Artificial Neural Networks

Outline

1. Introduction
2. Perceptron
3. The perceptron training rule
4. Gradient descent and the Delta Rule
5. Derivation of the gradient descent rule
6. Multilayer networks and the back-propagation algorithm
7. Remarks on the back-propagation algorithm

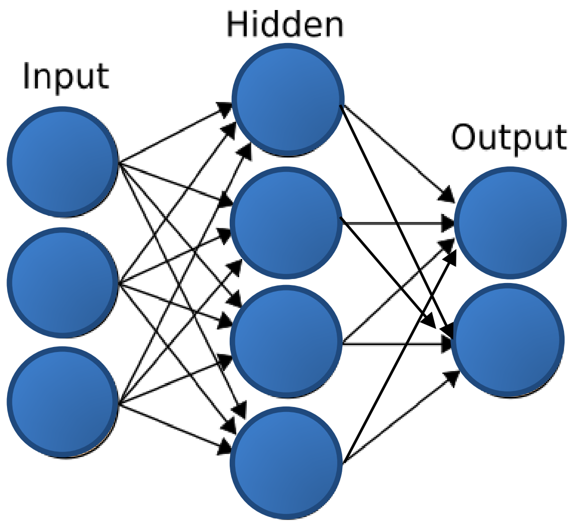
Videos

1. But what is a Neural Network? Deep learning, chapter 1.
2. Gradient descent, how neural networks learn | Deep learning, chapter 2
3. What is backpropagation really doing? | Deep learning, chapter 3
4. Backpropagation calculus | Deep learning, chapter 4

1. Introduction

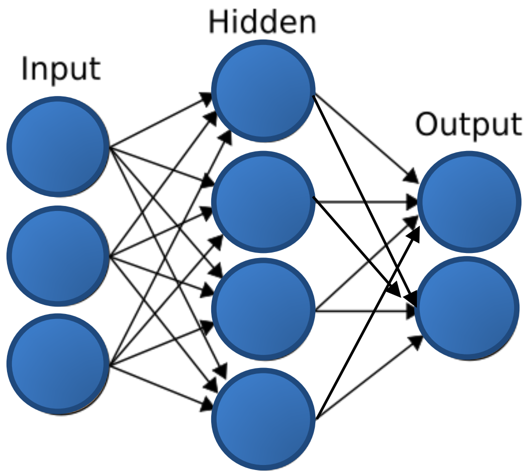
- Neural network learning methods provide a robust approach to approximating
  - real-valued,
  - discreet-valued, and
  - vector-valued target

  functions.



- For some types of problems, e.g. interpreting complex real-world sensor data, artificial neural networks are very effective.
- **Backpropagation method** has been successfully applied in many practical problems such as learning to recognize handwritten characters and faces.

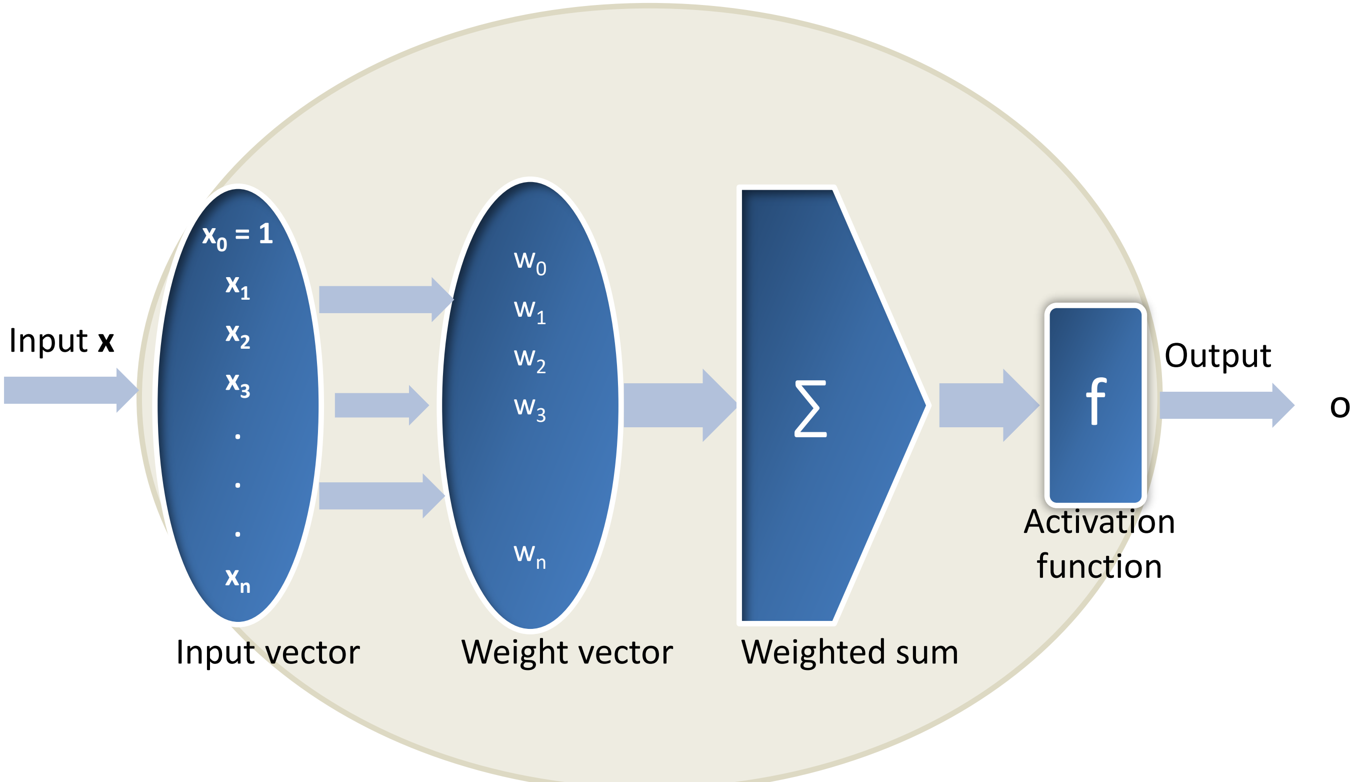
1. Introduction



- Each node (circle) corresponds to a single network unit.
- The arrows represent the inputs to a hidden unit or to an output unit.
- The four hidden units are "hidden" because their output is available only within the network and is not available as part of the global network output.
- Each of the hidden units computes a single real-valued output based on the weighted combination of its inputs.
- These hidden units are then used as inputs to the second layer of consisting of 2 output units.
- Each output unit normally has binary target values. For example, the two outputs may have target values (0,1) and (1,0) for a binary classification problem.
- There are 3×4 connections between input layer and hidden layer and 4×2 connections between hidden layer and output layer.
- Network learning corresponds to choosing a weight value for each of these connections.

