Neural Networks and Learning Systems
TBMI26 / 732A55
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Lecture 3

Supervised learning – Neural networks

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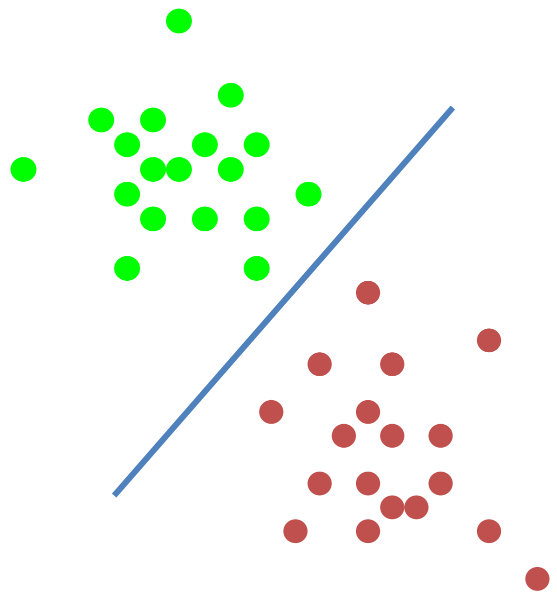
Recap - Supervised learning

- **Task:** Learn to predict/classify new data from labelled examples.
- **Input:** Training data examples $\{\mathbf{x}_i, y_i\}$ i=1...K, where $\mathbf{x}_i$ is a feature vector and y_i is a class label.
- **Output:** A function $f(\mathbf{x}; w_1,\ldots,w_N)$ that can predict the class label of $\mathbf{x}$.

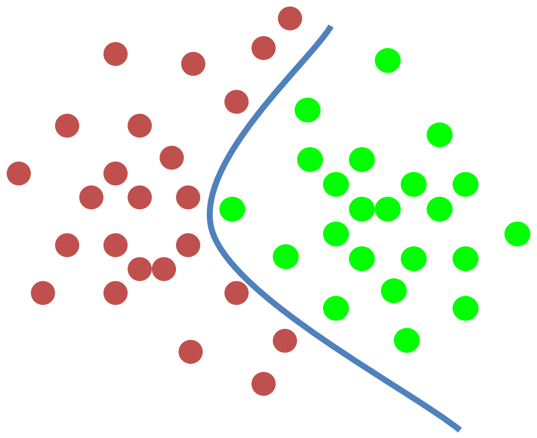
Find a function f and adjust the parameters $w_1,\ldots,w_N$ so that new feature vectors are classified correctly. Generalization!!

