{w}^T \boldsymbol{x}_i > 0 \\ -y_i \boldsymbol{x_i} & otherwise \end{cases}$ $\quad \eta = 0.5$
- $L_{x_0} = \max(0, -2) = 0$
- $L_{x_1} = \max(0, 1) = 1 \longrightarrow \boldsymbol{w} = \boldsymbol{w} + \eta y_i \boldsymbol{x_i} = \begin{bmatrix}0\\-1\\1\end{bmatrix} + 0.5 \cdot 1 \cdot \begin{bmatrix}1\\5\\4\end{bmatrix} = \begin{bmatrix}0.5\\1.5\\3\end{bmatrix}$
- $L_{x_2} = \max(0, 18.5) = 18.5 \longrightarrow \boldsymbol{w} = \boldsymbol{w} - \eta y_i \boldsymbol{x_i} = \begin{bmatrix}0.5\\1.5\\3\end{bmatrix} - 0.5 \cdot 1 \begin{bmatrix}1\\6\\3\end{bmatrix} = \begin{bmatrix}0\\-1.5\\1.5\end{bmatrix}$
- $L_{x_3} = \max(0, -3) = 0$ $\quad L_{x_0} = \max(0, -3) = 0 \longrightarrow \ldots$

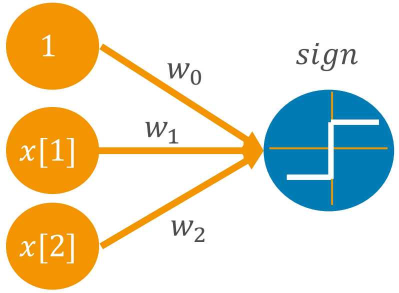


Perceptron

- How do you need to set the weights of a perceptron to seperate these points:

Class +1: $a = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad b = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad c = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

Class -1: $\mathrm{d} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$



- Which function does this perceptron then compute?

Start 5 4 3 2 1 End

History of the Perceptron

- Introduced by Frank Rosenblatt in **1958** [R58]
- Opponent: Marvin Minsky
  - Showed in **1969** that **XOR-Problem** cannot be solved with a perceptron [MP69]
  - The assumption that an extended perceptron could solve the problem proofed to be wrong.
    - AI winter
- Rumelhart and McClelland developed the multi-layer perceptron in **1986**
  - Two-layer perceptrons can represent all Boolean functions
    - Including XOR
  - Hard to train

The XOR Problem

- Can neural units compute simple functions of input?

AND			OR			XOR		
x1	x2	y	x1	x2	y	x1	x2	y
0	0	0	0	0	0	0	0	0
0	1	0	0	1	1	0	1	1
1	0	0	1	0	1	1	0	1
1	1	1	1	1	1	1	1	0

- Only a certain class of functions can be computed!
  -> Linear functions!

Perceptrons are Linear Classifiers

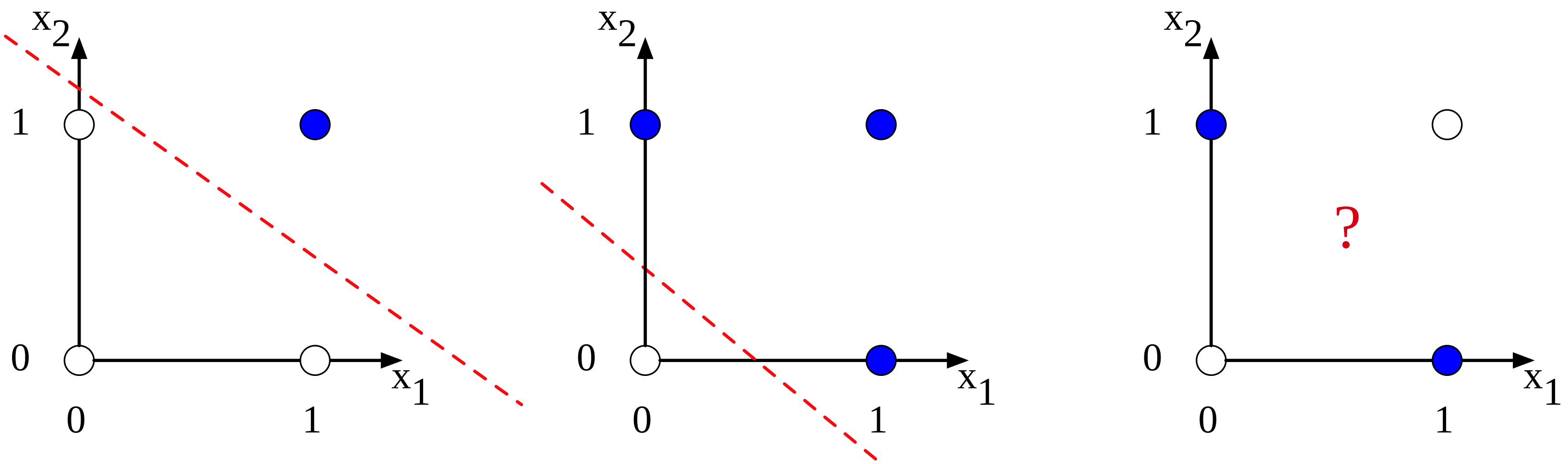
- Perceptron equation given x_1 and x_2, is the equation of a line

$$w_1 x_1 + w_2 x_2 + b = 0$$

  - in standard linear format: $x_2 = (-w_1/w_2)x_1 + (-b/w_2)$

- This line acts as a decision boundary
  - 0 if input is on one side of the line
  - 1 if on the other side of the line

Decision Boundaries



a) x_1 AND x_2 b) x_1 OR x_2 c) x_1 XOR x_2

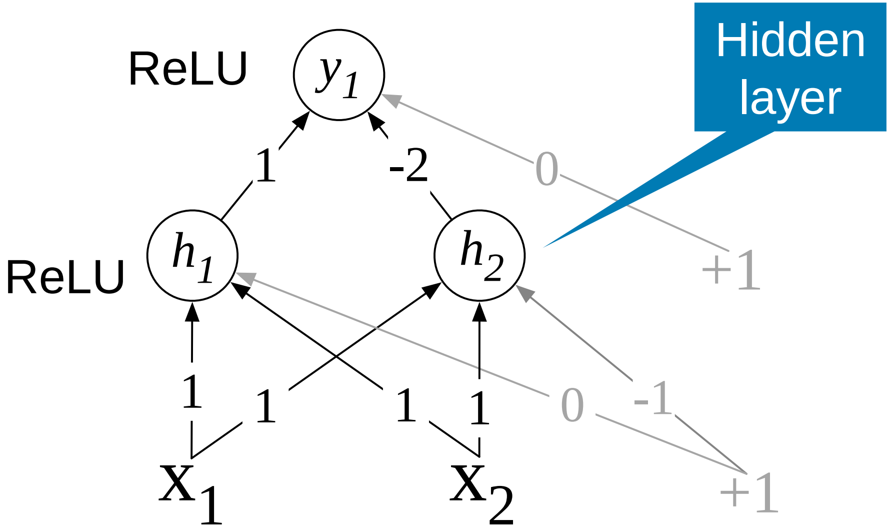
XOR is not a linearly separable function!

Solution to the XOR Problem

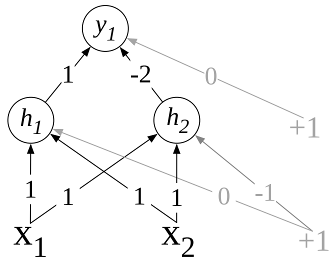
- XOR **can't** be calculated by a single perceptron
- XOR **can** be calculated by a layered network of units.

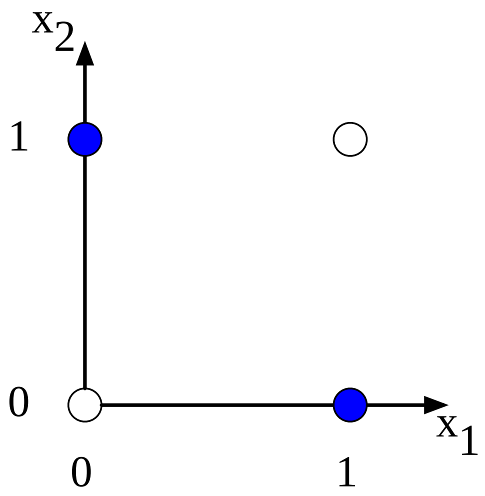
XOR

x1	x2	y
0	0	0
0	1	1
1	0	1
1	1	0

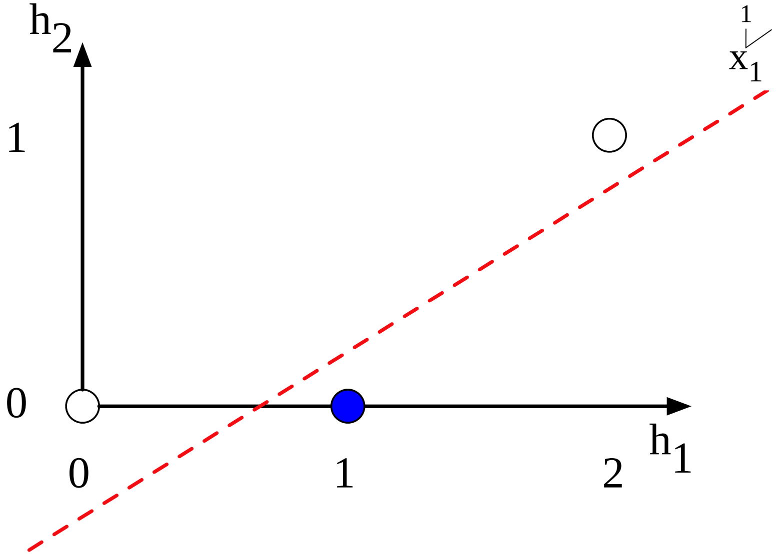


The Hidden Representation h





a) The original *x* space



b) The new (linearly separable) *h* space

(With learning: hidden layers will learn to form useful representations)