2. Perceptron

- One type of ANN system is based on a unit called **perceptron**.
- A perceptron takes a vector of real-valued inputs, calculates a linear combination of these inputs, then outputs a 1 if the result is greater than a threshold, -1 otherwise.



$$o = f(w_0x_0 + w_1x_1 + w_2x_2 + w_3x_3 + \ldots w_nx_n)$$

Perceptron

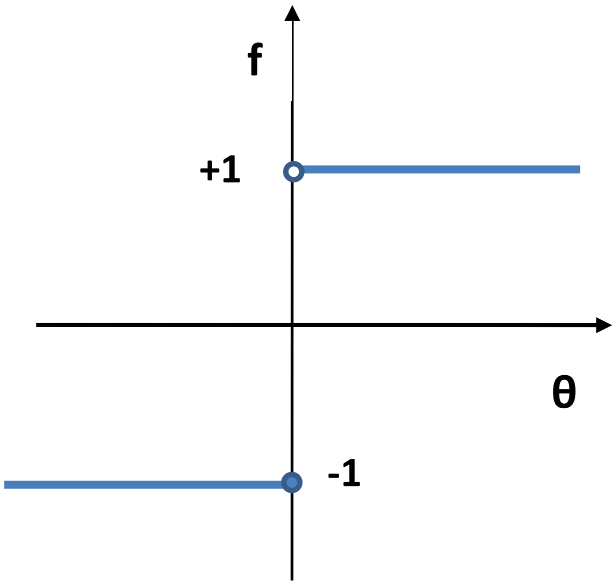
- Given an observation **x**, the prediction by the perceptron is computed by applying the <u>activation function</u> f to the linear combination of the predictors:

$$o = f(w_0x_0 + w_1x_1 + w_2x_2 + w_3x_3 + \dots w_nx_n)$$

- The function f maps the linear combination into the set $\mathbb{H} = \{-1,1\}$:
  - $f(\theta) = 1$ if $\theta > 0$

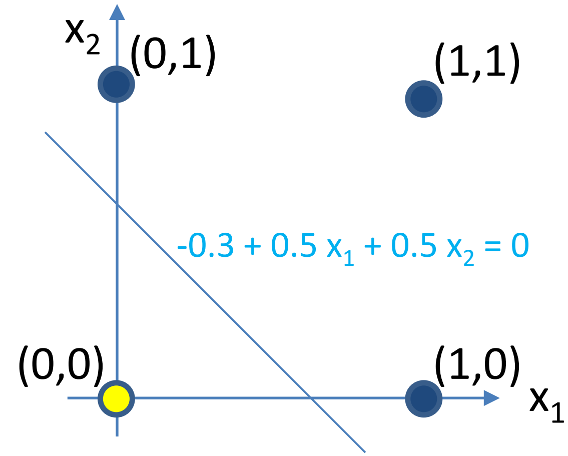
    $= -1$ otherwise

- w_0 is called the *distortion* or *bias* when x_0 is set to 1 for all data samples.



Representational power of perceptrons

- A single perceptron can be used to represent many Boolean functions:
  - AND: let w_0 = -0.8 and $w_1 = w_2$ = 0.5
  - OR: let w_0 = -0.3 and $w_1 = w_2$ = 0.5
  - AND and OR are special cases of m-of-n functions.
  - AND: m = n, OR: m = 1



- m-of-n function: if (m of the following n conditions are true), then ……
- Any m-of-n function is easily represented using a perceptron by setting all input weights to the same value and then setting the threshold accordingly.
- Perceptron can represent all primitive Boolean functions AND, OR, NAND, NOR.
- It cannot represent [XOR function](#).
- Every Boolean function can be represented by some network of perceptrons only two level deep.

3. The perceptron training rule

- **Training**: determine a weight vector that causes the perceptron to produce correct +1 or -1 output for each of the given training examples:
- Begin with a random weight and iteratively apply the perceptron to each training example.
- Modify the weights whenever the output is not correct.
- Weights are corrected as follows:
    - $\mathbf{w}_i \Leftarrow \mathbf{w}_i + \Delta\mathbf{w}$, where
    - $\Delta\mathbf{w} = \eta(t - o)\,\mathbf{x}_i$
- Here:
    - t is the target output of the current training example $\mathbf{x}_i$
    - o is the output generated by the perceptron
    - η is a positive learning constant usually set to a small value, e.g. 0.1.
    - $\mathbf{x}_i$ is the i-th data sample (n-dimensional vector).
    - $\Delta\mathbf{w}$ is the change in weight given the data sample $\mathbf{x}_i$

The perceptron training rule

Example.

- Classify 4 input patterns with known class membership:
  - $\mathbf{x_1} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\mathbf{x_2} = \begin{bmatrix} 1 \\ -0.5 \end{bmatrix}$ $\mathbf{x_3} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$ $\mathbf{x_4} = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$
  - $t_1 = t_3 = +1$ (Class 1)
  - $t_2 = t_4 = -1$ (Class 2)

- Assume learning rate $\eta = 0.5$, initial weight $\mathbf{w_1} = \begin{bmatrix} 1.75 \\ -2.5 \end{bmatrix}$

- Input patterns presented sequentially as $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$ and $\mathbf{x}_4$ in a complete training cycle (also called an **epoch**).

The perceptron training rule

Step 1: Pattern $\mathbf{x}_1$ as input

$$o_1 = f(w_{1,0}x_{1,0} + w_{1,1}x_{1,1}) = f\{ (1.75)(1) + (-2.5)(1) \} = f(-0.75) = -1$$

$$\Delta\mathbf{w} = \eta(t_1 - o_1)\,\mathbf{x}_1 = 0.5(1+1)\,\mathbf{x}_1 = \mathbf{x}_1$$

$$\mathbf{w_2} = \mathbf{w_1} + \Delta\mathbf{w}$$

$$= \begin{bmatrix}1.75\\-2.5\end{bmatrix} + \begin{bmatrix}1\\1\end{bmatrix} = \begin{bmatrix}2.75\\-1.5\end{bmatrix}$$

Step 2: Pattern $\mathbf{x}_2$ as input

$$o_2 = f(w_{2,0}x_{2,0} + w_{2,1}x_{2,1}) = f\{ (2.75)(1) + (-1.5)(-0.5) \} = f(3.5) = +1$$

$$\Delta\mathbf{w} = \eta(t_2 - o_2)\,\mathbf{x}_2 = 0.5(-1-1)\,\mathbf{x}_2 = -\,\mathbf{x}_2$$

$$\mathbf{w_3} = \mathbf{w_2} + \Delta\mathbf{w}$$

$$= \begin{bmatrix}2.75\\-1.5\end{bmatrix} + \begin{bmatrix}-1\\0.5\end{bmatrix} = \begin{bmatrix}1.75\\-1\end{bmatrix}$$

$$\mathbf{x_1} = \begin{bmatrix}1\\1\end{bmatrix} \quad \mathbf{x_2} = \begin{bmatrix}1\\-0.5\end{bmatrix} \quad \mathbf{x_3} = \begin{bmatrix}1\\3\end{bmatrix} \quad \mathbf{x_4} = \begin{bmatrix}1\\-2\end{bmatrix}$$

$t_1 = t_3 = +1$ (Class 1)

$t_2 = t_4 = -1$ (Class 2)

The perceptron training rule

Step 3: Pattern $\mathbf{x}_3$ as input

$$o_3 = f(w_{3,0}x_{3,0} + w_{3,1}x_{3,1}) = f\{ (1.75)(1) + (-1)(3) \} = f(-1.25) = -1$$

$$\Delta\mathbf{w} = \eta(t_3 - o_3)\,\mathbf{x}_3 = 0.5(1 + 1)\,\mathbf{x}_3 = \mathbf{x}_3$$

$$\mathbf{w}_4 = \mathbf{w}_3 + \Delta\mathbf{w}$$

$$= \begin{bmatrix} 1.75 \\ -1 \end{bmatrix} + \begin{bmatrix} 1 \\ 3 \end{bmatrix} = \begin{bmatrix} 2.75 \\ 2 \end{bmatrix}$$

Step 4: Pattern $\mathbf{x}_4$ as input

$$o_4 = f(w_{2,0}x_{2,0} + w_{2,1}x_{2,1}) = f\{ (2.75)(1) + (2)(-2) \} = f(-1.25) = -1$$

$$\Delta\mathbf{w} = \eta(t_4 - o_4)\,\mathbf{x}_4 = 0.5(-1 + 1)\,\mathbf{x}_4 = \mathbf{0}$$

$$\mathbf{w}_5 = \mathbf{w}_4$$

$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\quad \mathbf{x}_2 = \begin{bmatrix} 1 \\ -0.5 \end{bmatrix}$ $\quad \mathbf{x}_3 = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$ $\quad \mathbf{x}_4 = \begin{bmatrix} 1 \\ -2 \end{bmatrix}$

$t_1 = t_3 = +1$ (Class 1)

$t_2 = t_4 = -1$ (Class 2)

End of first epoch and there is no change in weights.

