Deep Learning

Feedforward neural networks: Multi Layer Perceptron

Technische Hochschule Rosenheim
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https://lme.tf.fau.de/

Overview

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- Perceptrons
- MLP-Training Basics
- MLP – Layer Abstraction
- Universal Approximation Theorem

Perceptrons

Real Neurons

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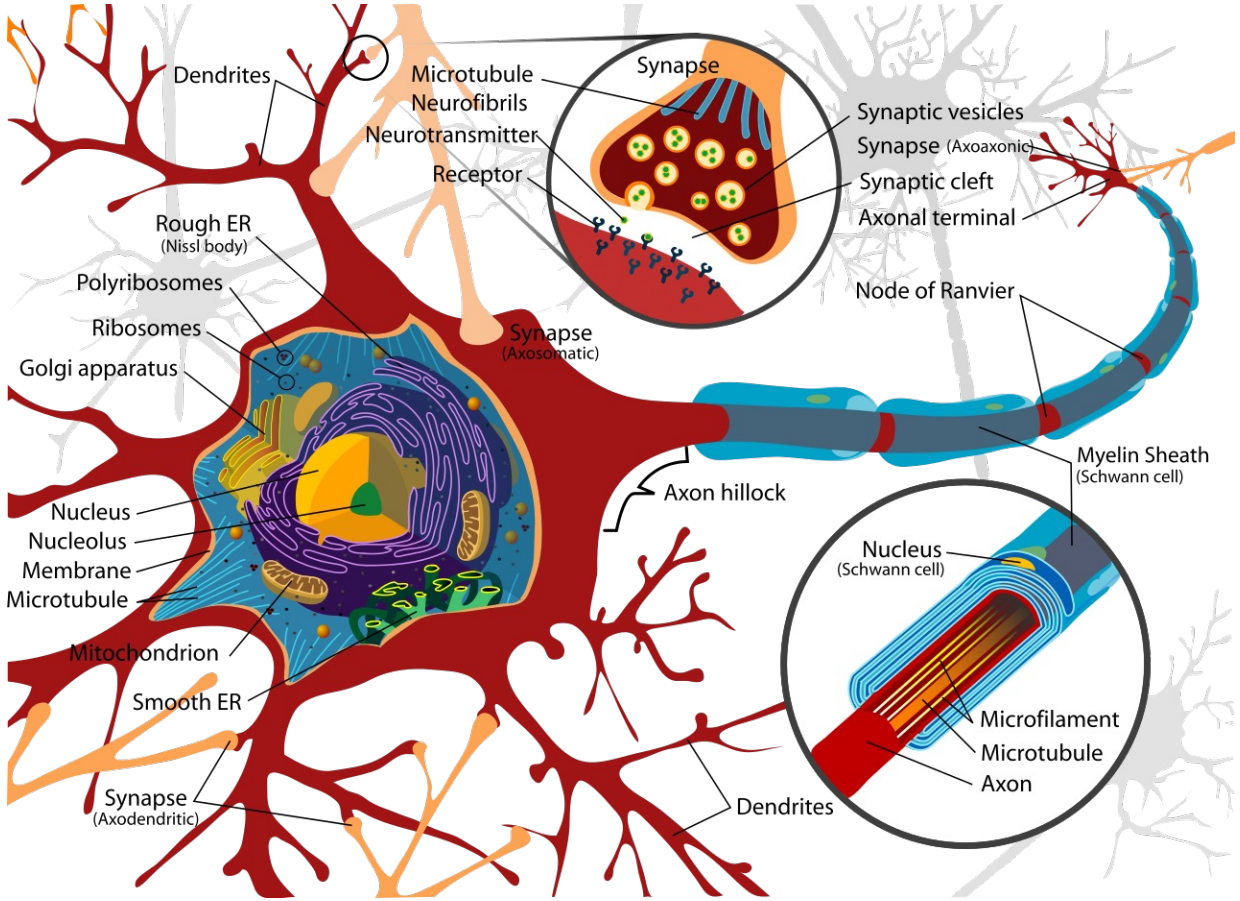
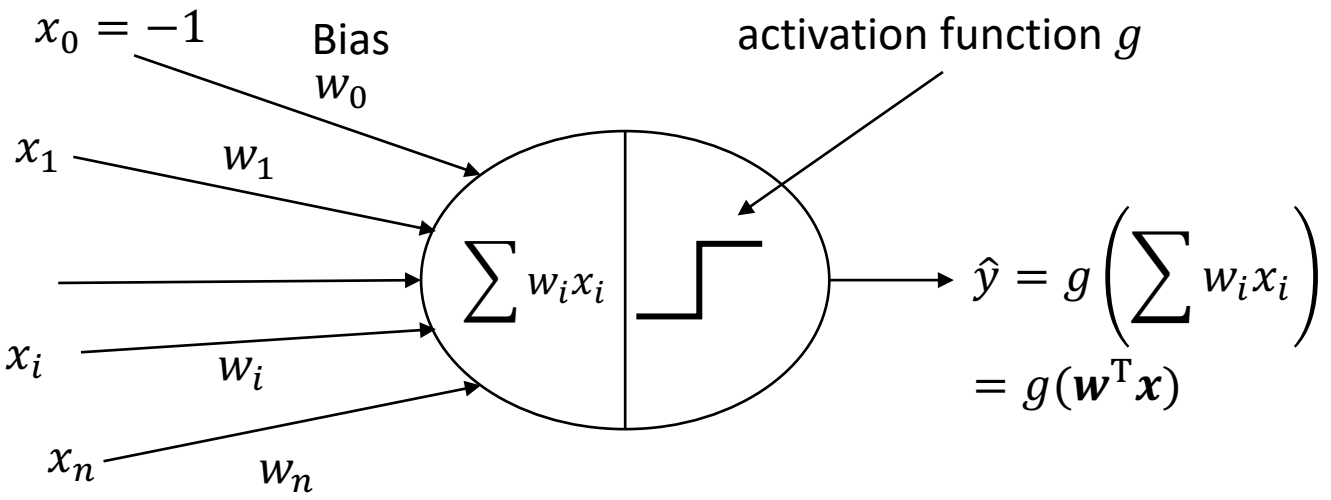
Human brain:

- 10^{11} Neurons
- more than 20 different types
- 10^{14} synapses (connections)
- Cycle time: 1-10 msec

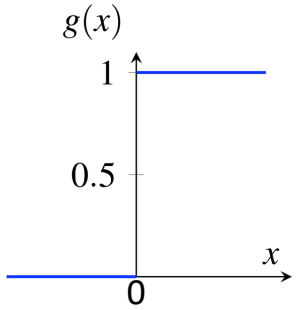


Rosenblatt's Perceptron

- simplified model of a real neuron
- by Frank Rosenblatt 1957
- binary classifier $y \in \{0, 1\}$
- $\boldsymbol{w} = (w_0, w_1, \ldots, w_n)$ set of weights (w_0: bias)
- $\boldsymbol{x} = (-1, x_1, \ldots, x_n)$ input feature vector
- Output: linear function of input + (non-linear) threshold



$$\hat{y} = \begin{cases} 1 & \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$



Bias

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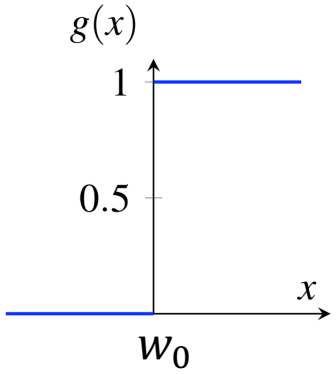
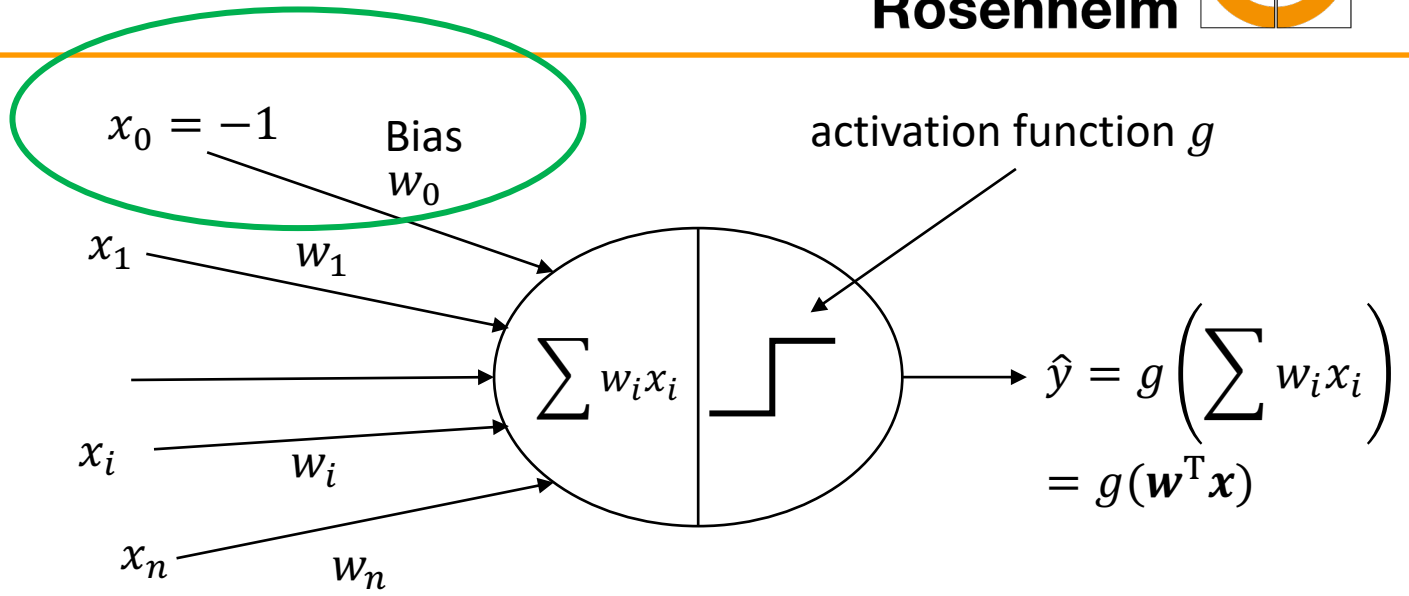
Decision threshold is always zero?
Can we set it to an arbitrary value?
YES: Bias weight = threshold position!

$$\hat{y} = \begin{cases} 1 & \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} > 0 \\ 0 & \text{otherwise} \end{cases}$$

$$\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} = \sum_{i=0}^{n} w_i x_i = w_0 x_0 + \sum_{i=1}^{n} w_i x_i = -w_0 + \sum_{i=1}^{n} w_i x_i$$

$$\sum_{i=0}^{n} w_i x_i > 0 \quad \longrightarrow \quad \sum_{i=1}^{n} w_i x_i > w_0$$



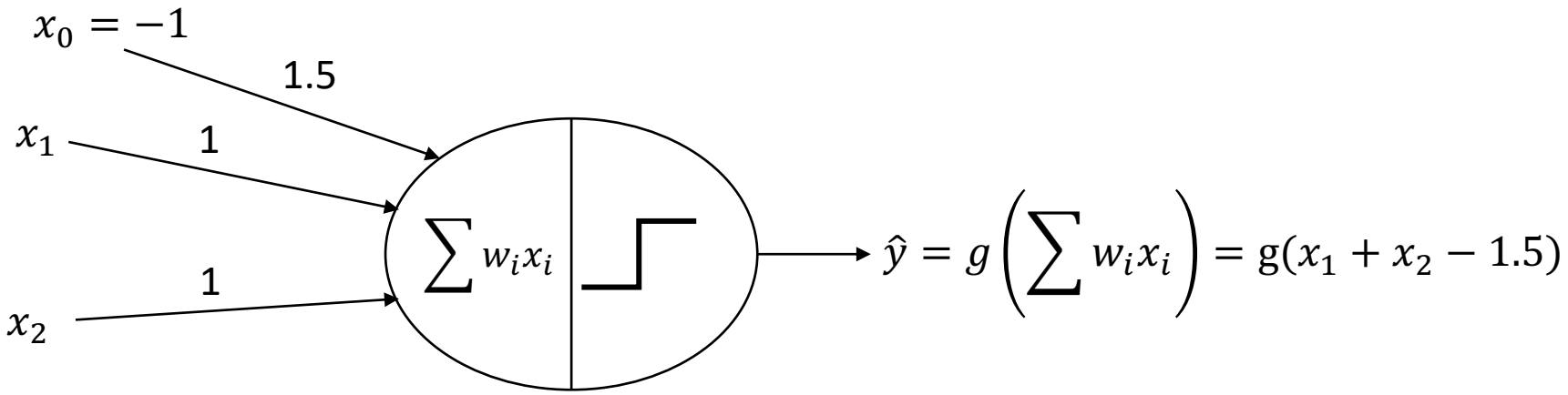


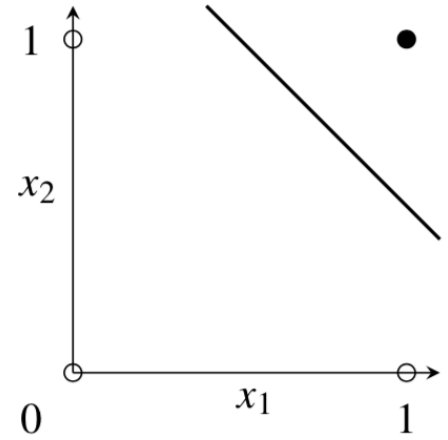
Why?