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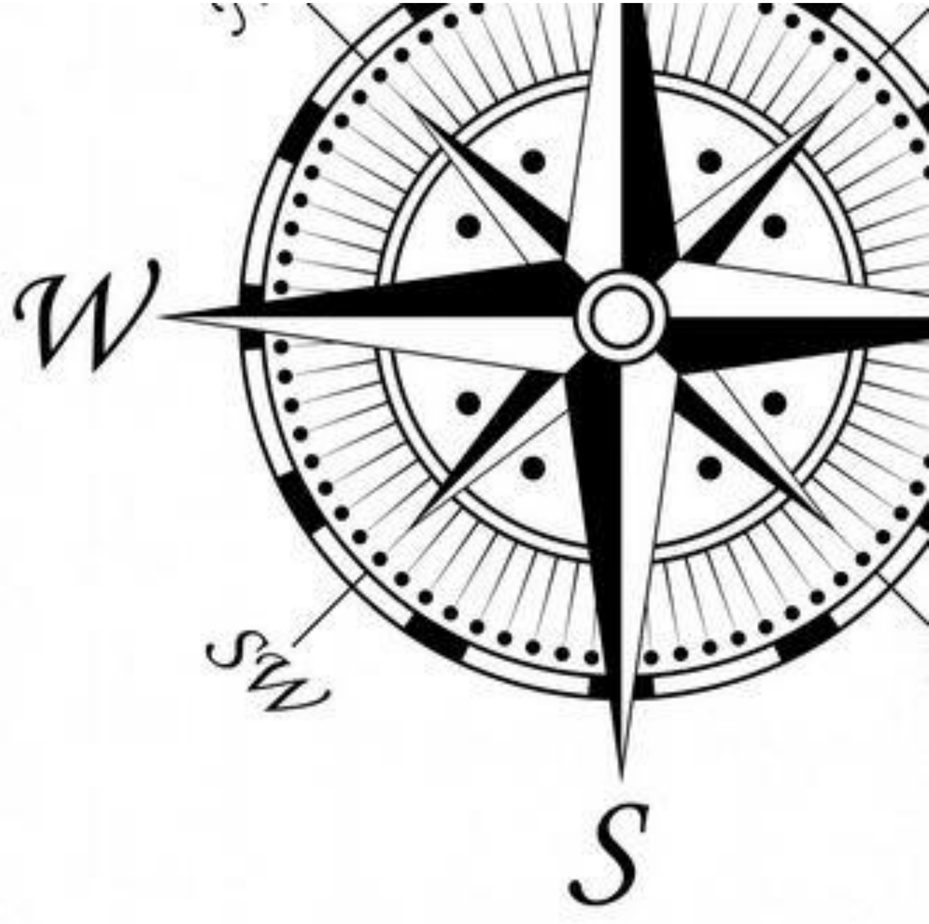
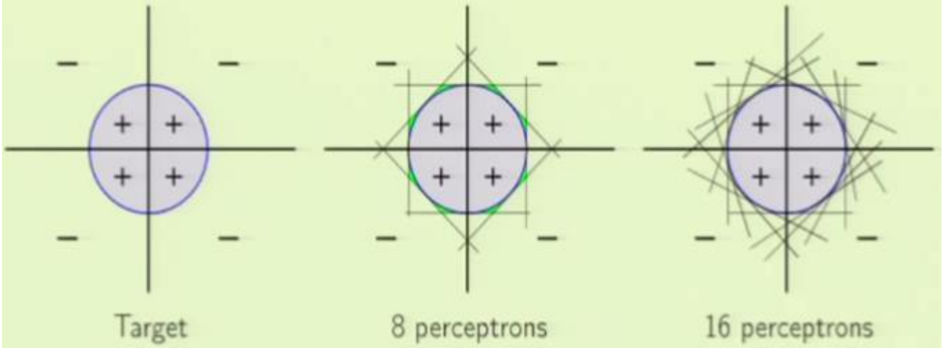


Multilayer Perceptron

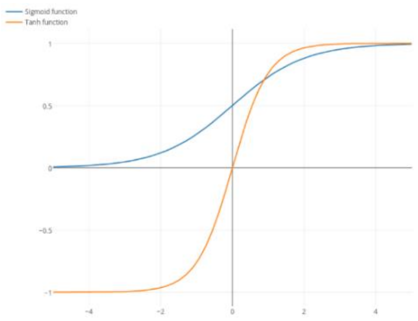
- Multilayer perceptrons (MLP) or multilayer neural networks or feedforward neural networks

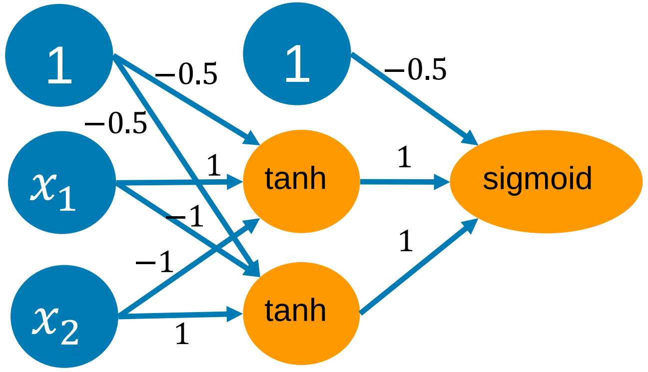


  – Generalization/Overfitting
  – High-dimensional
    $\longrightarrow$ Needs a lot of training examples
  – Hard to optimize
  – **But**: With two layers, all Boolean functions can be modeled!

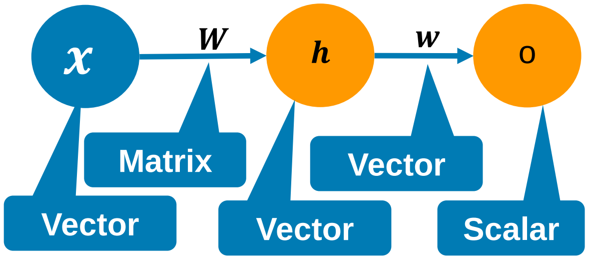
Multilayer Neural Networks

- Activation function: sigmoid or tanh



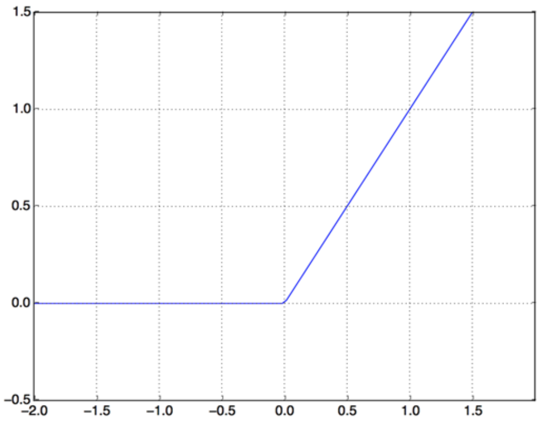


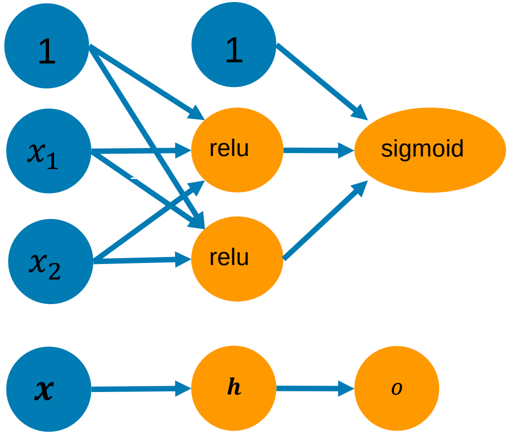
- Recap: compact representation
  - Omit bias/intercept terms
  - Node = input tensor or result of an activation function
  - Edge = parameters, which map input layer to output layer



Deep Feedforward Networks

- Activation function: relu
  - **Re**ctified **l**inear **u**nit





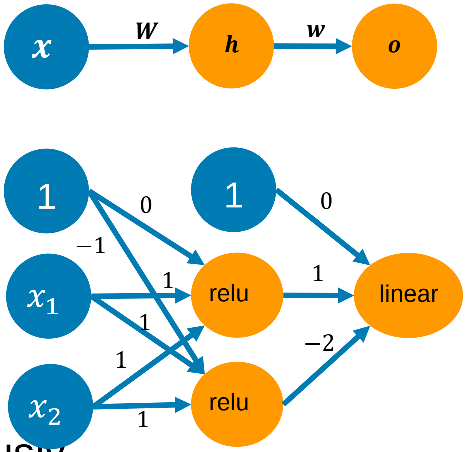
- XOR-Problem mit Deep Feedforward Networks:
  - $f(\boldsymbol{x};\boldsymbol{W},\boldsymbol{w}) = \boldsymbol{w}^T \max(0, \boldsymbol{W}^T\boldsymbol{x})$

XOR-Problem: Deep Feedforward Network

- XOR-Problem with deep feedforward networks:
  - $f(\boldsymbol{x};\boldsymbol{W},\boldsymbol{w}) = \boldsymbol{w}'^T \max(0, \boldsymbol{W}'^T\boldsymbol{x} + \boldsymbol{c}) + b$
  - $\underbrace{\boldsymbol{W}' = \begin{bmatrix}1 & 1\\1 & 1\end{bmatrix} \boldsymbol{c} = \begin{bmatrix}0\\-1\end{bmatrix}}\ \underbrace{\boldsymbol{w}' = \begin{bmatrix}1\\-2\end{bmatrix} \quad b = 0}$
  - $\boldsymbol{W} = \begin{bmatrix}0 & -1\\1 & 1\\1 & 1\end{bmatrix} \qquad \boldsymbol{w} = \begin{bmatrix}0\\1\\-2\end{bmatrix}$

Design matrix: One sample per row

$$\boldsymbol{X} = \begin{bmatrix}1 & 0 & 0\\1 & 0 & 1\\1 & 1 & 0\\1 & 1 & 1\end{bmatrix}$$