Linear separability

Linearly separable

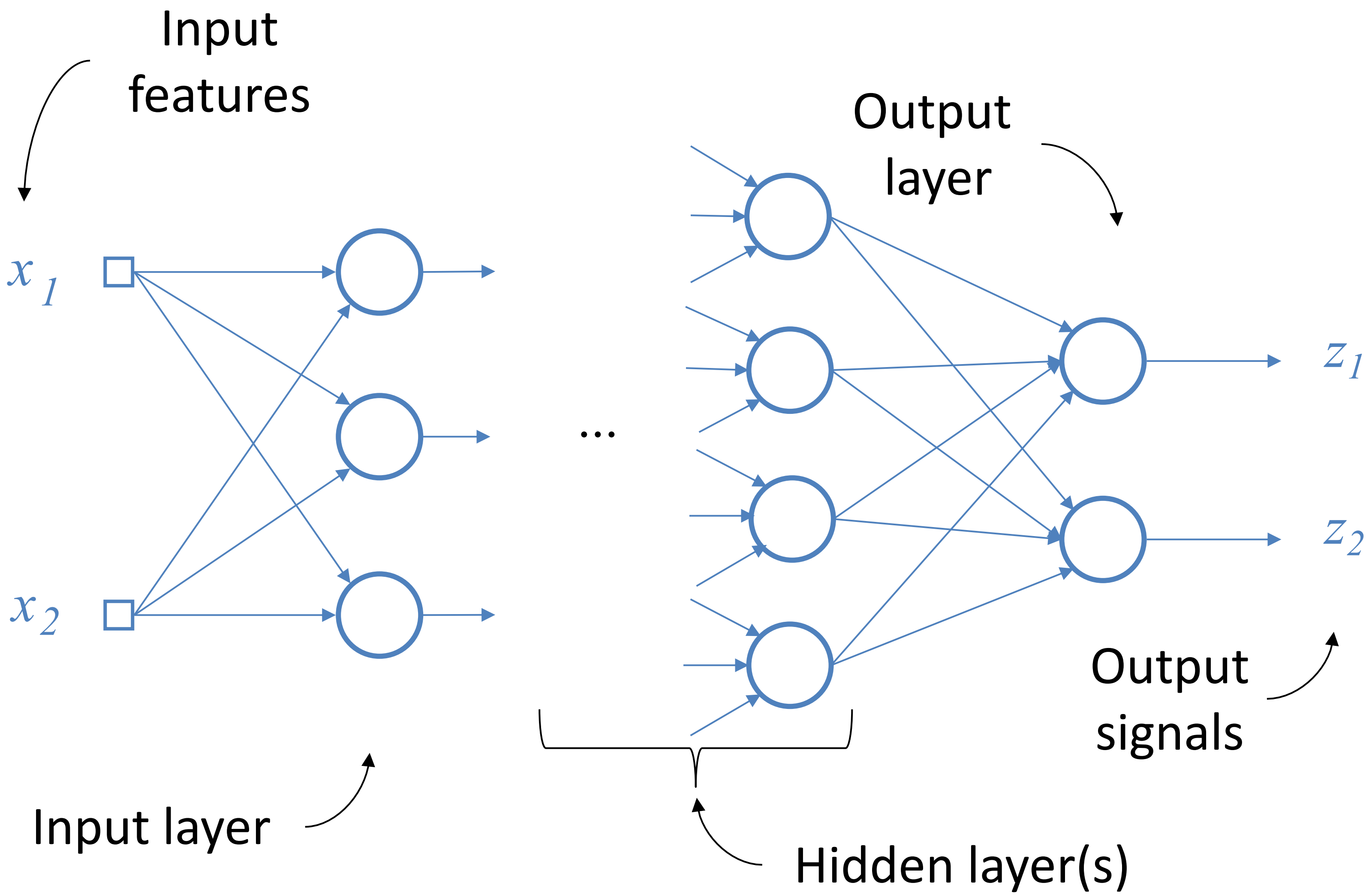


Non-linearly separable

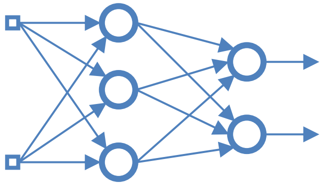


Neural Networks

a.k.a. the Multi-layer Perceptron



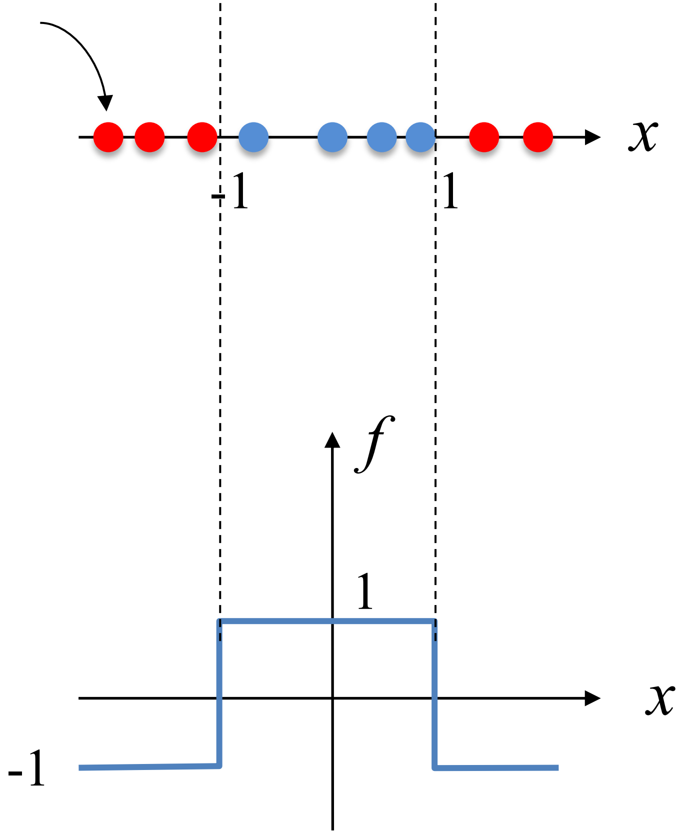
History of neural networks



- 1960’s: Large enthusiasm around the perceptron and “connectionism” (Frank Rosenblatt).
- 1969: Limitations of the perceptron pointed out in a paper by Minsky & Papert, e.g., the XOR problem.
- “Winter period” – little research
- 1980’s: Revival of connectionism and neural networks:
  - Multi-layer perceptrons can solve nonlinear problems (this was known before, but not how to train them!)
  - Back-propagation training algorithm
- 1990’s: Reduced interest, other methods seemed more promising
- 2010’s: Renewed interest – “Deep learning”

A simple 1D example

Training samples with only one feature value!

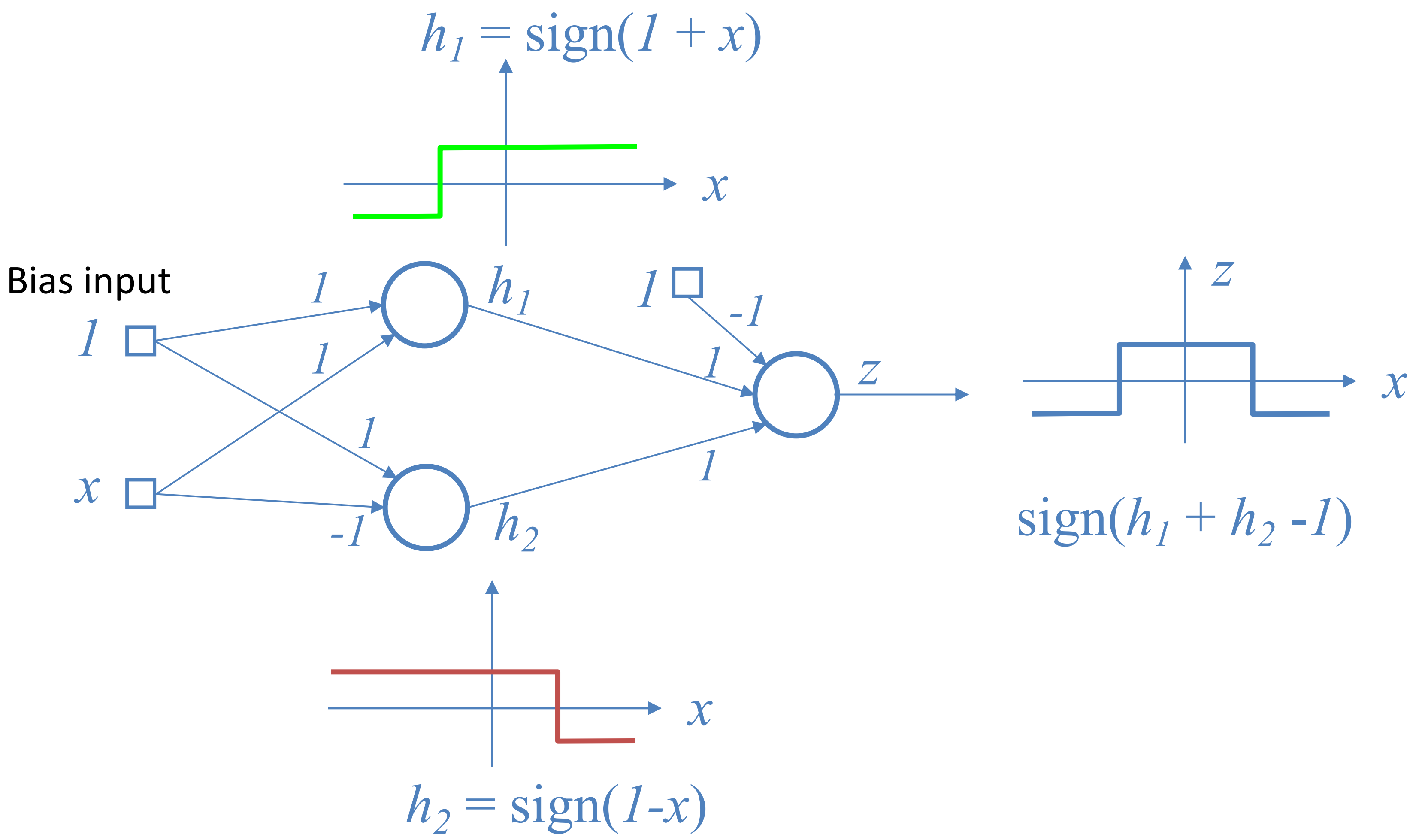


Not separable with a linear function!

