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# INF3490 - Biologically inspired computing

## Lecture 28th September 2016

Multi-Layer Neural Networks

Kai Olav Ellefsen

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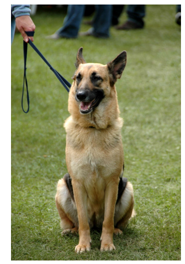
## Classification



Trained Classifier → "DOG"

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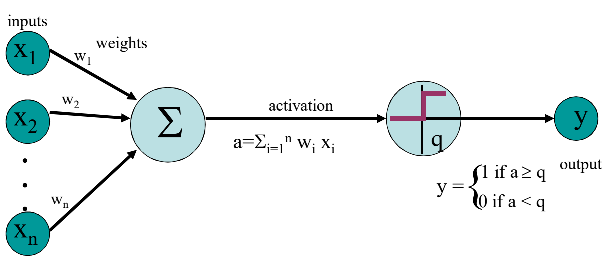
## Perceptron

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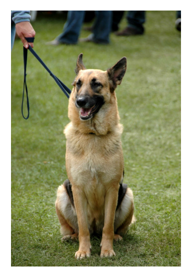
## Training a classifier (supervised learning)



Untrained Classifier → "CAT"

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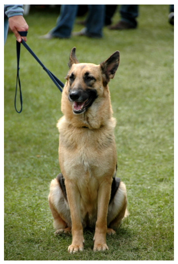
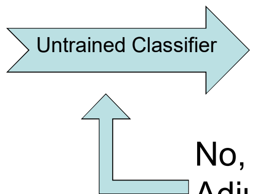
## Training a classifier (supervised learning)






“CAT”

No, it was a dog.
Adjust classifier parameters

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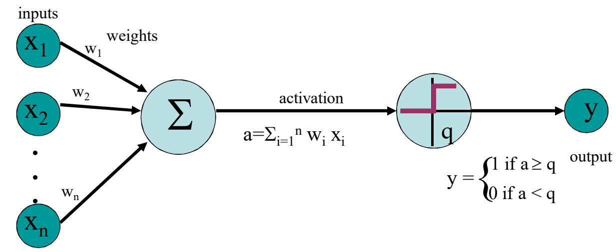
## Training a perceptron




Learning rate　　　Input

$$\Delta w_{ij} = \eta \cdot (t_j - y_j) \cdot x_i$$

Desired output　　　Actual output

Error



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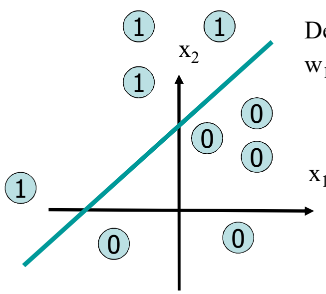
## Decision Surface




Decision line
$w_1 x_1 + w_2 x_2 = q$



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## A Quick Overview

- Linear Models are easy to understand.
- However, they are very simple.
  - They can only identify flat decision boundaries (straight lines, planes, hyperplanes, ...).
- ***Majority of interesting data are not linearly separable. Then?***

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## A Quick Overview

- ***Learning*** in the neural networks (NN) happens in the weights.
- **Weights** are associated with connections.
- Thus, it is sensible to add more connections to perform more complex computations.
- Two ways for non-lin. separation (not exclusive):
  - ***Recurrent Network***: connect the output neurons to the inputs with feedback connections.
  - ***Multi-layer perceptron network***: add neurons between the input nodes and the outputs.



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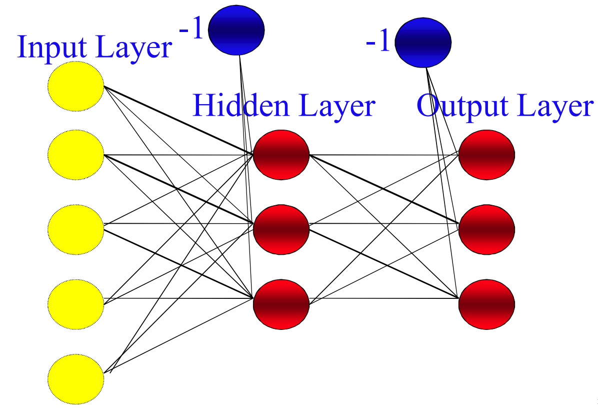
## Multi-Layer Perceptron (MLP)



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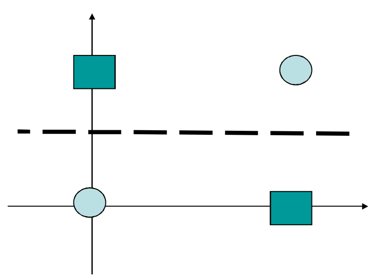
## XOR Problem



**XOR (Exclusive OR) Problem**

| A | B | Out |
|---|---|---|
| 0 | 0 | 0 |
| 0 | 1 | 1 |
| 1 | 0 | 1 |
| 1 | 1 | 0 |

*Perceptron does not work here.*

Single layer generates a linear decision boundary.