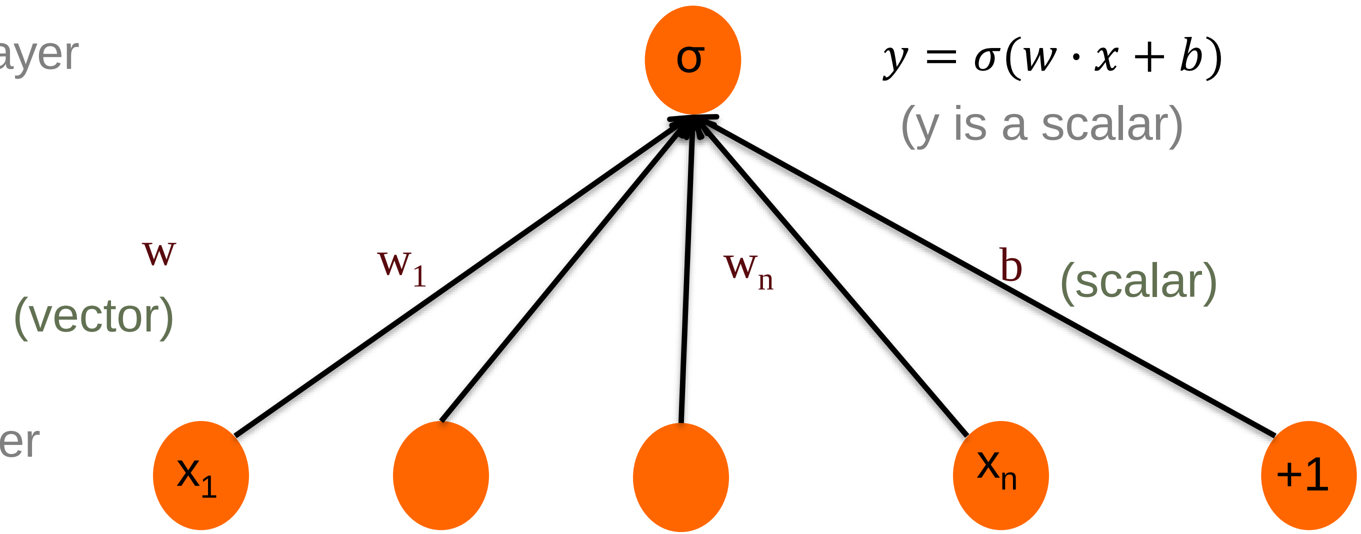
- Batch processing
  - Compute the output of the network for all four samples simultaneously
    - Forward pass
  - $\boldsymbol{XW} = \begin{bmatrix}0 & -1\\1 & 0\\1 & 0\\2 & 1\end{bmatrix} \quad \mathbf{H}' = \max(0, \boldsymbol{XW}) = \begin{bmatrix}0 & 0\\1 & 0\\1 & 0\\2 & 1\end{bmatrix} \quad \boldsymbol{H} = \begin{bmatrix}1 & 0 & 0\\1 & 1 & 0\\1 & 1 & 0\\1 & 2 & 1\end{bmatrix} \quad \mathbf{Hw} = \begin{bmatrix}0\\1\\1\\0\end{bmatrix}$

Binary Logistic Regression as a 1-layer Network

(we don't count the input layer in counting layers!)

Output layer
(σ node)

$y = \sigma(w \cdot x + b)$
(y is a scalar)



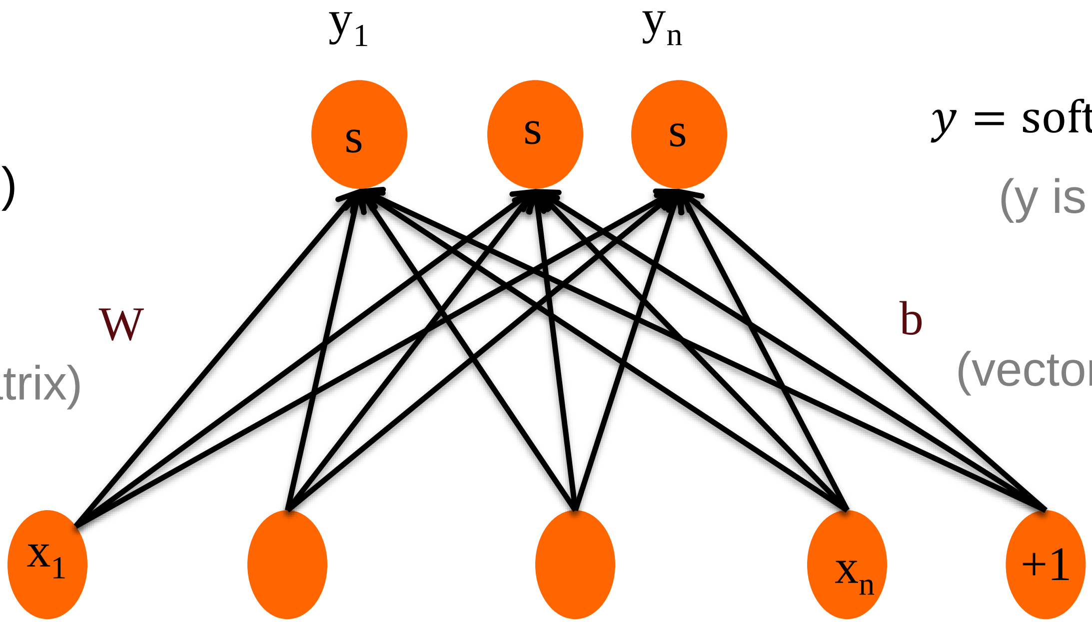
Input layer
vector x

Multinomial Logistic Regression as a 1-layer Network

Fully connected single layer network

Output layer
(softmax nodes)

Input layer
scalars



$$y = \mathrm{softmax}(Wx + b)$$

(y is a vector)

Softmax: a Generalization of Sigmoid

- For a vector *z* of dimensionality *k*, the softmax is:

$$\mathrm{softmax}(z) = \left[\frac{\exp(z_1)}{\sum_{i=1}^{k} \exp(z_i)}, \frac{\exp(z_2)}{\sum_{i=1}^{k} \exp(z_i)}, \ldots, \frac{\exp(z_k)}{\sum_{i=1}^{k} \exp(z_i)} \right]$$

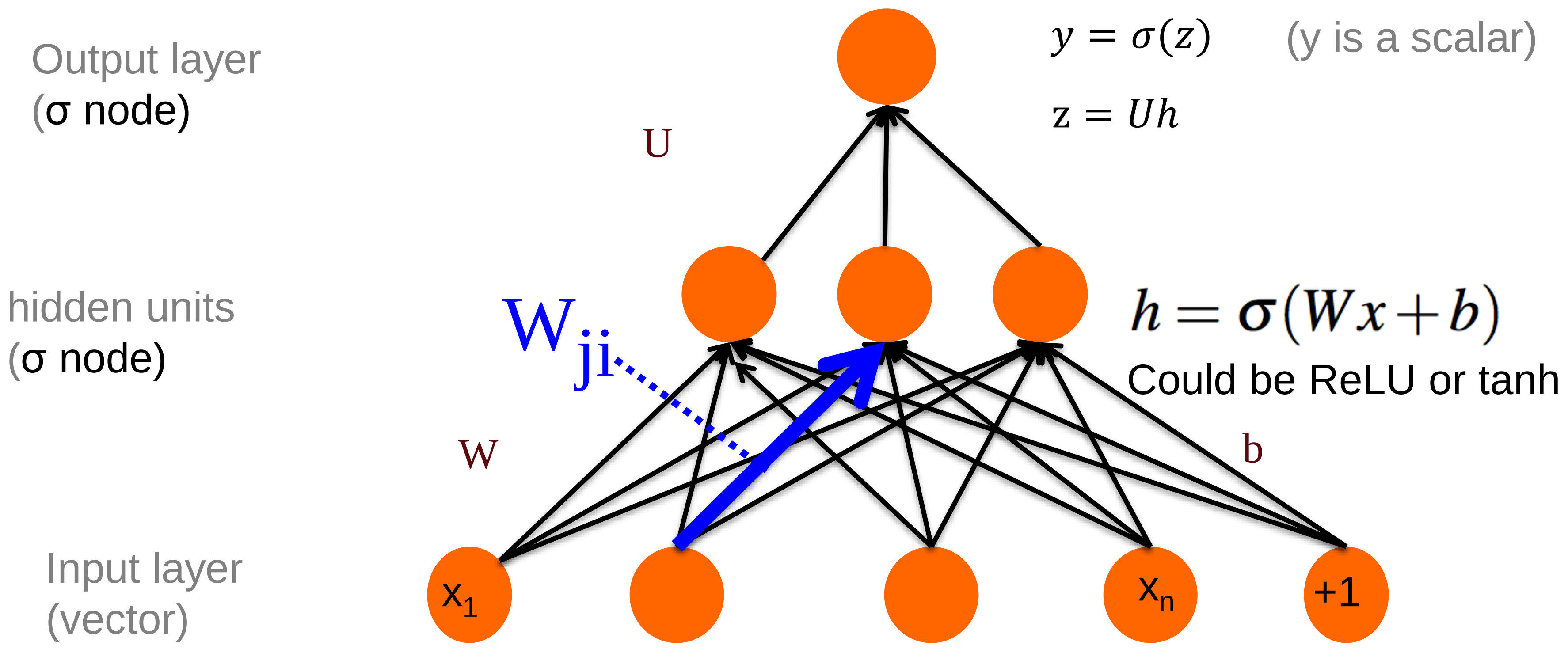
- Example:

$$\mathrm{softmax}(z_i) = \frac{\exp(z_i)}{\sum_{j=1}^{k} \exp(z_j)} \quad 1 \le i \le k$$

