

# Deep Learning

## Part I: Neural Networks

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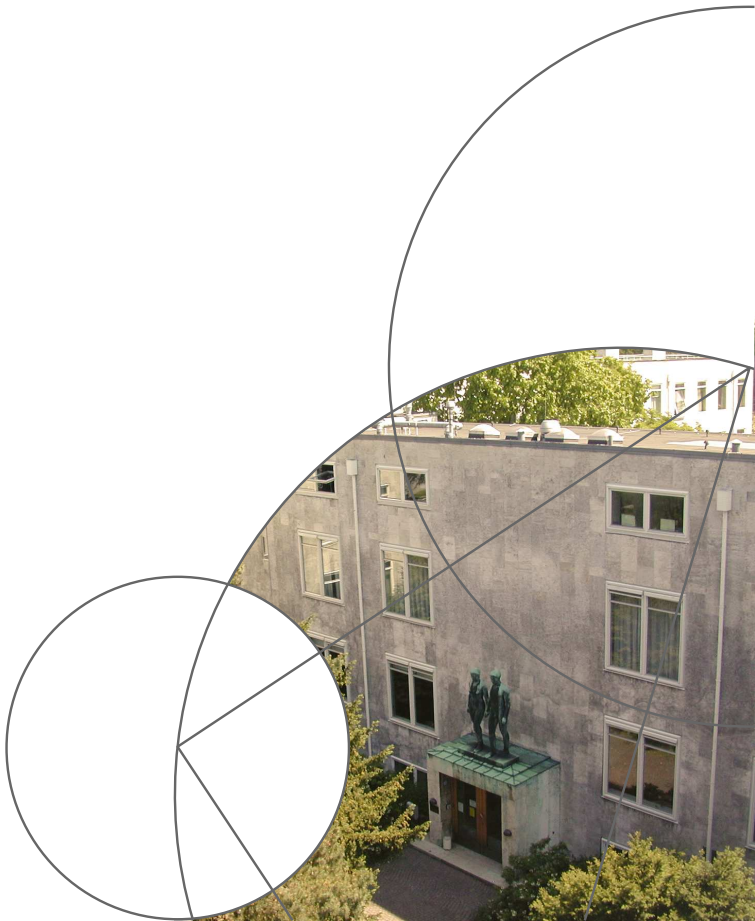

# Warm-up: Chain rule

The *chain rule* for computing the derivative of a composition of two functions,

$$\frac{\partial f(g(x))}{\partial x} = f'(g(x))g'(x)$$

with $f'(x) = \frac{\partial f(x)}{\partial x}$ and $g'(x) = \frac{\partial g(x)}{\partial x}$, can be extended to:

$$\frac{\partial f(g_1(x), g_2(x), \ldots, g_n(x))}{\partial x} = \sum_{i=1}^{n} \frac{\partial f(g_1(x), \ldots, g_n(x))}{\partial g_i(x)} \frac{\partial g_i(x)}{\partial x}$$

# Outline

1. Neural Networks
2. Loss Functions and Encoding
3. Backpropagation & Gradient-based Learning
4. Regularization

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# Neuroscience vs. machine learning

Two applications of neural networks:

**Computational neuroscience:** Modelling biological information processing to gain insights about biological information processing

**Machine learning:** Deriving learning algorithms (loosely) inspired by neural information processing to solve technical problems better than other methods

# Feed-forward artificial neural networks

Different classes of NNs exist:

- feed-forward NNs $\longleftrightarrow$ recurrent networks
- supervised $\longleftrightarrow$ unsupervised learning

We start with

- feed-forward NNs,
- regression and classification,
- supervised learning.

Neural network learning: Using data to adapt (train) the parameters (weights) of a mathematical model.

# Simple neuron models

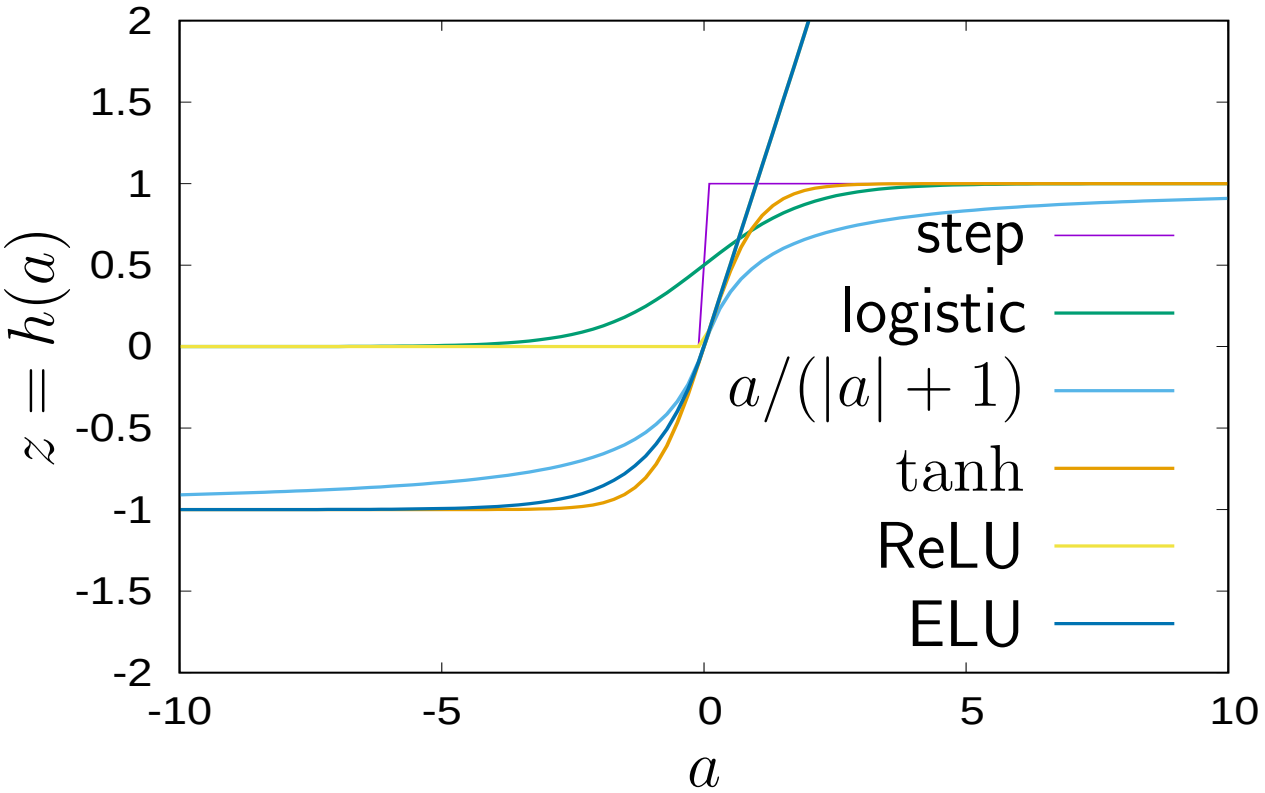
- Let the input be $x_1, \ldots, x_d$ collected in the vector $\boldsymbol{x} \in \mathbb{R}^d$.
- Let the output of neuron $i$ be denoted by $z_i(\boldsymbol{x})$. Often we omit writing the dependency on $\boldsymbol{x}$ to keep the notation uncluttered.
- "Integration": Computing weighted sum

$$a_i = \sum_{j=1}^{d} w_{ij} x_j + w_{i0}$$

  with bias (threshold, offset) parameter $w_{i0} \in \mathbb{R}$
- "Firing": Applying transfer function (activation function) $h$:

$$z_i = h(a_i) = h\left(\sum_{j=1}^{d} w_{ij} x_j + w_{i0}\right)$$

# Activation functions




Step / threshold:

$$h(a) = \mathbb{I}\{a > 0\}$$

Fermi / logistic:

$$h(a) = \frac{1}{1 + e^{-a}}$$

Hyperbolic tangens:

$$h(a) = \tanh(a)$$

Alternative sigmoid:

$$h(a) = \frac{a}{1 + |a|}$$

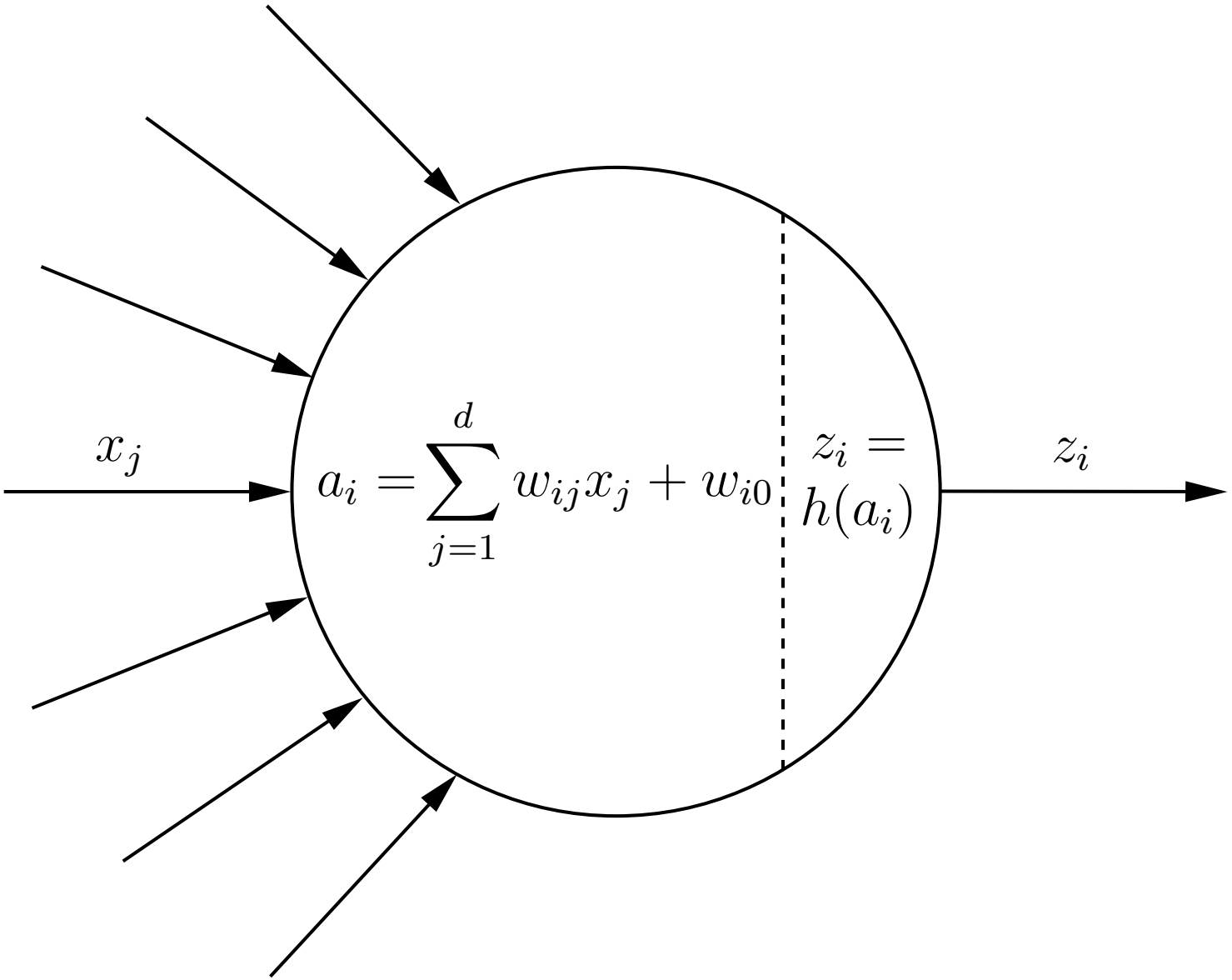
Rectified linear unit (ReLU):

$$h(a) = \max(0, a)$$

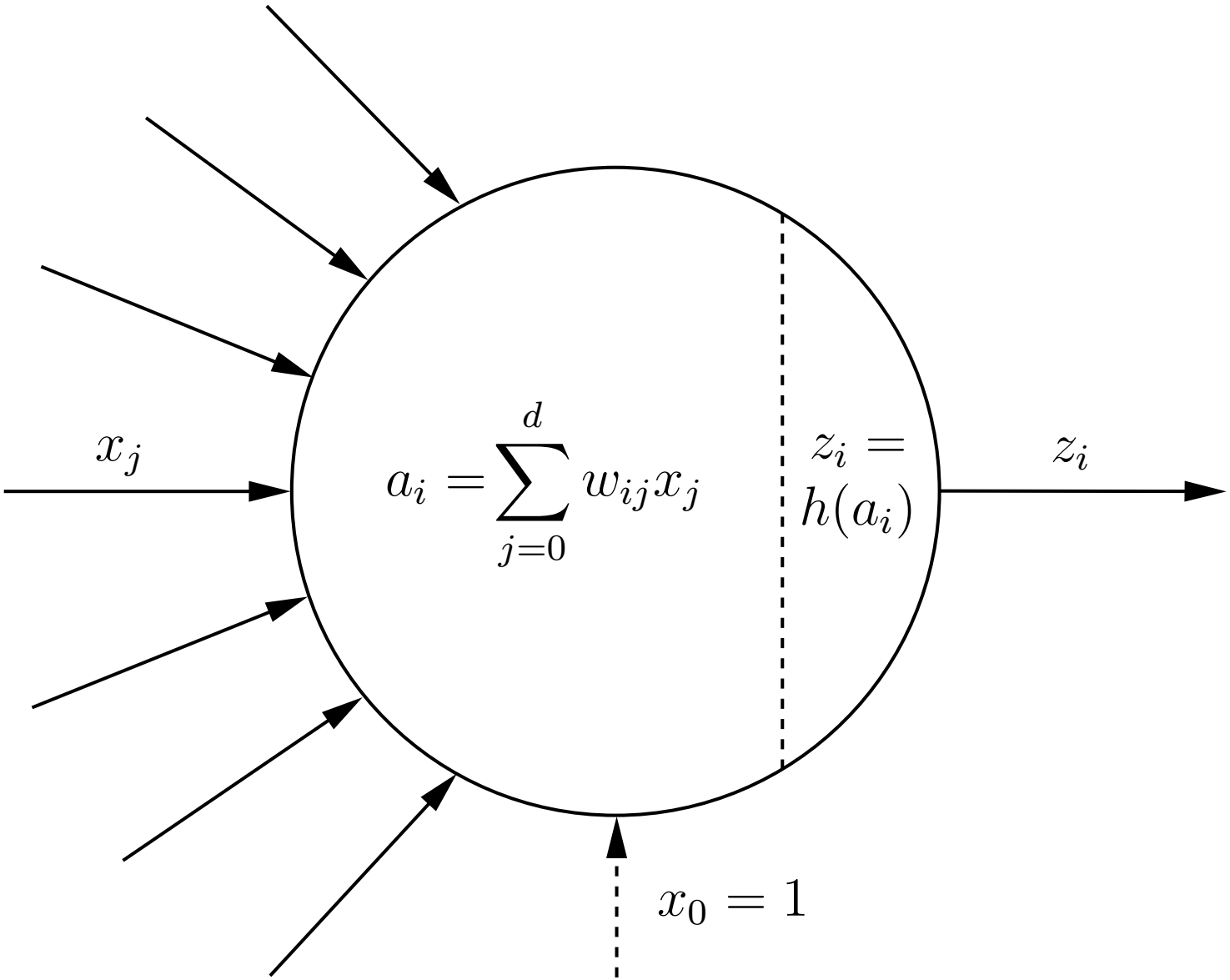
Exponential LU (ELU, $\alpha > 0$):