- The threshold becomes just another weight
- The weights are learned during training
- Thus, the threshold can be trained automatically

Example: Boolean AND

A perceptron can compute the Boolean AND-function:



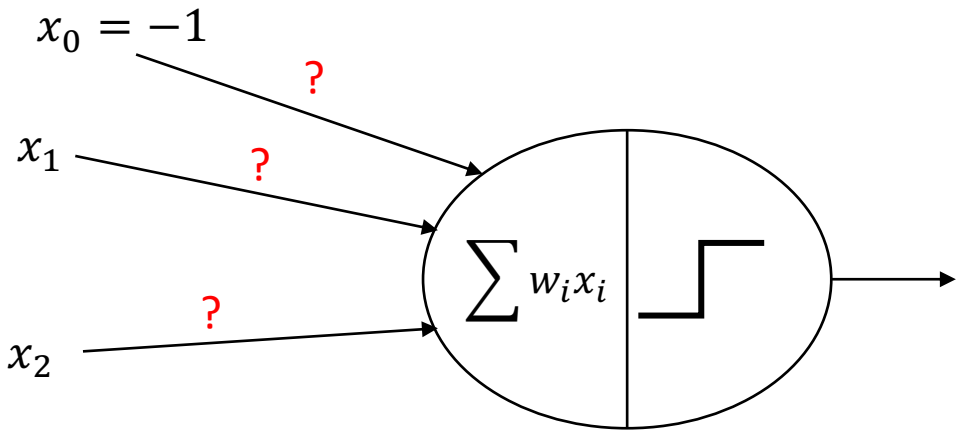


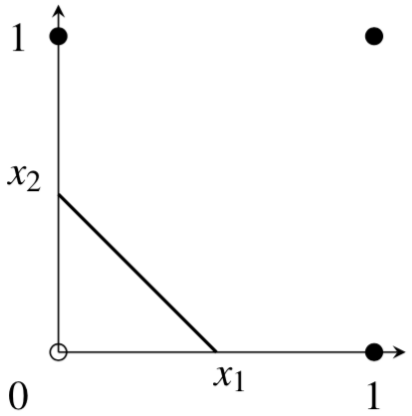
Could we use other weights?

x_1	x_2	$\sum w_i x_i$	$g\left(\sum w_i x_i\right)$
0	0	–1.5	0
0	1	–0.5	0
1	0	–0.5	0
1	1	0.5	1

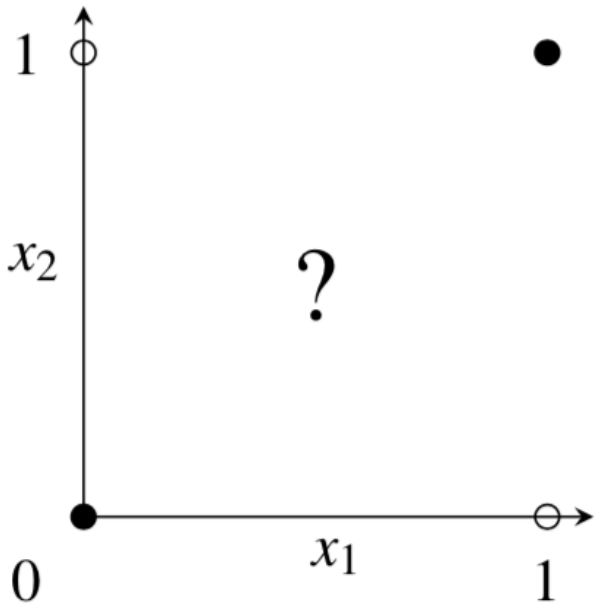
Exercise: Boolean OR

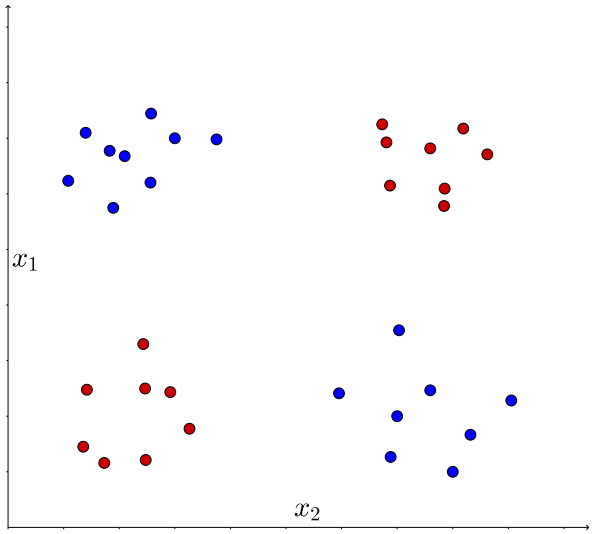
What would the weights look like for the Boolean OR-function?





Boolean XOR?





Observation: A single perceptron computes a linear separation of the feature space

Perceptron – Interpretation

$$f(\boldsymbol{x}) = -w_0 + \sum_{i=1}^{n} w_i x_i = \boldsymbol{w'}^{\mathrm{T}} \boldsymbol{x'} - w_0$$ is the equation of an n-dimensional hyperplane

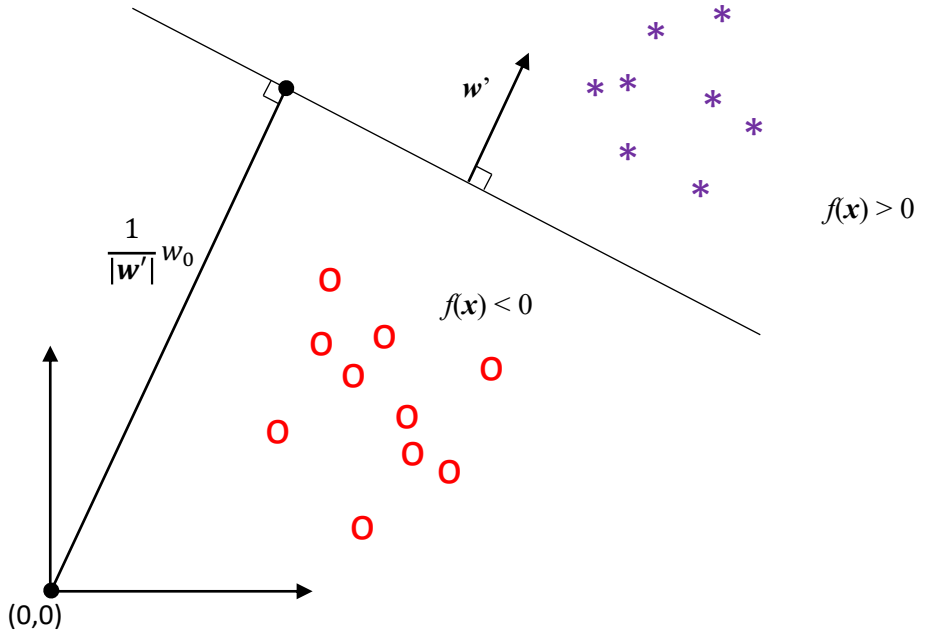
$\boldsymbol{w'} = (w_1, \ldots, w_n)$ set of weights without bias w_0
$\boldsymbol{x'} = (x_1, \ldots, x_n)$ input feature vector

- normal vector: $\boldsymbol{w'}$
  - point on plane: $f(\boldsymbol{x'}) = 0$
  - point above plane: $f(\boldsymbol{x'}) > 0$
  - point below plane: $f(\boldsymbol{x'}) < 0$
  - ”above” = in direction of plane normal

- Signed distance d of a point to hyperplane
  - normalize $\boldsymbol{w'}$, such that $|\boldsymbol{w'}| = 1$:

$$d = f'(\boldsymbol{x'}) = \frac{1}{|\boldsymbol{w'}|} f(\boldsymbol{x'}) = \frac{1}{|\boldsymbol{w'}|} \boldsymbol{w'}^{T} \boldsymbol{x'} - \frac{1}{|\boldsymbol{w'}|} w_0$$

  - distance of plane from origin: $\frac{1}{|\boldsymbol{w'}|} w_0$



P.S.: The perceptron decision rule looks exactly like the one for an SVM (Support Vector Machine)

Perceptron Training

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Can we learn the weights automatically?

- We need a training data set: $\mathcal{S} = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_m, y_m)\}$
- Weights $\boldsymbol{w} = (w_0, w_1, \ldots, w_n)$ initialized randomly

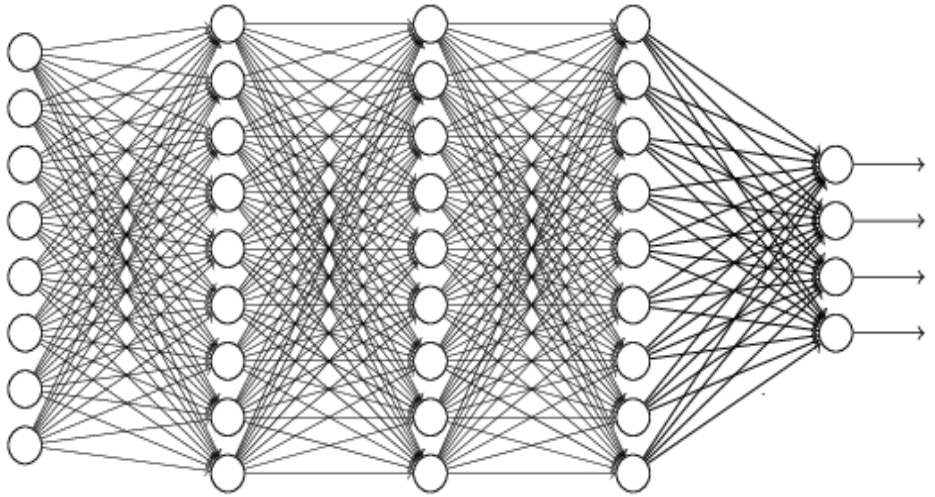
- Repeat until convergence or for a defined number of iterations:
  - for each training sample $(\boldsymbol{x}_e, y_e) \in \mathcal{S}$
    - compute output $\hat{y_e} = \mathrm{g}(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_e)$
    - compute residual error: $\varepsilon = y_e - \hat{y_e}$
    - update weights: $\boldsymbol{w} := \boldsymbol{w} + \alpha\, \varepsilon\, \boldsymbol{x}_e$

- α: **Learning Rate**, e.g., $\alpha = 0.1$

- this algorithm updates weights after each sample
- other strategies:
  - process all samples, sum changes, update weights after each iteration
  - process small batches, sum changes, then update

Multi-Layer Perceptron (MLP)

- How to obtain nonlinear decision boundaries? Use more than one neuron.
- Neurons are arranged in layers
- Layer i is (fully) connected with layer i+1
  - no connections within layer
  - no connections to any other layers
  - no feedback
- Information flow from one layer to the next: **feed-forward**
- network has no internal state



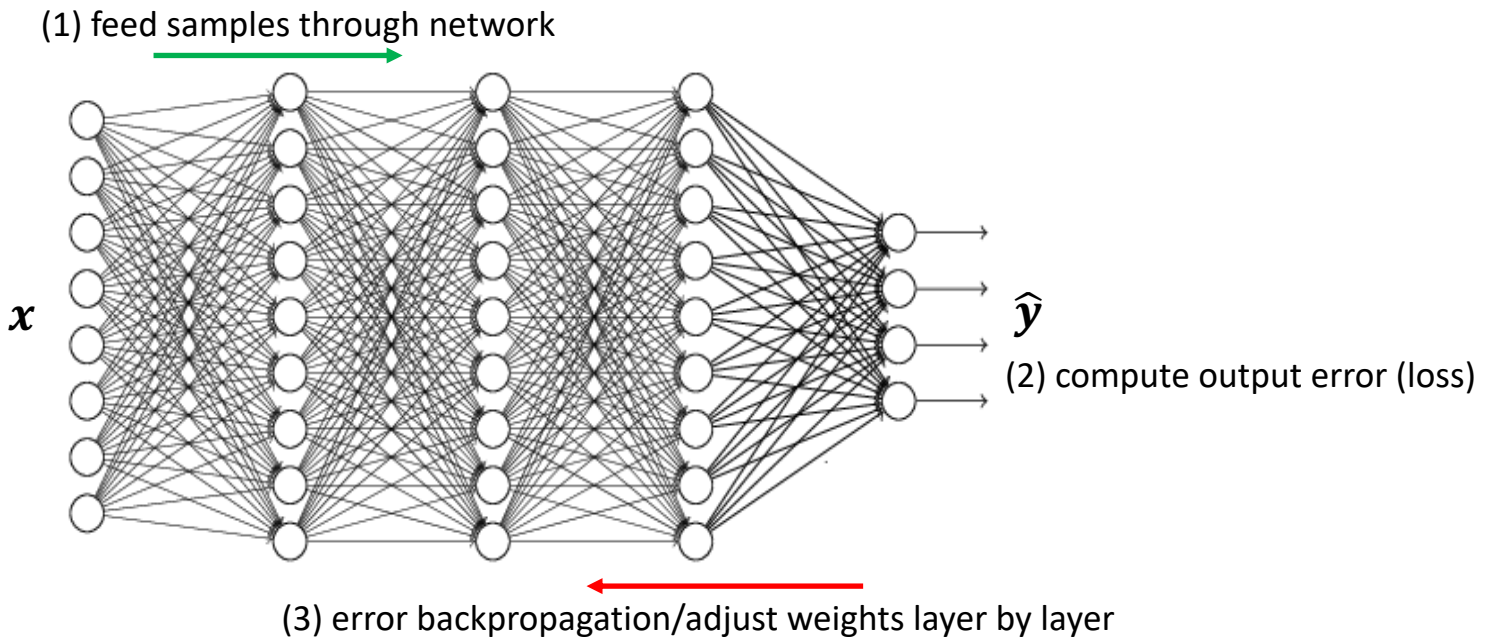
- number of input/output units is problem dependent
- number of layers/hidden units determined by developer
  - … we will discuss this in more detail later