$$z = [0.6, 1.1, -1.5, 1.2, 3.2, -1.1]$$

$$\mathrm{softmax}(z) = [0.055, 0.090, 0.006, 0.099, 0.74, 0.010]$$

Two-Layer Network with Scalar Output

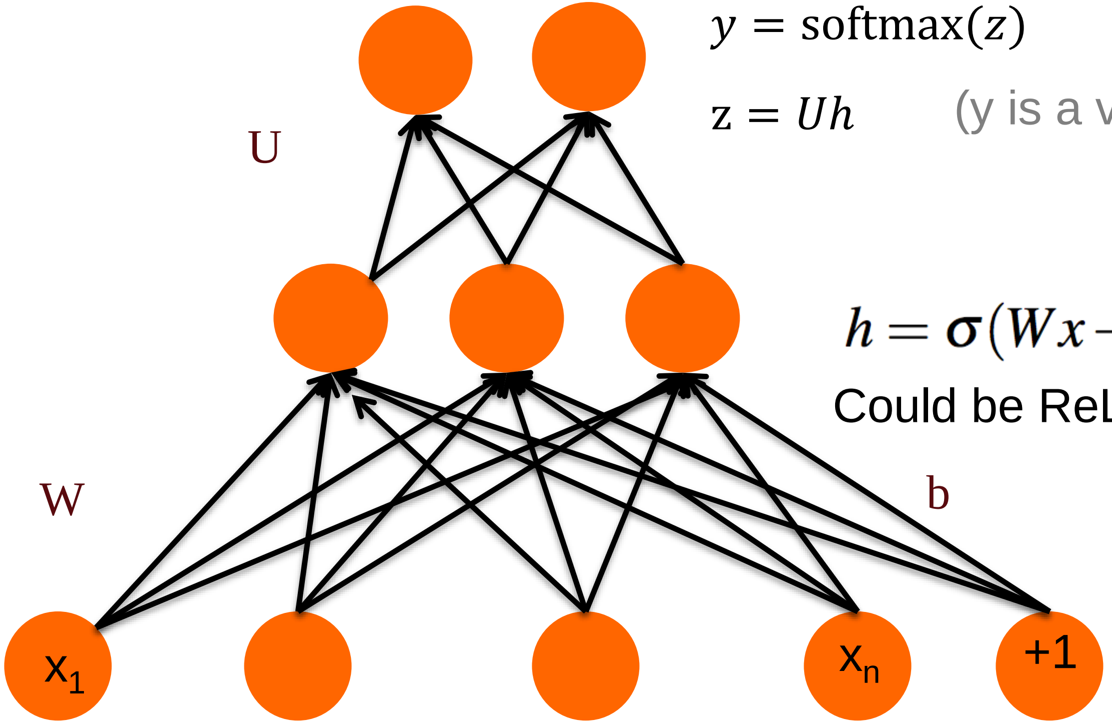


Two-Layer Network with Softmax Output

Output layer
(σ node)

hidden units
(σ node)

Input layer
(vector)



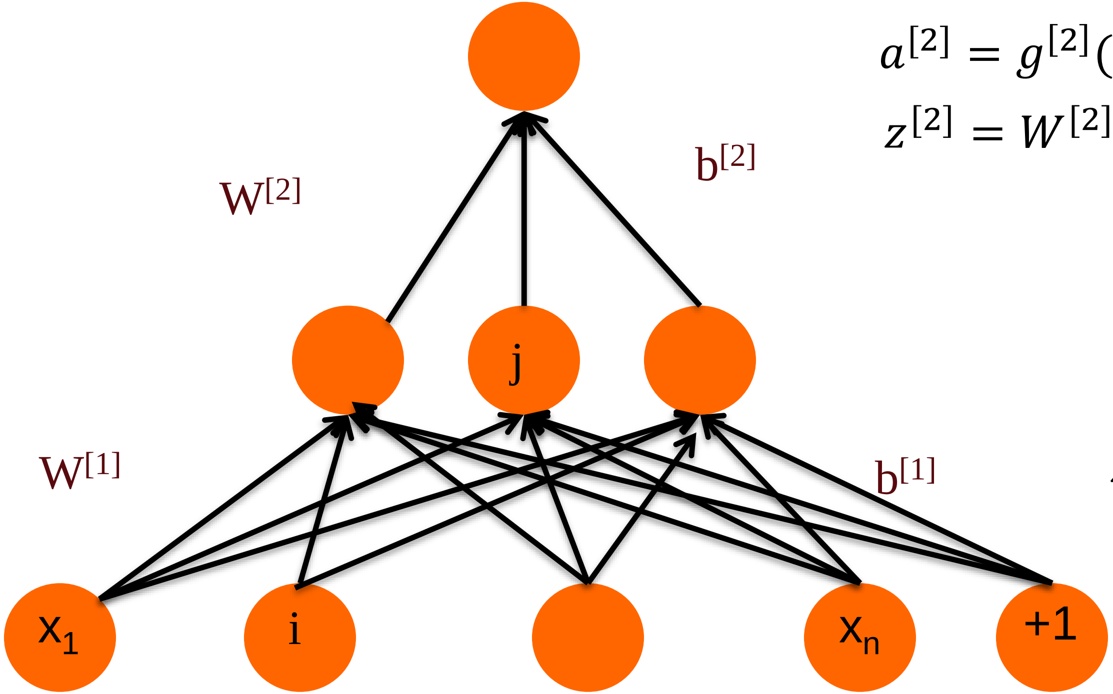
$y = \text{softmax}(z)$

$z = Uh$ (y is a vector)

$h = \sigma(Wx + b)$

Could be ReLU or tanh

Multi-layer Notation



$$y = a^{[2]}$$

$$a^{[2]} = g^{[2]}(z^{[2]})$$ sigmoid or softmax

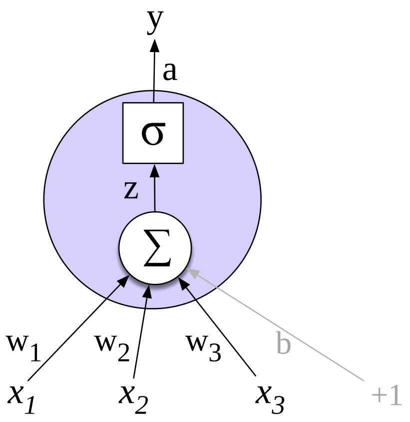
$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]}$$

$$a^{[1]} = g^{[1]}(z^{[1]})$$ ReLU

$$z^{[1]} = W^{[1]}a^{[0]} + b^{[1]}$$

$a^{[0]}$

Multi Layer Notation



$$
\begin{aligned}
z^{[1]} &= W^{[1]}a^{[0]} + b^{[1]} \\
a^{[1]} &= g^{[1]}(z^{[1]}) \\
z^{[2]} &= W^{[2]}a^{[1]} + b^{[2]} \\
a^{[2]} &= g^{[2]}(z^{[2]}) \\
\hat{y} &= a^{[2]}
\end{aligned}
$$

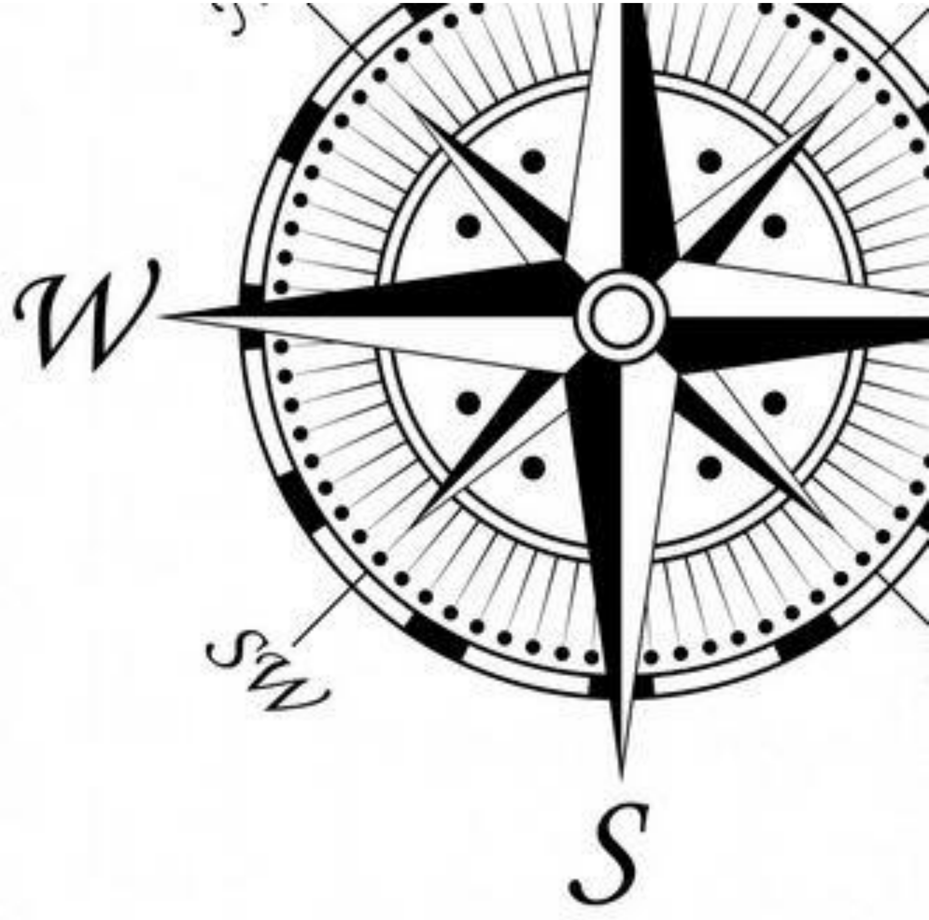
for i **in** 1..n

$$
\begin{aligned}
z^{[i]} &= W^{[i]}\, a^{[i-1]} + b^{[i]} \\
a^{[i]} &= g^{[i]}(z^{[i]})
\end{aligned}
$$