Is training complete? NO

The perceptron training rule

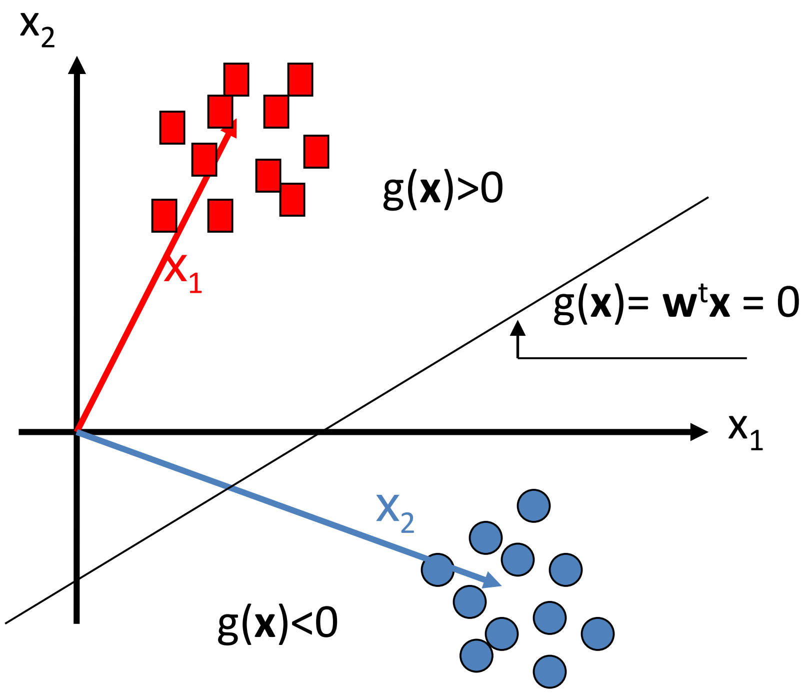
- Step 5 ($\mathbf{x}_1$) : $\mathbf{w}_6 = \mathbf{w}_5$
- Step 6 ($\mathbf{x}_2$) : $\mathbf{w}_7 = \begin{bmatrix} 1.75 \\ 2.5 \end{bmatrix}$
- Step 7-9 ($\mathbf{x}_3$, $\mathbf{x}_4$, $\mathbf{x}_1$) : $\mathbf{w}_{10} = \mathbf{w}_9 = \mathbf{w}_8 = \mathbf{w}_7$ (no adjustment)
- Step 10 ($\mathbf{x}_2$) : $\mathbf{w}_{11} = \begin{bmatrix} 0.75 \\ 3 \end{bmatrix}$ (final weights)
- It took 10 pattern presentations to find the solution.
- It can be verified:

$$\mathbf{Xw} = \begin{bmatrix} 1 & 1 \\ 1 & -0.5 \\ 1 & 3 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} 0.75 \\ 3 \end{bmatrix} = \begin{bmatrix} 3.75 \\ -0.75 \\ 9.75 \\ -5.25 \end{bmatrix}$$

$$f(\mathbf{Xw}) = \begin{bmatrix} 1 \\ -1 \\ 1 \\ -1 \end{bmatrix}$$

Perceptron

<u>Perceptron Convergence Theorem</u>: Perceptron learns correct dichotomization of two-class patterns in a finite number of steps, k, regardless of η and $\mathbf{w_0}$, provided classes are linearly separable, i.e., $\mathbf{w}^* = \mathbf{w}_{k+1} = \mathbf{w}_{k+2} = \mathbf{w}_{k+3}$ .....



4. Gradient descent and Delta Rule

- If samples are not linearly separable, perceptron rule may fail to converge.
- Delta rule converges toward a best-fit approximation to the target concept when the samples are not linearly separable.
- Key idea: **Gradient descent** to search the hypothesis space to find the best weights.
- Consider the case of a linear unit with no threshold, the output for input $\mathbf{x}_i$ is computed as

$$o_i = \mathbf{w}^t \mathbf{x}_i = w_1 x_{i1} + w_2 x_{i2} + \dots + w_n x_{in}$$

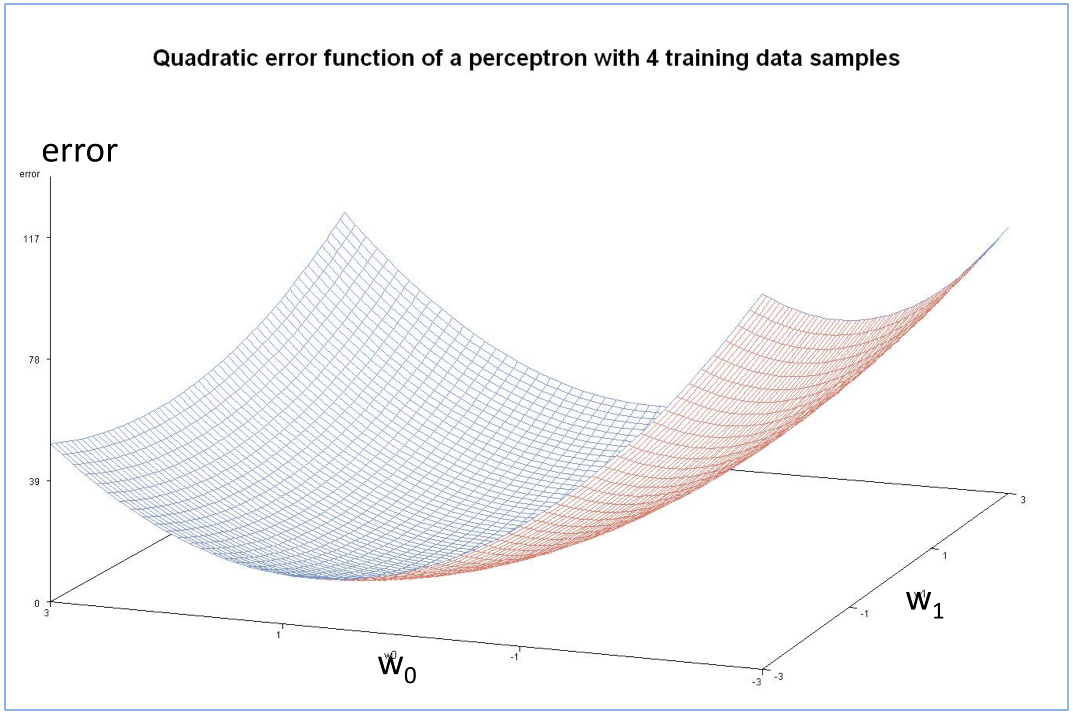
- The training error for the training data set is defined as

$$E(\mathbf{w}) = \tfrac{1}{2} \sum_d (t_d - o_d)^2$$

where t_d is the target value and o_d is the unit's output for input $\mathbf{x}_d$.

Visualizing the hypothesis space

- **Visualizing the hypothesis space**



- The axes w_0 and w_1 represent possible values of the two weights of a simple linear unit.
- The w_0,w_1 plane represents the entire hypothesis space.
- The vertical axis indicates the error E relative to the 4 training examples..
- Gradient descent search determines a weight vector that minimizes E by moving along the steepest descent direction along the error surface.

5. Derivation of the gradient descent rule.

Derivation of the gradient descent rule.