MLP-Training Basics

Training

Training = Determine weights

- define loss function L of output neurons
- minimize loss



Training as an Optimization Problem

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Objective: Find optimal weights $\boldsymbol{w}$ for all layers

- Abstraction: Consider the whole neural network as a function

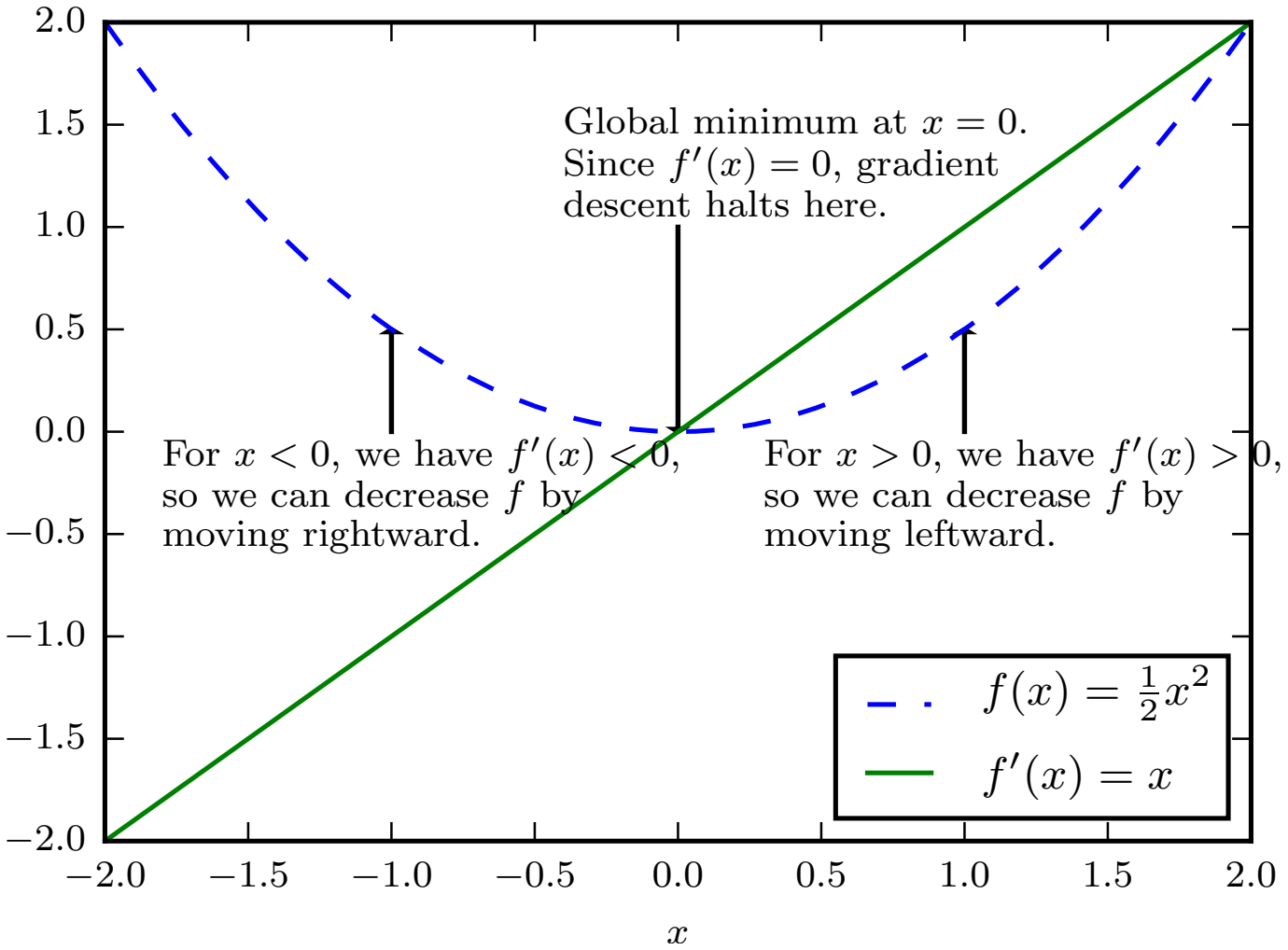
$$L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y})$$

- Consider all M training samples

$$\frac{1}{M} \sum_{m=1}^{M} L(\boldsymbol{w}, \boldsymbol{x}_m, \boldsymbol{y}_m)$$

- Minimize (with unknowns $\boldsymbol{w}$)
  - computing the first derivative and solving for zero crossings will not work (highly nonlinear)
  - method of choice: Gradient Descent

Gradient Descent Illustration

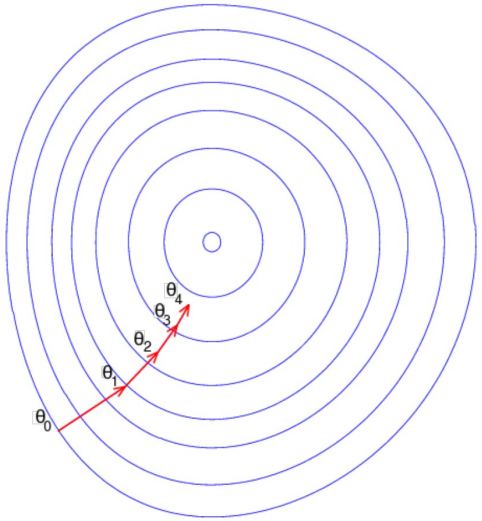


Gradient Descent

$$\frac{1}{M}\sum_{m=1}^{M} L(\boldsymbol{w}, \boldsymbol{x}_m, \boldsymbol{y}_m)$$

1. Initialize weights $\boldsymbol{w}$
2. Iterate until convergence (or for a defined number of iterations)

$$\boldsymbol{w}^{(k+1)} := \boldsymbol{w}^{(k)} - \alpha \nabla_{\boldsymbol{w}} \frac{1}{M}\sum_{m=1}^{M} L(\boldsymbol{w}, \boldsymbol{x}_m, \boldsymbol{y}_m)$$



α: **Learning Rate**

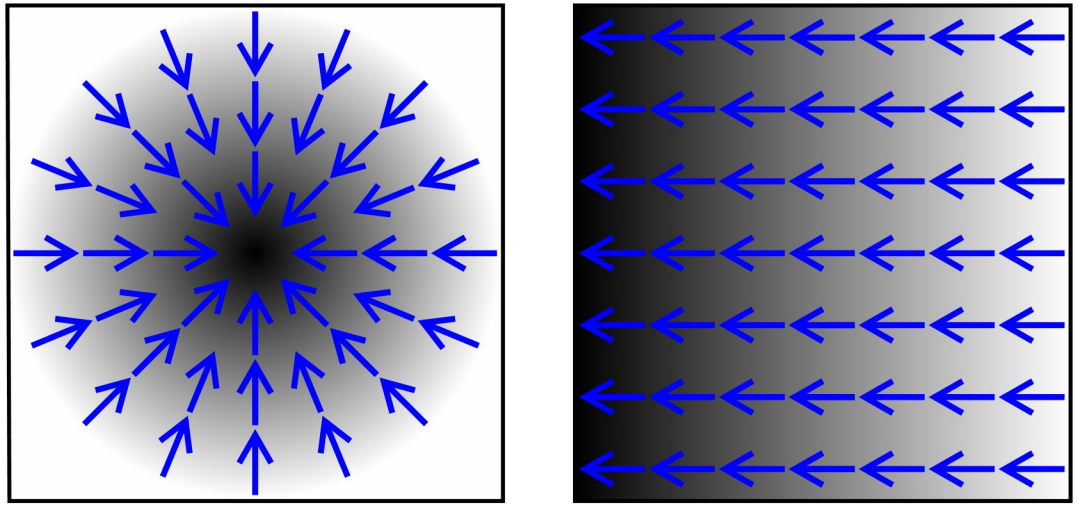
$$\nabla_x f(\boldsymbol{x}, \boldsymbol{y}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

Gradient of f

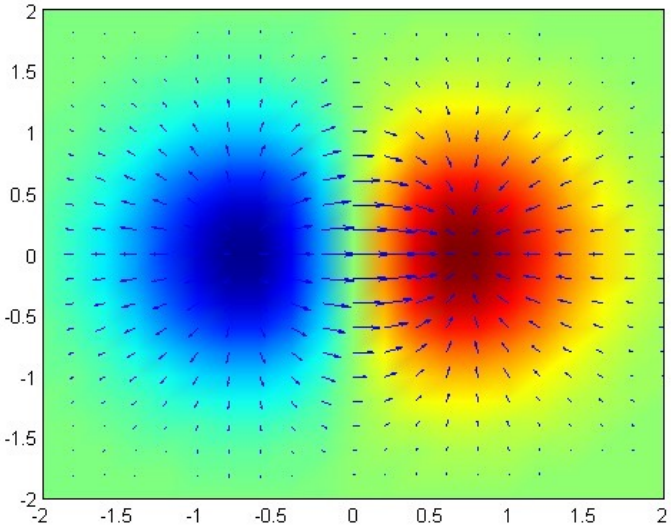
- vector direction: direction of steepest increase
- vector magnitude: rate/strength of increase

Gradient Illustration

Gradient of f
- vector direction: direction of steepest increase
- vector magnitude: rate/strength of increase

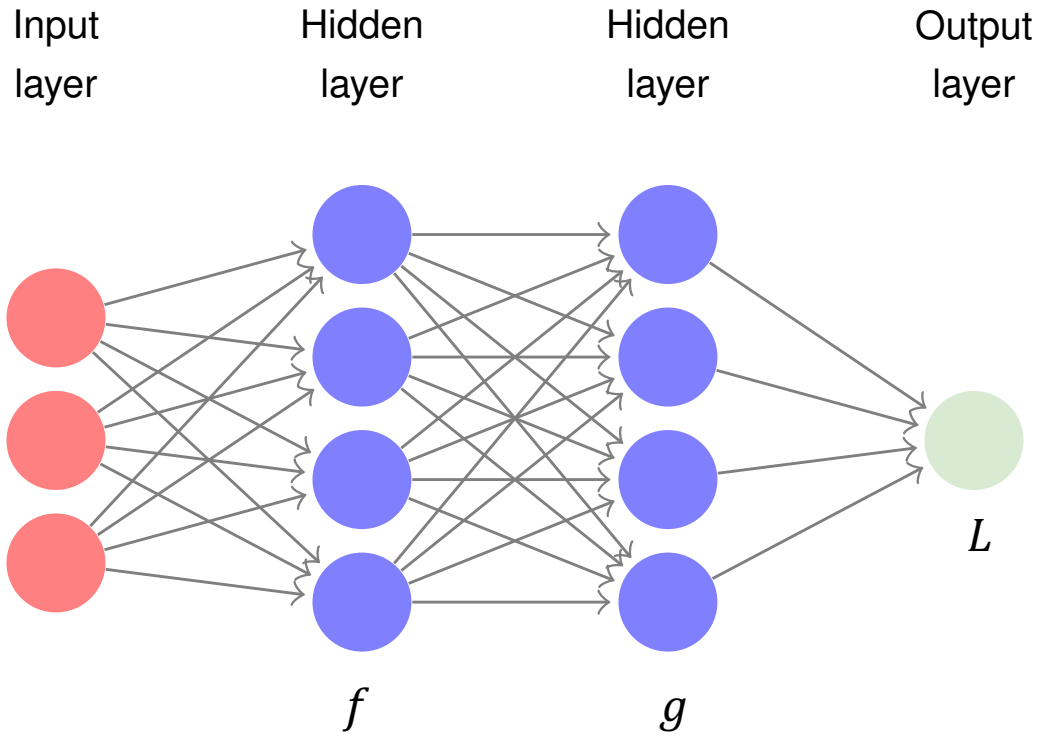


Function values in grayscale:
white = low values
dark = high values



Gradient of $f(x, y) = \frac{x}{e^{x^2+y^2}}$ as pseudo color plot
blue/cold = low values
red/hot = high values

What does this look like in a Neural Network?



A complex network can be looked at as composed functions:

$$L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) = L\big(g\big(f\big(\boldsymbol{x}, \boldsymbol{w}_f\big), \boldsymbol{w}_g\big), \boldsymbol{y}\big)$$

How do we Calculate Derivatives in a Neural Network?