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

# Single neuron with bias

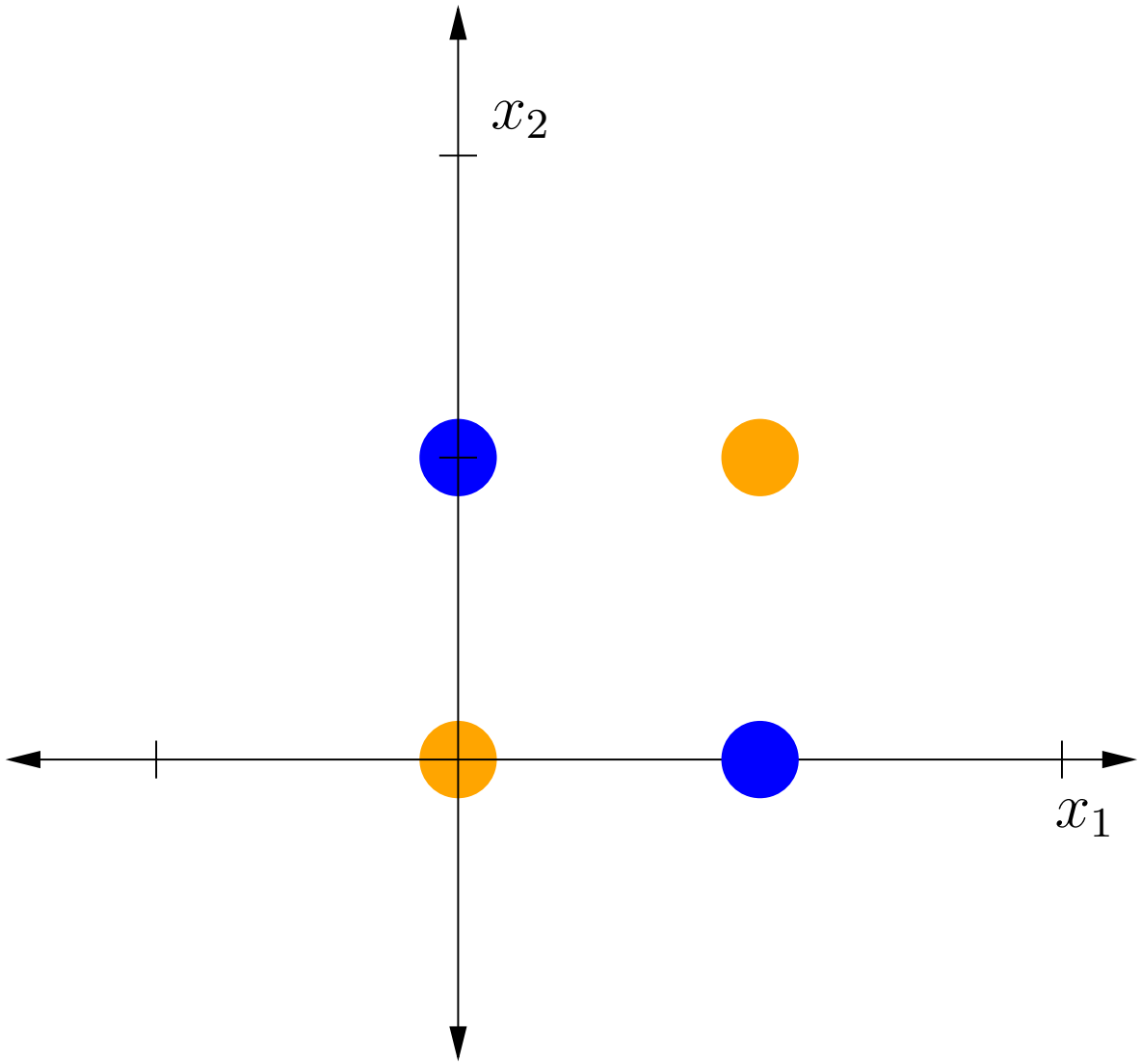



# Single neuron with implicit bias




# XOR

| $x_1$ | $x_2$ | $y$ |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |




# Simple neural network models

- Neural network (NN): Set of connected neurons
- NN can be described by a weighted directed graph
  - Neurons are the nodes/vertices and numbered by integers $V = \{0, 1, 2 \dots\}$
  - Connections between neurons are the edges $A$
  - Strength of connection $(j, i) \in A$ from neuron $j$ to neuron $i$ is described by weight $w_{ij}$
  - All weights are collected in weight vector $\boldsymbol{w}$
- Restriction to feed-forward NNs: We do not allow cycles in the connectivity graph
- NN represents mapping

$$f : \mathbb{R}^d \to \mathbb{R}^K$$

parameterized by $\boldsymbol{w}$: $f(\boldsymbol{x}; \boldsymbol{w})_i = \hat{y}_i$

# Notation I

- $d$ input neurons, $K$ output neurons, $M$ *hidden* neurons:

$$V_{\text{input}} = \{1, \ldots, d\}$$
$$V_{\text{hidden}} = \{d+1, \ldots, d+M\}$$
$$V_{\text{output}} = \{d+M+1, \ldots, d+M+K\}$$

That is:

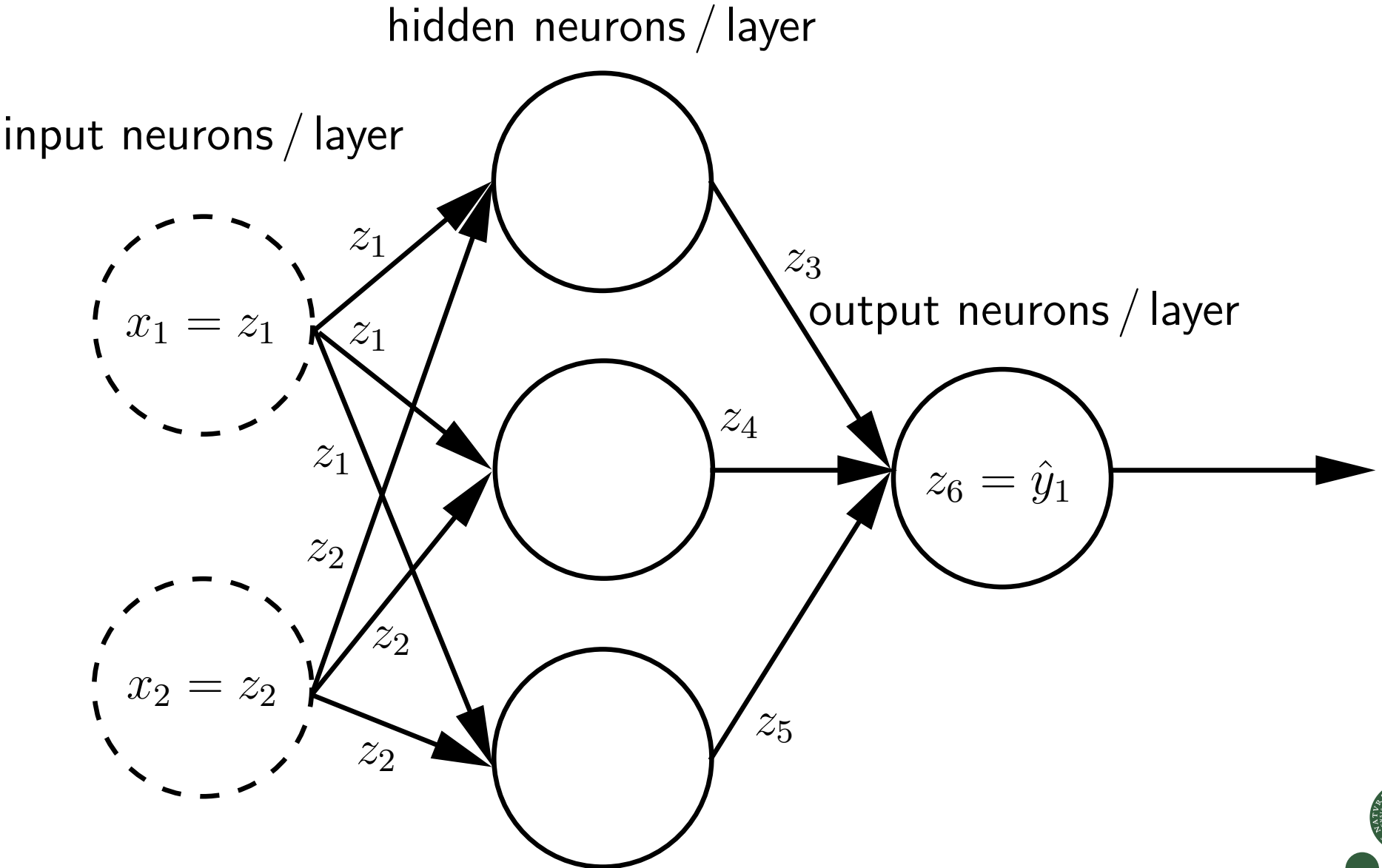
$$V = \{0\} \cup V_{\text{input}} \cup V_{\text{hidden}} \cup V_{\text{output}} = \{0, 1, 2 \ldots, d+M+K\}$$

- Activation function of neuron $i$ is denoted by $h_i$
  - $h_i(a) = a$ for $i \in \{0\} \cup V_{\text{input}}$
  - Typically $h_i \neq h_j$ for $i \in V_{\text{hidden}}$ and $j \in V_{\text{output}}$
- Neuron $i$ can get only input from neuron $j$ if $j < i$, this ensures that the graph is acyclic