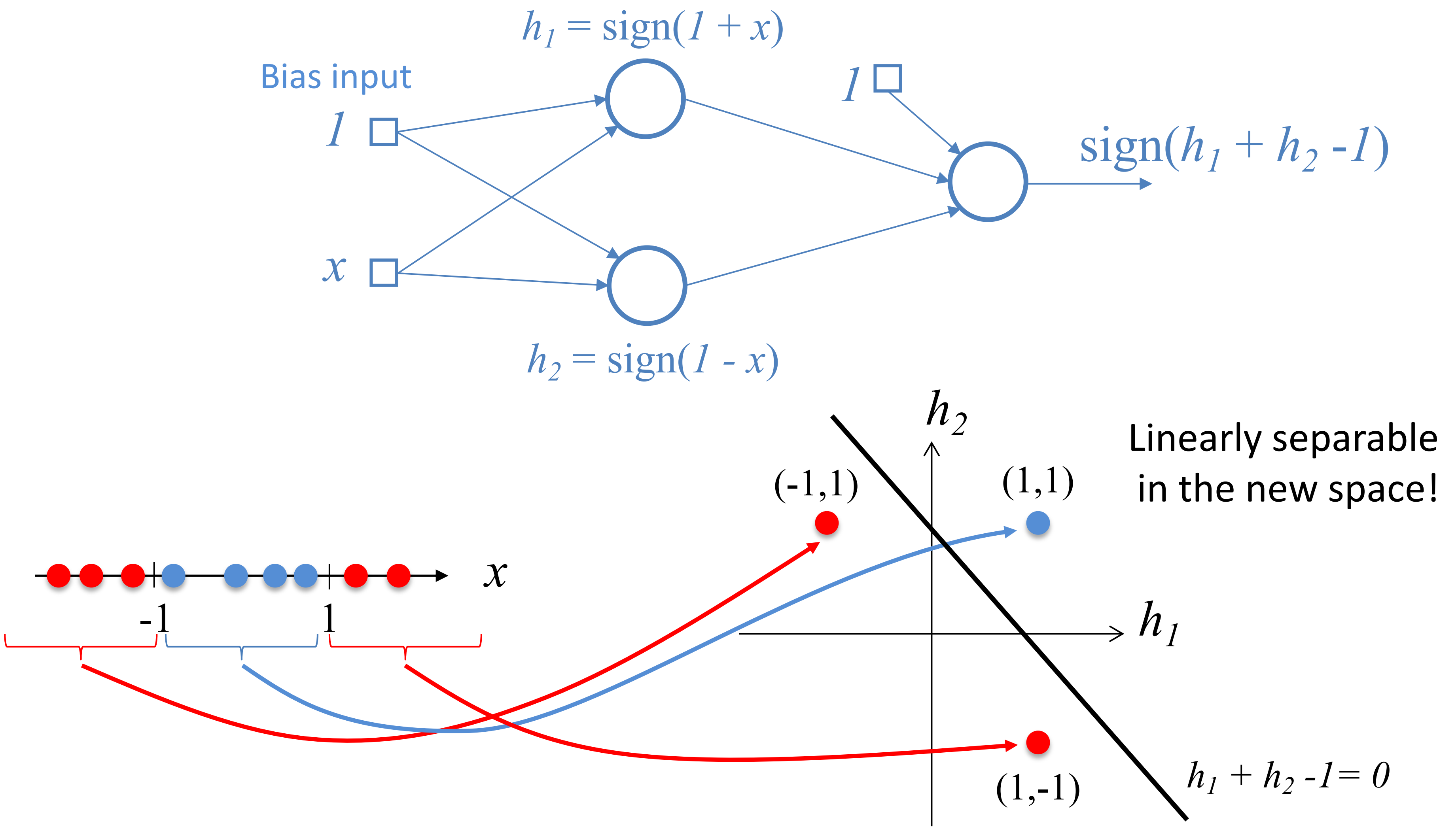
But with a nonlinear function!

$$f(x; w_0, \ldots, w_n) = \begin{cases} -1 & |x| > 1 \\ 1 & |x| < 1 \end{cases}$$

Example solution



Nonlinear mapping to a new feature space!

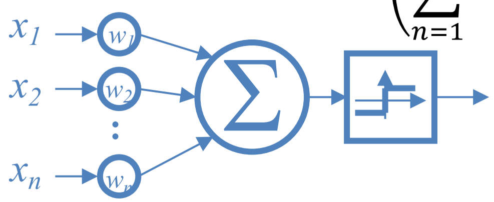


Key: The hidden layer(s)

- The output layer requires linear separability. The purpose of the hidden layers is to make the problem linearly separable!

- **Cover's theorem (1965):** The probability that classes are linearly separable increases when the features are nonlinearly mapped to a higher-dimensional feature space.