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Example

- function $\hat{y} = f(\boldsymbol{x}) = f(x_1, x_2) = (2x_1 + 3x_2)^2 + 3$
- evaluate $\frac{\partial}{\partial x_1} f(1, 3)$

Two methods:

- numerical derivative using finite differences
- analytic derivative

Numerical Computation Using Finite Differences

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Definition of derivative: $$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

This is asymmetric; due to finite precision, we prefer the symmetric definition:

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right)}{h}$$

Thus, we get the derivative at the exact position of x

Numerical Computation – Example

- function $\hat{y} = f(\boldsymbol{x}) = f(x_1, x_2) = (2x_1 + 3x_2)^2 + 3$
- evaluate $\frac{\partial}{\partial x_1} f(1,3)$

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right)}{h}$$

Set $h = 2 \cdot 10^{-2}$. We get

$$\frac{\partial}{\partial x_1} f(1,3) = \frac{(2(1 + 10^{-2}) + 9)^2 + 3 - ((2(1 - 10^{-2}) + 9)^2 + 3)}{2 \cdot 10^{-2}} = \frac{124.4404 - 123.5604}{2 \cdot 10^{-2}} = 43.999$$

(the exact value is 44)

Numerical Computation – Summary

- for practical purposes it often suffices to use $h = 1 \cdot 10^{-5}$
- for a more accurate derivative use $h = \sqrt[3]{\varepsilon_f} \cdot x$
  - ε_f is the fractional accuracy with which f is computed
    - for a simple function this is approximately the machine accuracy ($\varepsilon_m \approx 10^{-7}$ for 32 Bit floats)
    - for complex functions this may be considerably larger than machine accuracy
  - x is the position, where f is being evaluated
  - prevent division by zero when $x = 0$
- see [Pre07, pp.186-189] for more details

- easy to use
- we only need to be able to evaluate functions
  - can be computed for any function, even if we do not have the derivative
- however:
  - computationally inefficient
  - not as accurate as using the analytical derivative
- frequently used for validating implementations of analytical derivatives

Analytic Derivative – Example

- function $\hat{y} = f(\boldsymbol{x}) = f(x_1, x_2) = (2x_1 + 3x_2)^2 + 3$
- evaluate $\frac{\partial}{\partial x_1} f(1, 3)$

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = \frac{\partial}{\partial x_1}\left((2x_1 + 3x_2)^2 + 3\right)$$

$$= \frac{\partial}{\partial x_1}(2x_1 + 3x_2)^2 + \frac{\partial}{\partial x_1} 3 \qquad (2)$$

$$= \frac{\partial}{\partial x_1}(2x_1 + 3x_2)^2 \qquad (1)$$

$$= \frac{\partial}{\partial z} z^2 \; \frac{\partial}{\partial x_1}(2x_1 + 3x_2) \qquad (4) \text{ and } (2x_1 + 3x_2) = z$$

$$= 2z \cdot 2 = 2 \cdot (2x_1 + 3x_2) \cdot 2 = (8x_1 + 12x_2) \qquad (1) + (2)$$

$$\frac{\partial}{\partial x_1} f(1, 3) = (8 \cdot 1 + 12 \cdot 3) = 44$$

Required Rules:

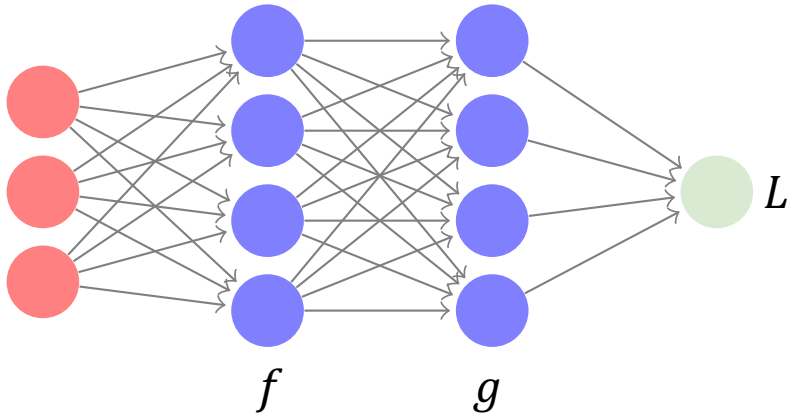
1. $\frac{d}{dx}\,\text{const} = 0$
2. $\frac{d}{dx}$ is a linear operation
3. Monomials: $\frac{d}{dx} x^n = n \cdot x^{n-1}$
4. Chain rule: $\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \cdot \frac{d}{dx} g(x)$

Analytic Derivative – Summary

- **chain rule** and **linearity** enable us to **decompose** complex functions
- analytic derivatives have to be calculated manually
- computationally more efficient and more precise than finite differences

Can we compute analytic gradients of the network loss function automatically?

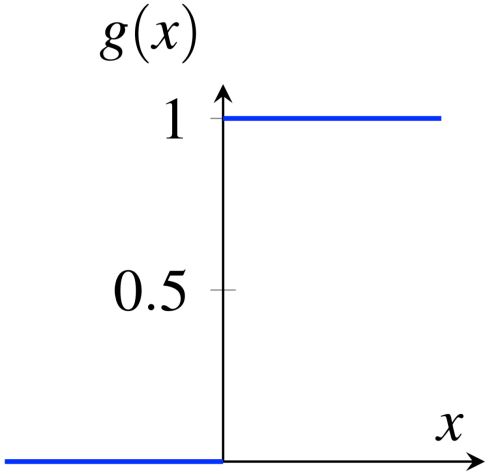
YES: Provided we have the analytic derivative of the activation function – just use chain rule and linearity



$$L(\boldsymbol{w}, \boldsymbol{x}, \boldsymbol{y}) = L\big(g\big(f\big(\boldsymbol{x}, \boldsymbol{w}_f\big), \boldsymbol{w}_g\big), \boldsymbol{y}\big)$$

Ooops – Activation Derivatives Required!

As activation we used the Heaviside step function:



$$g(x) = \begin{cases} 1 & x > 0 \\ 0 & \text{otherwise} \end{cases}$$

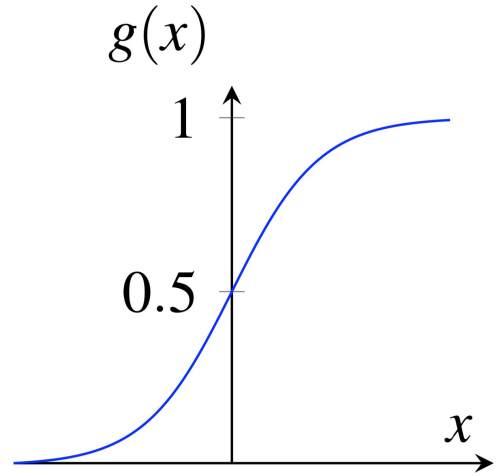
$$g'(x) = \delta(x)$$

replace activation

- not differentiable in the usual sense
- gradient vanishes almost everywhere

Unsuitable for gradient descent!

Sigmoid (also: logistic function)



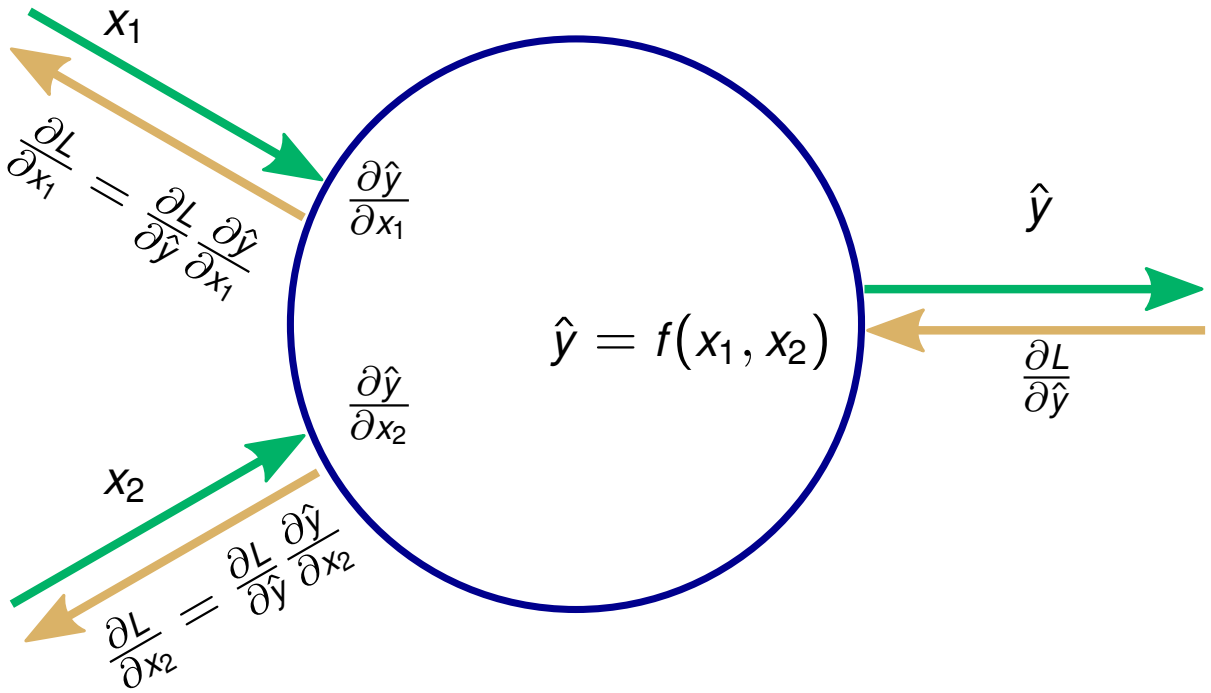
$$g(x) = \frac{1}{1 + e^{-x}}$$

$$g'(x) = g(x)(1 - g(x))$$

- smooth approximation of step function
- efficient computation of derivative
- gradient still vanishes eventually…

we will discuss other activation functions later

Backpropagation algorithm



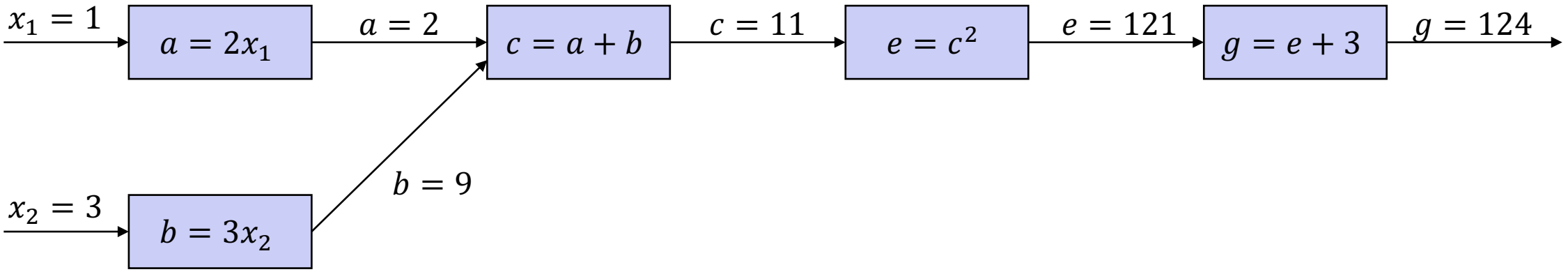
- does not show weights
- to train weights, we also require the derivatives w.r.t. the weights (for update in gradient descent)

1. Forward pass: Compute activations
2. Backward pass: Recursively apply chain rule

Backpropagation – Example / Forward Pass

- function $\hat{y} = f(\boldsymbol{x}) = f(x_1, x_2) = (2x_1 + 3x_2)^2 + 3$
- evaluate $\frac{\partial}{\partial x_1} f(1, 3)$

$$\frac{d}{dx} f(g(x)) = \frac{d}{dg} f(g) \cdot \frac{d}{dx} g(x)$$



Backpropagation – Example / Backward Pass

- function $\hat{y} = f(\boldsymbol{x}) = f(x_1, x_2) = (2x_1 + 3x_2)^2 + 3$
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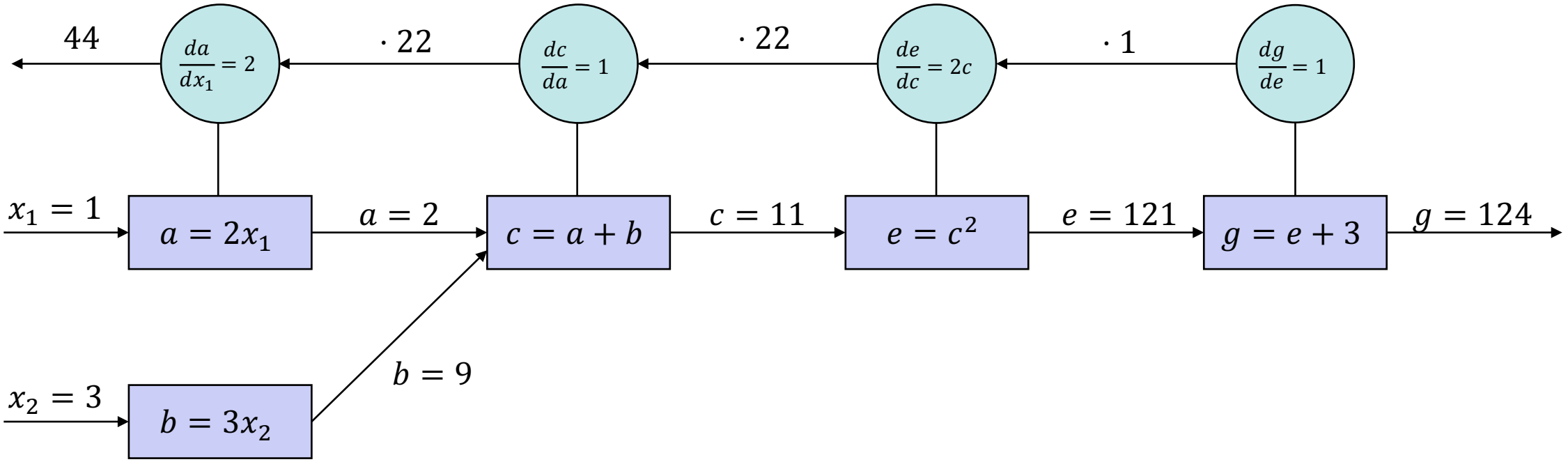
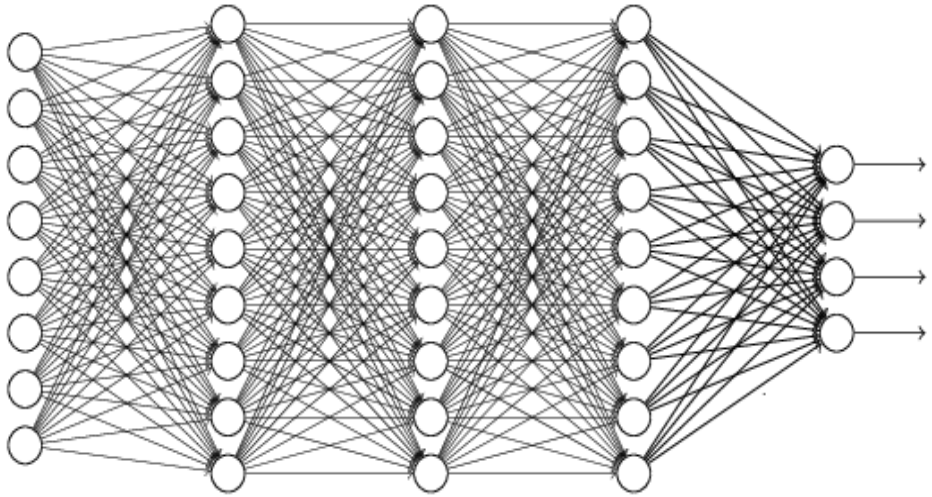