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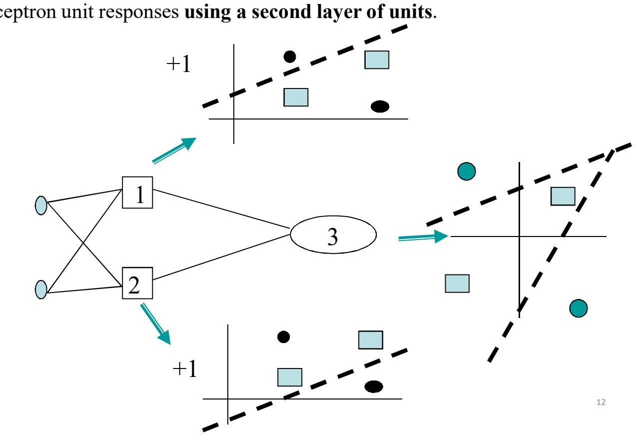
## Solution for XOR : Add a Hidden Layer !!

Minsky & Papert (1969) offered **solution to XOR problem** by combining perceptron unit responses **using a second layer of units**.



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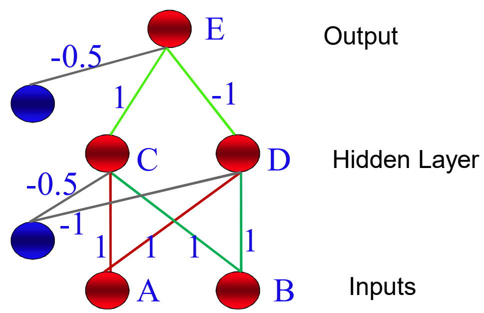
## XOR Again



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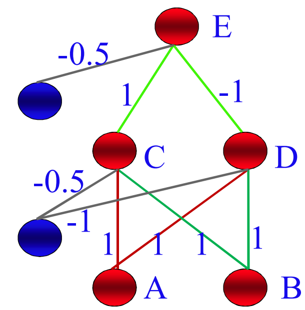
## XOR Again

| A | B | $C_{in}$ | $C_{out}$ | $D_{in}$ | $D_{out}$ | $E_{in}$ |
|---|---|---|---|---|---|---|
| 0 | 0 | -0.5 | 0 | -1 | 0 | -0.5 |
| 0 | 1 | 0.5 | 1 | 0 | 0 | 0.5 |
| 1 | 0 | 0.5 | 1 | 0 | 0 | 0.5 |
| 1 | 1 | 1.5 | 1 | 1 | 1 | -0.5 |

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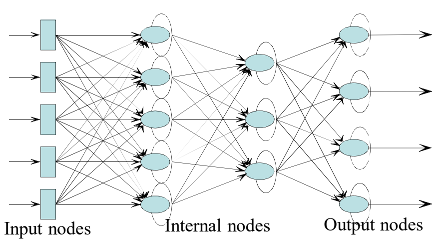
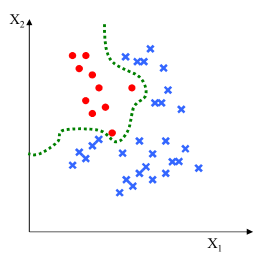
## MLP Decision Boundary – Nonlinear Problems, Solved!

In contrast to perceptrons, multilayer networks can learn not only multiple decision boundaries, but the boundaries may also be nonlinear.



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## Multilayer Network Structure

- A neural network with one or ***more*** layers of ***nodes*** between the input and the output nodes is called ***multilayer network***.
- The multilayer *network structure*, or *architecture*, or *topology*, consists of ***an input layer***, ***one or more hidden layers***, and ***one output layer***.
- The input nodes pass values to the first hidden layer, its nodes to the second and so until producing outputs.
    - A network with a layer of input units, a layer of hidden units and a layer of output units is a ***two-layer network***.
    - A network with two layers of hidden units is a ***three-layer network***, and so on.

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## Properties of the Multi-Layer Perceptron

- No connections within a single layer.
- No direct connections between input and output layers.
- Fully connected; all nodes in one layer connect to all nodes in the next layer.
- Number of output units need not equal number of input units.
- Number of hidden units per layer can be more or less than input or output units.

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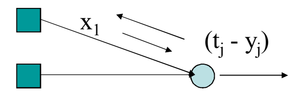
## How to Train MLP?

- How we can train the network, so that
  - The weights are adapted to generate correct (target answer)?




- In Perceptron, errors are computed at the output.
- In MLP,
  - Don't know which weights are wrong:
  - Don't know the correct activations for the neurons in the hidden layers.