- The direction of steepest descent along the hypothesis space can be obtained by computing the derivative of the error function E(**w**).
- The derivative (**gradient**) is

  $\nabla E(\mathbf{w}) \equiv [\partial E/\partial \mathbf{w}_0, \partial E/\partial \mathbf{w}_1, \ldots\ldots, \partial E/\partial \mathbf{w}_n]^t$

- The negative of this gradient gives the direction of steepest descent.
- The training rule for gradient descent is

  $\mathbf{w} \Leftarrow \mathbf{w} + \Delta\mathbf{w}$

  where: $\Delta\mathbf{w} = -\,\eta\, \nabla E(\mathbf{w})$

- Working on each component of the weight vector **w**, the training rule can be written as

  $\mathbf{w}_j \Leftarrow \mathbf{w}_j + \Delta\mathbf{w}_j$

  where: $\Delta\mathbf{w}_j = -\,\eta\, \partial E/\partial \mathbf{w}_j$

Derivation of the gradient descent rule.

Efficient gradient calculation.

- At each iteration we need to compute $\partial E/\partial \mathbf{w}_j$
- This can be done as follows:

$$\partial E/\partial \mathbf{w}_j = \partial/\partial \mathbf{w}_j \ \tfrac{1}{2} \sum_d (t_d - o_d)^2$$

$$= \tfrac{1}{2} \sum_d \partial/\partial \mathbf{w}_j \ (t_d - o_d)^2$$

$$= \tfrac{1}{2} \sum_d \ 2 (t_d - o_d) \ \partial/\partial \mathbf{w}_j (t_d - o_d)$$

$$= \tfrac{1}{2} \sum_d \ 2 (t_d - o_d) \ \partial/\partial \mathbf{w}_j (t_d - \mathbf{w}^t \mathbf{x}_d)$$

$$= \sum_d (t_d - o_d) (- \mathbf{x}_{d,j})$$

Eg. $\mathbf{x}_1 = \begin{bmatrix} 3 \\ -2 \end{bmatrix}$ $\quad t_1 = 1$

$$\partial/\partial \mathbf{w}_j (t_d - \mathbf{w}^t \mathbf{x}_d)$$
$$= \partial/\partial \mathbf{w}_j (1 - 3 \, w_1 + 2 \, w_2)$$

For $j = 1$, $\partial/\partial \mathbf{w}_1 (t_d - \mathbf{w}^t \mathbf{x}_d) = -3$

$j = 2$, $\partial/\partial \mathbf{w}_2 (t_d - \mathbf{w}^t \mathbf{x}_d) = 2$

- The weight update rule for gradient descent is then:

$$\Delta \mathbf{w}_j = - \eta \ \partial E/\partial \mathbf{w}_j$$

$$= \eta \sum_d (t_d - o_d) \mathbf{x}_{d,j}$$

Compare to weight update formula on page 9:

$$\Delta \mathbf{w} = \eta(t - o) \ \mathbf{x}_i$$

Derivation of the gradient descent rule.

The algorithm.

- Input: $(\mathbf{x}_d, t_d)$, d = 1,2, …. N, $\mathbf{x}_d$ is the vector of input values, t_d is its corresponding target value.
- Learning parameter: η
- Initialize each $\mathbf{w}_j$ to a small random value
- Until termination condition is met, do
  - Initialize each $\Delta \mathbf{w}_j$ to zero.
  - For each $(\mathbf{x}_d, t_d)$ in the data set, do
    - Input the data $\mathbf{x}_d$ to the unit and compute the output o_d
    - For each linear unit weight $\mathbf{w}_j$, do

$$\Delta \mathbf{w}_j \Leftarrow \Delta \mathbf{w}_j + \eta \, (t_d - o_d) \, \mathbf{x}_{d,j}$$

  - Update the weight $\mathbf{w}_j$

$$\mathbf{w}_j \Leftarrow \mathbf{w}_j + \Delta \mathbf{w}_j$$

Derivation of the gradient descent rule.

Termination condition could be one of the following:

- When the gradient is sufficiently small $\| \nabla E(\mathbf{w}) \| \leq \varepsilon$
- When the total error is sufficiently small $\sum_d (t_d - o_d)^2 \leq \varepsilon$
- When 2 consecutive weights are similar $\| \mathbf{w}^{k+1} - \mathbf{w}^{k} \|^2 \leq \varepsilon$
- When maximum iteration is reached $k \geq K$
- When the error on cross-validation set starts to increase

Derivation of the gradient descent rule.

Example.

- Tasting score of a certain processed cheese.
- The two predictors: scores for fat and salt (0 is the minimum amount and 1 is the maximum amount possible).
- The output: 1 indicates a test panel likes the cheese, 0 otherwise.

Observation	Fat score	Salt score	Acceptance
1	0.2	0.9	1
2	0.1	0.1	0
3	0.2	0.4	0
4	0.2	0.5	0
5	0.4	0.5	1
6	0.3	0.8	1

Derivation of the gradient descent rule.

Example.

- Let $\mathbf{w} = (1 \quad 1 \quad -1)^t$, where the 3rd component $\mathbf{w}_3 = -1$ is the bias
- The predictions and errors with these weights are as follows:

Obs. d	Fat score	Salt score		t_d	$o_d = w^t x_d$	$(t_d - o_d)^2$
	x					
1	0.2	0.9	1	1	(1)(0.2) + (1)(0.9) + (-1)(1) = 0.10	$(1-0.10)^2 = 0.81$
2	0.1	0.1	1	0	(1)(0.1) + (1)(0.1) + (-1)(1) = -0.80	$(0+0.80)^2 = 0.64$
3	0.2	0.4	1	0	(1)(0.2) + (1)(0.4) + (-1)(1) = -0.40	$(0+0.40)^2 = 0.16$
4	0.2	0.5	1	0	(1)(0.2) + (1)(0.5) + (-1)(1) = -0.30	$(0+0.30)^2 = 0.09$
5	0.4	0.5	1	1	(1)(0.4) + (1)(0.5) + (-1)(1) = -0.10	$(1+0.10)^2 = 1.21$
6	0.3	0.8	1	1	(1)(0.3) + (1)(0.8) + (-1)(1) = 0.10	$(1-0.10)^2 = 0.81$

$$\tfrac{1}{2} \sum (t_d - o_d)^2 = 1.86$$

Derivation of the gradient descent rule.

Example.

- Compute the weight correction vector $\Delta \mathbf{w}_j \Leftarrow \Delta \mathbf{w}_j + \eta\,(t_d - o_d)x_{d,j}$

Compute the sum:

$$(t_1 - o_1)\,\mathbf{x_1} + (t_2 - o_2)\,\mathbf{x_2} + (t_3 - o_3)\,\mathbf{x_3} + (t_4 - o_4)\,\mathbf{x_4} + (t_5 - o_5)\,\mathbf{x_5} + (t_6 - o_6)\,\mathbf{x_6} =$$

$$0.9\begin{pmatrix}0.2\\0.9\\1\end{pmatrix} + 0.8\begin{pmatrix}0.1\\0.1\\1\end{pmatrix} + 0.4\begin{pmatrix}0.2\\0.4\\1\end{pmatrix} + 0.3\begin{pmatrix}0.2\\0.5\\1\end{pmatrix} + 1.1\begin{pmatrix}0.4\\0.5\\1\end{pmatrix} + 0.9\begin{pmatrix}0.3\\0.8\\1\end{pmatrix}$$

$$= \begin{pmatrix}1.11\\2.47\\4.40\end{pmatrix}\begin{matrix}\leftarrow j = 1\\ \leftarrow j = 2\\ \leftarrow j = 3\end{matrix}$$

Derivation of the gradient descent rule.

Example.