Stability

What do these two systems have in common?

https://youtu.be/esfpcnQW6qs

- Both suffer from positive feedback
- This can lead to desaster



Backpropagation:
Long chains of float multiplications of potentially large and small numbers → positive feedback

Feedback Loop

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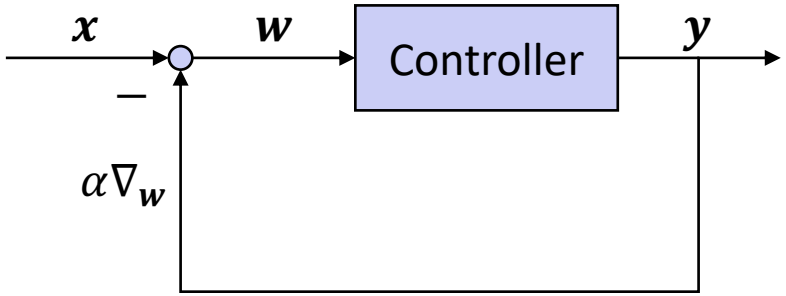
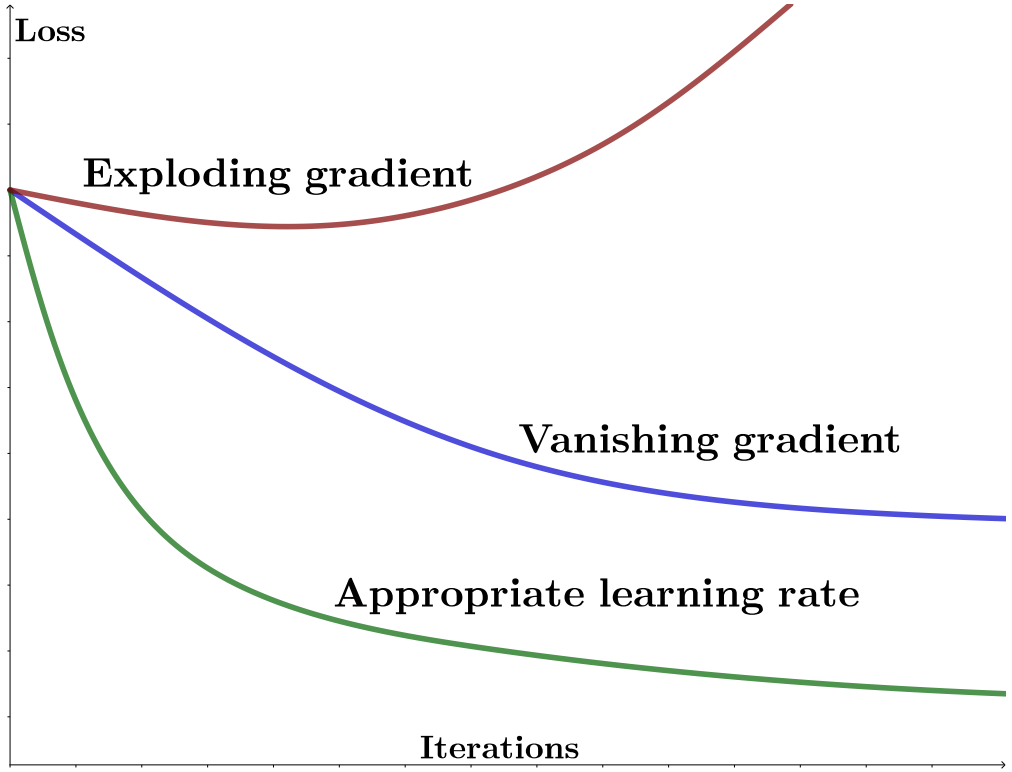
Analogy to control theory





- if α is too large → **positive feedback** → loss grows without bounds
- if α is too small → **negative feedback** → gradient vanishes
- choice of α is critical for learning

Backpropagation – Summary

- built around the **chain rule**
- uses a **forward pass** computing the function output
- and a **backward pass** for computing the gradient
- computationally very **efficient** by using a dynamic programming approach
  - store inputs and intermediate results during forward pass, so that they are available for backward pass

- product of partials → numerical **errors multiply**
- product of partials → **vanishing** or **exploding** gradient
  - can be mitigated to a certain degree by choosing other activation functions
    → we will discuss these later

MLP – Layer Abstraction

From Graphs of Nodes to Graphs of Layers

- we introduced layers but computed everything on individual nodes
- it is convenient to add further abstraction
  - more compact and clear notation
  - we can talk directly about gradients of entire layers
  - training is implemented on GPUs: matrix/vector notation required

Representing Connections

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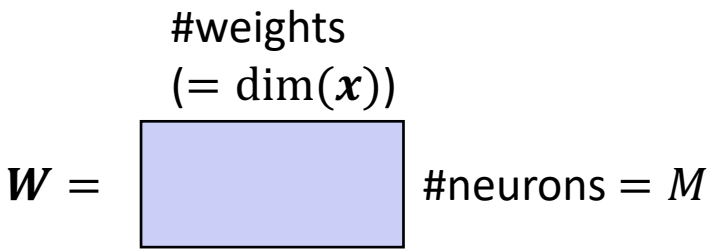
- recall a single neuron: $\hat{y} = g(\sum w_i x_i) = g(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x})$
- for simplicity of notation, we will use the identity mapping as activation – i.e., we omit g

- assume we have M neurons → M sets of weights $\boldsymbol{w}_m$ for $m \in \{1, \dots, M\}$.
- for each neuron we get $\hat{y}_m = \boldsymbol{w}_m^{\mathrm{T}}\boldsymbol{x}$
- we collect all outputs in a vector and all weights in a matrix:

$$\hat{\boldsymbol{y}} = \boldsymbol{W}\boldsymbol{x}$$



- this is known as a **fully connected layer**
- the non-linear activation g is then applied to each element of $\hat{\boldsymbol{y}}$

Backpropagation

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- we can formulate error backpropagation using matrix calculus
- the forward pass is: $\hat{\boldsymbol{y}} = \boldsymbol{W}\boldsymbol{x}$
- after the forward pass through all layers, we compute a loss that depends on our loss function L
- two gradients are required for the backward pass:
  - gradient with respect to **weights** for gradient descent: $\frac{\partial L}{\partial \boldsymbol{W}} = \frac{\partial L}{\partial \hat{\boldsymbol{y}}} \frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{W}} = \frac{\partial L}{\partial \hat{\boldsymbol{y}}} \boldsymbol{x}^{\mathrm{T}}$ (this is a matrix)
  - gradient with respect to **inputs** for backpropagation: $\frac{\partial L}{\partial \boldsymbol{x}} = \frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{x}} \frac{\partial L}{\partial \hat{\boldsymbol{y}}} = \boldsymbol{W}^{\mathrm{T}} \frac{\partial L}{\partial \hat{\boldsymbol{y}}}$ (this is a vector)

order to be consistent with matrix multiplication

Matrix Notation – Single Layer Example

- assume we have simple network with no activation function. Forward pass: $\hat{\boldsymbol{y}} = \boldsymbol{W}\boldsymbol{x}$
- we want to find weights minimizing the following loss function (L_2 loss):

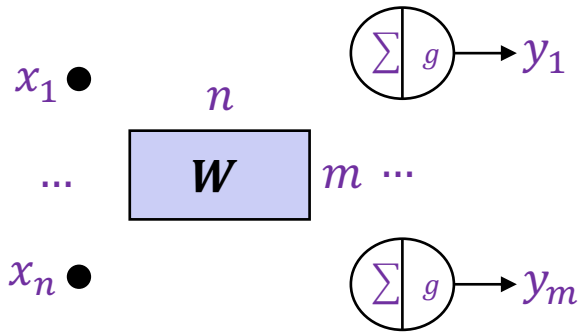
$$L(\boldsymbol{x}, \boldsymbol{W}, \boldsymbol{y}) = \frac{1}{2}\|\hat{\boldsymbol{y}} - \boldsymbol{y}\|_2^2 = \frac{1}{2}(\hat{\boldsymbol{y}} - \boldsymbol{y})^{\mathrm{T}}(\hat{\boldsymbol{y}} - \boldsymbol{y}) = \frac{1}{2}(\boldsymbol{W}\boldsymbol{x} - \boldsymbol{y})^{\mathrm{T}}(\boldsymbol{W}\boldsymbol{x} - \boldsymbol{y})$$

- we get
  - $\frac{\partial L}{\partial \hat{\boldsymbol{y}}} = \hat{\boldsymbol{y}} - \boldsymbol{y} = \boldsymbol{W}\boldsymbol{x} - \boldsymbol{y}$
  - gradient with respect to weights:

$$\underset{m \times n}{\frac{\partial L}{\partial \boldsymbol{W}}} = \underset{m \times 1}{\frac{\partial L}{\partial \hat{\boldsymbol{y}}}} \underset{1 \times n}{\frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{W}}} = (\boldsymbol{W}\boldsymbol{x} - \boldsymbol{y})\boldsymbol{x}^{\mathrm{T}}$$

  - gradient with respect to inputs:

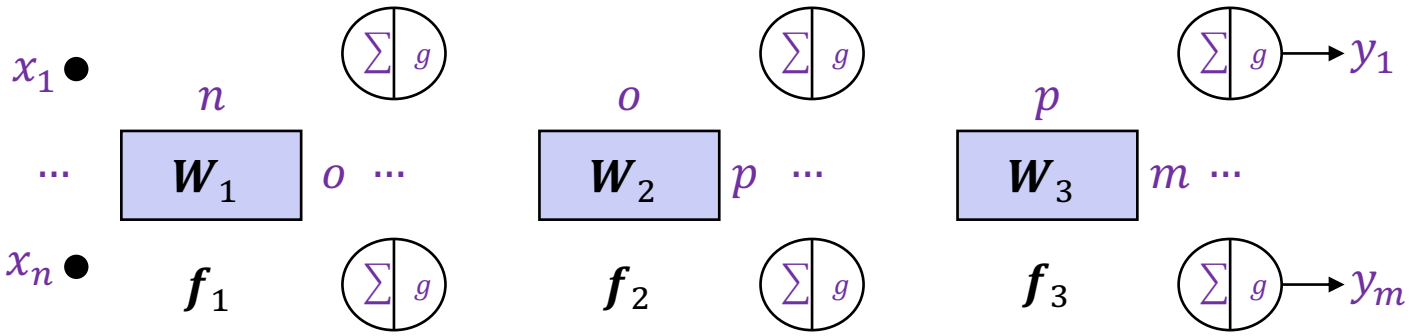
$$\underset{n \times 1}{\frac{\partial L}{\partial \boldsymbol{x}}} = \underset{n \times m}{\frac{\partial L}{\partial \hat{\boldsymbol{y}}}} \underset{m \times 1}{\frac{\partial \hat{\boldsymbol{y}}}{\partial \boldsymbol{x}}} = \boldsymbol{W}^{\mathrm{T}}(\boldsymbol{W}\boldsymbol{x} - \boldsymbol{y})$$



Linear Network in Matrix Notation

- now we add two more layers: $\hat{\boldsymbol{y}} = \boldsymbol{f}_3\left(\boldsymbol{f}_2\left(\boldsymbol{f}_1(\boldsymbol{x})\right)\right) = \boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x}$

this is why non-linear activation is required:
without, this will collapse to a single layer!