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## Then…

**The problem is**: ***How to train Multi Layer Perceptrons??***

**Solution**: Backpropagation Algorithm (Rumelhart and colleagues,1986)



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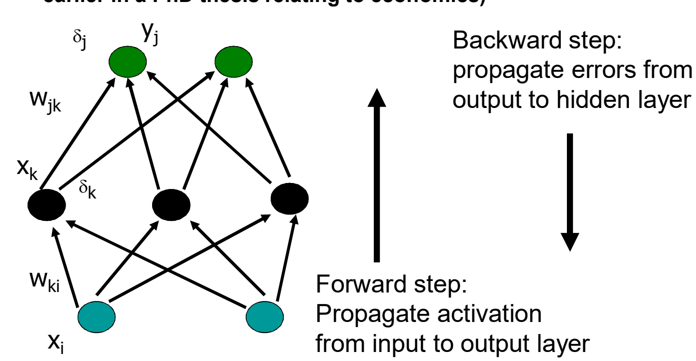
## Backpropagation

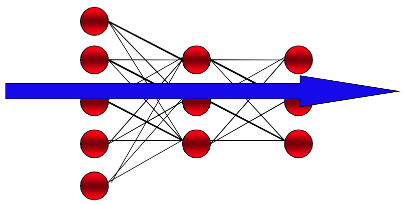
***Rumelhart, Hinton and Williams (1986)*** **(though actually invented earlier in a PhD thesis relating to economics)**



## Training MLPs

**Forward Pass**

1. Put the input values in the input layer.
2. Calculate the activations of the hidden nodes.
3. Calculate the activations of the output nodes.



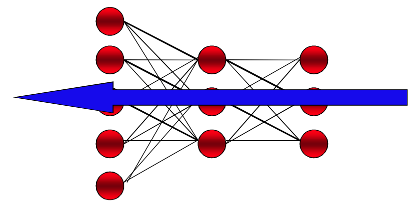




## Training MLPs

**Backward Pass**

1. Calculate the output errors
2. Update last layer of weights.
3. Propagate error backward, update hidden weights.
4. Until first layer is reached.







## Error Function

- Single scalar function for entire network.
- Parameterized by weights (objects of interest).
- Multiple errors of different signs should not cancel out.
- ***Sum-of-squares error:***

$$E(\mathbf{w}) = \frac{1}{2}\sum_k (t_k - y_k)^2 = \frac{1}{2}\sum_k \left(t_k - \sum_i w_{ik}x_i\right)^2$$





## Back Propagation Algorithm

- The backpropagation training algorithm uses the ***gradient descent*** technique to **minimize the *mean square difference*** between the desired and actual outputs.
- The network is trained initially selecting ***small random weights*** and then presenting all training data incrementally.
- ***Weights*** are ***adjusted*** after every trial until they ***converge*** and the error is reduced to an acceptable value.

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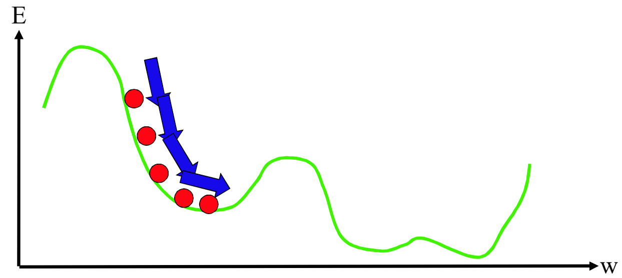
## Gradient Descent




$$\Delta w_{ik} = -\eta \frac{\partial E}{\partial w_{ik}}$$

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## Error Terms

- Need to differentiate the **error function**
- The full calculation is presented in the book.
- Gives us the following *error terms* (deltas)
  - For the outputs

$$\delta_k = (y_k - t_k) g'(a_k)$$

  - For the hidden nodes

$$\delta_i = g'(u_i) \sum_k \delta_k w_{ik}$$

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## Update Rules

- This gives us the necessary update rules
  - For the weights connected to the outputs:

$$w_{jk} \leftarrow w_{jk} - \eta \delta_k z_j$$

  - For the weights on the hidden nodes:

$$v_{ij} \leftarrow v_{ij} - \eta \delta_j x_i$$

  - The learning rate $\eta$ depends on the application. Values between 0.1 and 0.9 have been used in many applications.