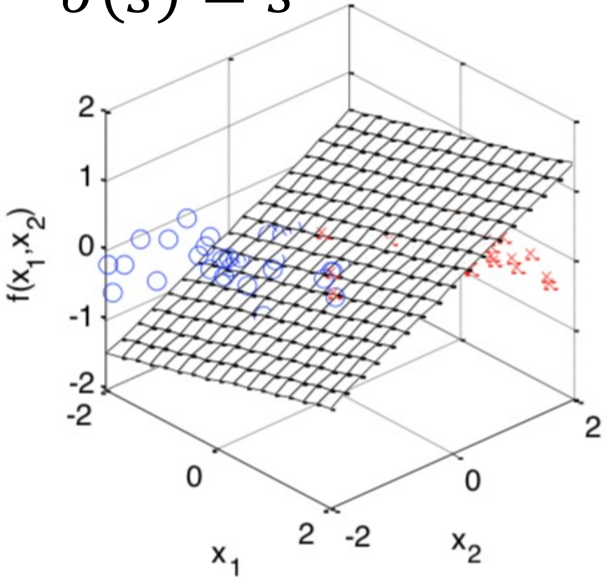
The Perceptron Revisited



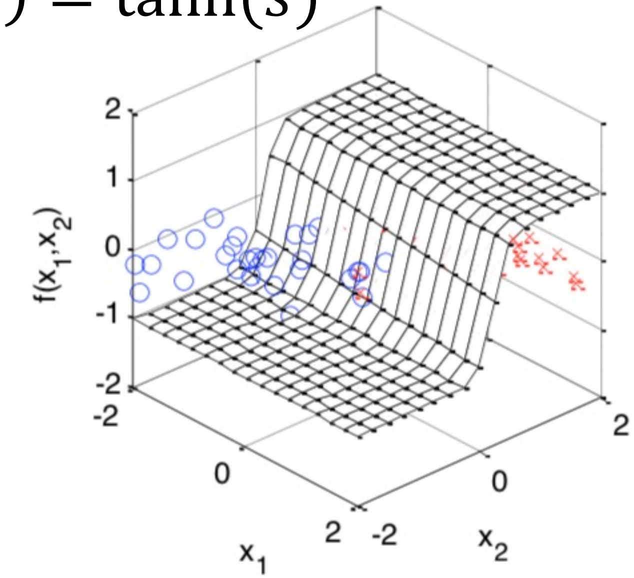
Minimize the following loss function:

$$\varepsilon(\mathbf{w}) = \underbrace{\sum_{k=1}^{K}}_{\text{\# training examples}} \left(\sigma\left(\underbrace{\sum_{n=1}^{N}}_{\text{\# inputs}} w_n x_{nk} - w_0\right) - y_k\right)^2$$

$\sigma(s) = s$

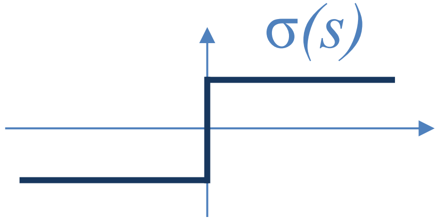


$\sigma(s) = \tanh(s)$



Some nonlinear activation functions

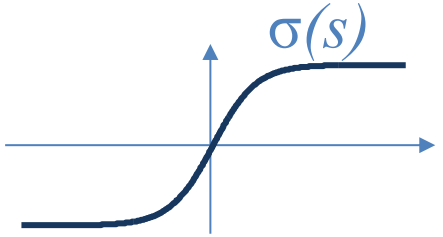
- Step/sign function



Not differentiable – cannot be optimized!
(by gradient search)

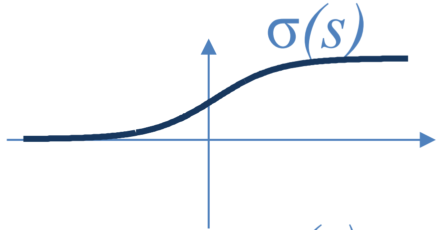
- Hyperbolic tangent

$$\sigma(s) = \tanh(s) \quad \sigma' = 1 - \tanh^2(s) = 1 - \sigma^2$$



- The Fermi-function

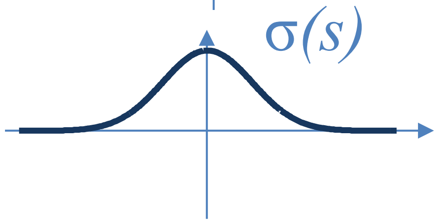
$$\sigma(s) = \frac{1}{1+e^{-s}} \quad \sigma' = \sigma(1-\sigma)$$



Sigmoid functions

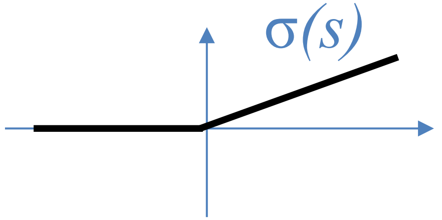
- Gaussian function

$$\sigma(s;\gamma) = e^{-\frac{s^2}{\gamma^2}} \quad \sigma'(s;\gamma) = -\frac{2s}{\gamma}\sigma$$



- Rectifying Linear Unit (ReLU)

$$\sigma(s) = \max(0, s) \quad \sigma' = \begin{cases} 0, & s < 0 \\ 1, & s \geq 0 \end{cases}$$