- Let the learning parameter η = 0.1, then $\mathbf{w} \Leftarrow \mathbf{w} + \Delta\mathbf{w}$

$$\mathbf{w}^{new} = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} + 0.1 \begin{pmatrix} 1.11 \\ 2.47 \\ 4.40 \end{pmatrix} = \begin{pmatrix} 1.111 \\ 1.247 \\ -0.56 \end{pmatrix}$$

where: $\Delta\mathbf{w} = -\eta \nabla E(\mathbf{w})$

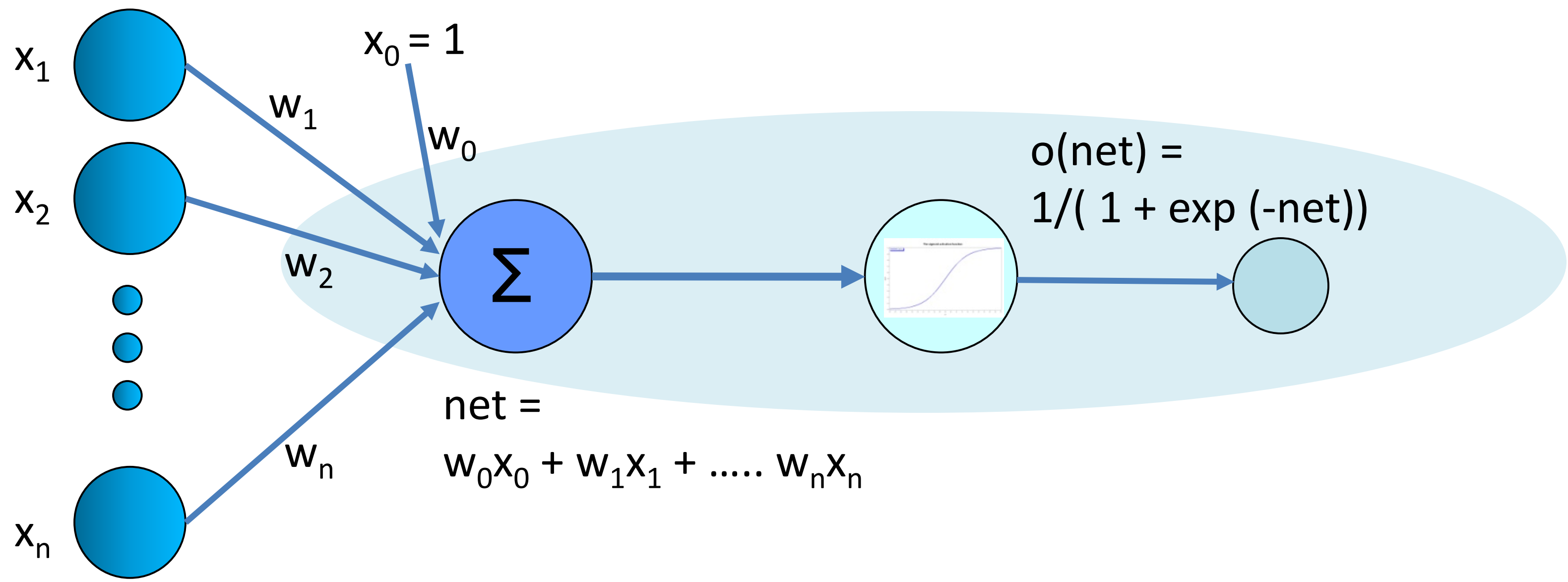
$\frac{1}{2} \sum (t_d - o_d)^2 = 0.28$

Obs. d	Fat score	Salt score		t_d	$o_d = w^t x_d$	$(t_d - o_d)^2$
	x					
1	0.2	0.9	1	1	(1.111)(0.2) + (1.247)(0.9) + (-0.56)(1) = 0.78	$(1-0.78)^2$ = 0.0464
2	0.1	0.1	1	0	(1.111)(0.1) + (1.247)(0.1) + (-0.56)(1) = -0.32	$(0+0.32)^2$ = 0.1051
3	0.2	0.4	1	0	(1.111)(0.2) + (1.247)(0.4) + (-0.56)(1) = 0.16	$(0-0.16)^2$ = 0.0259
4	0.2	0.5	1	0	(1.111)(0.2) + (1.247)(0.5) + (-0.56)(1) = 0.29	$(0-0.29)^2$ = 0.0816
5	0.4	0.5	1	1	(1.111)(0.4) + (1.247)(0.5) + (-0.56)(1) = 0.51	$(1-0.51)^2$ = 0.2422
6	0.3	0.8	1	1	(1.111)(0.3) + (1.247)(0.8) + (-0.56)(1) = 0.77	$(1-0.77)^2$ = 0.0525

6. Multilayer networks and the backpropagation algorithm

A differentiable threshold unit.

- Multiple layers of cascaded linear units still produce only linear function.
- Networks capable of representing highly nonlinear function are preferred.
- A unit giving a nonlinear function of its inputs as output is the **sigmoid unit**:



Multilayer networks and the back-propagation algorithm

A differentiable threshold unit.

- The sigmoid unit computes its output o as

  $o = \sigma(\mathbf{w}^T\mathbf{x})$, where σ is the sigmoid activation function:

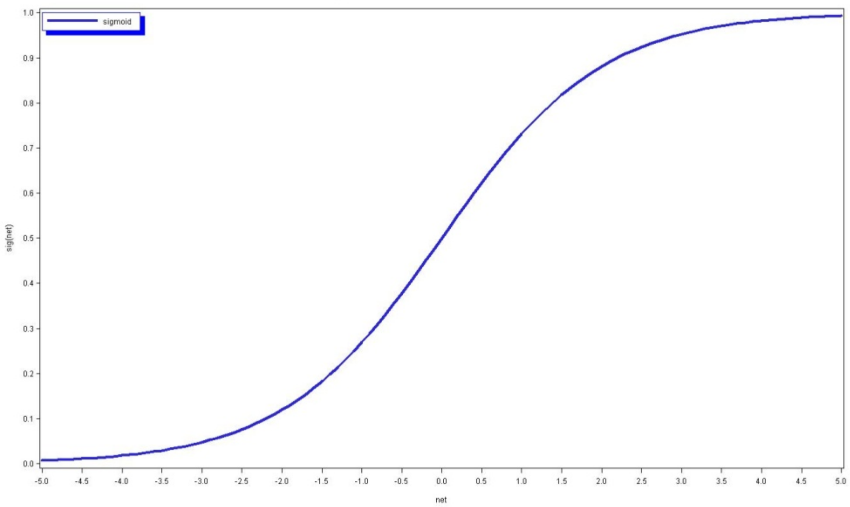
  $\sigma(y) = 1/(1 + \exp(-y)) = 1/(1 + e^{-y})$

- The derivative of the sigmoid function is

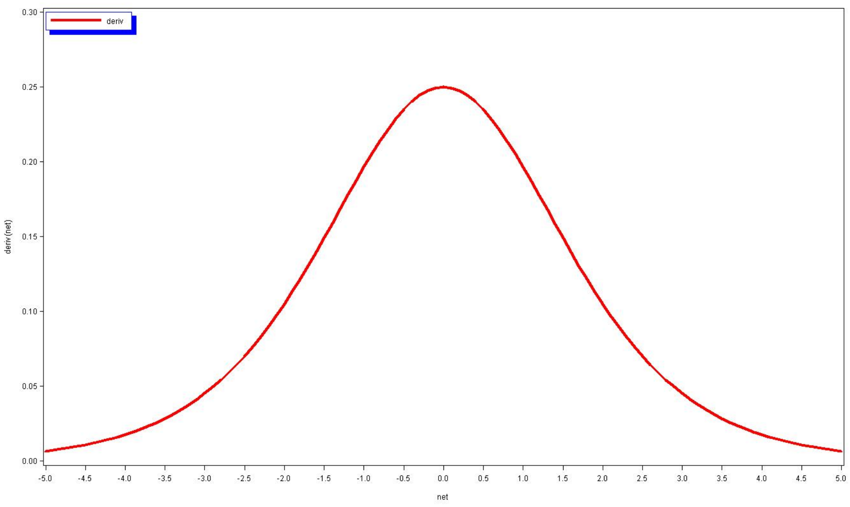
  $\sigma'(y) = \sigma(y)(1 - \sigma(y))$

- The function is often referred to as the **squashing function**.