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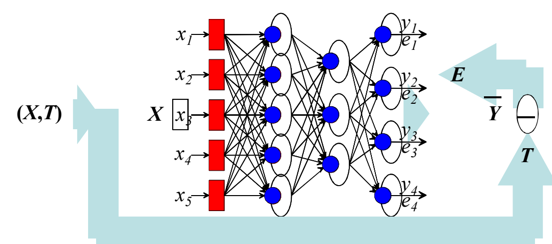
## BackPropagation Algorithm

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## Algorithm (sequential)

1. Apply an input vector and calculate all activations, *a* and *u*
2. Evaluate deltas for all output units:

$$\delta_k = (y_k - t_k)\, g'(a_k)$$

3. Propagate deltas backwards to hidden layer deltas:

$$\delta_i = g'(u_i) \sum_k \delta_k w_{ik}$$

4. Update weights:

$$w_{jk} \leftarrow w_{jk} - \eta \delta_k z_j$$

$$v_{ij} \leftarrow v_{ij} - \eta \delta_j x_i$$

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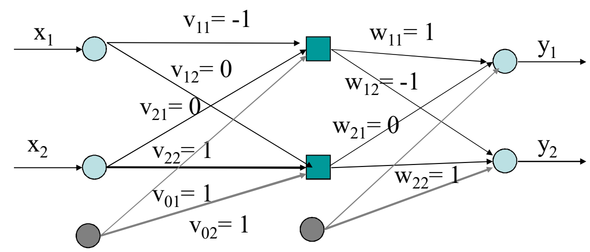
## Example: Backpropagation




Use identity activation function (ie g(a) = a) for simplicity of example



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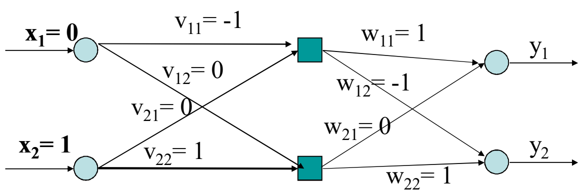
## Example: Backpropagation

All biases set to 1. Will not draw them for clarity.

Learning rate h = 0.1




Have input [0 1] with target [1 0].



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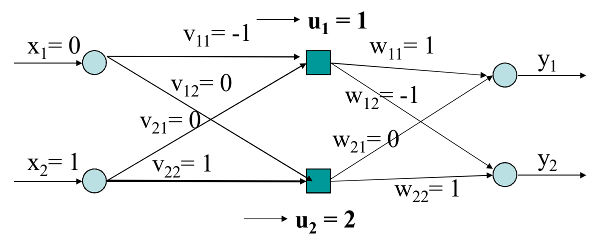
## Example: Backpropagation

Forward pass. Calculate 1st layer activations:




$u_1$ = -1x0 + 0x1 +1 = 1

$u_2$ = 0x0 + 1x1 +1 = 2

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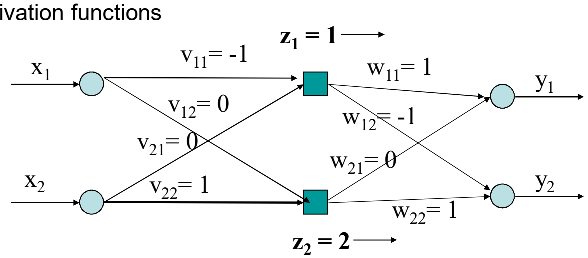
## Example: Backpropagation

Calculate first layer outputs by passing activations through activation functions




$z_1 = g(u_1) = 1$

$z_2 = g(u_2) = 2$



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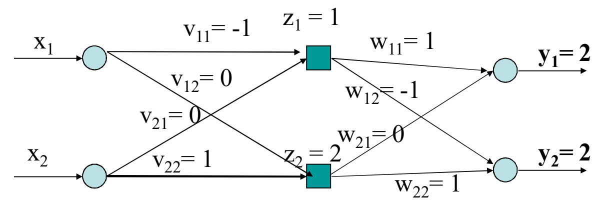
## Example: Backpropagation

Calculate 2[nd] layer outputs (weighted sum through activation functions):




$y_1 = a_1 = 1\text{x}1 + 0\text{x}2 + 1 = 2$

$y_2 = a_2 = -1\text{x}1 + 1\text{x}2 + 1 = 2$



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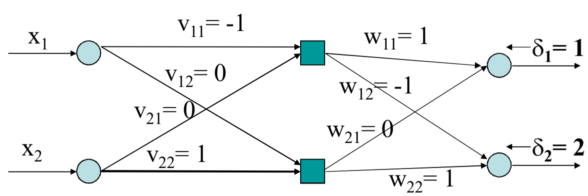
## Example: Backpropagation

Backward pass:

$$\delta_k = (y_k - t_k)\, g'(a_k)$$




Target =[1, 0] so $t_1 = 1$ and $t_2 = 0$. So:

$\delta_1 = (y_1 - t_1) = 2 - 1 = 1$

$\delta_2 = (y_2 - t_2) = 2 - 0 = 2$



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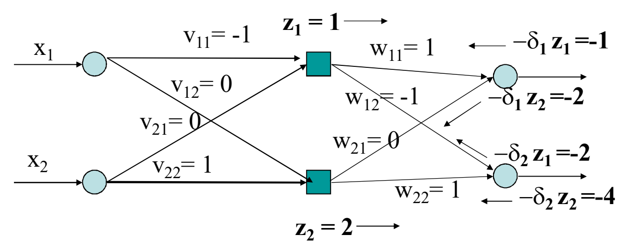
## Example: Backpropagation

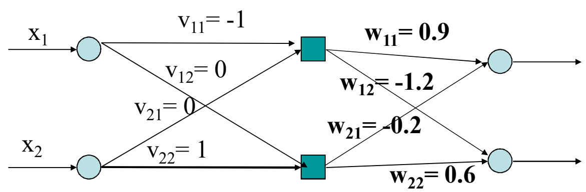
Calculate weight changes for 1[st] layer:




$$w_{jk} \leftarrow w_{jk} - \eta \delta_k z_j$$

## Example: Backpropagation

Weight changes will be:



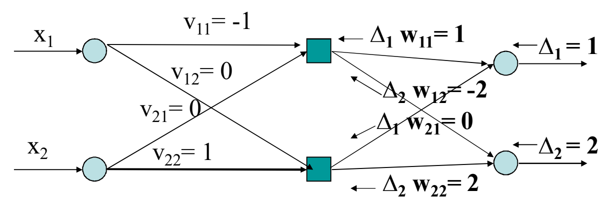

$$w_{jk} \leftarrow w_{jk} - \eta \delta_k z_j$$





## Example: Backpropagation

Calculate hidden layer deltas:



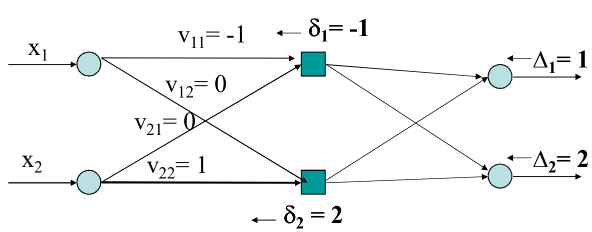

$$\delta_i = g'(u_i) \sum_k \Delta_k w_{ik}$$





## Example: Backpropagation

Deltas propagate back: $\delta_i = g'(u_i) \sum_k \Delta_k w_{ik}$



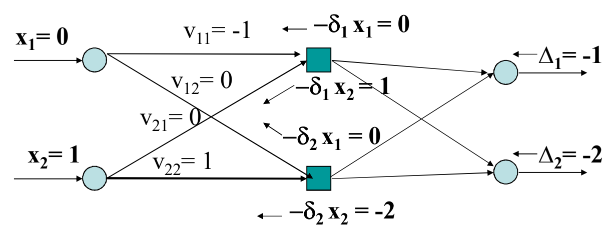

$\delta_1 = 1 - 2 = -1$
$\delta_2 = 0 + 2 = 2$





## Example: Backpropagation

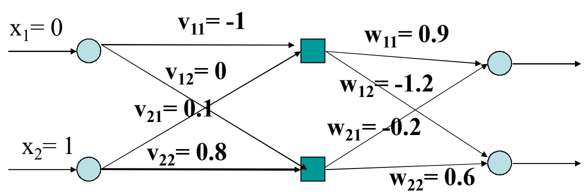
And are multiplied by inputs




$$v_{ij} \leftarrow v_{ij} - \eta \delta_j x_i$$

## Example: Backpropagation

Finally change weights: $v_{ij} \leftarrow v_{ij} - \eta \delta_j x_i$




Note that the weights multiplied by the zero input are unchanged as they do not contribute to the error

We have also changed biases (not shown)



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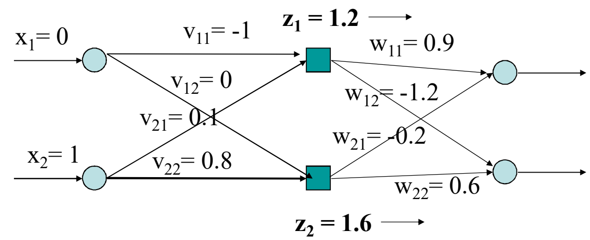
## Example: Backpropagation

Now go forward again (would normally use a new input vector):



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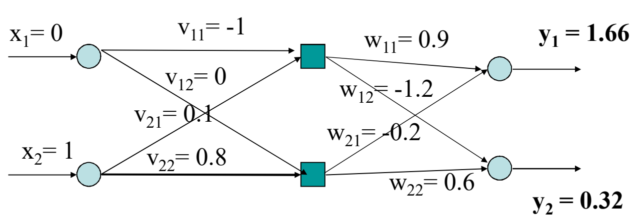
## Example: Backpropagation