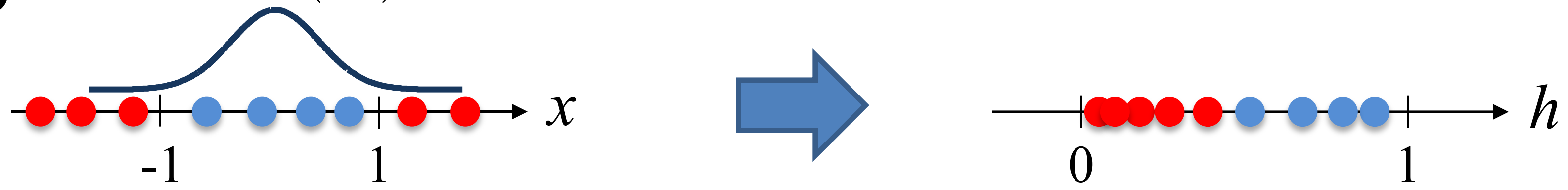


Example - Radial Basis Functions

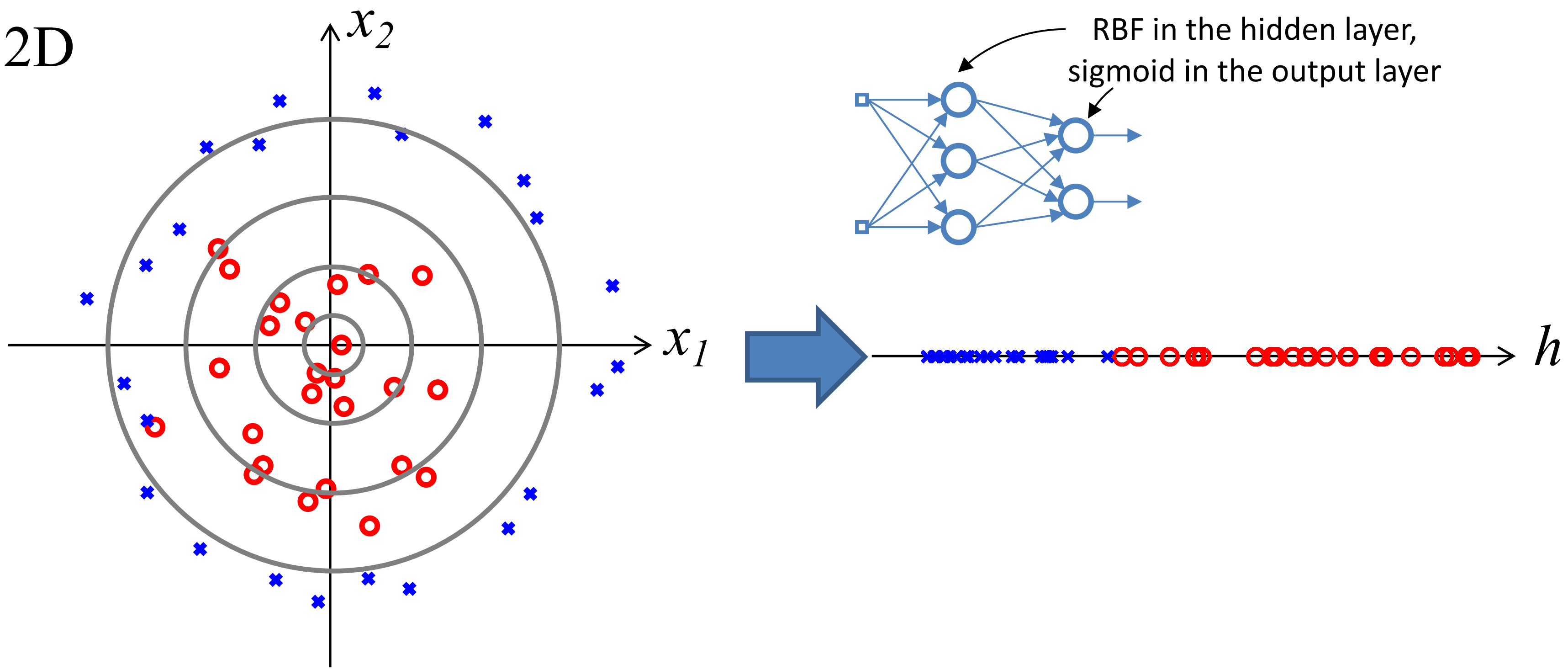
For example a Gaussian

1D

$h = \sigma(\|\mathbf{x}\|)$

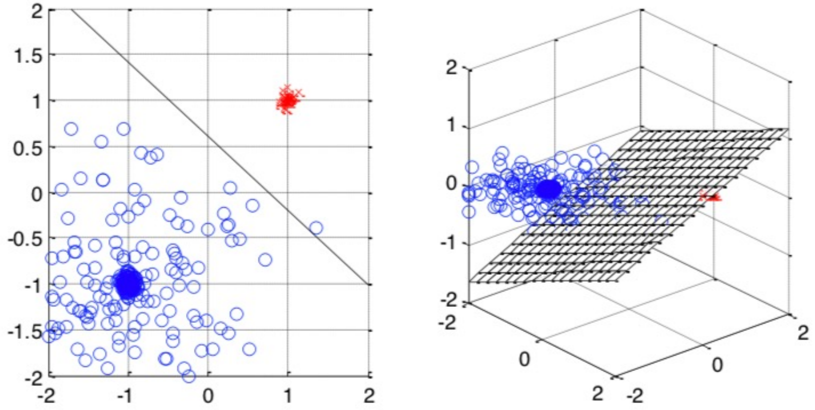


2D



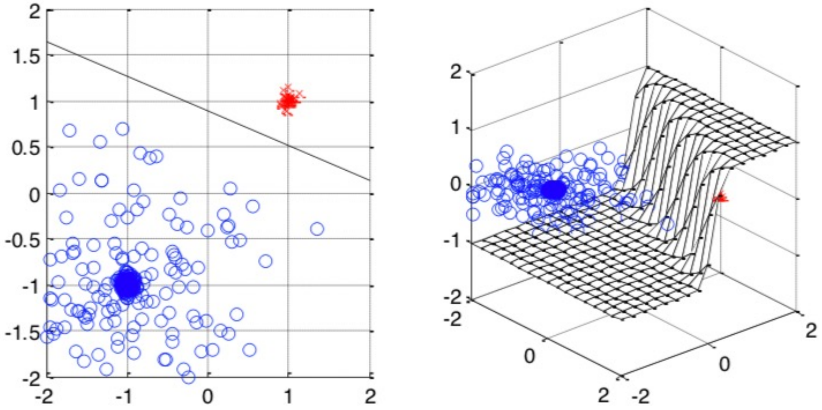
Example - tanh

$$\sigma(s) = s$$



Same as in lecture 2!

$$\sigma(s) = \tanh(s)$$



Updated optimization algorithm

$$\varepsilon(\mathbf{w}) = \sum_{k=1}^{K}\left(\sigma\left(\sum_{n=1}^{N} w_n x_{nk} - w_0\right) - y_k\right)^2$$

$$\frac{\partial\varepsilon}{\partial w_i} = 2\sum_{k=1}^{K}\left(\sigma\left(\sum_{n=1}^{N} w_n x_{nk} - w_0\right) - y_k\right)\sigma'\left(\sum_{n=1}^{N} w_n x_{nk} - w_0\right)x_{ik}$$

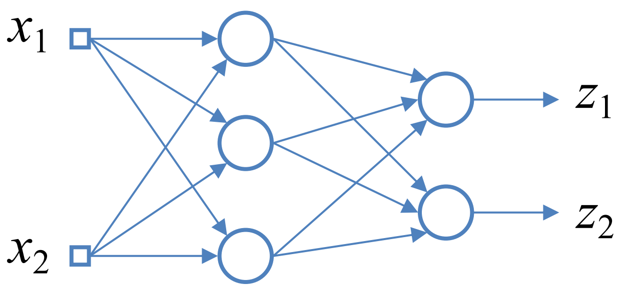
Gradient descent:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta\frac{\partial\varepsilon}{\partial\mathbf{w}} \quad (\text{Eq.}1)$$