# Notation II

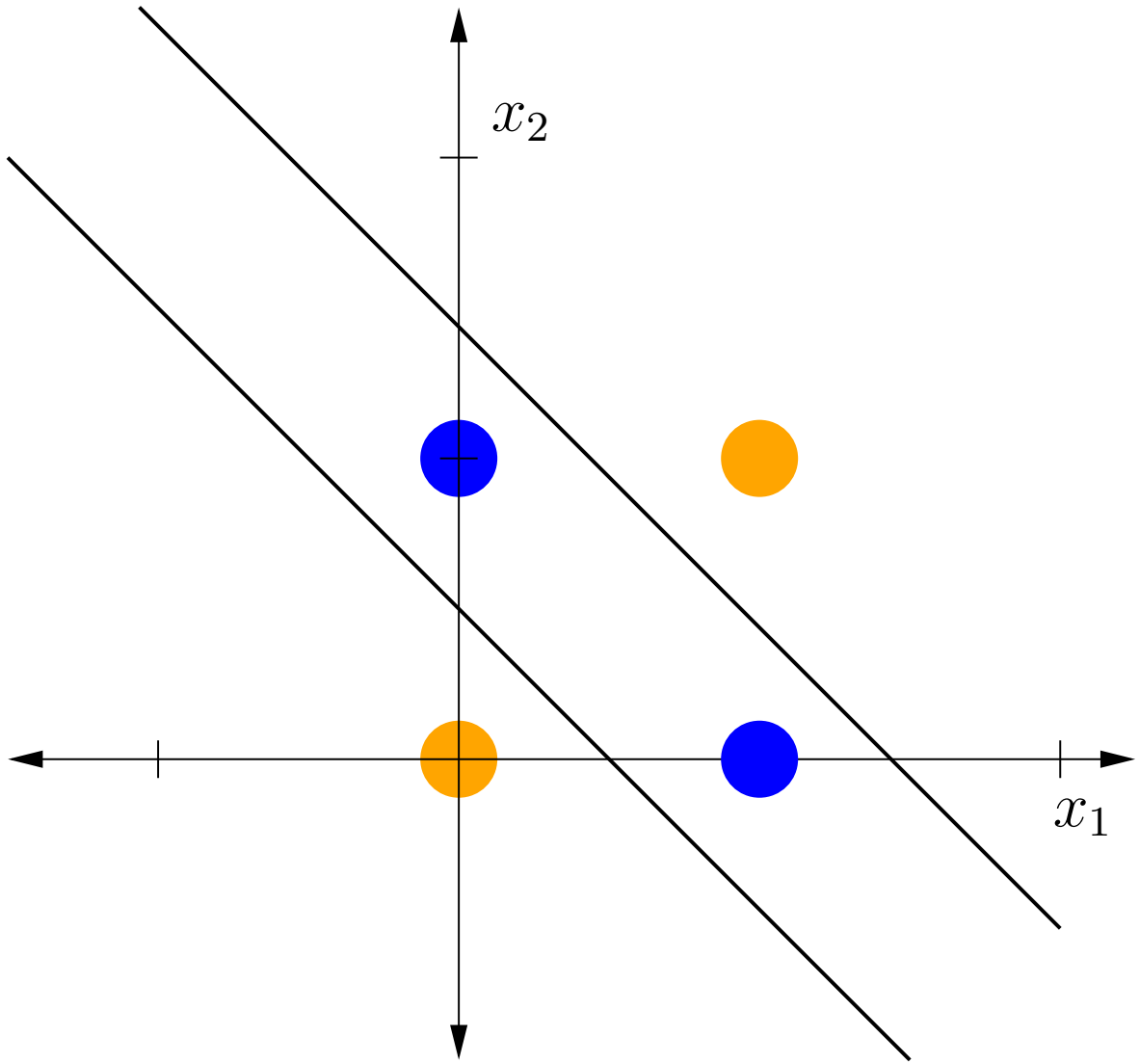
- Activation of neuron $i > 1$ is $a_i = \sum_{(j,i)\in A} w_{ij} z_j$
- Output of neuron $i$ is denoted by $z_i$
- $z_i(a_i) = h_i(a_i)$
  - $z_0(\cdot) = 1$ ($w_{i0} z_0$ is the bias parameter of neuron $i$)
  - $z_i(\cdot) = x_i$ for $i \in V_{\text{input}} = \{1, \ldots, d\}$
- Output of the network: $f(\boldsymbol{x}; \boldsymbol{w}) = \begin{pmatrix} z_{M+d+1} \\ z_{M+d+2} \\ \vdots \\ z_{M+d+K} \end{pmatrix} = \begin{pmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_K \end{pmatrix}$

# Multi-layer perceptron network

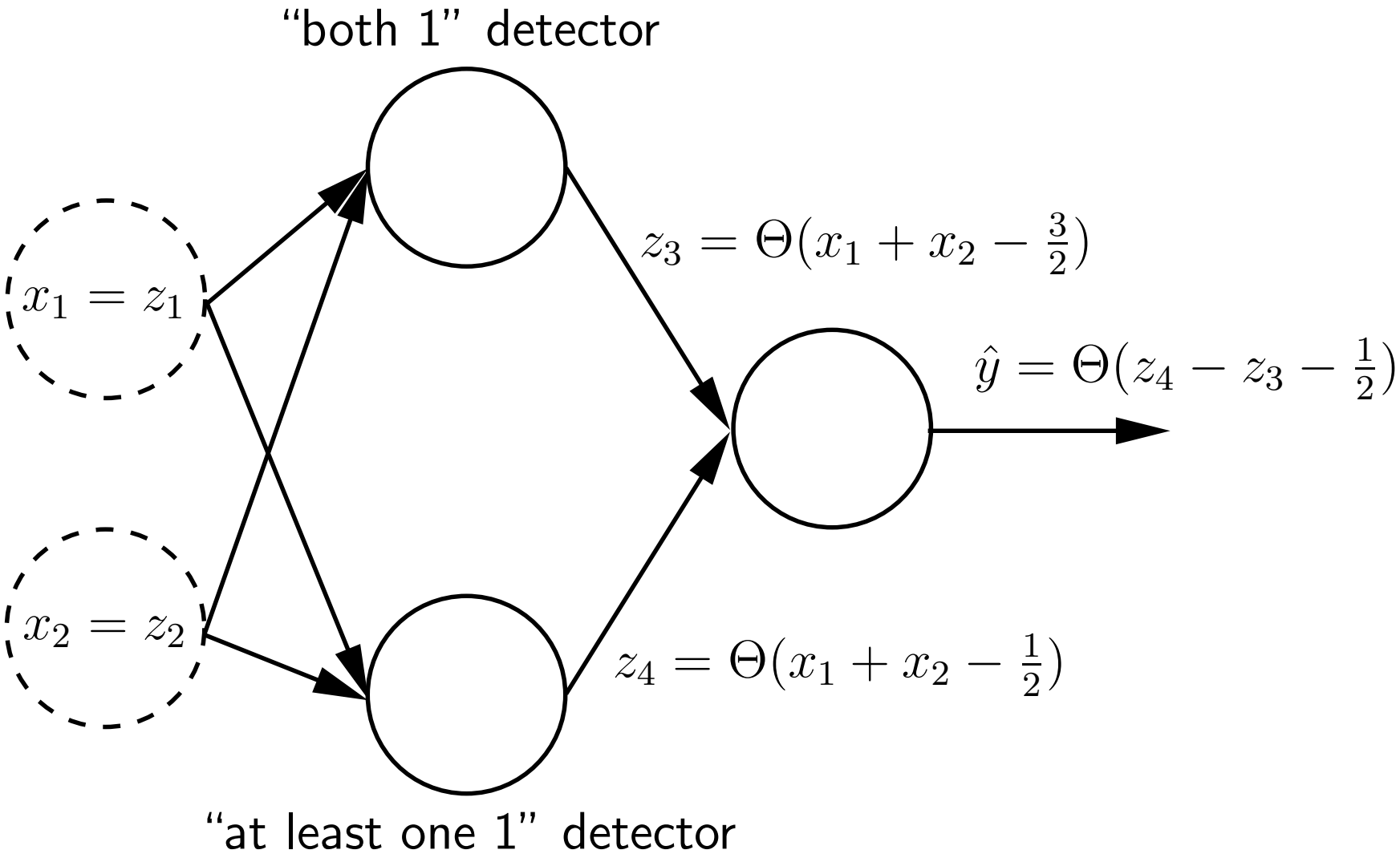



# XOR revisited

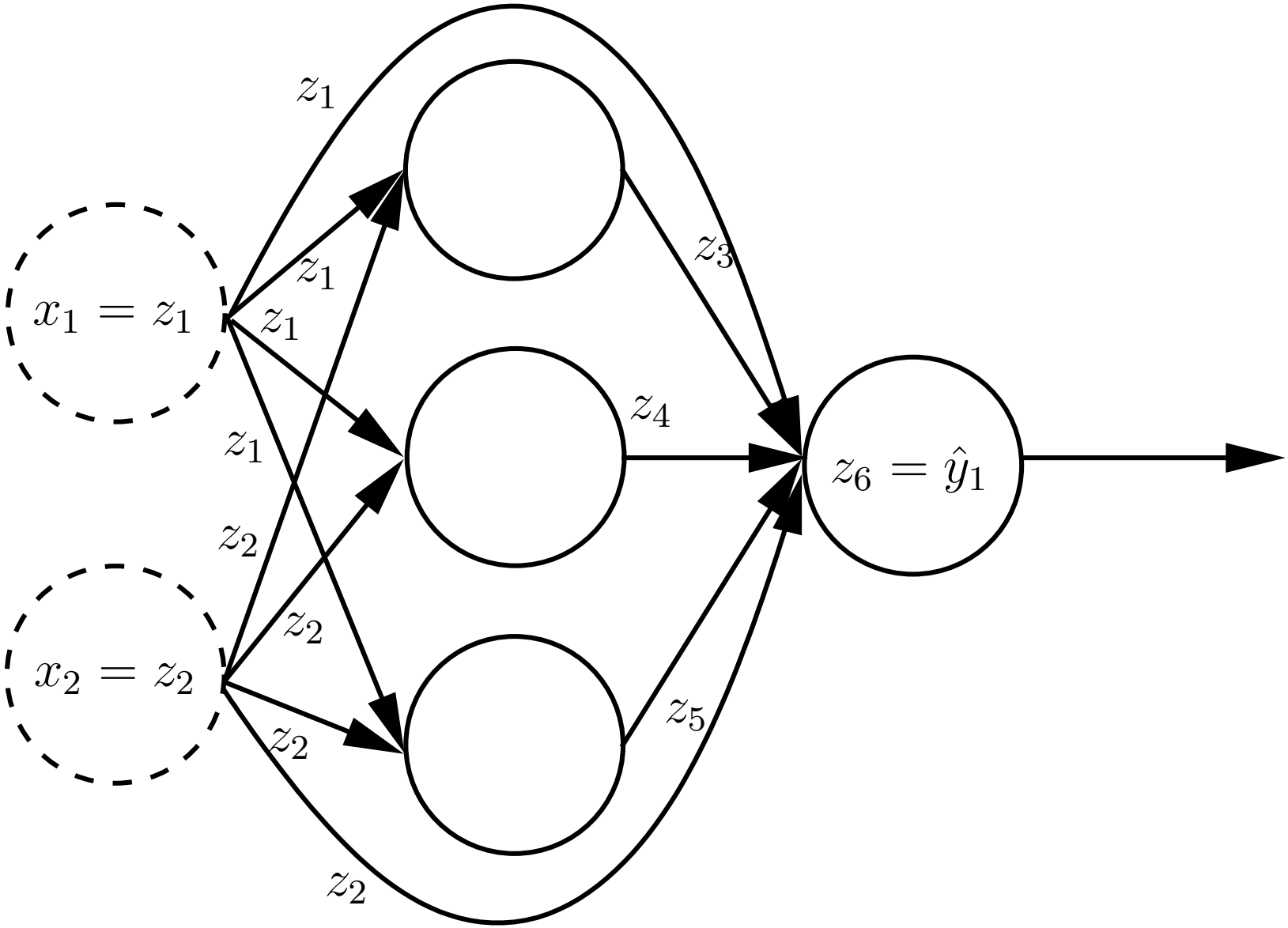
| $x_1$ | $x_2$ | $y$ |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |




# Multi-layer perceptron solving XOR




# Multi-layer perceptron network with shortcuts

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# Regression

- NN shall learn function

$$f : \mathbb{R}^d \to \mathbb{R}^K$$

  $\Rightarrow d$ input neurons, $K$ output neurons
- Training data $S = \{(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_N, \boldsymbol{y}_N)\}$, $\boldsymbol{x}_i \in \mathbb{R}^d$, $\boldsymbol{y}_i \in \mathbb{R}^K$, $1 \leq i \leq N$
- Sum-of-squares error

$$E = \frac{1}{2} \sum_{n=1}^{N} \| f(\boldsymbol{x}_n; \boldsymbol{w}) - \boldsymbol{y}_n \|^2 = \frac{1}{2} \sum_{n=1}^{N} \sum_{i=1}^{K} ([f(\boldsymbol{x}_n; \boldsymbol{w})]_i - [\boldsymbol{y}_n]_i)^2$$

- Usually linear output neurons: $h_i(a) = a$ for $i \in V_{\text{output}}$

# Sum-of-squares and maximum likelihood

W.l.o.g. $d = 1$, $S = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\}$. We assume that the observations $t$ given an input $\boldsymbol{x}$ are normally distributed (with variance $s^2$) around the model $f(\boldsymbol{x}; \boldsymbol{w})$:

$$p(y|\boldsymbol{x}; \boldsymbol{w}) = \frac{1}{s\sqrt{2\pi}} \exp \frac{-(y - f(\boldsymbol{x}; \boldsymbol{w}))^2}{2s^2}$$

Likelihood and negative log-likelihood:

$$p(S|\boldsymbol{w}) = \prod_{n=1}^{N} \frac{1}{s\sqrt{2\pi}} \exp \frac{-(y_n - f(\boldsymbol{x_n}; \boldsymbol{w}))^2}{2s^2}$$

$$-\ln p(S|\boldsymbol{w}) = \frac{1}{2s^2} \sum_{n=1}^{N} (y_n - f(\boldsymbol{x_n}; \boldsymbol{w}))^2 + N \ln(s\sqrt{2\pi})$$

As blue terms are independent of $\boldsymbol{w}$, minimizing the sum-of-squares error corresponds to maximum likelihood estimation under the Gaussian noise assumption.

# Binary classification

For binary classification, assume $\mathcal{Y} = \{0, 1\}$, the output is in $[0, 1]$, and the target follows a Bernoulli distribution:

$$p(y|\boldsymbol{x}; \boldsymbol{w}) = f(\boldsymbol{x}; \boldsymbol{w})^y [1 - f(\boldsymbol{x}; \boldsymbol{w})]^{1-y} = \begin{cases} f(\boldsymbol{x}) & \text{for } y = 1 \\ 1 - f(\boldsymbol{x}) & \text{for } y = 0 \end{cases}$$

Negative logarithm of $p(S|\boldsymbol{w}) = \prod_{n=1}^{N} p(y_n|\boldsymbol{x}_n; \boldsymbol{w})$ leads to *cross-entropy* error function:

$$-\ln p(S|\boldsymbol{w}) = -\sum_{n=1}^{N} \{y_n \ln f(\boldsymbol{x}_n; \boldsymbol{w}) + (1 - y_n) \ln(1 - f(\boldsymbol{x}_n; \boldsymbol{w}))\}$$

Use sigmoid mapping to $[0, 1]$ as output activation function.

# Multi-class classification: One-hot

For $K$ classes, use one-hot encoding ($1$ out of $K$ encoding):

- The $j$th component of $\boldsymbol{y}_i$ is one, if $\boldsymbol{x}_i$ belongs to the $j$th class, and zero otherwise.
- Example: If $K = 4$ and $\boldsymbol{x}_i$ belongs to third class, then $\boldsymbol{y}_i = (0, 0, 1, 0)^\mathsf{T}$.

With $\sum_{k=1}^{K} [f(\boldsymbol{x}; \boldsymbol{w})]_k = 1$ and $\forall k : [f(\boldsymbol{x}; \boldsymbol{w})]_k \geq 0$

$$p(\boldsymbol{y}|\boldsymbol{x}; \boldsymbol{w}) = \prod_{k=1}^{K} [f(\boldsymbol{x}; \boldsymbol{w})]_k^{[\boldsymbol{y}]_k}$$

gives negative log likelihood (cross-entropy for multiple classes):

$$-\ln p(S|\boldsymbol{w}) = -\sum_{n=1}^{N} \sum_{k=1}^{K} [\boldsymbol{y}_n]_k \ln [f(\boldsymbol{x}_n; \boldsymbol{w})]_k$$

# Multi-class classification: Soft-max

The *soft-max* activation function

$$[f(\boldsymbol{x};\boldsymbol{w})]_j = \sigma(a_{M+d+j}) = \frac{\exp a_{M+d+j}}{\sum_{k=1}^{K} \exp a_{M+d+k}}$$

naturally extends the logistic function to multiple classes and ensures that $\sum_{j=k}^{K}[f(\boldsymbol{x};\boldsymbol{w})]_k = 1$.

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# Gradient descent

- Consider learning by iteratively changing the weights

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + \Delta\boldsymbol{w}^{(t)}$$

- Simplest choice is (steepest) gradient descent

$$\Delta\boldsymbol{w}^{(t)} = -\eta\nabla E|_{\boldsymbol{w}^{(t)}}$$

  with learning rate $\eta > 0$

- Often a *momentum term* is added to improve the performance

$$\Delta\boldsymbol{w}^{(t)} = -\eta\nabla E|_{\boldsymbol{w}^{(t)}} + \mu\Delta\boldsymbol{w}^{(t-1)}$$

  with momentum parameter $\mu \geq 0$

# Backpropagation I

Let the activation functions be differentiable. From

$$z_i = h(a_i) \qquad a_i = \sum_{(j,i)\in A} w_{ij} z_j$$

$$E = \sum_{n=1}^{N} E^n \qquad \text{e.g.} \qquad \sum_{n=1}^{N} \underbrace{\frac{1}{2}\|\boldsymbol{y}_n - f(\boldsymbol{x}_n; \boldsymbol{w})\|^2}_{E^n}$$

we get for $(j, i) \in A$ the partial derivatives:

$$\frac{\partial E}{\partial w_{ij}} = \sum_{n=1}^{N} \frac{\partial E^n}{\partial w_{ij}}$$

In the following, we derive $\frac{\partial E^n}{\partial w_{ij}}$; the index $n$ is omitted to keep the notation uncluttered (i.e., we write $E$ for $E^n$, $\boldsymbol{x}$ for $\boldsymbol{x}_n$, etc.).