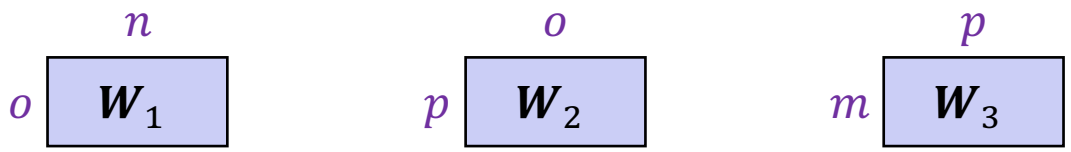


- loss function: $L(\boldsymbol{x}, \boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2}\|\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y}\|_2^2$

Linear Network in Matrix Notation

- now we add two more layers: $\hat{\boldsymbol{y}} = \boldsymbol{f}_3\left(\boldsymbol{f}_2\left(\boldsymbol{f}_1(\boldsymbol{x})\right)\right) = \boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x}$
- loss function: $L(\boldsymbol{x}, \boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2}\|\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y}\|_2^2$
- gradient of last layer: $\frac{\partial L}{\partial \boldsymbol{W}_3} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{W}_3} = (\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y})(\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x})^{\mathrm{T}}$

$m \times p$ $\quad$ $m \times 1$ $\quad$ $1 \times p$

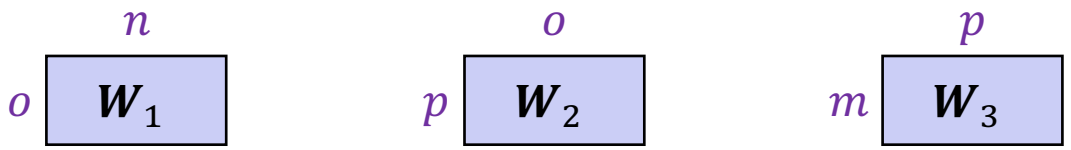


Linear Network in Matrix Notation

- now we add two more layers: $\hat{\boldsymbol{y}} = \boldsymbol{f}_3\left(\boldsymbol{f}_2\left(\boldsymbol{f}_1(\boldsymbol{x})\right)\right) = \boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x}$
- loss function: $L(\boldsymbol{x}, \boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2}\|\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y}\|_2^2$
- deeper gradients: $\frac{\partial L}{\partial \boldsymbol{W}_2} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{W}_2} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{f}_2}\frac{\partial \boldsymbol{f}_2}{\partial \boldsymbol{W}_2} = \boldsymbol{W}_3^{\mathrm{T}}(\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y})(\boldsymbol{W}_1\boldsymbol{x})^{\mathrm{T}}$

order to be consistent with matrix multiplication

$p \times o$ $\quad$ $p \times m$ $\quad$ $m \times 1$ $\quad$ $1 \times o$



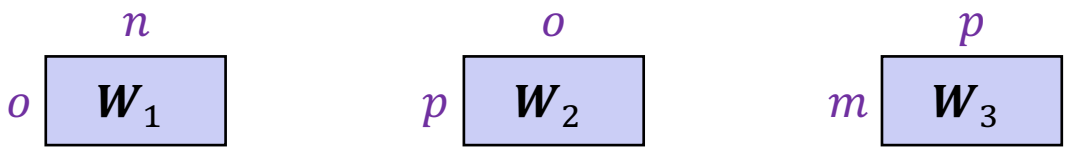
Linear Network in Matrix Notation

- now we add two more layers: $\hat{\boldsymbol{y}} = \boldsymbol{f}_3\left(\boldsymbol{f}_2\left(\boldsymbol{f}_1(\boldsymbol{x})\right)\right) = \boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x}$
- loss function: $L(\boldsymbol{x}, \boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2}\|\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y}\|_2^2$

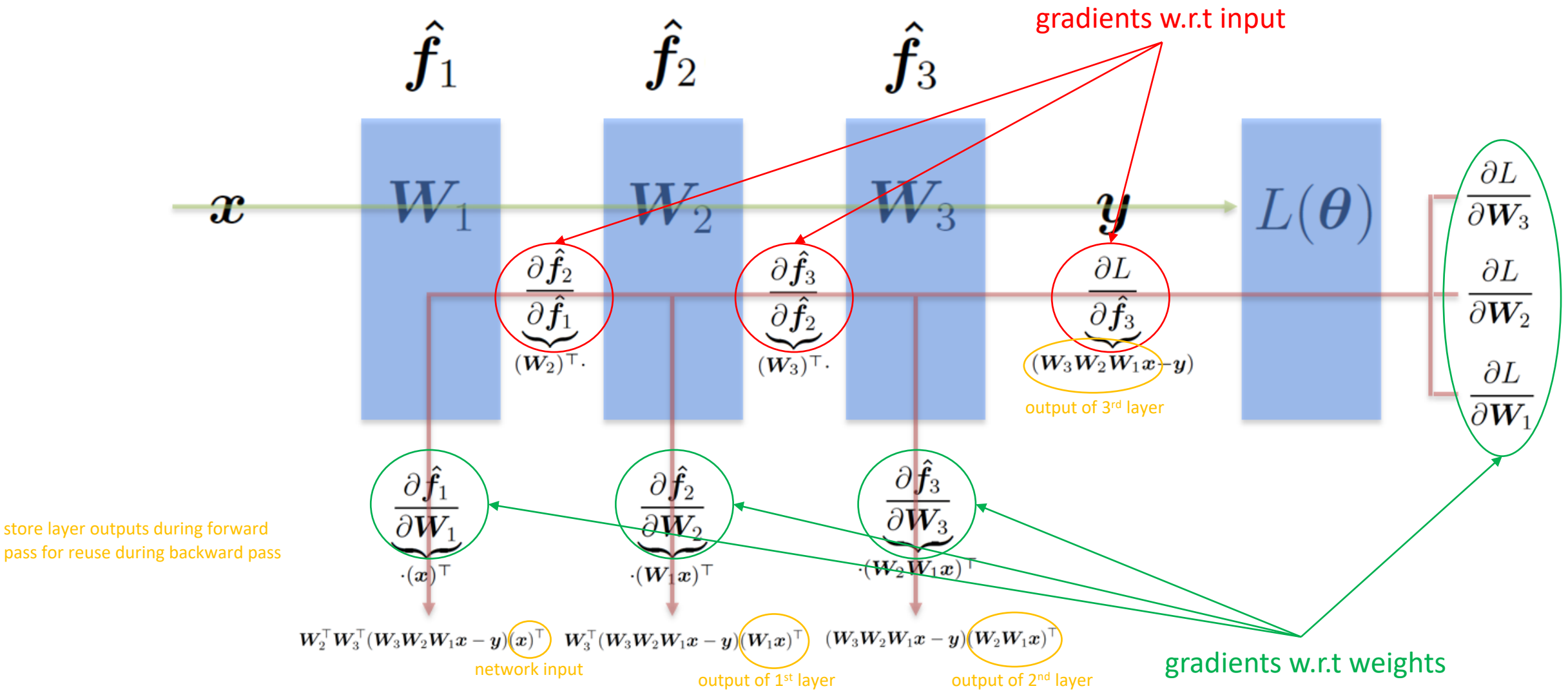
- deeper gradients:

order to be consistent with matrix multiplication

$$\underset{o \times n}{\frac{\partial L}{\partial \boldsymbol{W}_1}} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{W}_1} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{f}_2}\frac{\partial \boldsymbol{f}_2}{\partial \boldsymbol{W}_1} = \frac{\partial L}{\partial \boldsymbol{f}_3}\frac{\partial \boldsymbol{f}_3}{\partial \boldsymbol{f}_2}\frac{\partial \boldsymbol{f}_2}{\partial \boldsymbol{f}_1}\frac{\partial \boldsymbol{f}_1}{\partial \boldsymbol{W}_1} = \underset{o \times p}{\boldsymbol{W}_2^{\mathrm{T}}}\underset{p \times m}{\boldsymbol{W}_3^{\mathrm{T}}}\underset{m \times 1}{(\boldsymbol{W}_3\boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} - \boldsymbol{y})}\underset{1 \times n}{\boldsymbol{x}^{\mathrm{T}}}$$



Linear Network in Matrix Notation



Universal Approximation Theorem

Universal Approximation Theorem

A **single hidden layer** is already sufficient to be a **universal function approximator**

- Proof by [Hor89, Hor91, Cyb89]; for a more recent paper see [Kra21]
- Let $\varphi(\cdot)$ be a non-constant, bounded and monotonically increasing function
- For any $\varepsilon > 0$ and any continuous function f defined on a compact subset of $\mathbb{R}^m$ there exists an integer N, real constants v_i, b_i and real vectors $\boldsymbol{w}_i \in \mathbb{R}^m$ such that

#neurons in hidden layer

activation function

input vector

Bias

$$F(\boldsymbol{x}) = \sum_{i=1}^{N} v_i \varphi(\boldsymbol{w}_i^{\mathrm{T}} \boldsymbol{x} + b_i) \quad \text{with} \quad |F(\boldsymbol{x}) - f(\boldsymbol{x})| < \varepsilon$$

2nd layer of weights

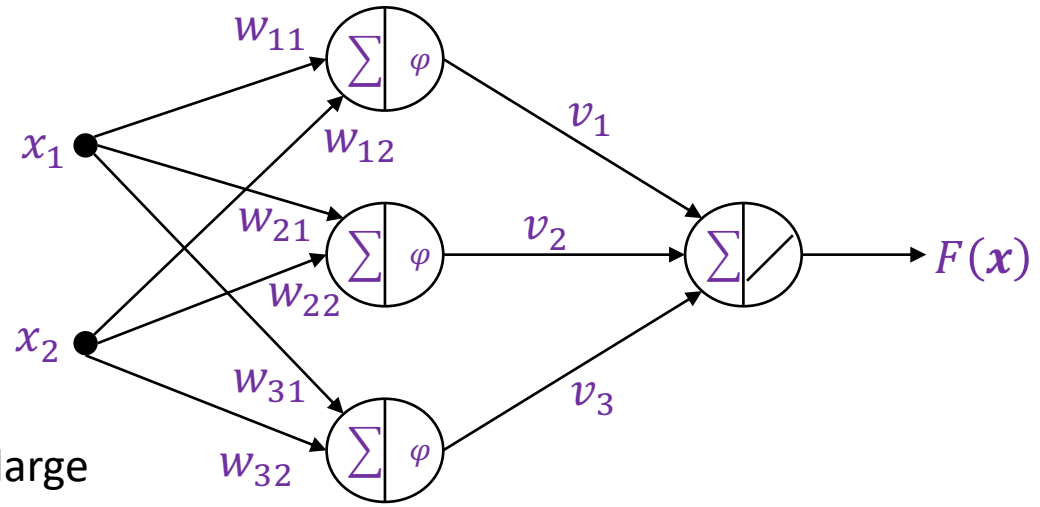
first layer of weights (input – hidden)

only a **single** hidden layer is required!

Example:

$\boldsymbol{x} = (x_1, x_2)$

$\boldsymbol{w}_1 = (w_{11}, w_{12}), \boldsymbol{w}_2 = (w_{21}, w_{22}), \boldsymbol{w}_3 = (w_{31}, w_{32})$

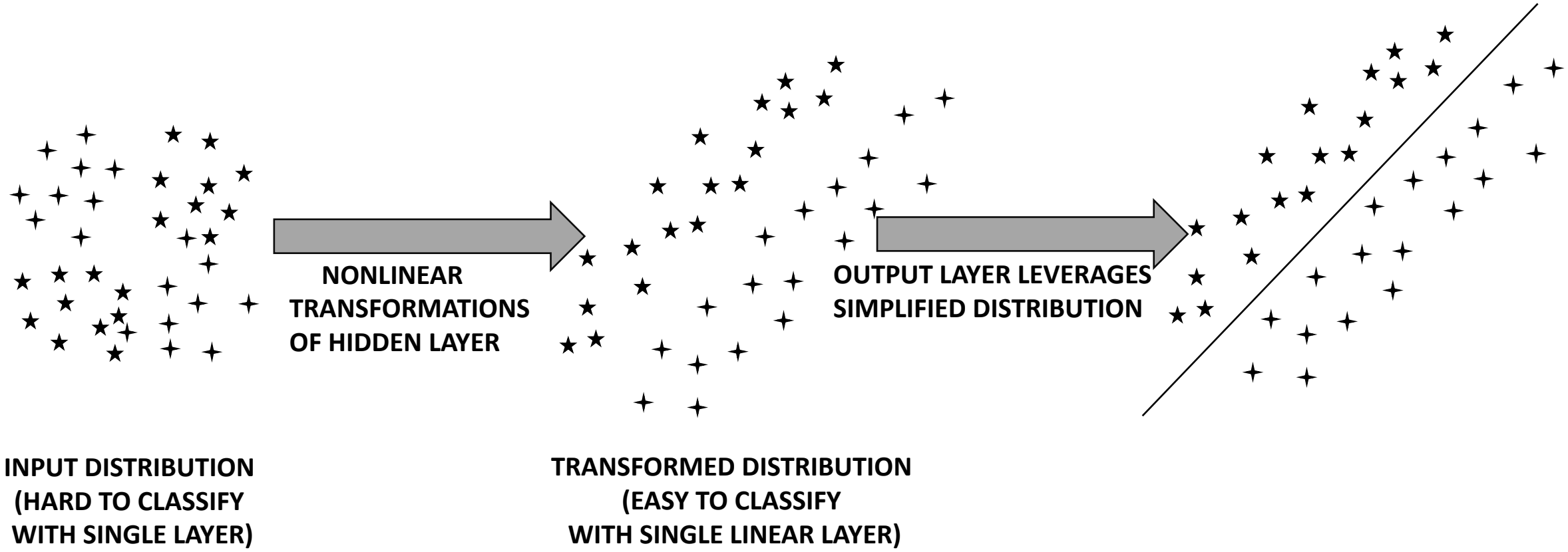


Observations:

- f can be approximated with arbitrary accuracy – just increase N
- it does not say anything about how to choose N, so ε may be quite large
- no nonlinear activation is required in the output neuron

Feature Engineering by Hidden Layer

A **single hidden layer** is also sufficient to train arbitrary (including non-contiguous) class boundaries [Mak89]