Algorithm:

1. Start with a random **w**
2. Iterate Eq. 1 until convergence

Training multi-layer neural networks



Loss function

\# training examples   # output nodes

$$\varepsilon(\mathbf{w}) = \sum_{k=1}^{K} \sum_{m=1}^{M} \left[y_{mk} - z_{mk}(\mathbf{w}) \right]^2$$

all weights   desired output   actual output

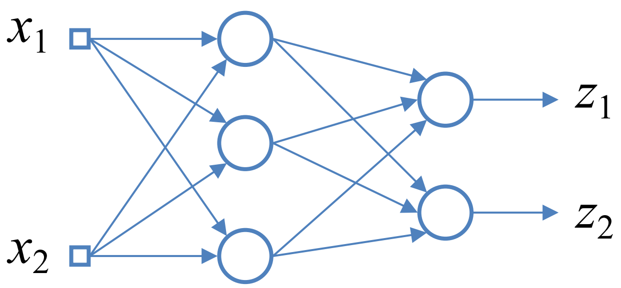
Stochastic gradient descent

Update using one (K=1) training example

$$\varepsilon(\mathbf{w}) = \sum_{m=1}^{M} \left[y_m - z_m(\mathbf{w}) \right]^2$$

$$w_{ij}^{t+1} = w_{ij}^{t} - \eta \frac{\partial \varepsilon}{\partial w_{ij}}$$

From node i to node j
in a layer



The chain rule

$$f(g(x)) \qquad\qquad f(g(x),h(x))$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x} \qquad\qquad \frac{\partial f}{\partial x} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial x} + \frac{\partial f}{\partial h}\frac{\partial h}{\partial x}$$

Example:

$$f(x;w) = \sigma(\underbrace{wx}_{s}) \rightarrow \frac{\partial f}{\partial w} = \frac{\partial f}{\partial s}\frac{\partial s}{\partial w} = \sigma'(x,w)\cdot x$$

Note that the activation function σ must be differentiable. This is why the step function does not work with back propagation!

Automatic Differentiation

- Any algorithm that is defined by a sequence of arithmetic operations can be automatically differentiated by repeatedly applying the chain rule!
- This is the basis for error back propagation

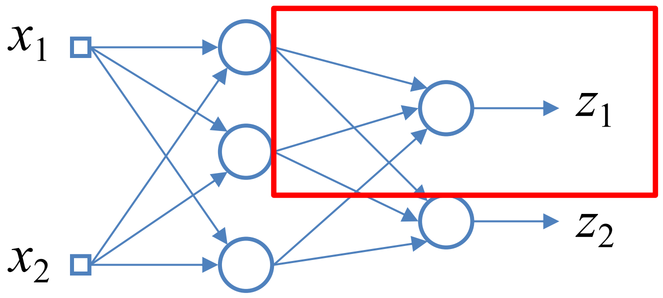
- (Note that this is different from numeric and analytical differentiation)

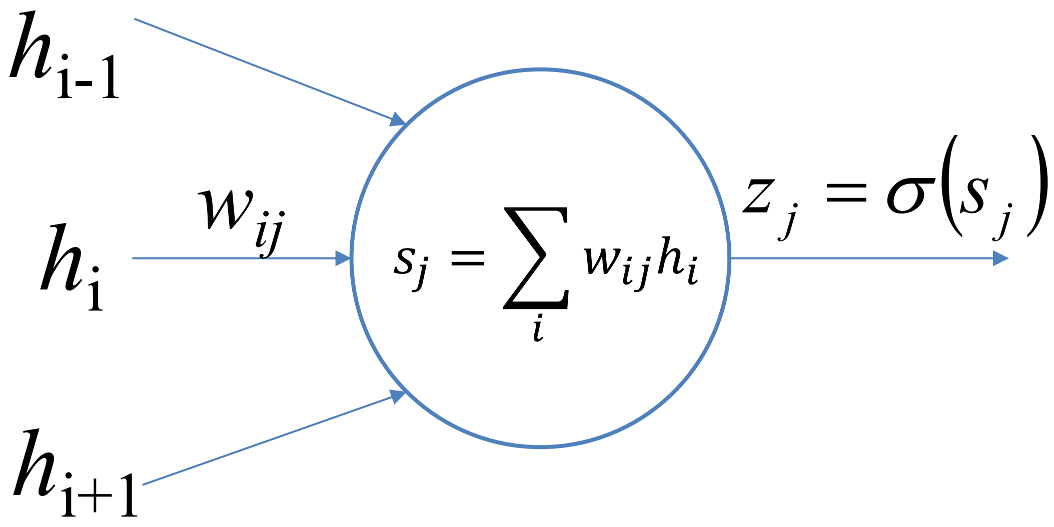
The error back propagation algorithm

- an exercise of the chain rule!

$$\frac{\partial \varepsilon}{\partial w_{ij}} = \frac{\partial \varepsilon}{\partial z_j}\frac{\partial z_j}{\partial w_{ij}} = \frac{\partial \varepsilon}{\partial z_j}\frac{\partial z_j}{\partial s_j}\frac{\partial s_j}{\partial w_{ij}}$$

$$\varepsilon(\mathbf{w}) = \sum_{m=1}^{M}\left[y_m - z_m(\mathbf{w})\right]^2$$





Back propagation, cont.

$$\varepsilon(\mathbf{w}) = \sum_{m=1}^{M}\left[y_m - z_m(\mathbf{w})\right]^2 \qquad \frac{\partial \varepsilon}{\partial w_{ij}} = \frac{\partial \varepsilon}{\partial z_j}\frac{\partial z_j}{\partial s_j}\frac{\partial s_j}{\partial w_{ij}}$$

$$\frac{\partial \varepsilon}{\partial z_j} = -2\left(y_j - z_j\right)$$

$$\frac{\partial z_j}{\partial s_j} = \sigma'\left(s_j\right) = 1 - \sigma\left(s_j\right)^2 = 1 - z_j^2$$

