Neural Networks and Learning Systems
TBMI26 / 732A55
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Lecture 3

Supervised learning – Neural networks

Magnus Borga
magnus.borga@liu.se

Recap - Supervised learning

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

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

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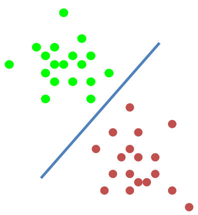
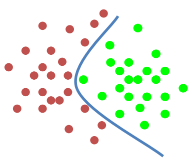
Linear separability

Linearly separable



Non-linearly separable



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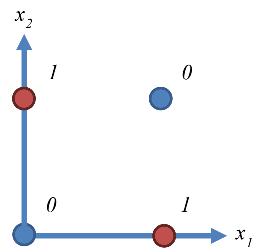
The XOR problem

x_1	x_2	f
0	0	0
0	1	1
1	0	1
1	1	0



Not linearly separable!

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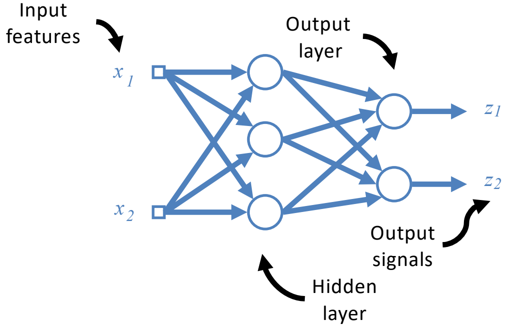
Multi-layer perceptron

a.k.a Neural Network



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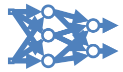
History of neural networks



- 1960's: Large enthusiasm around the perceptron and "connectionism" (Frank Rosenblatt).
- 1969: Limitations of the perceptron made clear 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 networks 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"

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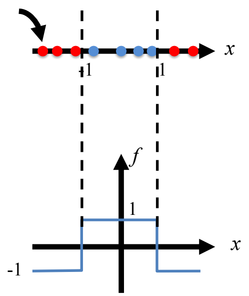
A simple 1D example

Training samples with only one feature value!



Not separable with a linear function!

But with a nonlinear function!

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

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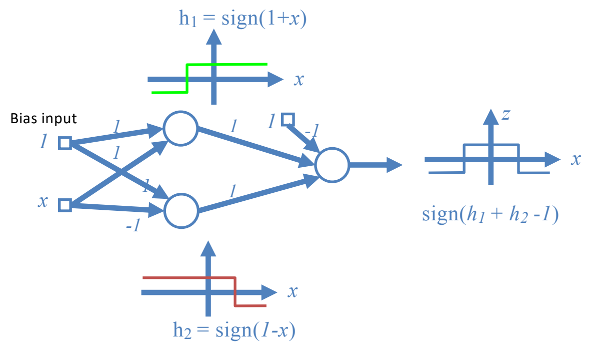
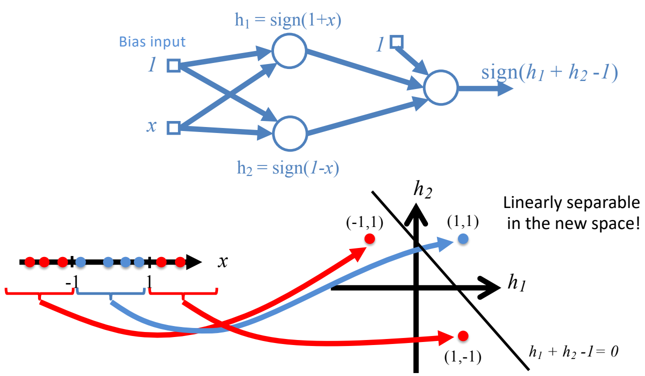
Example solution



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.