# Backpropagation II

We want

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial E}{\partial a_i} \frac{\partial a_i}{\partial w_{ij}}$$

and define:

$$\delta_i := \frac{\partial E}{\partial a_i}$$

With

$$\frac{\partial a_i}{\partial w_{ij}} = z_j$$

we get:

$$\frac{\partial E}{\partial w_{ij}} = \delta_i z_j$$

# Backpropagation III

For an output unit $i \in V_{\text{output}} = \{M+d+1, \ldots, M+d+K\}$ we have:

$$\delta_i = \frac{\partial E}{\partial a_i} = \frac{\partial z_i}{\partial a_i}\frac{\partial E}{\partial z_i} = h_i'(a_i)\frac{\partial E}{\partial z_i}$$

If $h_i(a) = a$, i.e., the output is linear and $h_i'(a) = 1$, and $E = \frac{1}{2}\|f(\boldsymbol{x};\boldsymbol{w}) - \boldsymbol{y}\|^2$, we get:

$$E = \frac{1}{2}\sum_{i=1}^{K}([f(\boldsymbol{x};\boldsymbol{w})]_i - y_i)^2 = \frac{1}{2}\sum_{i \in V_{\text{output}}}(z_i - y_{i-M-d})^2$$

$$\delta_i = \frac{\partial}{\partial z_i}\frac{1}{2}\sum_{j \in V_{\text{output}}}(z_j - y_{j-M-d})^2 = \frac{\partial}{\partial z_i}\frac{1}{2}(z_i - y_{i-M-d})^2 \Rightarrow$$

$$\delta_i = z_i - y_{i-M-d}$$

# Backpropagation IV

Fort the $\delta$ of a hidden unit $i \in V_{\text{hidden}} = \{d+1, \ldots, M+d\}$, we need the chain rule again

$$\delta_i = \frac{\partial E}{\partial a_i} = \sum_{k=i+1}^{M+d+K} \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial a_i} = \sum_{k=i+1}^{M+d+K} \frac{\partial E}{\partial a_k} \frac{\partial a_k}{\partial z_i} \frac{\partial z_i}{\partial a_i}$$

and obtain:

$$\delta_i = h_i'(a_i) \sum_{k \text{ with } (i,k)\in A} w_{ki}\delta_k$$

# Backpropagation V

For each training pattern $(\boldsymbol{x}, \boldsymbol{y})$:

- *Forward pass (determines output of network given $\boldsymbol{x}$):*
  1. Compute $z_{d+1}, \ldots, z_{d+M+K}$ in sequential order
  2. $z_{M-K+1}, \ldots, z_M$ define $f(\boldsymbol{x}; \boldsymbol{w})$
- *Backward pass (determines partial derivatives):*
  1. After a forward pass, compute $\delta_{d+1}, \ldots, \delta_{d+M+K}$ in reverse order
  2. Compute the partial derivatives for $(j, i) \in A$ according to $\partial E / \partial w_{ij} = \delta_i z_j$

# Other error functions

For an output unit $M + d < i \leq d + M + K$ we get

$$\delta_i = z_i - y_{i-M-d}$$

for

- Sum-of-squares error and linear output neurons
- Cross-entropy error and single logistic output neuron
- Cross-entropy error for multiple classes and soft-max output

# Linear algebra notation I (and a special layer definition)

- Layers collect neurons getting the same input and perform the same type of computation
- Layer $l$ gets only input from layers $l' < l$
- The activation function of layer $l$ is $h^{(l)}$
- Inputs (external inputs as well as outputs from other neurons) to layer $l$ are gathered in vector $\boldsymbol{x}^{(l)}$, the outputs of the neurons in layer $l$ in vector $\boldsymbol{h}^{(l)}$

$\rightarrow$ If the outputs of layer $l$ are the only inputs to layer $l+1$, we have $\boldsymbol{h}^{(l)} = \boldsymbol{x}^{(l+1)}$

# Linear algebra notation II

- Denoting the weights of the $i$th neuron in layer $l$ by $\boldsymbol{w}_i^{(l)}$ and its bias by $b_i^{(l)}$ we get $h_i^{(l)}(\boldsymbol{x}) = h^{(l)}\left(\left[\boldsymbol{w}_i^{(l)}\right]^\mathsf{T}\boldsymbol{x} + b_i^{(l)}\right)$
- We stack the $\boldsymbol{w}_i^{(l)}$ of all neurons in layer $l$ in matrix $\boldsymbol{W}^{(l)}$ and their bias parameters in vector $\boldsymbol{b}^{(l)}$ and write

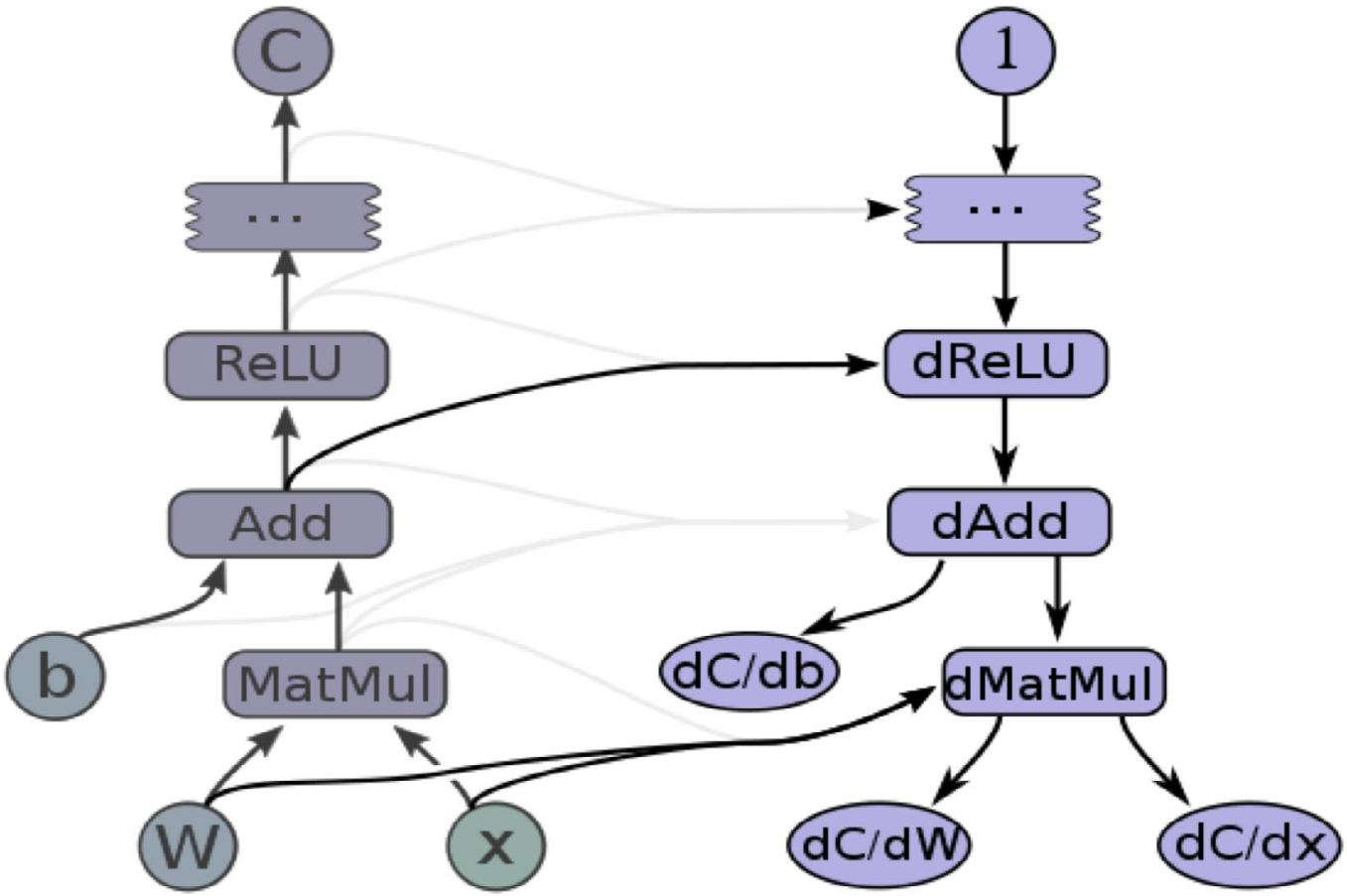
$$\boldsymbol{h}^{(l)}\left(\boldsymbol{x}^{(l)}\right) = h^{(l)}\left(\boldsymbol{W}^{(l)}\boldsymbol{x}^{(l)} + \boldsymbol{b}^{(l)}\right) \qquad \text{[great for GPU]}$$

  where $h^{(l)}$ acts component-wise
- Assume implicit bias parameters and a batch of inputs $\boldsymbol{x}_1^{(l)}, \ldots, \boldsymbol{x}_B^{(l)}$ gathered as rows in a data matrix $\boldsymbol{X}^{(l)}$, the output of the layer can be computer for the full batch as:

$$\boldsymbol{H}^{(l)}\left(\boldsymbol{X}^{(l)}\right) = h^{(l)}\left(\boldsymbol{W}^{(l)}\left[\boldsymbol{X}^{(l)}\right]^\mathsf{T}\right) \qquad \text{[great for GPU]}$$

# Symbolic differentiation

Many modern machine learning frameworks can compute gradients automatically:




Abadi et al. TensorFlow: Large-Scale Machine Learning on Heterogeneous Distributed Systems. *arXiv:1603.04467*, 2016