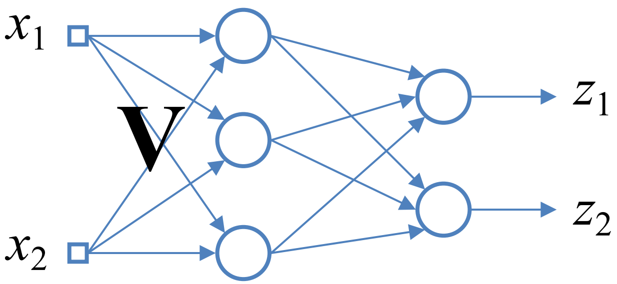
If $\sigma(s) = \tanh(s)$ is used!

$$\frac{\partial s_j}{\partial w_{ij}} = h_i$$

(input i to unit j)

Updating the hidden layer(s)

$$\frac{\partial \varepsilon}{\partial v_{ij}} = ?$$



$$\varepsilon(\mathbf{v}) = \sum_{m=1}^{M} \left[y_m - z_m(\mathbf{v}) \right]^2$$

A weight in a hidden layer affects **all** output nodes!

$$\varepsilon\left(z_1(\mathbf{v}), \ldots, z_M(\mathbf{v})\right)$$

$$\frac{\partial \varepsilon}{\partial v_{ij}} = \sum_{k=1}^{M} \frac{\partial \varepsilon}{\partial z_k} \frac{\partial z_k}{\partial v_{ij}} = \ldots. \quad \text{Exercise!}$$

Chain rule! Continue expanding!

Back propagation – Summary

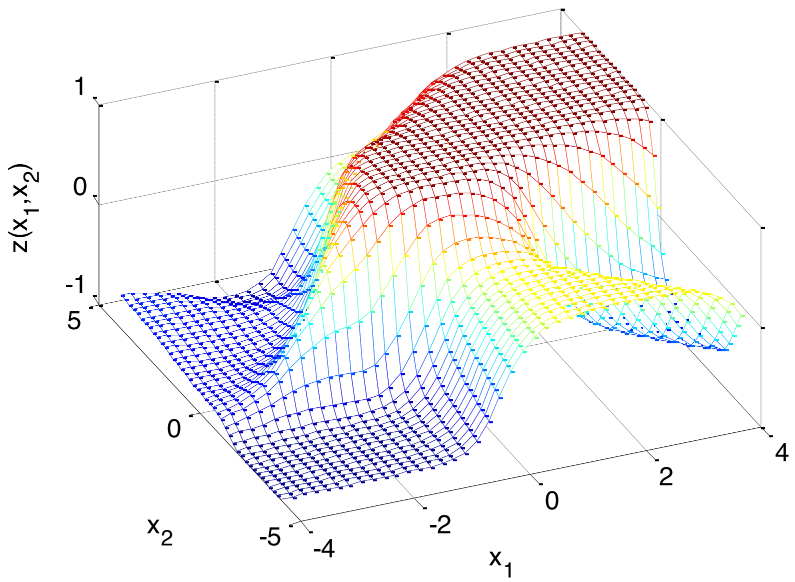
- Two phases:
  - Forward propagation: Propagate a training example through the network
  - Backward propagation: Propagate the error relative to the desired output backwards in the net and update parameter weights.
- Batch update: update after all examples have been presented.

$$\Delta w_{ij} = -\eta \sum_{k=1}^{K} \frac{\partial \varepsilon(k)}{\partial w_{ij}}$$

Decision boundaries

Neural networks can produce
very complex class boundaries!

$$z(x_1, x_2)$$



$$f(x_1, x_2) = sign(z(x_1, x_2))$$

What about more than 2 classes?

Multiple outputs each representing likelihood for a certain class

Softmax

$$\sigma(\mathbf{z})_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$$

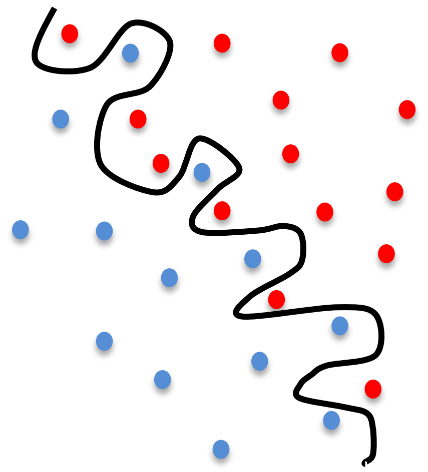
- Normalized exponential function
- Gives a vector $\mathbf{z}$ where the components' sum is one
- Enables the components of $\mathbf{z}$ to interpreted as probabilities
- Smooth version of the *argmax* function

Pros and cons of neural networks

- A multi-layer neural network can learn any class boundaries.
- The large number of parameters is a problem:
  - Local optima → suboptimal performance
  - Overfitting → poor generalization
  - Slow convergence → long training times

Overfitting

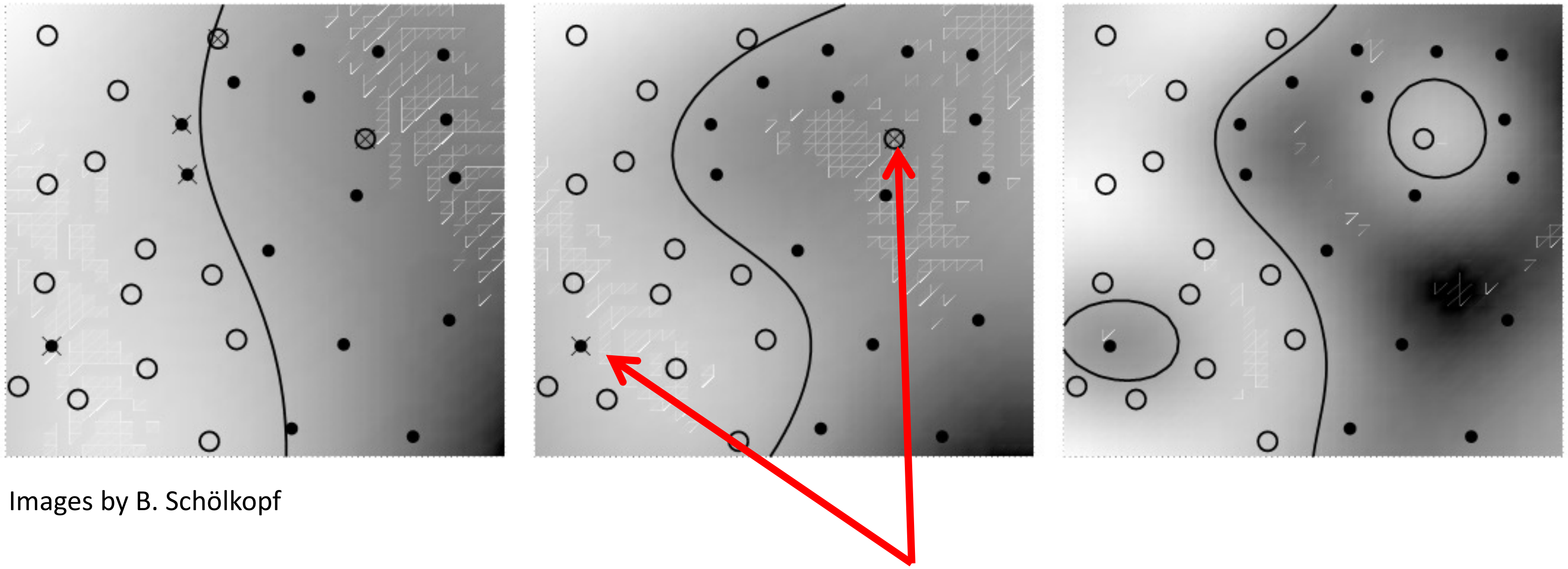
- The large number of parameters makes it possible to produce overly complicated boundaries.