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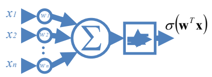
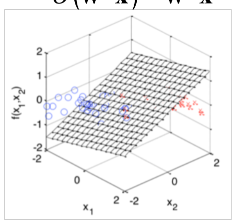
The Perceptron Revisited



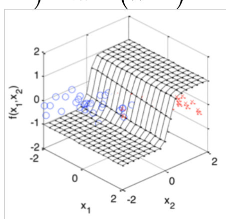
Minimize the following cost function

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\sigma(\mathbf{w}^T\mathbf{x}_i) - y_i\right)^2$$

$$\sigma(\mathbf{w}^T\mathbf{x}) = \mathbf{w}^T\mathbf{x}$$



$$\sigma(\mathbf{w}^T\mathbf{x}) = \tanh(\mathbf{w}^T\mathbf{x})$$



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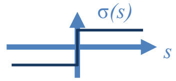
Nonlinear activation functions

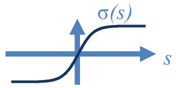
- Step/sign function

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



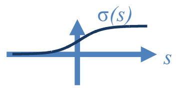
- Hyperbolic tangent

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



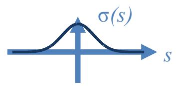
- The Fermi-function

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



- Gaussian function

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



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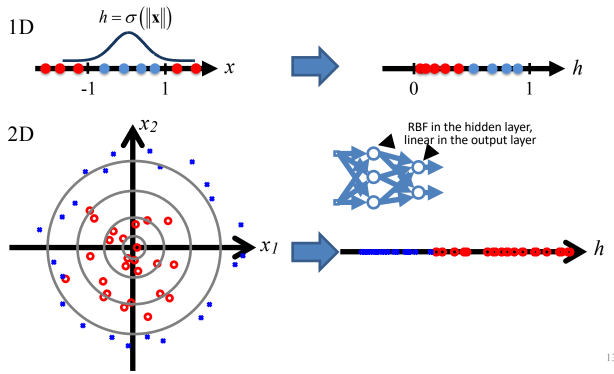
Example - Radial Basis Functions

For example a Gaussian



Updated minimization algorithm

$$\varepsilon(\mathbf{w}) = \sum_{i=1}^{N} \left(\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i \right)^2$$

$$\frac{\partial \varepsilon}{\partial \mathbf{w}} = 2 \sum_{i=1}^{N} \left(\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i \right) \sigma'(\mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i$$

Gradient descent:

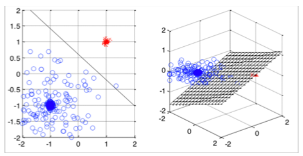
$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta \frac{\partial \varepsilon}{\partial \mathbf{w}} \quad \text{(Eq.1)}$$

Algorithm:

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

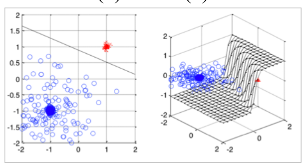
Example

$\sigma(s) = s$

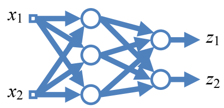


Same as in lecture 2!

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



Training multi-layer neural networks



Cost 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

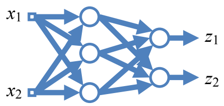
Stochastic gradient descent

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



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The chain rule

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

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

Examples:

$$f(x) = \sin(x^2) \qquad \frac{\partial f}{\partial x} = \cos(x^2)2x$$

$$f(x) = x^2 \sin(x) \qquad \frac{\partial f}{\partial x} = 2x\sin(x) + x^2\cos(x)$$

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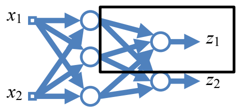
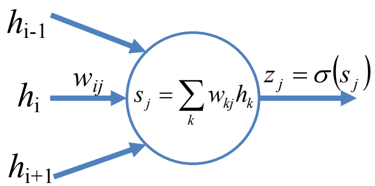
The error back propagation algorithm

\- an exercise of the chain rule!