# Mini-batch learning

**Batch learning:** Compute the gradients over all $N$ training samples and update

$$\Delta \boldsymbol{w}^{(t)} = -\eta \nabla E|_{\boldsymbol{w}^{(t)}}$$

**Mini-batch learning:** Choose a subset
$S_m = \{(\boldsymbol{x}_{i_1}, \boldsymbol{y}_{i_1}), \ldots, (\boldsymbol{x}_{i_B}, \boldsymbol{y}_{i_B})\}$,
$1 \leq i_1 \leq \cdots \leq i_B \leq N$, and update

$$\Delta \boldsymbol{w}^{(t)} = -\eta \sum_{(\boldsymbol{x}_n, \boldsymbol{y}_n) \in S_B} \nabla E^n|_{\boldsymbol{w}^{(t)}}$$

typically with a smaller learning rate $\eta$

# "Vanishing gradient"

- Derivative of $h(a) = \frac{1}{1+\exp(-a)}$ is upper bounded by 0.25.
- What is the derivative of the rectified linear unit (ReLU) $h(a) = \max(0, a)$ for $a < 0$ and $a > 0$, respectively?
- Consider a deep neural network with many layers and

$$\delta_i = h_i'(a_i) \sum_{k=i+1}^{M+d+K} w_{ki}\delta_k \quad .$$

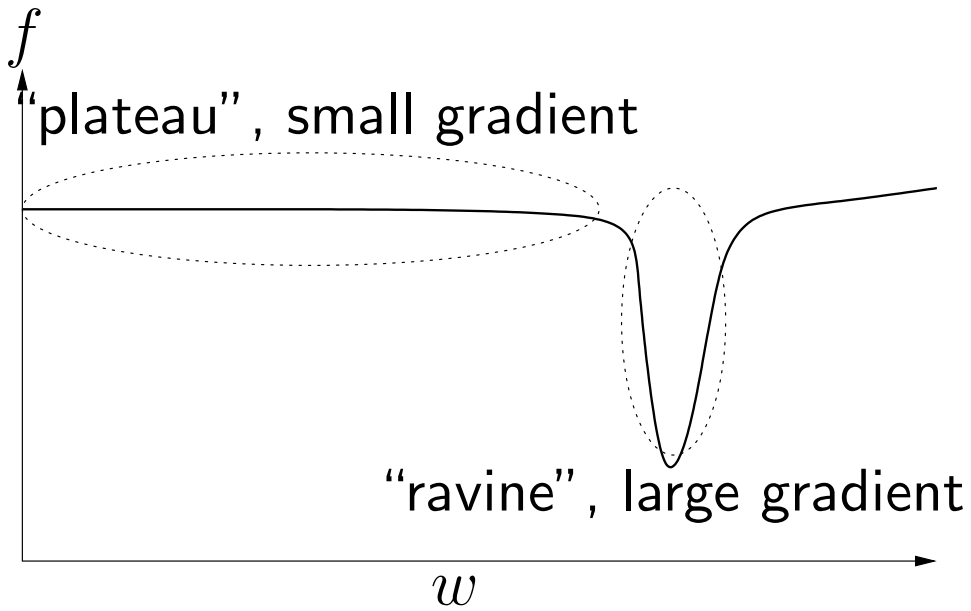
What happens to the magnitude of $\delta_i$ with increasing number of layers between neuron $i$ and the output?

# Efficient gradient-based optimization

- Vanilla steepest-descent is usually not the best choice for (batch) gradient-based learning
- Many powerful gradient-based search techniques exist
- Recent method for online/mini-batch learning: Adam (from "adaptive moments")

Kingma, Ba. Adam: A Method for Stochastic Optimization. *ICLR*, 2015

# Basic problem




- The idea is – instead of directly using the magnitude of the partial derivative – to adjust the update in the direction of the partial derivative for each weight individually based on feedback from previous iterations.

# Rescaling by second raw moment I

- Goal: Iterative minimization of $f(\boldsymbol{w})$
- Taylor approximation:

$$f(\boldsymbol{w} + \boldsymbol{\Delta w}) \approx f(\boldsymbol{w}) + \boldsymbol{\Delta w}^\mathsf{T} \nabla f(\boldsymbol{w})$$

leads to update step $\boldsymbol{w}_i^{(t+1)} \leftarrow \boldsymbol{w}_i^{(t)} + \boldsymbol{\Delta w}^{(t)}$ in iteration $t$

$$\boldsymbol{\Delta w}^{(t)} = \operatorname{argmin}_{\boldsymbol{\Delta w}} \left\{ \boldsymbol{\Delta w}^\mathsf{T} \nabla f(\boldsymbol{w}^{(t)}) \quad \text{s.t.} \quad \|\boldsymbol{\Delta w}^{(t)}\| \leq \alpha \right\} \ ,$$

where $\alpha$ defines a trust region (in which we trust the approximation)

- Solution is co-linear with gradient and has maximum length:

$$\boldsymbol{\Delta w}^{(t)} = -\alpha \frac{\nabla f(\boldsymbol{w}^{(t)})}{\|\nabla f(\boldsymbol{w}^{(t)})\|}$$

# Rescaling by second raw moment II

- We have unbiased estimates $\nabla \tilde{f}(\boldsymbol{w}^{(t)})$ instead of $\nabla f(\boldsymbol{w}^{(t)})$, typically gradients computed on mini-batches:

$$\boldsymbol{\Delta w} = -\alpha \frac{\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w}^{(t)})]}{\|\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w}^{(t)})]\|} = -\alpha \frac{\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w}^{(t)})]}{\sqrt{\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w}^{(t)})]^{\mathsf{T}} \mathbb{E}[\nabla \tilde{f}(\boldsymbol{w}^{(t)})]}}$$

- Concretele, for neural networks $\nabla_i \tilde{f}(\boldsymbol{w}^{(t)})$ is the partial derivative of the error function estimate (the error over a mini-batch) w.r.t. weight $w_i$ at iteration $t$

# Rescaling by second raw moment III

Now we do the following ...

- Replace $\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})^\mathsf{T}]\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})]$ by $\mathbb{E}[(\nabla \tilde{f}(\boldsymbol{w}))^2]$. We have

  $$\mathbb{E}[(\nabla \tilde{f}(\boldsymbol{w}))^2] = \mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})^\mathsf{T} \nabla \tilde{f}(\boldsymbol{w})] \geq E[\nabla \tilde{f}(\boldsymbol{w})^\mathsf{T}]\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})] \ ,$$

  which might increase numerical stability.
- Add a positive constant $\epsilon$ to $\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})^2]$ to avoid division by zero.
- Consider each weight $w_i$ independently.
- Use a running average ($\beta \in ]0, 1]$)

  $$v_i^{(t+1)} = (1 - \beta) v_i^{(t)} + \beta \left( \nabla_i \tilde{f}(\boldsymbol{w}^{(t)}) \right)^2$$

  as estimate for $\mathbb{E}[\nabla \tilde{f}(\boldsymbol{w})^2]$.

# RMSprop

. . . then we arrive at the RMSprop update rule:

$$w_i^{(t+1)} \leftarrow w_i^{(t)} - \alpha \frac{\nabla_i \tilde{f}(\boldsymbol{w}^{(t)})}{\sqrt{v_i^{(t+1)} + \epsilon}}$$

Tieleman, Hinton. Lecture 6.5. RMSPROP: Divide the gradient by a running average of its recent magnitude. *COURSERA: Neural Networks for Machine Learning*, 2012

Lafond, Vasilache, Bottou. Diagonal Rescaling For Neural Networks. *arXiV:1705.09319*

# Adam algorithm

**Algorithm 1:** Adam algorithm

1 init. $\boldsymbol{w}^{(0)}, \beta_1, \beta_2, \alpha, \epsilon$; $t \leftarrow 1$; $\boldsymbol{v}^{(0)}, \hat{\boldsymbol{v}}^{(0)}, \boldsymbol{m}^{(0)}, \hat{\boldsymbol{m}}^{(0)} \leftarrow \mathbf{0}$

2 **while** *stopping criterion not met* **do**

3  **foreach** $w_i$ **do**

4  $g_i^{(t)} \leftarrow \nabla_i \tilde{f}(\boldsymbol{w}^{(t)})$

5  $m_i^{(t+1)} \leftarrow \beta_1 \cdot m_i^{(t)} + (1-\beta_1) \cdot g_i^{(t)}$

6  $v_i^{(t+1)} \leftarrow \beta_2 \cdot v_i^{(t)} + (1-\beta_2) \cdot \left(g_i^{(t)}\right)^2$

7  $\hat{m}_i^{(t+1)} \leftarrow m_i^{(t+1)} / (1-\beta_1^t)$

8  $\hat{v}_i^{(t+1)} \leftarrow v_i^{(t+1)} / (1-\beta_2^t)$

9  $w_i^{(t+1)} \leftarrow w_i^{(t)} - \alpha \cdot \hat{m}_i^{(t+1)} / \left(\sqrt{\hat{v}_i^{(t+1)}} + \epsilon\right)$

10  $t \leftarrow t+1$

$^t$: power of $t$; $^{(t)}$: iteration step $t$

# Adam default values

| parameter | range | default | comment |
|---|---|---|---|
| $\beta_1$ | $[0, 1[$ | $0.9$ | first moment learning rate |
| $\beta_2$ | $[0, 1[$ | $0.999$ | second raw moment learning rate |
| $\epsilon$ | $\mathbb{R}^+$ | $10^{-8}$ | avoid devision by zero |
| $\alpha$ | $\mathbb{R}^+$ | $0.001$ | learning rate<br>upper bound on update |