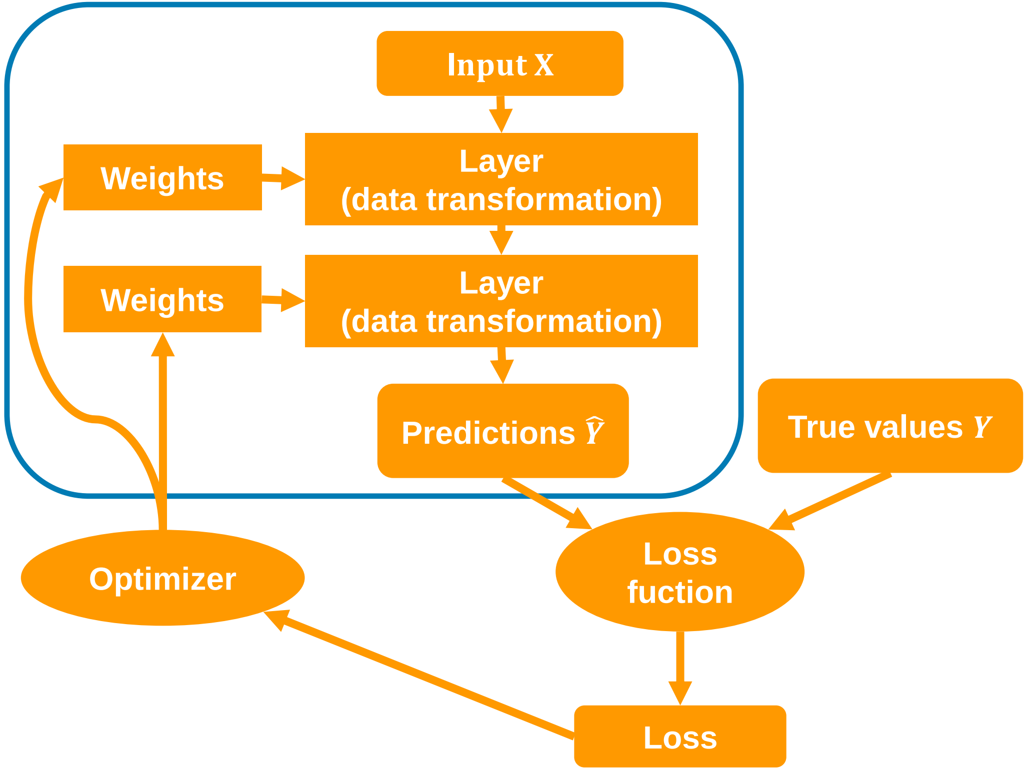
$$\hat{y} = a^{[n]}$$

Topics Today

1. Neural Network Unit
2. The Perceptron
3. Feedforward Neural Networks
4. **Gradient-Based Optimization**
5. Backprop(agation Algorithm)
6. Summary



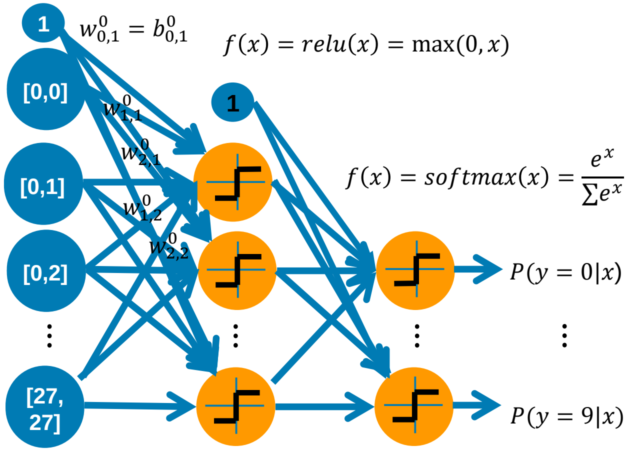
What Happens in a Neural Network?



What Happens in a Layer?

```
output = f(x)= f(dot(W, input) + b)
```

- W and b are tensors.
  - W are the **weights** or **parameters** of a layer and need to be trained / learned.
  - b can be merged into W by using a constant 1 as pseudo input
- At the beginning, weights are randomly initialized.
  - The network has not learned any meaningful representation or transormation and therefore no good mapping from input to output.



$$W^0 = \begin{bmatrix} w^0_{0,1} & \cdots & w^0_{28,1} \\ \vdots & \ddots & \vdots \\ w^0_{0,512} & \cdots & w^0_{28,512} \end{bmatrix}$$

How to Train a Network?

1. Randomly choose k training samples x (**mini batch**).
   - Alternative:
     - Batch (all training samples)
     - Stochastisic (one training sample)

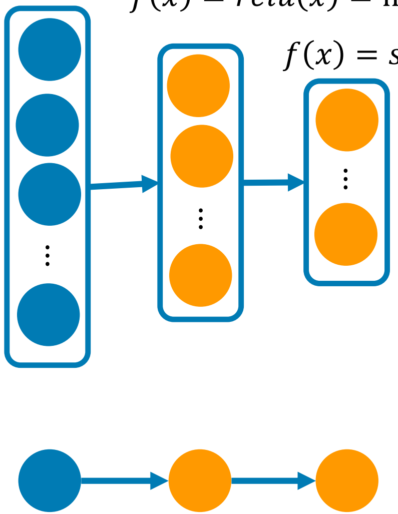
2. Compute the network‘s output $\hat{y}$ for input x.

3. Compute the **loss** of the network on the batch, i.e. the discrepancy between the predicition $\hat{y}$ and the actual value y

$$Loss = L(\hat{y}, y)$$

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

$$f(x) = softmax(x) = \frac{e^x}{\sum e^x}$$



4. Update the weights in a way that reduces the loss a little

Loss Functions

- Mean absolute error
  - $MAE = \frac{\sum_{i=1}^{n} |y_i - \hat{y}_i|}{n}$
- Mean squared error
  - $MSE = \frac{\sum_{i=1}^{n} |y_i - \hat{y}_i|^2}{n}$
- Binary cross entropy
  - $BCE = -(y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i))$
- Hinge loss
  - $Hinge = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$
- Categorical cross entropy
  - $CE = -\sum_C \boldsymbol{y}_i \log(\hat{\boldsymbol{y}}_i)$
- Kullback Leibler divergence
  - $KL(P, Q) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)}$

- Which loss functions for
  1. Regression problem
     - Input tensor $\boldsymbol{x} \rightarrow \mathbb{R}$
  2. Binary classification
     - Input tensor $\boldsymbol{x} \rightarrow [0,1]$ (can also be $\mathrm{x} \rightarrow [-1,1]$)
  3. (Single-label), multi-class classification
     - Input tensor $\boldsymbol{x} \rightarrow \boldsymbol{y}$, with y =binary vector and $|y| = 1$
  4. Multi-label, (multi-class) classification
     - Input tensor $\boldsymbol{x} \rightarrow \boldsymbol{y}$, with y =binary vector

How to Update the Weights I?

- Naive appraoch:
1. Choose a training **sample** randomly
2. Compute the **loss**
3. Choose a weight randomly
4. Update this weight **randomly**, keep all other weights fixed
5. Compute the **loss** again
    - If loss lower, keep weight and go to step 3.
    - If loss higher, go back to step 4.
    - If all weights are updated, go back to step 1.
    - If all samples were used for training, repeat whole process (i times)

- Way too **inefficient**!
  - Theoretically possible
  - Possible: Finding only **local minimum**

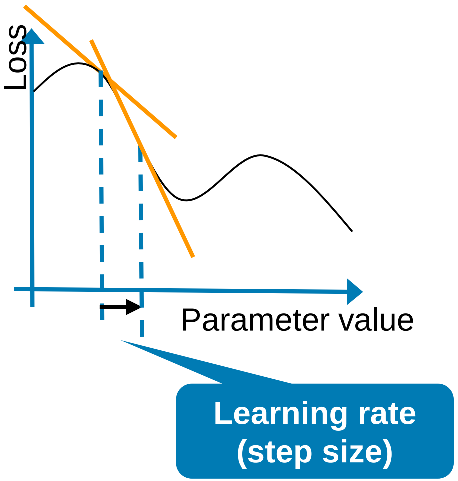
How to Update the Weights II?

- Analytical appraoch:
  1. Compute the derivative / gradient of the loss function $L(W)$
  2. Identify all W^* with $L'(W^*) = 0$
  3. Compute the loss for all W^*
  4. Select the W^* for which $L(W^*)$ is minimal
     - Globle minimum

- Not **efficiently** solvable!
  - If more than a few weights are involved
  - Typically: millions of weights!

Stochastic Gradient Descent (SGD)

- (true) **SGD**
  - Just like naive approach, only updates of weights not random
  - Updates are based on derivative / gradient
  - Stochastic, since samples are chosen randomly from training set



Batch and Mini-Batch SGD

- **Batch SGD**
  - Similar to SGD, but instead of using only one sample, compute loss on all training samples
    - Updates of weights much more accurate
    - Computation much more **expensive**
- **Mini-batch SGD**
  - Compromise between looking at all samples and only one sample
  - Simulaneously evaluating a small set of samples
    - Typically 8, 16, 32, 64, 128 or 256
- **Learning rate** is an important (hyper-) parameter
  - Variations:
    - Adaptive learning rate
      - Higher order derivatives (**momentum**)

The Backpropagation Algorithm

- SGD needs the derivative / gradient of the loss function for each weight
- Typically, a NN consists of many tensor operations

```
f(W1, W2, W3) = a(W1, b(W2, c(W3)))
```

  - For each single one it is easy to compute the gradient
- **Chain rule**:

$$f = u \circ v : V \to \mathbb{R}$$
$$(u \circ v)'(x_0) = u'\big(v(x_0)\big) \cdot v'(x_0)$$

- **Backpropagation Algoritm**
  - Application of chain rule to compute gradient of NN
  - Start with loss at the last (output) layer of the network and compute backwards the proportion that each weight contributed to this loss (backpropagation).
  - Implemented in Keras using symbolic differentiation
    - A gradient function for the chain of derivatives maps network parameter values (weights) to the respective gradients.

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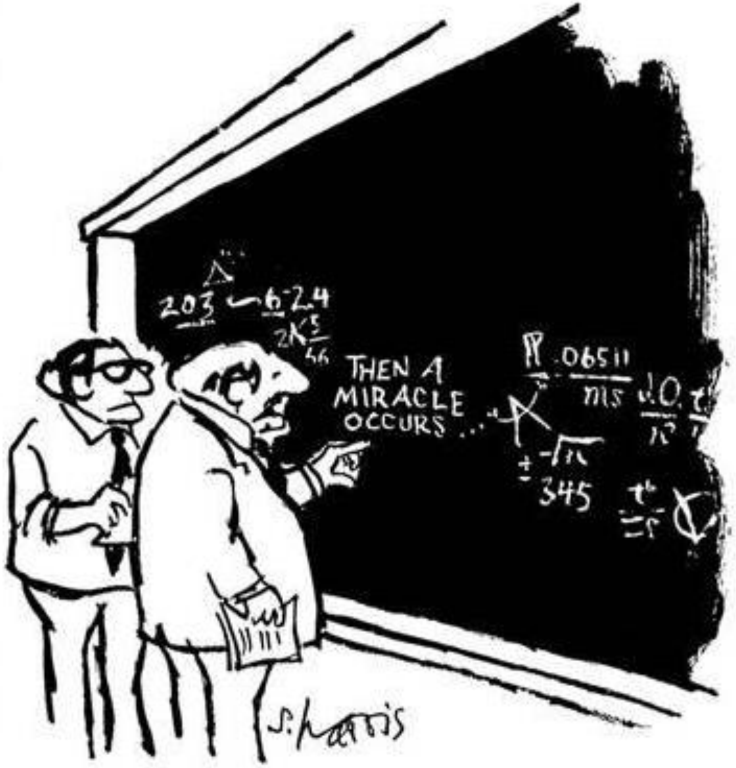
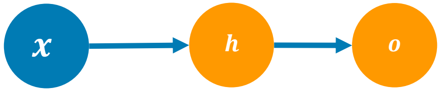


"I think you should be more explicit here in step two."