Now go forward again (would normally use a new input vector):




Outputs now closer to target value [1, 0]



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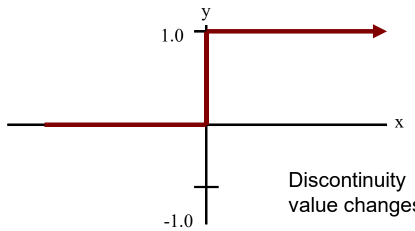
## Activation Function

- We need to compute the derivative of activation function *g*
- What do we want in an activation function?
  - Differentiable
  - Nonlinear (more powerful)
  - Bounded range (for numerical stability)

## Hard Limit Function

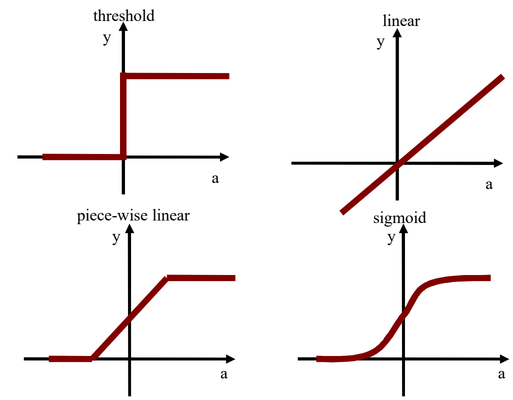



Discontinuity where the value changes from *0* to 1.





## A Quick Overview (Activation Functions)

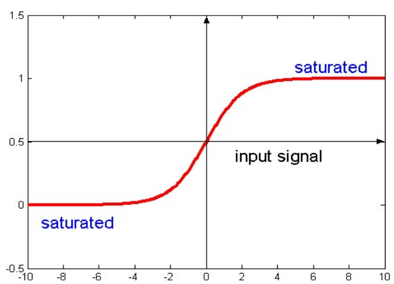







## Sigmoidal Function - Common in MLP

$$g(a_i) = \frac{1}{1+\exp(-k\,a_i)} = \frac{1}{1+e^{-k\,a_i}}$$




- Where *k* is a positive constant.
- The sigmoidal function gives a value in range of 0 to 1.
- Alternatively can use *tanh(ka)* which is same shape but in range –1 to 1.





## Network Training

- Training set shown repeatedly until stopping criteria are met.
- ***When should the weights be updated?***
  - After all inputs seen (***batch***)
  - After each input is seen (***sequential***)
  - Both ways, **need many epochs** - passes through the whole dataset

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## Batch Training

Update weights → Insert all training data → Calculate average error → Calculate deltas → Update weights

- One loop is called an **epoch**
- More accurate estimate of gradient
- Faster convergence to local optimum



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## Sequential Training

Update weights → Insert one training data → Calculate error → Calculate deltas → Update weights

- Simpler to program
- Can avoid local optima



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## Compromise: Minibatch

Update weights → Insert one minibatch → Calculate average error → Calculate deltas → Update weights

- Split all data into N minibatches
- Feed each minibatch to the network
- Shuffle data and repat

- May lead to the benefits of both batch-learning and sequential learning:
  - Rapid convergence
  - Avoiding local minima



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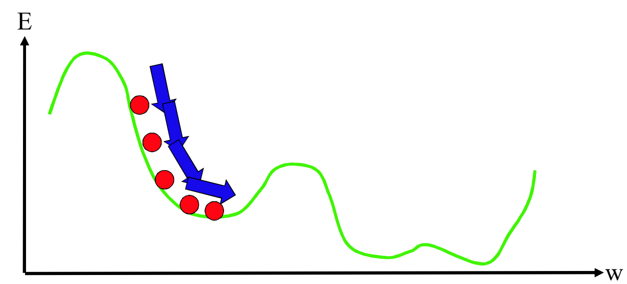
## Risk: Gradient descent takes us to local minimum




$$\Delta w_{ik} = -\eta \frac{\partial E}{\partial w_{ik}}$$

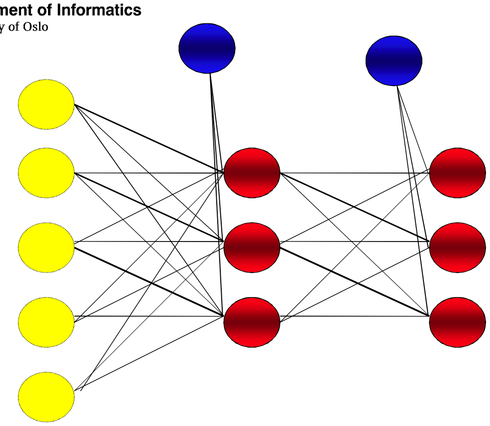
## How can we avoid the local minimum?