The sigmoid activation function



The derivative of the sigmoid activation function



Multilayer networks and the back-propagation algorithm

A differentiable threshold unit.

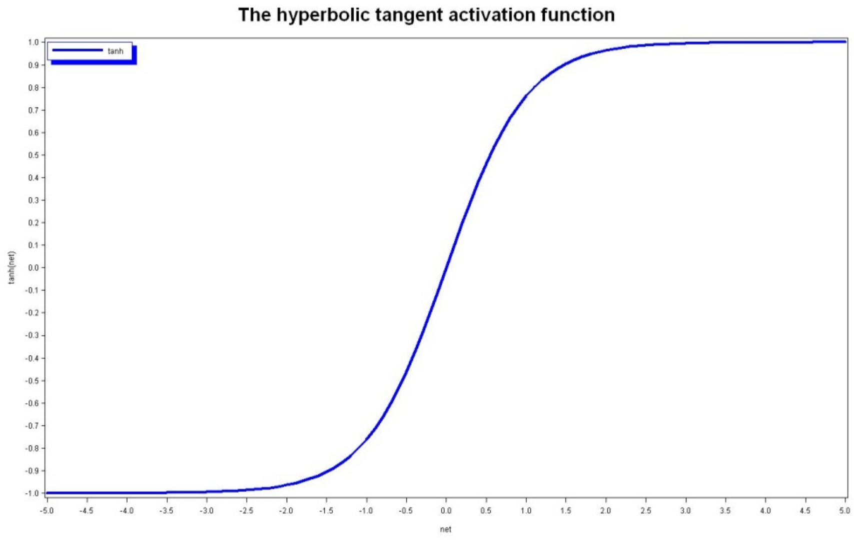
- The function tanh(y) is sometimes used in place of the sigmoid activation function:

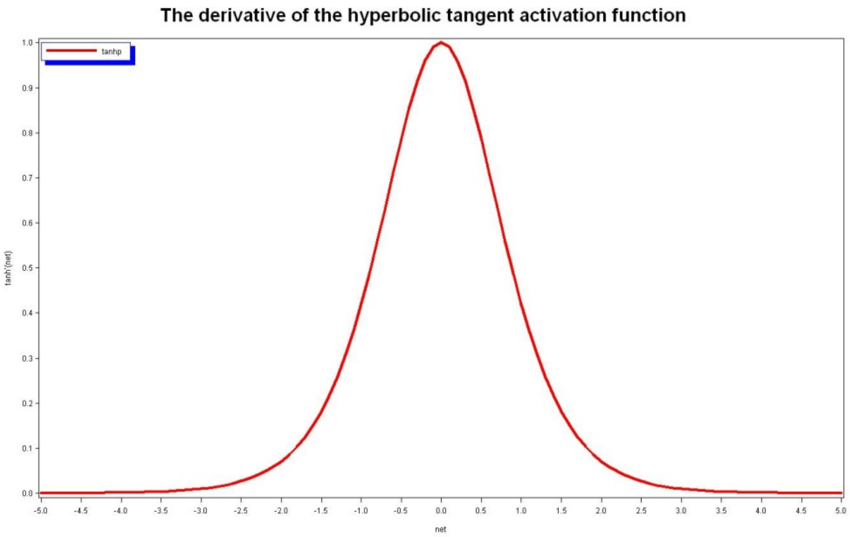
  o = tanh($\mathbf{w}^T\mathbf{x}$) , where tanh(y) is the **hyperbolic tangent** activation function:

  $$\tanh(y) = (e^{y} - e^{-y})/(e^{y} + e^{-y}) = 2\,\sigma(2y) - 1$$

- The derivative of tanh(y) is

  $$\tanh'(y) = 1 - \tanh(y)^2$$



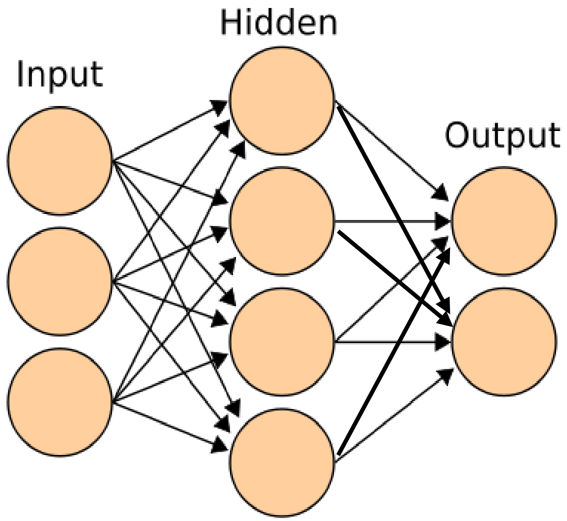


- σ(y) and tanh(y) are examples of activation function/gain function/transfer function/squashing function.

Multilayer networks and the back-propagation algorithm

The back-propagation algorithm.

Each training example is denoted as (**z**,**d**) where **z** is the vector of input values, and **d** is the vector of target network values.



- η is the learning rate (e.g. 0.5)
- I is the number of input units (= 3)
- J is the number of hidden units
- K is the number of output units
- **W** is the weight matrix for connections from hidden units to output units, with K rows and J columns (2 × 4)
- **V** is the weight matrix for connections from input units to hidden units, with J rows and I columns (4 × 3)
- **y** is a vector of hidden unit activations, J rows (= 4)
- **o** is a vector of output unit activations, K rows (= 2)

Multilayer networks and the back-propagation algorithm

The back-propagation algorithm
(Stochastic gradient descent with sigmoid activation function).

- Step 1. Choose E_{max}, $\eta > 0$. Set $q \Leftarrow 1$, $p \Leftarrow 1$, $E \Leftarrow 0$. Initialize **W**, **V** randomly.
- Step 2. Present the input data: $\mathbf{z} \Leftarrow \mathbf{z}_p$, $\mathbf{d} \Leftarrow \mathbf{d}_p$ and compute

  $y_j \Leftarrow f(\mathbf{v}_j^T \mathbf{z})$ for $j = 1, 2, \ldots. J$ and

  $o_k \Leftarrow f(\mathbf{w}_k^T \mathbf{y})$ for $k = 1, 2, \ldots. K$
- Step 3. Compute the error: $E \Leftarrow \frac{1}{2} (\mathbf{d}_k - \mathbf{o}_k)^2 + E$ for $k = 1,2, \ldots K$
- Step 4. Compute error signal vectors δ_o and δ_y for output and hidden layer units:

  $\delta_{ok} = (\mathbf{d}_k - \mathbf{o}_k)(1 - \mathbf{o}_k)\mathbf{o}_k$ for $k = 1, 2, \ldots K$

  $\delta_{yj} = \mathbf{y}_j(1 - \mathbf{y}_j) \sum_{k=1}^{K} \delta_{ok}\mathbf{w}_{kj}$ for $j = 1, 2, \ldots J$
- Step 5. Update output layer and hidden layer weights:

  $\mathbf{w}_{kj} \Leftarrow \mathbf{w}_{kj} + \eta\, \delta_{ok}\, \mathbf{y}_j$ for $k = 1, 2, \ldots K$ and $j = 1, 2, \ldots J$

  $\mathbf{v}_{ji} \Leftarrow \mathbf{v}_{ji} + \eta\, \delta_{yj}\, \mathbf{z}_i$ for $j = 1, 2, \ldots J$ and $i = 1, 2, \ldots I$
- Step 6. If $p < P$ then $p \Leftarrow p + 1$, $q \Leftarrow q + 1$, go to Step 2.
- Step 7. If $E < Emax$, stop. Output W, V, q, and E. Else $E \Leftarrow 0$,$p \Leftarrow 1$, go to Step 2.