MLP – Properties

A MLP can

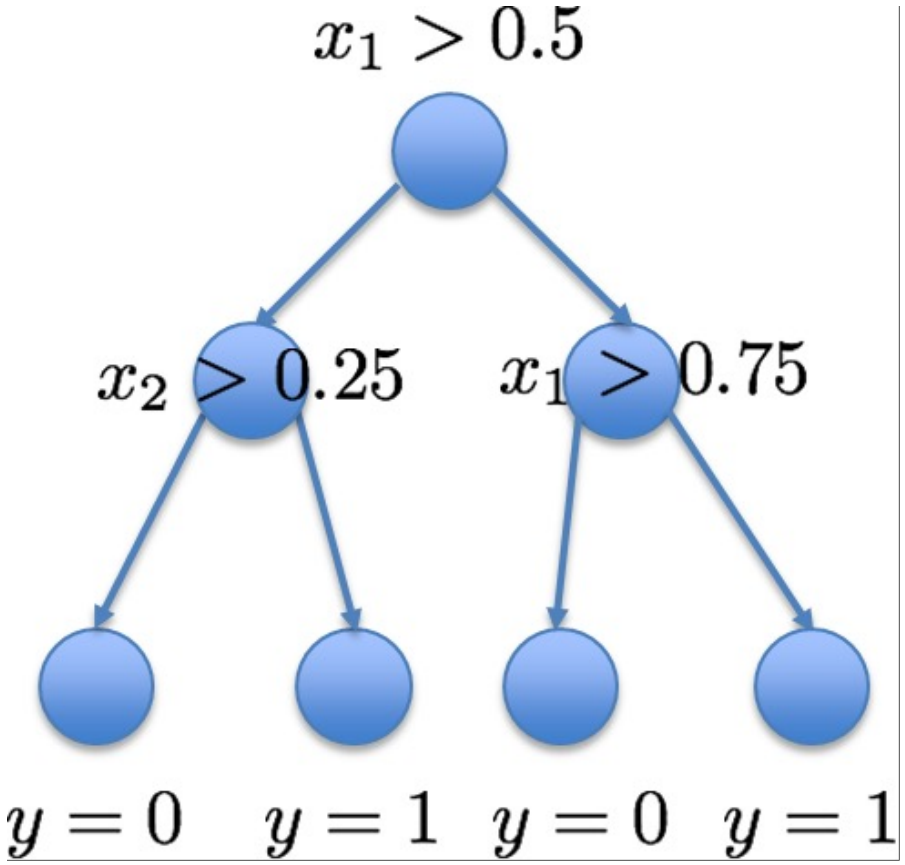
- compute any Boolean function (AND, OR, XOR, …)
- approximate any non-linear function
- define arbitrary class boundaries
- do supervised learning using a sample set (Error Backpropagation)

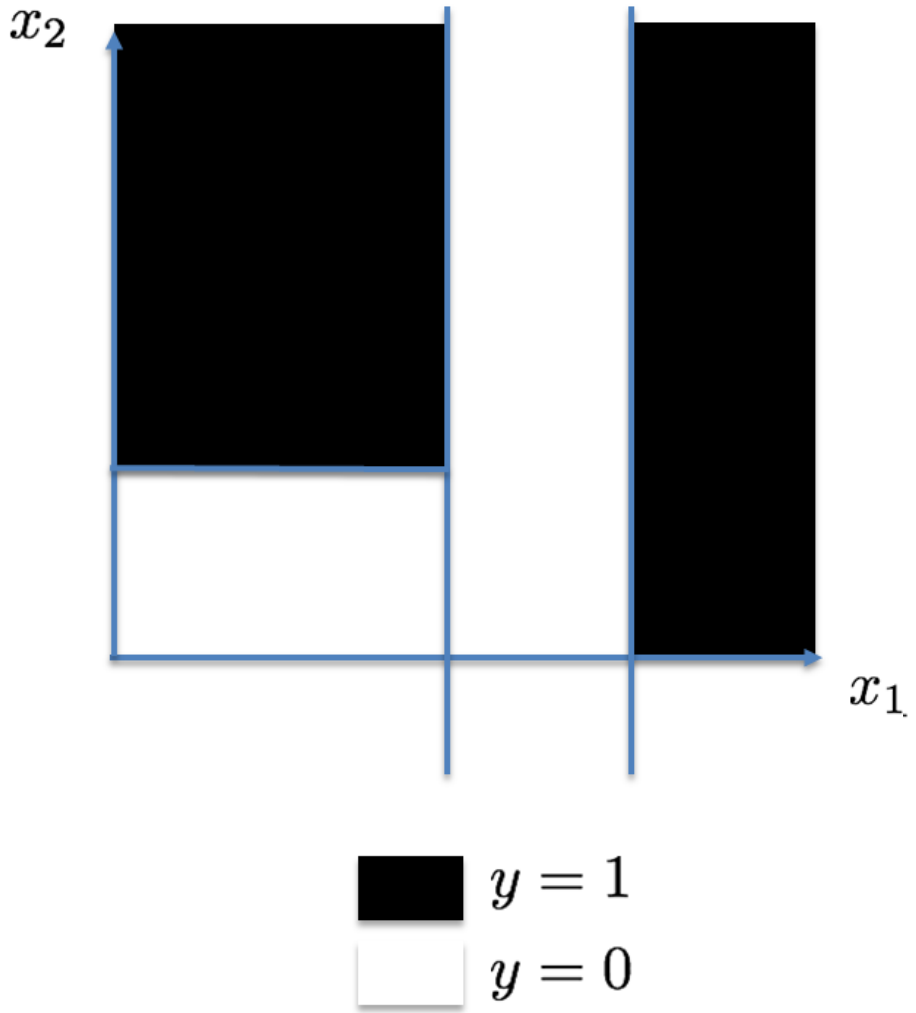
- 2 layers of weights (= 1 hidden layer of neurons) are sufficient for
  - any compact continuous function (= on closed and bounded intervals)
  - arbitrary (including non-contiguous) class boundaries [Mak89]
  - a finite number of neurons in the hidden layer suffices; however, a lot of neurons may be required in that layer
- using 3 layers of weights, the function intervals can be unbounded

So: Why would we need Deep Learning then?

A MLP is not Turing complete!

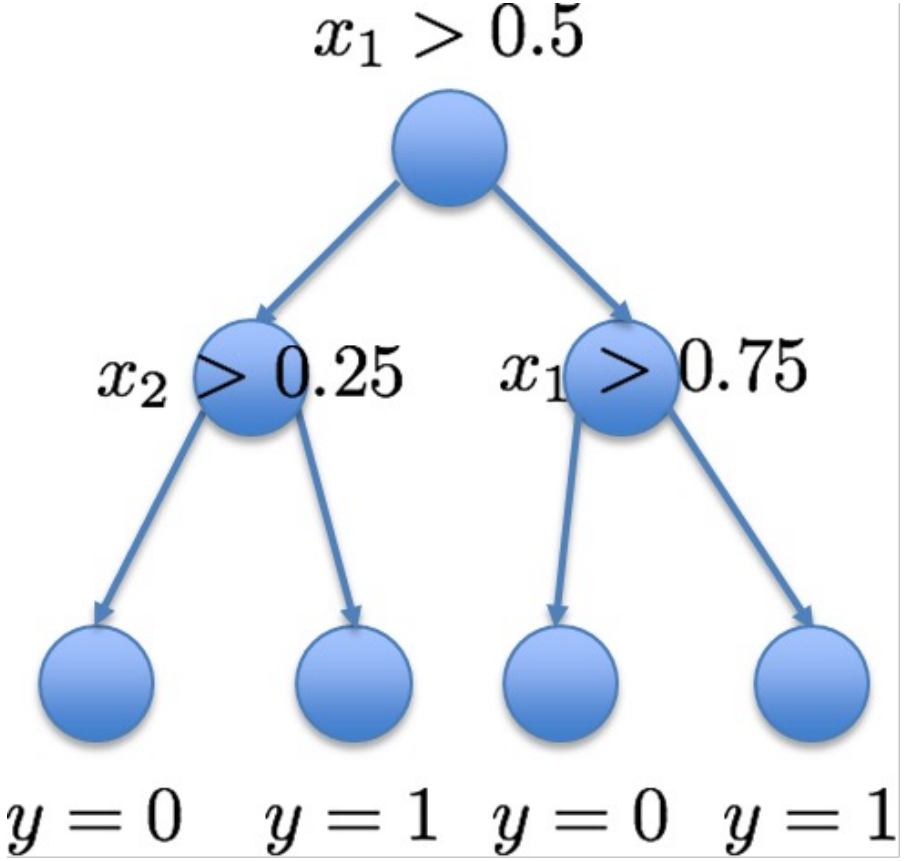
Example: Decision Tree

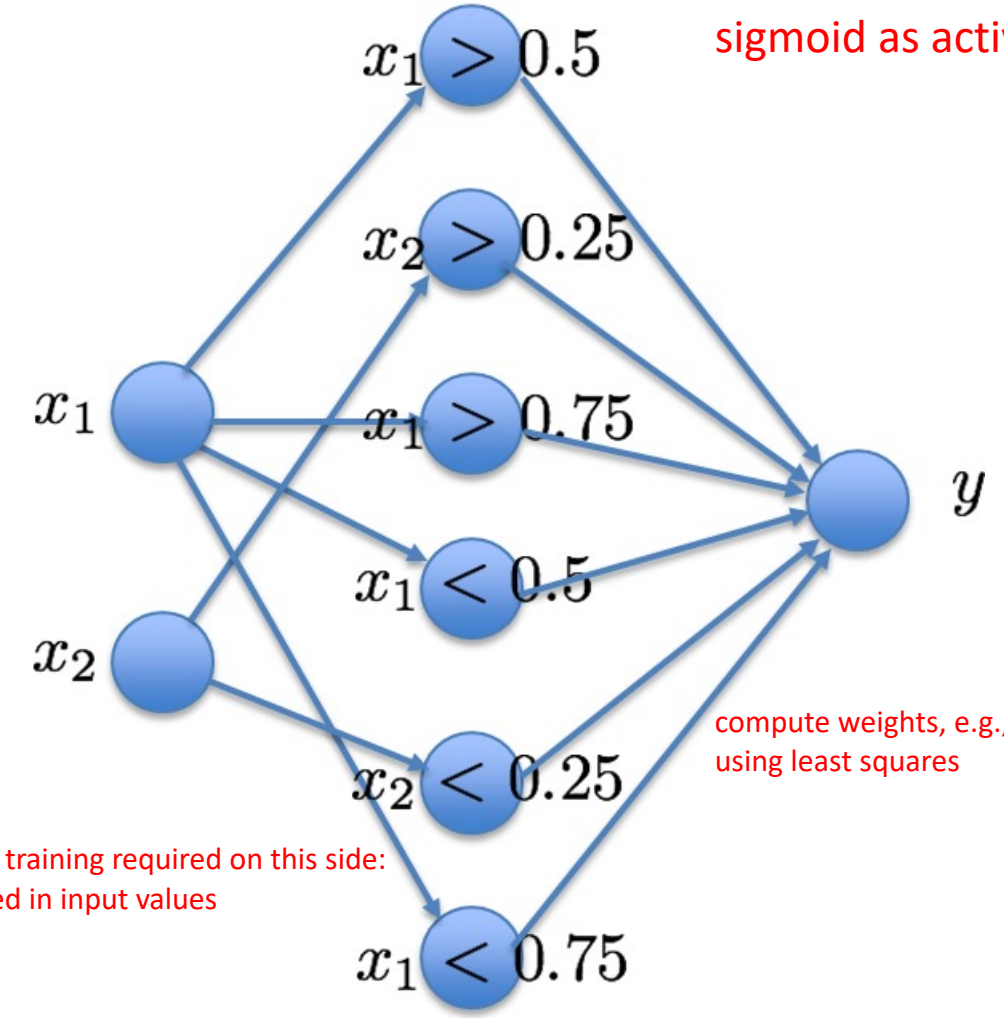




Example: Decision Tree

A neural network is an universal approximator →
We can transform the decision tree into a network:



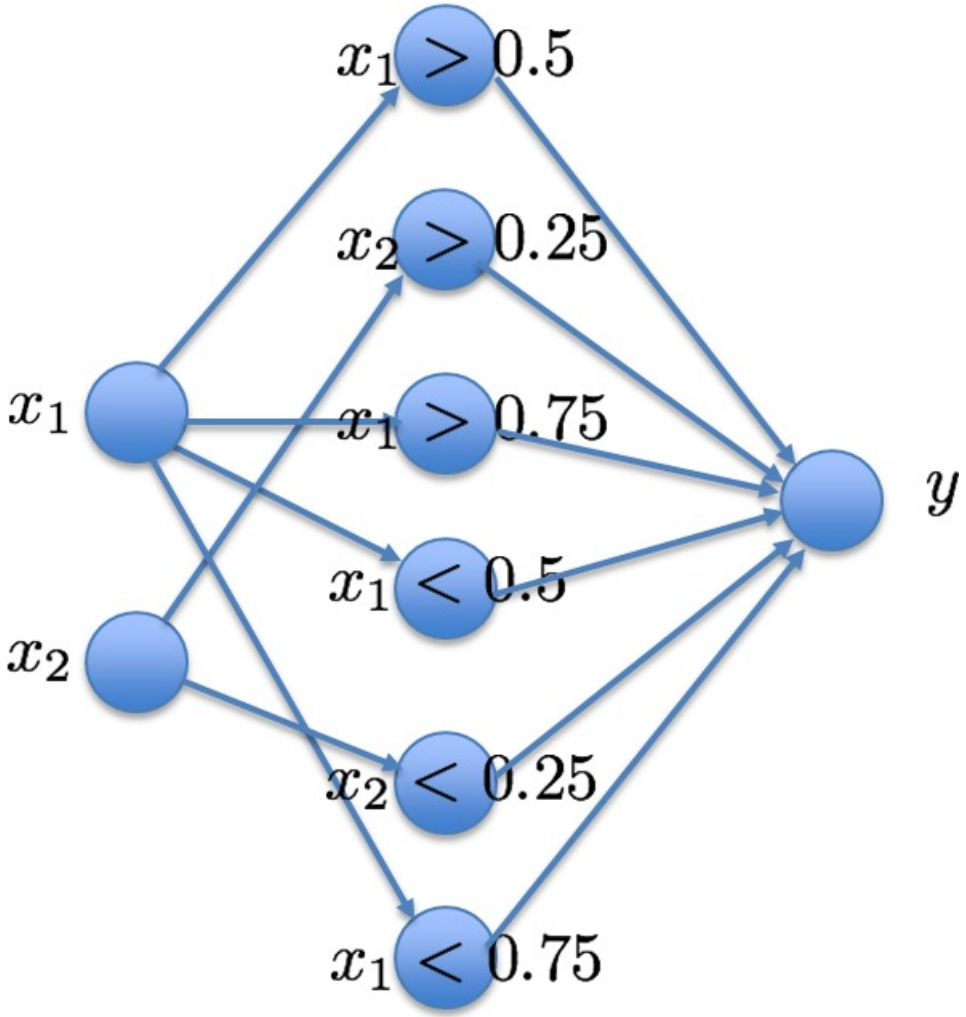


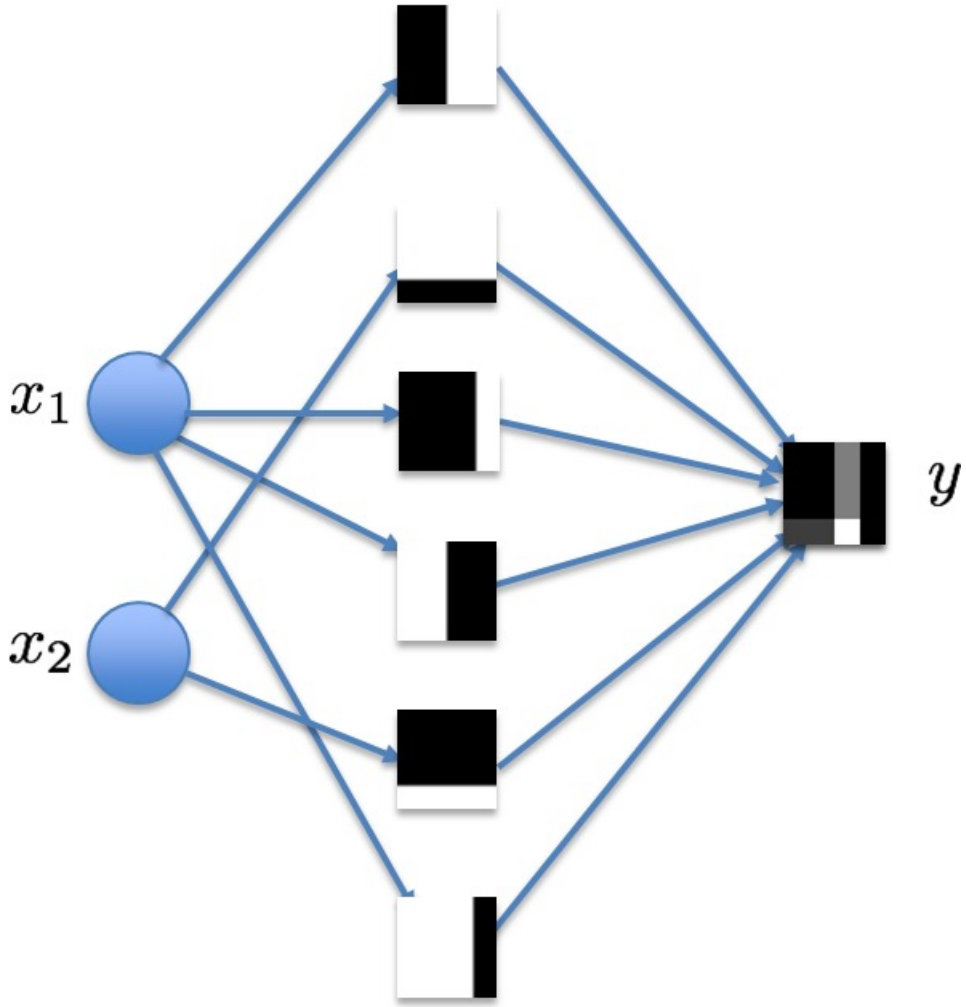
sigmoid as activation

compute weights, e.g., using least squares

no training required on this side: feed in input values

Example: Decision Tree





Example: Decision Tree

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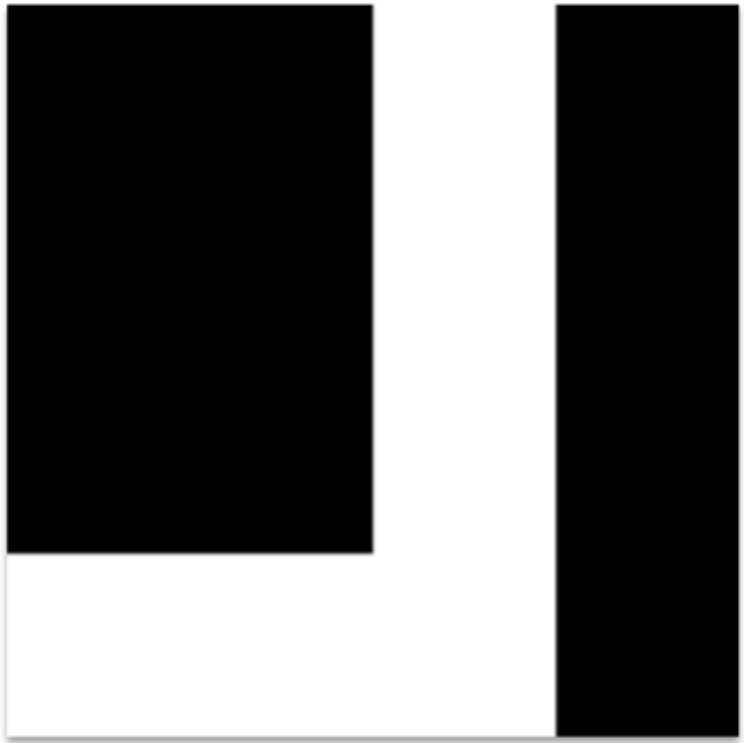
output of decision tree

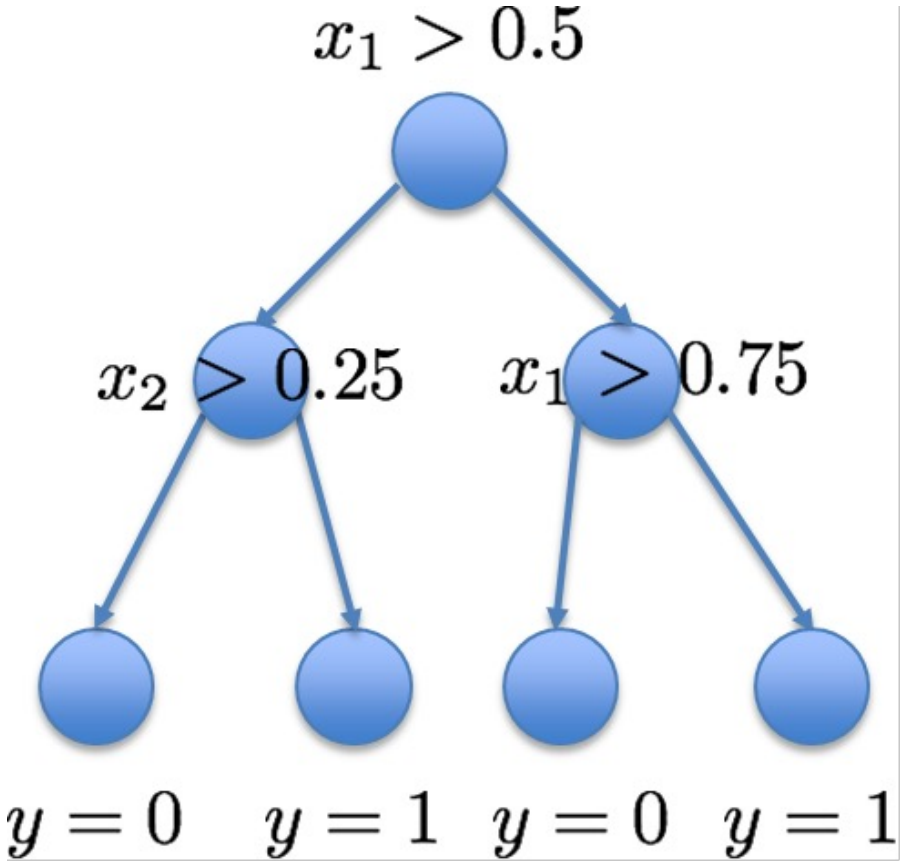


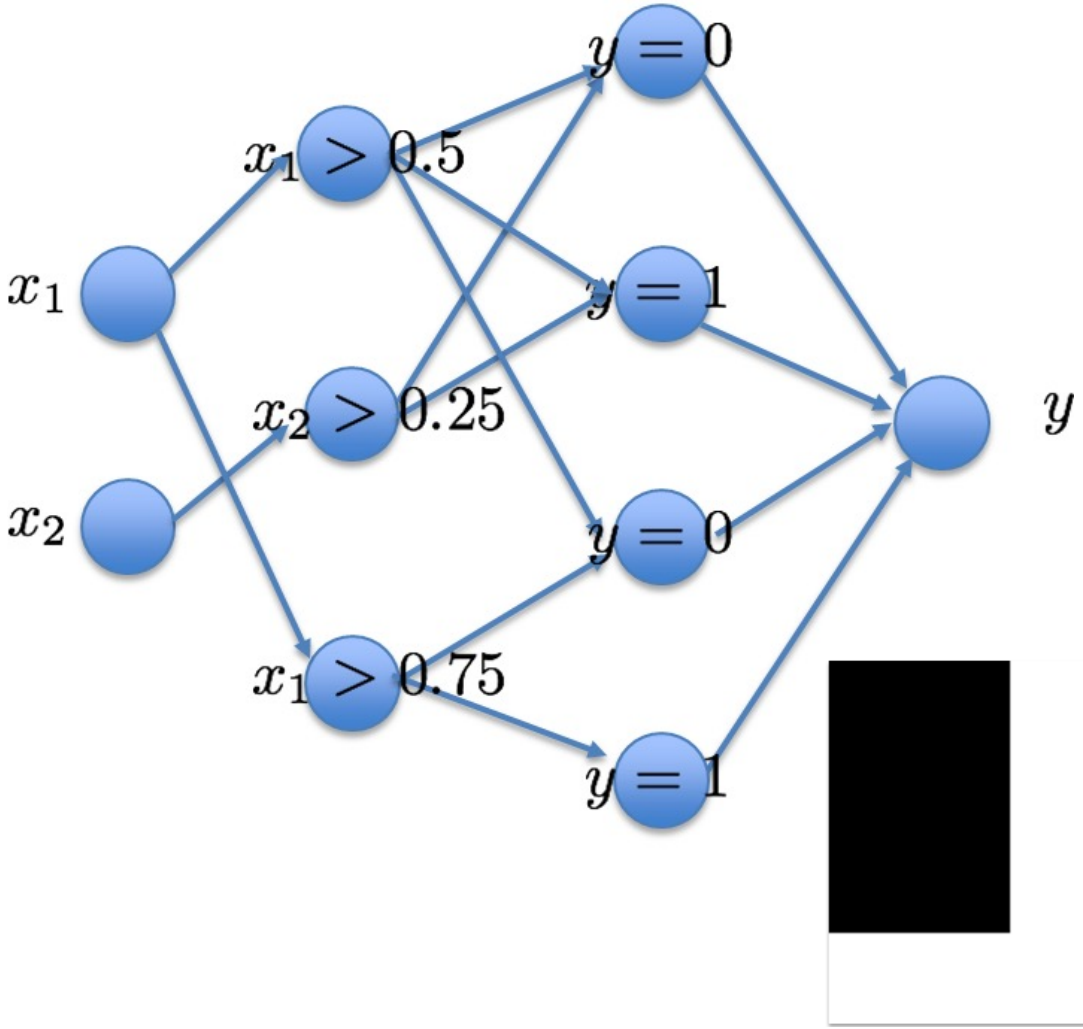
approximation of neural network with six neurons:

this is a quite hard problem – we would have to increase the number of neurons in the layer considerably to obtain a low-error approximation

Example: Decision Tree

add another layer





Depth vs. Width – Further Results

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- newer proofs regarding deep networks with ReLU activation [Lu17, Han17]:
  - deep networks require less neurons than flat ones (for the same approximation quality)
  - they showed that
    - any continuous function with d-dimensional input and k-dimensional output can be approximated with arbitrary accuracy
    - using $d + k$ neurons in all hidden layers.
    - less than $d + k$ neurons are never sufficient, no matter how deep the network gets.

- for practical purposes
  - more neurons and deeper networks may be desirable, as the training may converge faster (or at all).
  - strictly speaking we do not have continuous functions anyway:
    - the number of training samples are always finite,
    - we have only discrete samples of the function at certain positions

Summary

- MLPs are a universal function approximator
- gradient descent is the default training algorithm for deep learning
- backpropagation allows for computing gradients efficiently

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