Computation of Gradients

- **Forward pass**
  - For feedforward neural nets
    - Computation of $\hat{y}$ given input $\boldsymbol{x}$
  - During training: Additionally computation of
    - Error / Loss function $J(\boldsymbol{\theta})$
  - Batch processing possible
    - Simultaneously computing $J(\boldsymbol{\theta})$ for multiple input samples $\boldsymbol{X}$

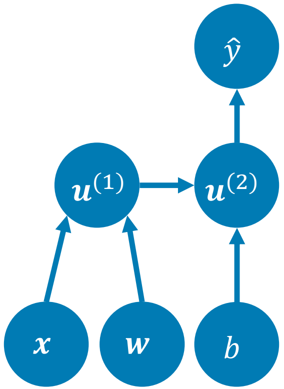


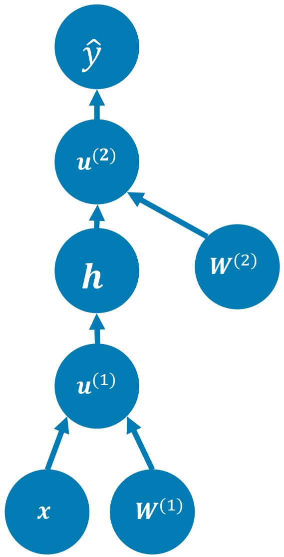
$\boldsymbol{\theta} = \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{w}$

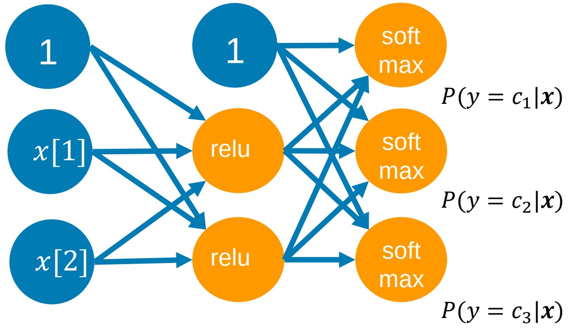
- **Backpropagation algorithm** (Rumelhart et al., 1986)
  - short: backprop
  - Propagation of the error back through the network to compute the gradients
  - **Backward pass**
  - Actual learning is done via gradient descent

Computational Graphs

Logistic regression $\hat{y} = \sigma(\boldsymbol{x}^T \boldsymbol{w} + b)$







Fully connected feed forward network

$$\hat{\boldsymbol{y}} = softmax\{\boldsymbol{h}\boldsymbol{W}^{(2)}\}$$
$$= softmax\{\max\{0, \boldsymbol{x}\boldsymbol{W}^{(1)}\}\boldsymbol{W}^{(2)}\}$$

Input: 2d, i.e. 2 features

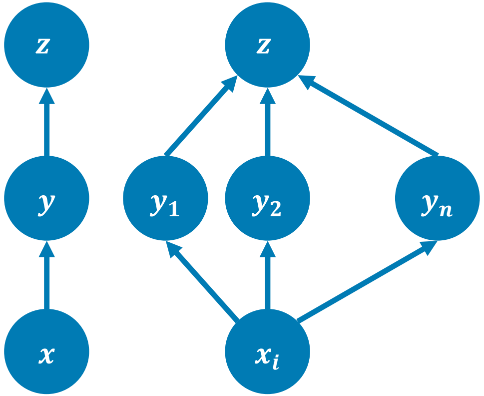
output: Probabilities for each of the three exclusive classes

Chain Rule

- Given $g, f\colon \mathbb{R} \to \mathbb{R}$
  - $y = g(x)$
  - $z = f\big(g(x)\big) = f(y)$

- Chain rule

$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$



- In case of vectors $\quad g\colon \mathbb{R}^m \to \mathbb{R}^n \qquad f\colon \mathbb{R}^n \to \mathbb{R}$
  - $\boldsymbol{x} \in \mathbb{R}^m;\ \boldsymbol{y} \in \mathbb{R}^n; \boldsymbol{y} = g(\boldsymbol{x});\ z = f(\boldsymbol{y})$

$$\frac{\partial z}{\partial x_i} = \sum_{j=1}^{n} \frac{\partial z}{\partial y_j}\frac{\partial y_j}{\partial x_i}$$

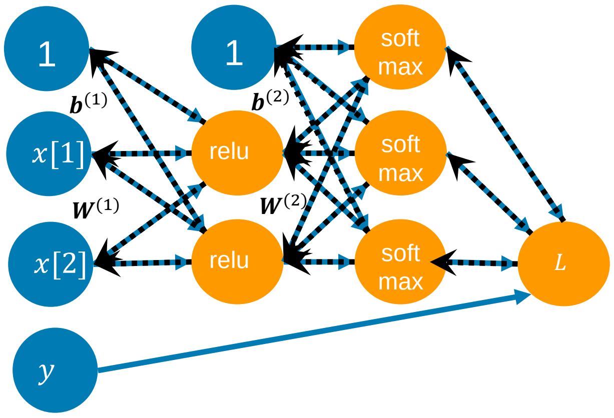
$$\nabla_{\boldsymbol{x}} z = \left(\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}\right)^T \nabla_{\boldsymbol{y}} z$$

$\boldsymbol{n \times m}$ **Jacobi-Matrix**

$\boldsymbol{n \times m}$ **Jacobi-Matrix**

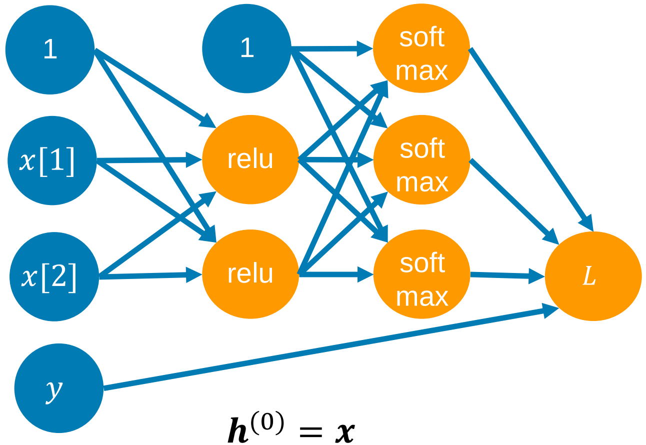
Graphical Representation

- For epoche 1 to k:
  - For each training sample / batch of samples:
    - Forward pass
    - Computation of loss function
    - Backward pass
    - Update of weights (gradient descent)



The Algorithm: Forward Pass

- Input:
  - Network depth l
  - $\boldsymbol{W}^{(i)}, i \in \{1, \dots, l\}$
  - $\boldsymbol{b}^{(i)}, i \in \{1, \dots, l\}$
  - $\boldsymbol{x}$ input data
  - $\boldsymbol{y}$ target data
- Output
  - Value of the loss function at position $\boldsymbol{x}$



$$
\begin{aligned}
&\boldsymbol{h}^{(0)} = \boldsymbol{x} \\
&\boldsymbol{for}\ k = 1, \dots, l\ \boldsymbol{do} \\
&\qquad \boldsymbol{a}^{(k)} = \boldsymbol{b}^{(k)} + \boldsymbol{W}^{(k)} \boldsymbol{h}^{(k-1)} \\
&\qquad \boldsymbol{h}^{(k)} = f\left(\boldsymbol{a}^{(k)}\right) \\
&\boldsymbol{end\ for} \\
&\hat{\boldsymbol{y}} = \boldsymbol{h}^{(l)} \\
&J = L(\hat{\boldsymbol{y}}, \boldsymbol{y}) + \lambda \Omega(\boldsymbol{\theta})
\end{aligned}
$$

Regularization;
$\boldsymbol{\theta} = \textbf{all weights} + \textbf{bias terms}$

The Algorithm: Backward Pass

- Output: The gradients of all activations $\boldsymbol{a}^{(k)}$
- Afterwards, update the weights
  - E.g. using gradient descent

$$
\begin{aligned}
&\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y}) \\
&\boldsymbol{for}\ k = l, l-1, \ldots, 1\ \boldsymbol{do} \\
&\qquad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'\left(\boldsymbol{a}^{(k)}\right) \\
&\qquad \nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\boldsymbol{\theta}) \\
&\qquad \nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g} \boldsymbol{h}^{(k-1)T} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\boldsymbol{\theta}) \\
&\qquad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)T} \boldsymbol{g} \\
&\boldsymbol{end\ for}
\end{aligned}
$$

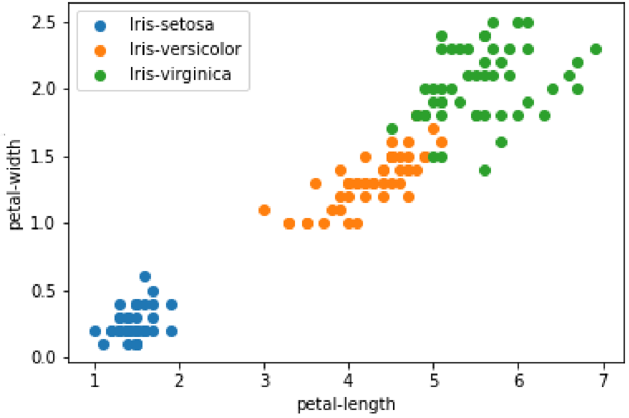
Gradient of output layer

Gradient before non-linear activation; ⊙ element-wise multiplication

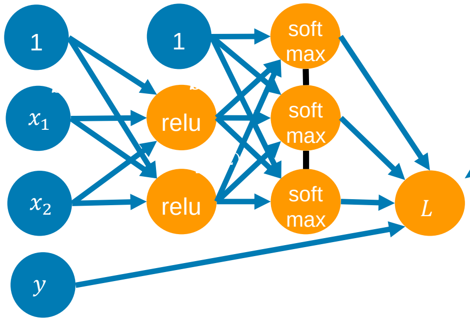
Gradients of weights and bias terms of layer k