Multilayer networks and the back-propagation algorithm

The back-propagation algorithm

(Stochastic gradient descent with <u>sigmoid activation function</u>).

- Step 1. Choose E_{max}, $\eta > 0$. Set $q \Leftarrow 1$, $p \Leftarrow 1$, $E \Leftarrow 0$. Initialize **W**, **V** randomly.

  - E_{max} is a stopping condition, stop training if $E < E_{max}$
  - $\eta > 0$ is the learning rate
  - q is a counter: total number of weights updates
  - p is an index, data sample d_p is presented to the network at this iteration.
  - E is the accumulated error at this iteration.

- Step 2. Present the input data: $\mathbf{z} \Leftarrow \mathbf{z}_p$, $\mathbf{d} \Leftarrow \mathbf{d}_p$ and compute

  $y_j \Leftarrow f(\mathbf{v}_j^T\mathbf{z})$ for j = 1, 2, …. J and

  $o_k \Leftarrow f(\mathbf{w}_k^T\mathbf{y})$ for k = 1, 2, …. K

  - **d** is the target output (target features) and **z** is the input (descriptive features)
  - $\mathbf{v}_j$ is the vector weight from the input to hidden unit j
  - $\mathbf{y}_j$ is the activation value at hidden unit j
  - $\mathbf{w}_k$ is the vector weight from the hidden units to output unit k
  - $\mathbf{o}_k$ is the activation value at output unit k

Multilayer networks and the back-propagation algorithm

The back-propagation algorithm (continued).

- Step 3. Compute the error: $E \Leftarrow ½ (\mathbf{d}_k – \mathbf{o}_k)^2 + E$ for k = 1,2, … K

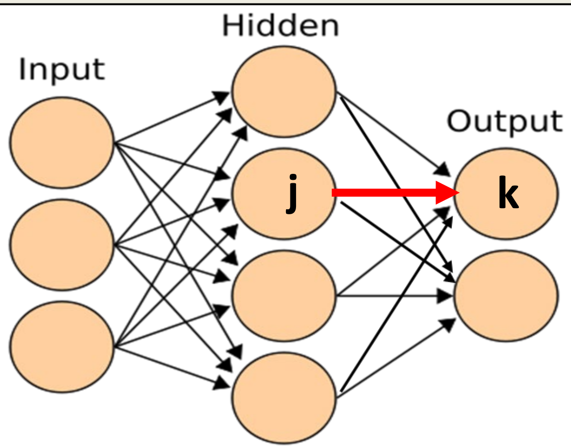
  - The difference between the target output and predicted output at output unit k is error $d_k – o_k$.
  - Accumulate sum of squared errors in E.

- Step 4. Compute error signal vectors δ_o and δ_y for output and hidden layer units:

$$\delta_{ok} = (\mathbf{d}_k - \mathbf{o}_k)(1 - \mathbf{o}_k)\mathbf{o}_k \quad \text{for } k = 1, 2, \ldots K$$

  - For the output unit, since $o_k \Leftarrow f(\mathbf{w}_k^T\mathbf{y}) = \sigma(\mathbf{w}_k^T\mathbf{y})$, we want to compute the partial derivative of E with respect to w_{kj}, where w_{kj} is the weight from hidden unit j to output unit k

$$\begin{aligned}
\partial E/\partial \mathbf{w}_{kj} &= \partial/\partial \mathbf{w}_{kj}\, ½ (\mathbf{d}_k – \mathbf{o}_k)^2 \\
&= (\mathbf{d}_k – \mathbf{o}_k)\, \partial/\partial \mathbf{w}_{kj} (\mathbf{d}_k – \mathbf{o}_k) \\
&= (– 1)(\mathbf{d}_k – \mathbf{o}_k)(1 – \mathbf{o}_k)\mathbf{o}_k\ \partial/\partial \mathbf{w}_{kj} (\mathbf{w}_k^T\mathbf{y}) \\
&= (– 1)(\mathbf{d}_k – \mathbf{o}_k)(1 – \mathbf{o}_k)\mathbf{o}_k\ \mathbf{y}_j \\
&= – \delta_{ok}\, \mathbf{y}_j
\end{aligned}$$



Multilayer networks and the back-propagation algorithm

The back-propagation algorithm (continued).

- Step 4. Compute error signal vectors δ_o and δ_y for output and hidden layer units:

$$\delta_{yj} = \mathbf{y}_j(1 - \mathbf{y}_j) \sum_{i=1}^{K} \delta_{ok}\mathbf{w}_{kj} \text{ for } j = 1, 2, \ldots J$$

◦ For the hidden unit j, $y_j \Leftarrow f(\mathbf{v}_j^T\mathbf{z}) = \sigma(\mathbf{v}_j^T\mathbf{z})$, we compute the partial derivative of E with respect to v_{ji}, where v_{ji} is the weight from input unit i to output unit j

$$\partial E/\partial \mathbf{v}_{ji} = \partial/\partial \mathbf{v}_{ji} \tfrac{1}{2} (\mathbf{d}_k - \mathbf{o}_k)^2 \text{ for } k = 1, 2 \ldots. K$$

$$= \tfrac{1}{2} \sum_{i=1}^{K} \partial/\partial \mathbf{v}_{ji} (\mathbf{d}_k - \mathbf{o}_k)^2$$

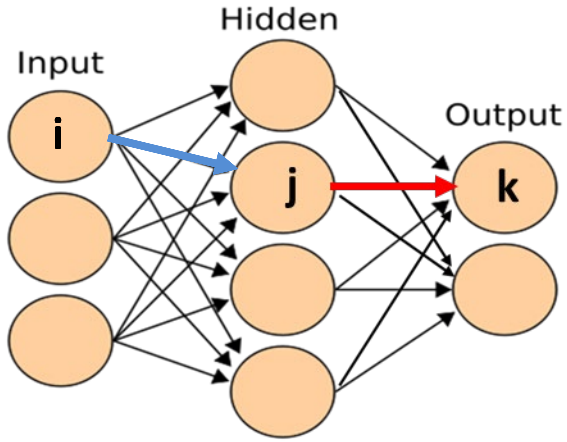
$$= \sum_{i=1}^{K} (\mathbf{d}_k - \mathbf{o}_k)\, \partial/\partial \mathbf{v}_{kj} (\mathbf{d}_k - \mathbf{o}_k)$$

$$= (-1) \sum_{i=1}^{K} (\mathbf{d}_k - \mathbf{o}_k)(1 - \mathbf{o}_k)\mathbf{o}_k\, \partial/\partial \mathbf{v}_{ji} (\mathbf{w}_k^T\mathbf{y})$$

$$= (-1) \sum_{i=1}^{K} \delta_{ok}\, \partial/\partial \mathbf{v}_{ji} (\mathbf{w}_k^T\mathbf{y})$$

$$= (-1)(1 - \mathbf{y}_j)\mathbf{y}_j \sum_{i=1}^{K} \delta_{ok}\mathbf{w}_{kj}\, \partial/\partial \mathbf{v}_{ji} (\mathbf{v}_j^T\mathbf{z})$$

$$= -\delta_{yj}\, z_i$$



Recall: $\delta_{ok} = (\mathbf{d}_k - \mathbf{o}_k)(1 - \mathbf{o}_k)\mathbf{o}_k$
and $\delta_{yj} = \mathbf{y}_j(1 - \mathbf{y}_j) \sum_{k=1}^{K} \delta_{ok}\mathbf{w}_{kj}$