- Initialize training many times with random weights
- Use **momentum:**

$$w_{ij} \leftarrow w_{ij} - \eta \Delta_j z_i + \alpha \Delta w_{ij}^{t-1}$$







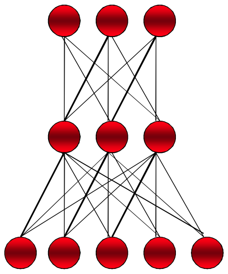
# PRACTICAL ISSUES





## Amount of Training

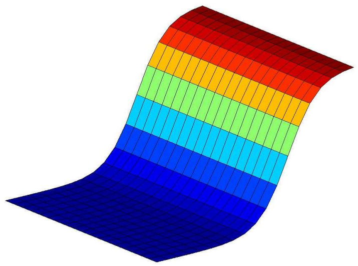
- How much training data is needed?
  - Count the weights
  - Rule of thumb: use 10 times more data than the number of weights



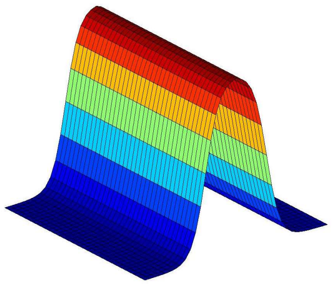




## How many hidden layers do we need?



Output of one sigmoid



Addition of two sigmoids

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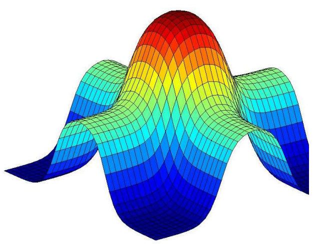
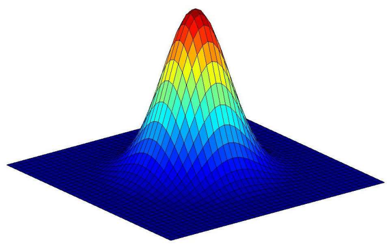
## How many hidden layers do we need?

Addition of more ridges:
Localised response





Addition of two ridges
Unique maximum



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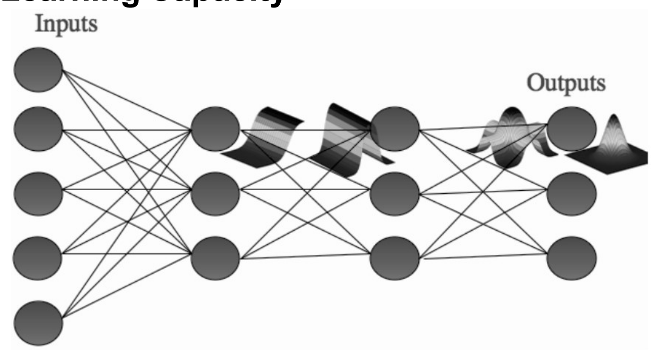
## Learning Capacity




Universal approximation theorem: Any continuous function can be approximated by a neural network with a single hidden layer



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## Network Topology

- How many layers?
- How many neurons per layer?
- No good answers
  - At most 3 weight layers, usually 2
  - Test several different networks
- Possible types of adaptive algorithms (not default in MLP):
  - start from a large network and successively remove some neurons and links until network performance degrades.
  - begin with a small network and introduce new neurons until performance is satisfactory.



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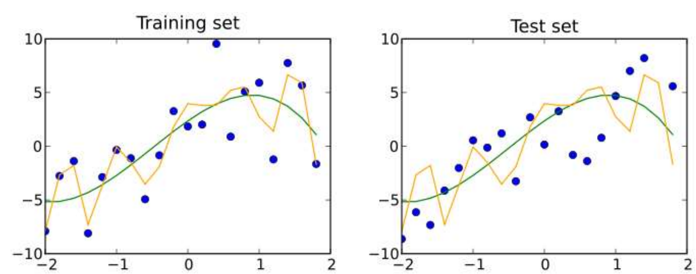


## GENERALIZATION, TRAINING AND TESTING

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## Generalisation

- Aim of neural network learning:
  - ***Generalise from training examples to all possible inputs.***
- The objective of learning is to achieve good ***generalization*** to new cases; we cannot train on all possible data.
- Under-training is ***bad***.
- Over-training is also ***bad.***

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## Generalisation - example

Given: training images and their categories

What are the categories of these test images?

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## Overfitting

- Overfitting occurs when a model begins to learn the **bias** of the training data rather than learning to generalize.
- Overfitting generally occurs when a model is excessively complex in relation to the amount of data available.
- A model which overfits the training data will generally have poor predictive performance, as it can exaggerate minor fluctuations in the data.