- A too good fit to the training data can perform poorly for new cases, i.e. worse generalization properties!

Overfitting – Example

Increasing classifier flexibility

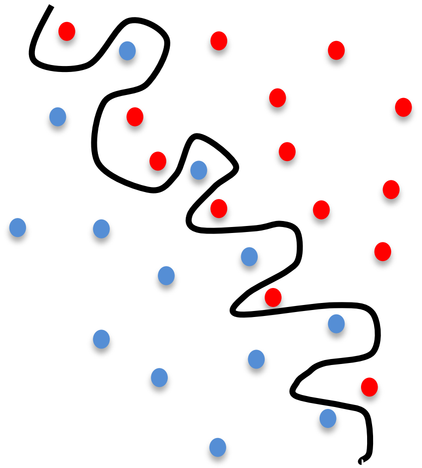


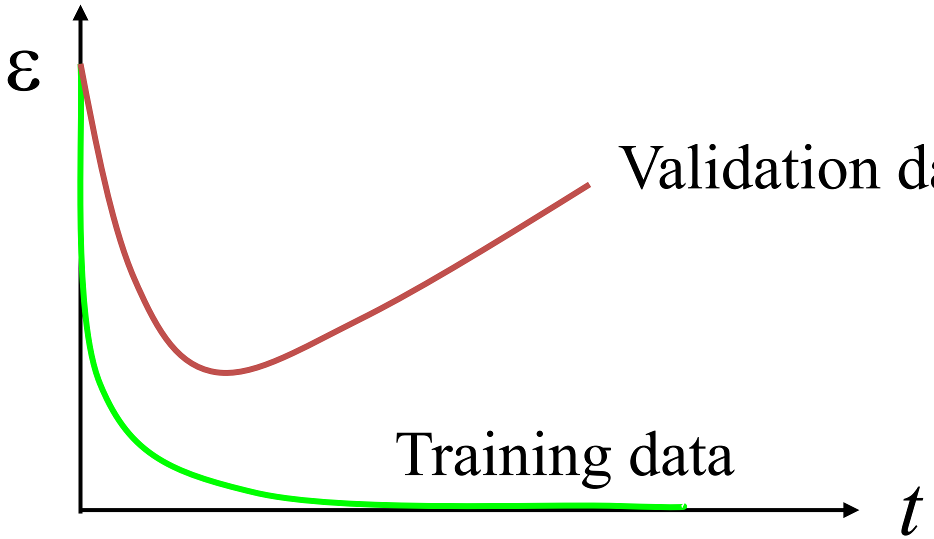
Images by B. Schölkopf

Outliers/incorrect labels?

Over-fitting

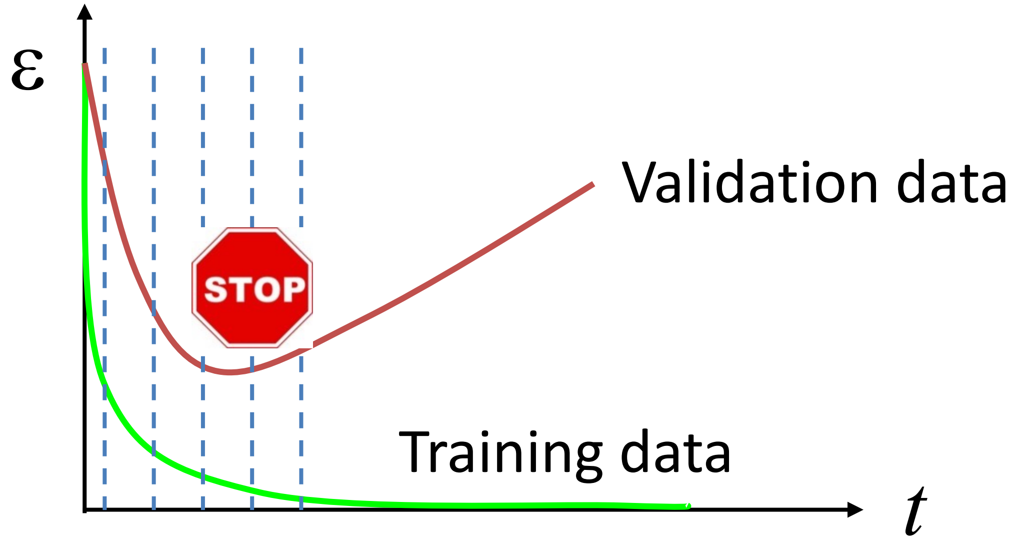
- The error on training data *always* decreases with increased training
- The error on validation data (the generalization error) decreases in the beginning, but can then start to increase if over-fitting occurs!





Preventing overfitting in neural networks

- **Early stopping:**
  Pause training regularly and calculate the performance on the validation data.
- Caution: Validation data becomes training data! Will bias evaluation.
- That's why we need a third dataset for testing – the test data



Training – Validation –Testing