Propagation of the gradients to the activations of the next lower layer

Walk-Through Example: Iris Dataset




```
>>> from sklearn.datasets import load_iris
>>> data = load_iris()
>>> list(data.target_names)
['setosa', 'versicolor', 'virginica']
```



Binary cross-entropy:

$$L = BCE(\hat{y}, y) = -(ylog(\hat{y}) + (1-y)log(1-\hat{y}))$$

Cross-entropy:

$$L = CE(\hat{y}, y) = -\sum_C y_i log(\hat{y}_i)$$

Cross-entropy considering also negative samples:

$$L = CE(\hat{y}, y) = -\sum_C y_i log(\hat{y}_i)\,(1-y_i)log(1-\hat{y}_i)$$

Walk-Through Example: Forward Pass

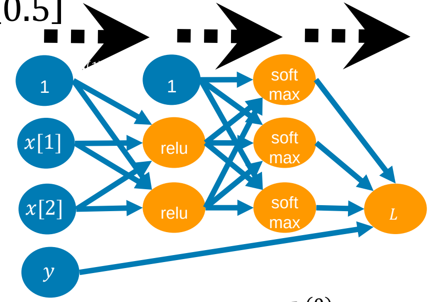
- Initializing the weights

Different Initializations possible

$$\boldsymbol{W}^{(1)} = \begin{bmatrix} 0.1 & -0.2 \\ 0.4 & 0.6 \end{bmatrix} \quad \boldsymbol{b}^{(1)} = \begin{bmatrix} 0.2 \\ -0.3 \end{bmatrix} \quad \boldsymbol{W}^{(2)} = \begin{bmatrix} 0.3 & -0.3 \\ 0.2 & 0.1 \\ 0.3 & -0.2 \end{bmatrix} \quad \boldsymbol{b}^{(2)} = \begin{bmatrix} -0.1 \\ -0.5 \\ -0.4 \end{bmatrix}$$

- First training sample $\boldsymbol{x}^{(1)} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.8 \\ 0.5 \end{bmatrix} \quad \boldsymbol{y}^{(1)} = \begin{bmatrix} 1.0 \\ 0.0 \\ 0.0 \end{bmatrix} \quad \boldsymbol{h}^{(0)} = \begin{bmatrix} 1.8 \\ 0.5 \end{bmatrix}$
  - $\boldsymbol{a}^{(1)} = \begin{bmatrix} 0.2 \\ -0.3 \end{bmatrix} + \begin{bmatrix} 0.1 & -0.2 \\ 0.4 & 0.6 \end{bmatrix} \begin{bmatrix} 1.8 \\ 0.5 \end{bmatrix} = \begin{bmatrix} 0.28 \\ 0.72 \end{bmatrix}$
  - $\boldsymbol{h}^{(1)} = relu\left(\begin{bmatrix} 0.28 \\ 0.72 \end{bmatrix}\right) = \begin{bmatrix} 0.28 \\ 0.72 \end{bmatrix}$
  - $\boldsymbol{a}^{(2)} = \begin{bmatrix} -0.1 \\ -0.5 \\ -0.4 \end{bmatrix} + \begin{bmatrix} 0.3 & -0.3 \\ 0.2 & 0.1 \\ 0.3 & -0.2 \end{bmatrix} \begin{bmatrix} 0.28 \\ 0.72 \end{bmatrix} = \begin{bmatrix} -0.23 \\ -0.37 \\ -0.46 \end{bmatrix}$
  - $\boldsymbol{o}^{(2)} = \text{softmax}\left(\begin{bmatrix} -0.23 \\ -0.37 \\ -0.46 \end{bmatrix}\right) = \begin{bmatrix} 0.38 \\ 0.32 \\ 0.30 \end{bmatrix} = \hat{\boldsymbol{y}}$
  - $J = CE\left(\begin{bmatrix} 0.38 \\ 0.32 \\ 0.30 \end{bmatrix}, \begin{bmatrix} 1.0 \\ 0.0 \\ 0.0 \end{bmatrix}\right) = -(\log(0.38) + \log(1 - 0.32) + \log(1 - 0.30)) = 0.74$

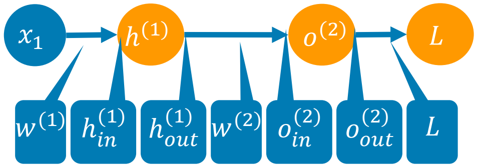
Considers also negative samples



$\boldsymbol{h}^{(0)} = \boldsymbol{x}$
$\boldsymbol{for}\ k = 1, \dots, l\ \boldsymbol{do}$
$\quad \boldsymbol{a}^{(k)} = \boldsymbol{b}^{(k)} + \boldsymbol{W}^{(k)} \boldsymbol{h}^{(k-1)}$
$\quad \boldsymbol{h}^{(k)} = f\left(\boldsymbol{a}^{(k)}\right)$
$\boldsymbol{end\ for}$
$\hat{\boldsymbol{y}} = \boldsymbol{h}^{(l)} = \boldsymbol{o}^{(l)}$
$J = L(\hat{\boldsymbol{y}}, \boldsymbol{y}) + \lambda\Omega(\boldsymbol{\theta})$

https://github.com/Prakashvanapalli/TensorFlow/blob/master/Blogposts/Backpropogation_with_Images.ipynb

Walk-Through Example: Backward Pass I

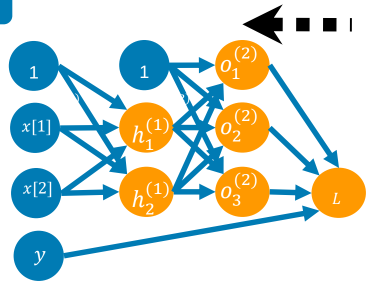


- Loss for $\boldsymbol{x}^{(1)} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.8 \\ 0.5 \end{bmatrix}$

  $$L = CE\left(\begin{bmatrix} 0.38 \\ 0.32 \\ 0.30 \end{bmatrix}, \begin{bmatrix} 1.0 \\ 0.0 \\ 0.0 \end{bmatrix}\right) = 0.74$$

- Reminder: chain rule

  $$\frac{\partial L}{\partial W^{(1)}} = \frac{\partial L}{\partial o_{out}} \frac{\partial o_{out}}{\partial o_{in}} \frac{\partial o_{in}}{\partial h_{out}} \frac{\partial h_{out}}{\partial h_{in}} \frac{\partial h_{in}}{\partial W^{(1)}}$$



- Gradient of loss function:

- $$\frac{\partial L}{\partial o_{out}} = \begin{bmatrix} \frac{\partial L}{\partial o_{1,out}} \\ \frac{\partial L}{\partial o_{2,out}} \\ \frac{\partial L}{\partial o_{3,out}} \end{bmatrix} = \begin{bmatrix} -1 \cdot (1 \cdot \frac{1}{0.38} + (1-1) \cdot \frac{1}{1-0.38}) \\ -1 \cdot (0 \cdot \frac{1}{0.32} + (1-0) \cdot \frac{1}{1-0.32}) \\ -1 \cdot (0 \cdot \frac{1}{0.30} + (1-0) \cdot \frac{1}{1-0.30}) \end{bmatrix} = \begin{bmatrix} -2.63 \\ -1.47 \\ -1.43 \end{bmatrix}$$

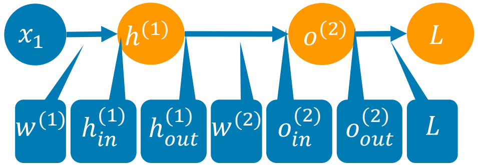
Partial derivative of cross-entropy:

$$\frac{\partial L}{\partial \hat{y}_i} = -1 \cdot (y_i \frac{1}{\hat{y}_i} + (1 - y_i) \frac{1}{1 - \hat{y}_i})$$

$\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y})$
$\boldsymbol{for}\ k = l, l-1, \ldots, 1\ \boldsymbol{do}$
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'(\boldsymbol{a}^{(k)})$
$\quad \nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g} \boldsymbol{h}^{(k-1)T} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)T} \boldsymbol{g}$
$\boldsymbol{end\ for}$

Hadamard product

Walk-Through Example: Backward Pass II

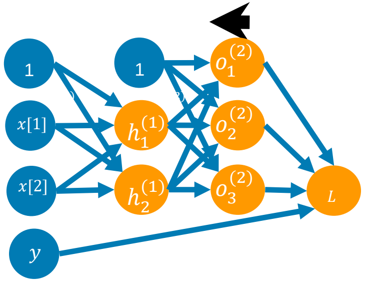


- Gradient of the output of the output layer

$$\frac{\partial o_{out}}{\partial o_{in}} = \begin{bmatrix} \frac{\partial o_{1,out}^{(2)}}{\partial o_{1,in}^{(2)}} \\ \frac{\partial o_{2,out}^{(2)}}{\partial o_{2,in}^{(2)}} \\ \frac{\partial o_{3,out}^{(2)}}{\partial o_{3,in}^{(2)}} \end{bmatrix} = \begin{bmatrix} \frac{e^{-0.23} \cdot (e^{-0.37} + e^{-0.46})}{(e^{-0.23} + e^{-0.37} + e^{-0.46})^2} \\ \frac{e^{-0.37} \cdot (e^{-0.23} + e^{-0.46})}{(e^{-0.23} + e^{-0.37} + e^{-0.46})^2} \\ \frac{e^{-0.46} \cdot (e^{-0.23} + e^{-0.37})}{(e^{-0.23} + e^{-0.37} + e^{-0.46})^2} \end{bmatrix} = \begin{bmatrix} 0.23 \\ 0.22 \\ 0.21 \end{bmatrix}$$

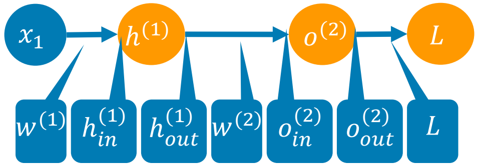
Partrial derivative of softmax:

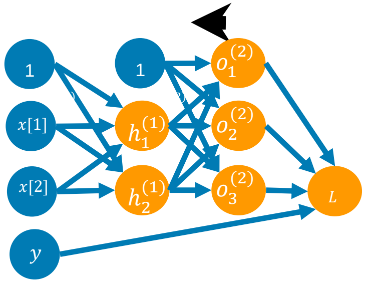
$$\frac{\partial o_{i,out}^{(2)}}{\partial o_{i,in}^{(2)}} = \frac{e^{o_{i,in}^{(2)}} \cdot \sum_{j \neq i} e^{o_{j,in}^{(2)}}}{\left(\sum_j e^{o_{j,in}^{(2)}}\right)^2}$$



$\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y})$
$\boldsymbol{for}\ k = l, l-1, \dots, 1\ \boldsymbol{do}$
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'(\boldsymbol{a}^{(k)})$
$\quad \nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g} \boldsymbol{h}^{(k-1)T} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)T} \boldsymbol{g}$
$\boldsymbol{end\ for}$

Walk-Through Example: Backward Pass III





- Gradient of the input of the output layer with respect to weights $W^{(2)}$

$$\frac{\partial o_{1,in}^{(2)}}{\partial W_{1,1}^{(2)}} = \frac{\partial o_{2,in}^{(2)}}{\partial W_{1,2}^{(2)}} = \frac{\partial o_{3,in}^{(2)}}{\partial W_{1,3}^{(2)}} = 0.28 \quad \frac{\partial o_{1,in}^{(2)}}{\partial W_{2,1}^{(2)}} = \frac{\partial o_{2,in}^{(2)}}{\partial W_{2,2}^{(2)}} = \frac{\partial o_{3,in}^{(2)}}{\partial W_{2,3}^{(2)}} = 0.72$$

Partial derivative:

$$\frac{\partial \boldsymbol{o}_{1,in}^{(2)}}{\partial \boldsymbol{W}_{1,1}^{(2)}} = \frac{\partial\left(\boldsymbol{h}_1^{(1)} \boldsymbol{W}_{1,1}^{(2)} + \boldsymbol{h}_2^{(1)} \boldsymbol{W}_{2,1}^{(2)} + \boldsymbol{b}_1^{(2)}\right)}{\partial \boldsymbol{W}_{1,1}^{(2)}} = \boldsymbol{h}_{1,out}^{(1)}$$

$\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y})$
$\boldsymbol{for}\ k = l, l-1, \dots, 1\ \boldsymbol{do}$
  $\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'\left(\boldsymbol{a}^{(k)}\right)$
  $\nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\boldsymbol{\theta})$
  $\nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g} \boldsymbol{h}^{(k-1)T} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\boldsymbol{\theta})$
  $\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)T} \boldsymbol{g}$
$\boldsymbol{end\ for}$

Walk-Through Example: Backward Pass IV

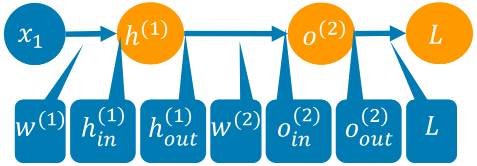
$$\frac{\partial L}{\partial W^{(2)}} = \frac{\partial L}{\partial o_{out}}\frac{\partial o_{out}}{\partial o_{in}}\frac{\partial o_{in}}{\partial W^{(2)}} = \begin{bmatrix} \frac{\partial L}{\partial o_{1,out}}\frac{\partial o_{1,out}}{\partial o_{1,in}}\frac{\partial o_{1,in}}{\partial W^{(2)}_{1,1}} & \frac{\partial L}{\partial o_{1,out}}\frac{\partial o_{1,out}}{\partial o_{1,in}}\frac{\partial o_{1,in}}{\partial W^{(2)}_{2,1}} \\ \frac{\partial L}{\partial o_{2,out}}\frac{\partial o_{2,out}}{\partial o_{2,in}}\frac{\partial o_{2,in}}{\partial W^{(2)}_{1,2}} & \frac{\partial L}{\partial o_{2,out}}\frac{\partial o_{2,out}}{\partial o_{2,in}}\frac{\partial o_{2,in}}{\partial W^{(2)}_{2,2}} \\ \frac{\partial L}{\partial o_{3,out}}\frac{\partial o_{3,out}}{\partial o_{13in}}\frac{\partial o_{3,in}}{\partial W^{(2)}_{1,3}} & \frac{\partial L}{\partial o_{3,out}}\frac{\partial o_{3,out}}{\partial o_{13in}}\frac{\partial o_{3,in}}{\partial W^{(2)}_{2,3}} \end{bmatrix}$$

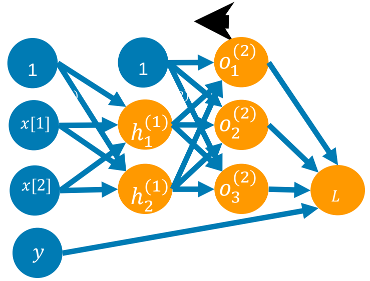
$$\frac{\partial L}{\partial W^{(2)}} = \begin{bmatrix} -2.63 \cdot 0.23 \cdot 0.28 & -2.63 \cdot 0.23 \cdot 0.72 \\ -1.47 \cdot 0.22 \cdot 0.28 & -1.47 \cdot 0.22 \cdot 0.72 \\ -1.43 \cdot 0.21 \cdot 0.28 & -1.43 \cdot 0.21 \cdot 0.72 \end{bmatrix}$$

- Gradient descent with learning rate $\lambda = 0.5$ results in new weights:

$$\boldsymbol{W}^{(2)} = \begin{bmatrix} 0.3 & -0.3 \\ 0.2 & 0.1 \\ 0.3 & -0.2 \end{bmatrix} \qquad \nabla_{\boldsymbol{W}^{(2)}}\boldsymbol{L} = \begin{bmatrix} -0.17 & -0.44 \\ -0.09 & -0.23 \\ -0.08 & -0.22 \end{bmatrix}$$

$$\boldsymbol{W}'^{(2)} = \boldsymbol{W}^{(2)} - \lambda\nabla_{\boldsymbol{W}^{(2)}}\boldsymbol{L} = \begin{bmatrix} 0.39 & -0.08 \\ 0.25 & 0.22 \\ 0.34 & -0.09 \end{bmatrix}$$

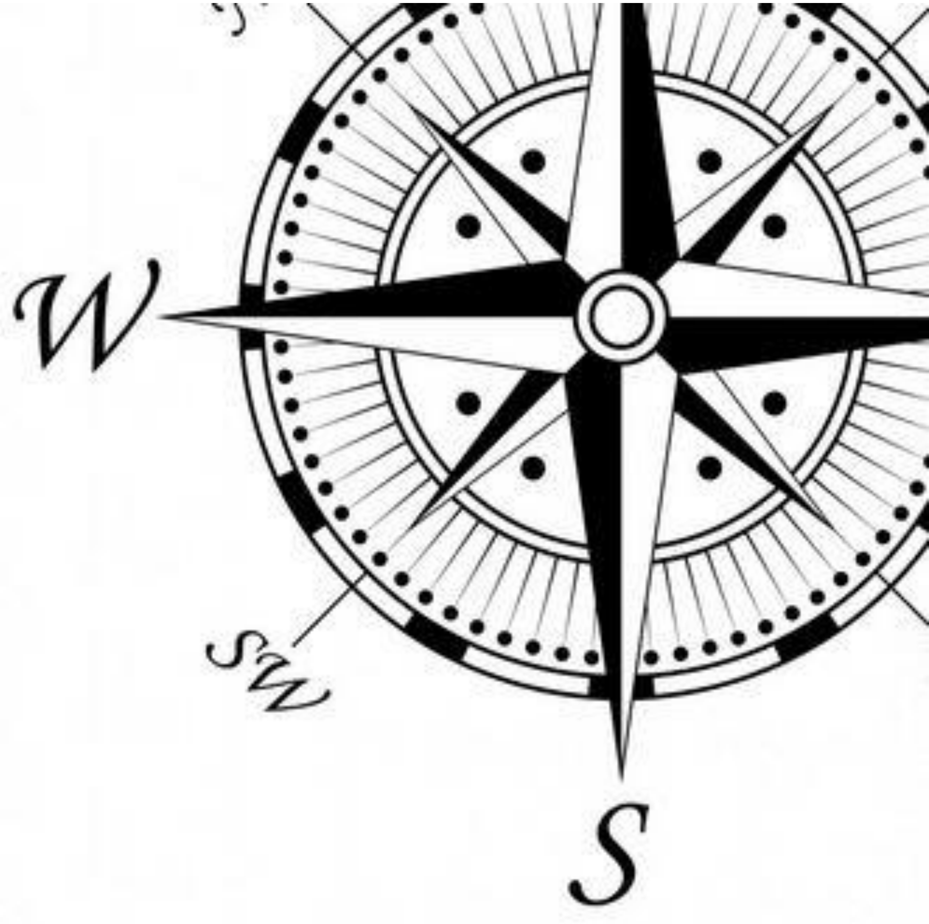




$\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y})$
for $k = l, l-1, \ldots, 1$ ***do***
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'(\boldsymbol{a}^{(k)})$
$\quad \nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g}\boldsymbol{h}^{(k-1)T} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\boldsymbol{\theta})$
$\quad \boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)T} \boldsymbol{g}$
end for

Topics Today

1. Neural Network Unit
2. The Perceptron
3. Feedforward Neural Networks
4. Gradient-Based Optimization
5. Backprop(agation Algorithm)
6. **Summary**



Summary

- Will be filled out during next session!

Learning Goals for this Chapter

- Know how the perceptron works
- Explain the need for multiple layers
- Understand gradient-based optimization
- Describe the components of deep neural networks
- Understand and apply the backpropagation algorithm

- Relevant chapters
  - P2, P3
  - S3 (2021) https://www.youtube.com/watch?v=X0Jw4kgaFlg

References

- [R58] Rosenblatt, F. (1958). The perceptron: a probabilistic model for information storage and organization in the brain. *Psychological review*, *65*(6), 386.
- [MP69] Minsky, M., & Papert, S. (1969). An introduction to computational geometry. *Cambridge tiass., HIT*, *479*(480), 104.