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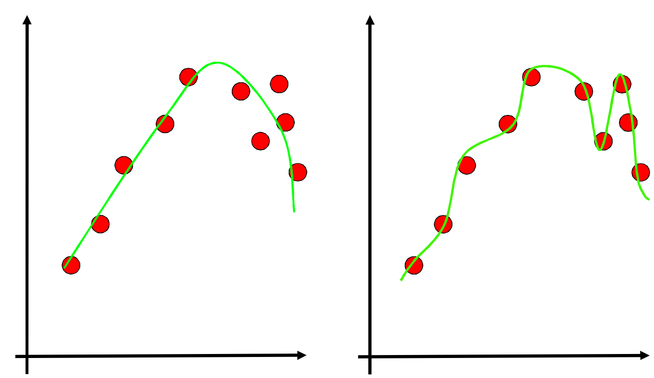
## Overfitting



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## Overfitting

- The training data contains information about the regularities in the mapping from input to output.
- Training data also contains **bias**:
  - There is ***sampling bias***. There will be accidental regularities due to the finite size of the training set.
  - The target values may also be unreliable or noisy.
- When we fit the model, it cannot tell which regularities are relevant and which are caused by sampling error.
  - So it fits both kinds of regularity.
  - If the model is very flexible it can model the sampling error really well. ***This is not what we want***.



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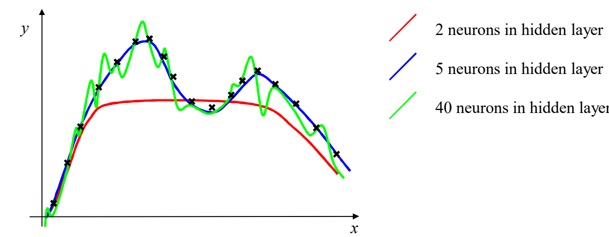
## The Problem of Overfitting

- Approximation of the function $y = f(x)$ :



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## The Solution: Cross-Validation

To maximize generalization and avoid overfitting, split data into three sets:

- **Training set**: Train the model.
- **Validation set**: Judge the model's generalization ability during training.
- **Test set**: Judge the model's generalization ability after training.



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## Validation set

- Data unseen by training algorithm – not used for backpropagation.
- Network is not trained on this data, so we can use it to measure generalization ability.
- Goal is to maximize generalization ability, so we should minimize the error on this data set.

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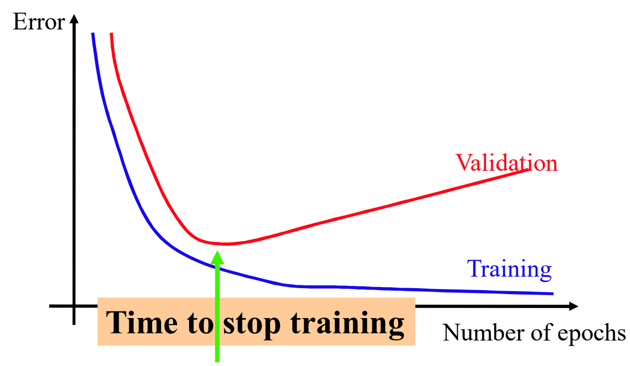
## Early Stopping



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### Testing set

- Data unseen during training and validation.
- Has no influence on when to stop training.
- With early stopping, we've maximized the ability to generalize **to the validation set**;
- To judge the final result, we should measure its ability to generalize to completely unseen data.



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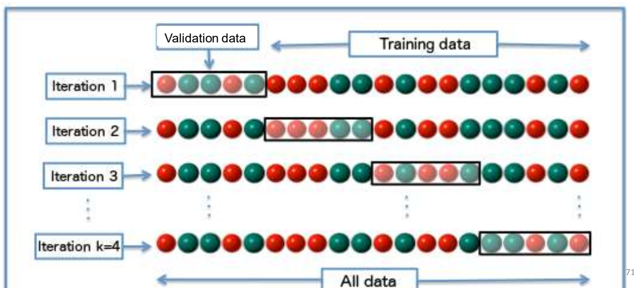
## k-Fold Cross Validation

- Validation and testing leaves less training data.
- Solution: repeat over many different splits.




Source: Wikimedia Commons



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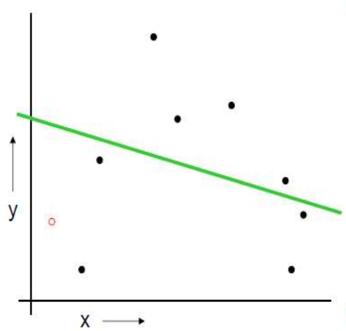
## Leave-one-out Cross Validation




For k=1 to R

1. Let $(x_k, y_k)$ be the $k^{th}$ record
2. Temporarily remove $(x_k, y_k)$ from the dataset
3. Train on the remaining R-1 datapoints
4. Note your error $(x_k, y_k)$

When you've done all points, report the mean error.