- $\beta_1$ controls learning approximation of gradient's mean
- $\beta_2$ controls learning approximation of gradient components' $2^{\text{nd}}$ raw moments
- $(1 - \beta_1^t)$ and $(1 - \beta_2^t)$ compensate for initialization bias
- $\epsilon$ avoids devision by zero (let's ignore it in the following)

# Adam: Observations I

- $m_i^{(t+1)}$ and $v_i^{(t+1)}$ are exponential moving averages
- Assume that the mini-batch gradients $\boldsymbol{g}^{(t)}$ ($\boldsymbol{g}^{(t)}$ collects all $g_i^{(t)}$) are drawn from distributions $p^{(t)}$, i.e., $\boldsymbol{g}^{(t)} \sim p^{(t)}$
- Assume $g_i^{(t)}$ stationary ($p^{(t)} = p$, $t = 1, \dots$):
  - $\mathbb{E}\{\hat{m}_i^{(t+1)}\} = \mathbb{E}\{g_i\}$
  - $\mathbb{E}\{\hat{v}_i^{(t+1)}\} = \mathbb{E}\{g_i^2\}$
    (see slide "Adam: Initialization bias correction")
- Under the stationary assumption:

$$\sqrt{\mathbb{E}\{g_i^2\}} = \sqrt{\mathbb{E}\{|g_i|^2\}} \geq \sqrt{\mathbb{E}\{|g_i|\}^2} = \mathbb{E}\{|g_i|\} \geq \left|\mathbb{E}\{g_i\}\right|$$

# Adam: Observations II

- Assuming $g_i^{(t)}$ stationary, $(1-\beta_1) = \sqrt{1-\beta_2}$, and $\epsilon = 0$, we have
  - $\hat{m}_i^{(t+1)} / \sqrt{\hat{v}_i^{(t+1)}}$ approximates $\mathbb{E}\{g_i\} / \sqrt{\mathbb{E}\{g_i^2\}}$
  - $\left|\mathbb{E}\{g_i\} / \sqrt{\mathbb{E}\{g_i^2\}}\right| = \left|\mathbb{E}\{g_i\}\right| / \sqrt{\mathbb{E}\{g_i^2\}} \leq 1$
  - $\alpha$ upper bounds the steps (for $(1-\beta_1) \leq \sqrt{1-\beta_2}$)
- Observation: $\left|\mathbb{E}\{g_i\}\right|$ is upper bounded by $\mathbb{E}\{|g_i|\}$ and reaches this bound if all $g_i$ have the same signs (assuming that the signs are the only difference in the sampled $g_i$). The latter is the case if the steps for that weight go in the same direction – and accordingly the learning rate can be large.

# Adam: Initialization bias correction

- We have:

$$v_i^{(t+1)} = (1-\beta_2)\sum_{i=1}^{t}\beta_2^{t-i}\left(g_i^{(i)}\right)^2 = (1-\beta_2)\sum_{i=0}^{t-1}\beta_2^{t-i-1}\left(g_i^{(i+1)}\right)^2$$

Assume $\mathbb{E}\{\left(g_i^{(t)}\right)^2\}$ to be stationary and recall from geometric series that $\sum_{i=0}^{t-1}\alpha^i = (1-\alpha^t)/(1-\alpha)$:

$$\mathbb{E}\{v_i^{(t+1)}\} = \mathbb{E}\left\{(1-\beta_2)\sum_{i=0}^{t-1}\beta_2^{t-i-1}\left(g_i^{(i+1)}\right)^2\right\}$$

$$= \mathbb{E}\{\left(g_i\right)^2\}(1-\beta_2)\sum_{i=0}^{t-1}\beta_2^{t-i-1}$$

$$= \mathbb{E}\{\left(g_i\right)^2\}(1-\beta_2)\sum_{i=0}^{t-1}\beta_2^{i} = \mathbb{E}\{\left(g_i\right)^2\}(1-\beta_2^t)$$

# Outline

1 Neural Networks

2 Loss Functions and Encoding

3 Backpropagation & Gradient-based Learning

4 Regularization

# Weight-decay

- The smaller the weights, the "more linear" is the neural network function.
- Thus, small $\|\boldsymbol{w}\|$ corresponds to smooth functions.
- Therefore, one can penalize large weights by optimizing

$$E + \gamma \frac{1}{2} \|\boldsymbol{w}\|^2$$

  with regularization hyperparameter $\gamma \geq 0$.
- Note: the weights of linear output neurons should not be considered when computing the norm of the weight vector.

# Early stopping

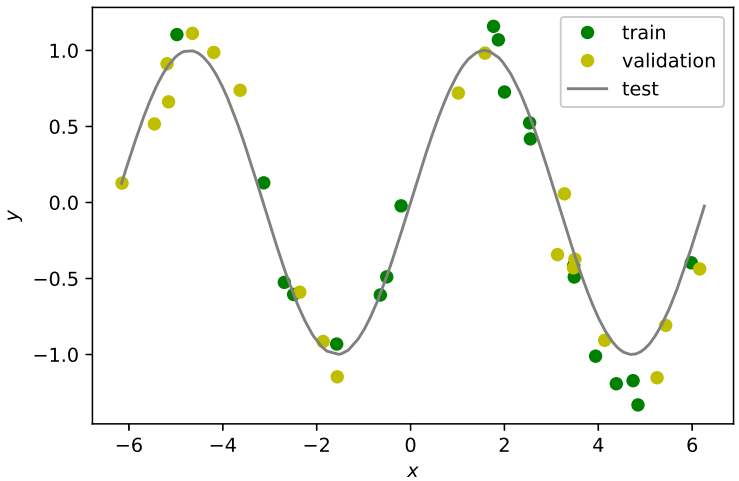
*Early-stopping*: the learning algorithm

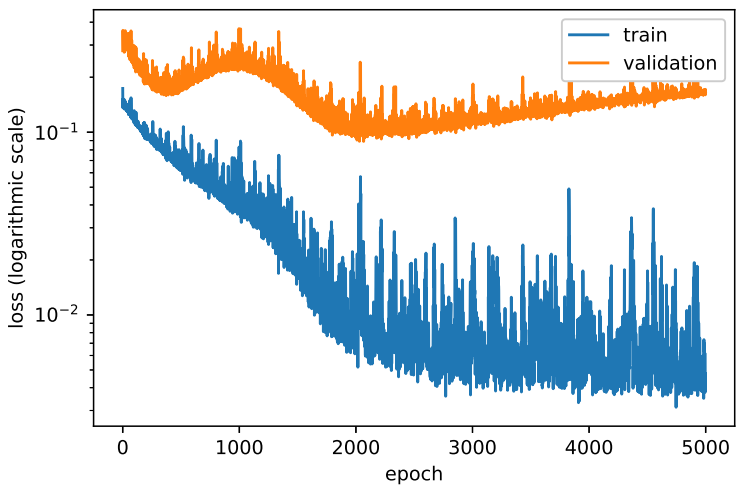
- partitions sample $S$ into training $S_{\text{train}}$ and validation $S_{\text{val}}$ data
- produces iteratively a sequence of hypotheses

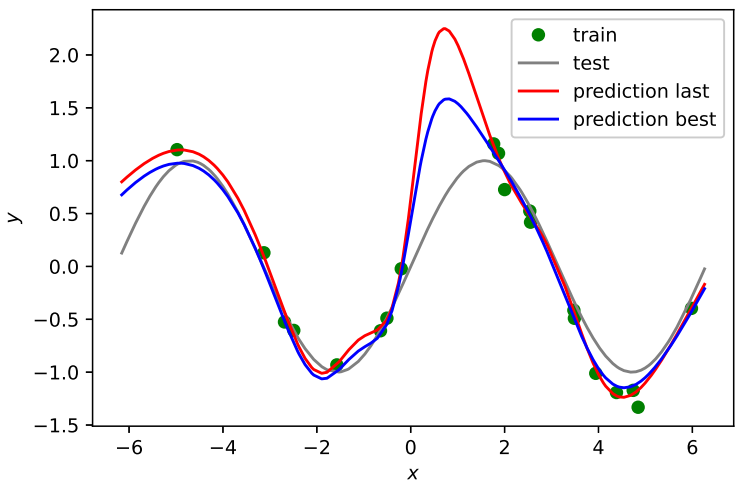
$$h_1, h_2, h_3, \ldots$$

  based on $S_{\text{train}}$
- monitors empirical risk $\mathcal{R}_{S_{\text{val}}}(h_i)$ on the validation data
- outputs the hypothesis $h_i$ minimizing $\mathcal{R}_{S_{\text{val}}}(h_i)$.

# Early stopping example



# The secrets of successful shallow NN training

- Normalize the data component-wise to zero-mean and unit variance
- Use a single layer with "enough neurons"
- Magnitude of the weights is more important for the complexity of a layer than number of neurons (assuming sigmoidal activation functions):
  - Start with small weights
  - Employ early stopping
- Try shortcuts