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

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





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Back propagation, cont.

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

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

$$\frac{\partial z_j}{\partial s_j} = \sigma'(s_j) = 1 - \sigma(s_j)^2 = 1 - z_j^2$$ If σ(s) = tanh(s) is used!

$$\frac{\partial s_j}{\partial w_{ij}} = h_i$$ (input *i* to unit *j*)

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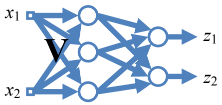
Updating the hidden layer

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



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

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

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

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

Chain rule! Continue expanding!

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Back propagation – Summary

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

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

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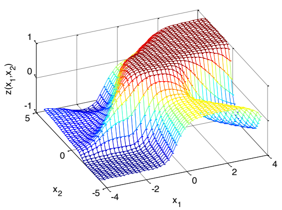
Decision boundaries

Neural networks can produce very complex class boundaries!

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



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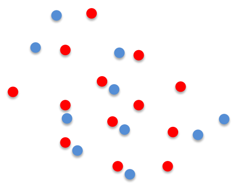
Reminder - Magic is not possible!

No neural network, however complex, can separate inseparable classes!



Finding and extracting suitable features are the critical problems in machine learning!

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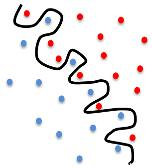
Pros and cons of neural networks

- 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

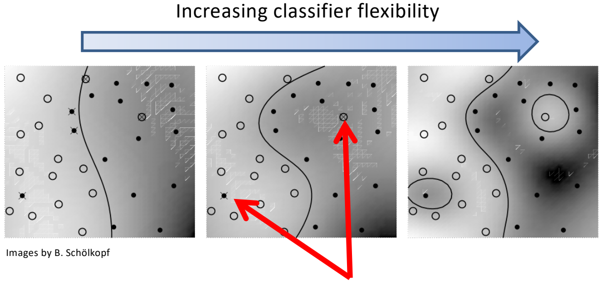
Overfitting

- 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!

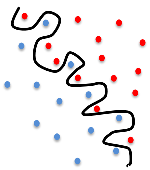
Example

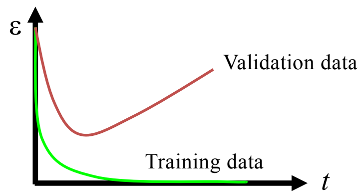


Images by B. Schölkopf

Over-fitting

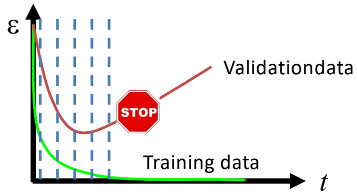
- The error on training data *always* decreases with increased training
- The error on validation data (the generalization error) decreases in the beginning, but can then start to increase if over-fitting occurs!





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



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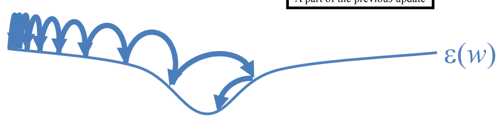
Faster convergence

- Normalize input features, e.g. to the range [-1,1].
- Separate and adaptive step length η for each weight:
  - If the derivative has the same sign in several consecutive steps, η should increase. If the derivative change sign, η should decrease.
- Introduce a *momentum term*:

$$\Delta w_{ji}(t) = \underbrace{\alpha \Delta w_{ji}(t-1)}_{\boxed{\text{A part of the previous update}}} - \eta \frac{\partial \varepsilon(t)}{\partial w_{ji}}$$



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How many layers?

- 1 hidden layer is enough to produce any classification boundary.
- Complex boundaries more compactly obtained with many non-linear layers - less nodes in total compared to 1-layer solution.
- With ordinary 'backprop' training, no performance advantage with many hidden layers.
  - Vanishing gradient problem: Error gradients become very small for early layers in the network → weights are not updated.

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