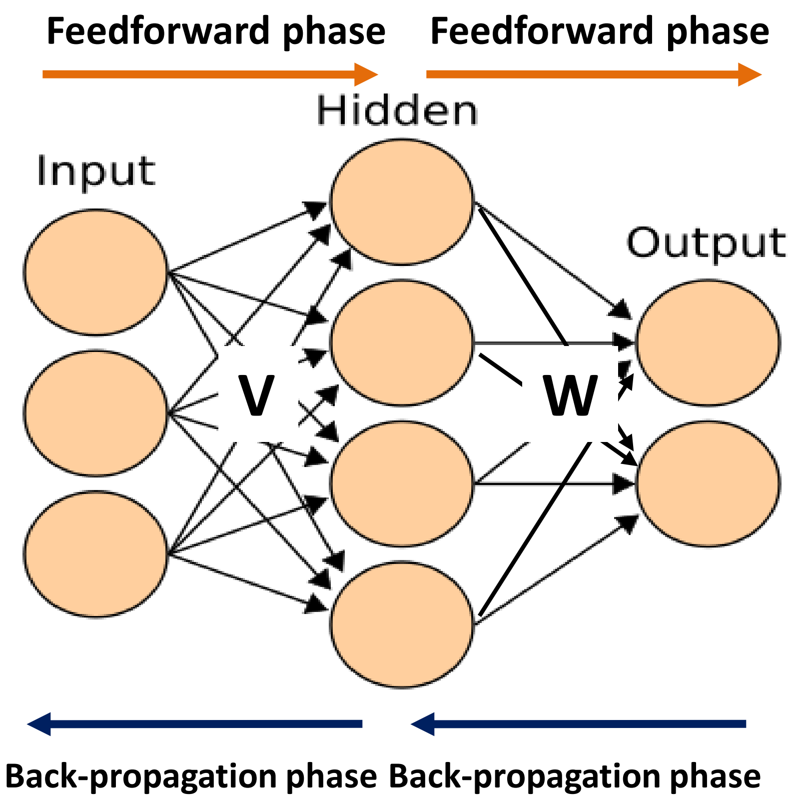
Multilayer networks and the back-propagation algorithm

The back-propagation algorithm (continued).

- Step 5. Update output layer and hidden layer weights:

$$\mathbf{w}_{kj} \Leftarrow \mathbf{w}_{kj} + \eta\, \delta_{ok}\, \mathbf{y}_j \text{ for } k = 1, 2, \dots K \text{ and } j = 1, 2, \dots J$$

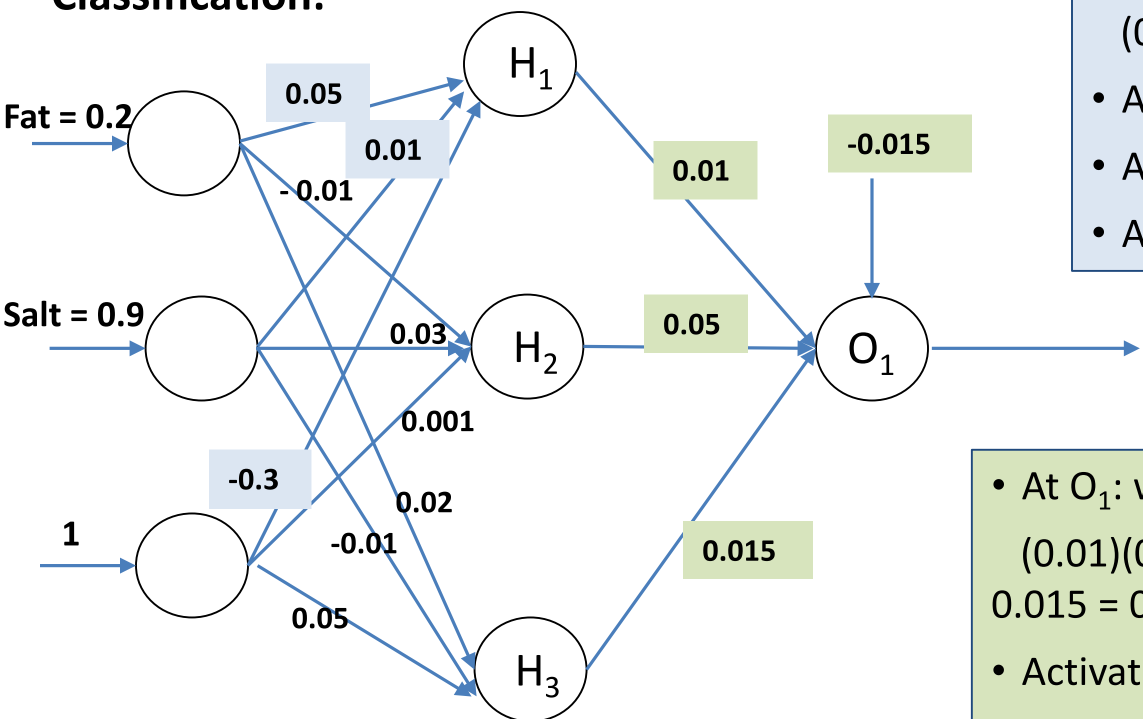
$$\mathbf{v}_{ji} \Leftarrow \mathbf{v}_{ji} + \eta\, \delta_{yj}\, \mathbf{z}_i \text{ for } j = 1, 2, \dots J \text{ and } i = 1, 2, \dots I$$



Multilayer networks and the back-propagation algorithm

The back-propagation algorithm (feedforward phase).

Classification:



- At H_1: $w_1x_1 + w_2x_2 + w_3x_3 =$ $(0.05)(0.2) + (0.01)(0.9) – 0.3 = -0.281$
- Activation value H_1: $1/(1 + e^{0.281}) = 0.430$
- Activation value H_2: $1/(1 + e^{-0.026}) = 0.506$
- Activation value H_3: $1/(1 + e^{-0.045})= 0.511$

- At O_1: $w_1x_1 + w_2x_2 + w_3x_3 + bias =$ $(0.01)(0.430) + (0.05)(0.506) + (0.015)(0.511) – 0.015 = 0.0223$
- Activation value O_1: $1/(1 + e^{-0.0223}) = 0.506$
- If we use a cut-off of 0.5, we classify this sample as Class 1 because 0.506 > 1

7. Remarks on the backpropagation algorithm

Convergence and local minima

- The BP algorithm implements a gradient descent search through the space of possible weights.
- It iteratively reduces the error E between the training sample target values and the network outputs.
- The error surface may contain many local minima and BP may be trapped in a local minimum.
- BP is a very effective function approximation method.
- A local minimum with respect to one weight will not necessarily be a local minimum with respect to other weights: more weights might provide more “escape routes” for gradient descent.
- More local minima are expected to exist in the region of the weight space representing more complex nonlinear function. It is hoped that when the network weights reach this region, they are already close enough to the global minimum.

Remarks on the backpropagation algorithm

Avoiding local minima

- Use **stochastic gradient** instead of true gradient descent:
  - Stochastic approximation descents a different error surface for each training example relying on the average of these to approximate the gradient with respect to full training set.
  - Use a <u>subset</u> of training data samples to update the weights.
  - Patterns can be <u>randomized</u> within each training cycle rather then submitted for training as a fixed sequence.
- Train multiple networks using the same data:
  - Initialize each network with different random weights.
  - Select the network with the best performance over a separate validation set, or
  - Form a committee of networks whose output is the (possibly weighted) average of the individual network outputs.

Remarks on the backpropagation algorithm

Representational power of feedforward networks

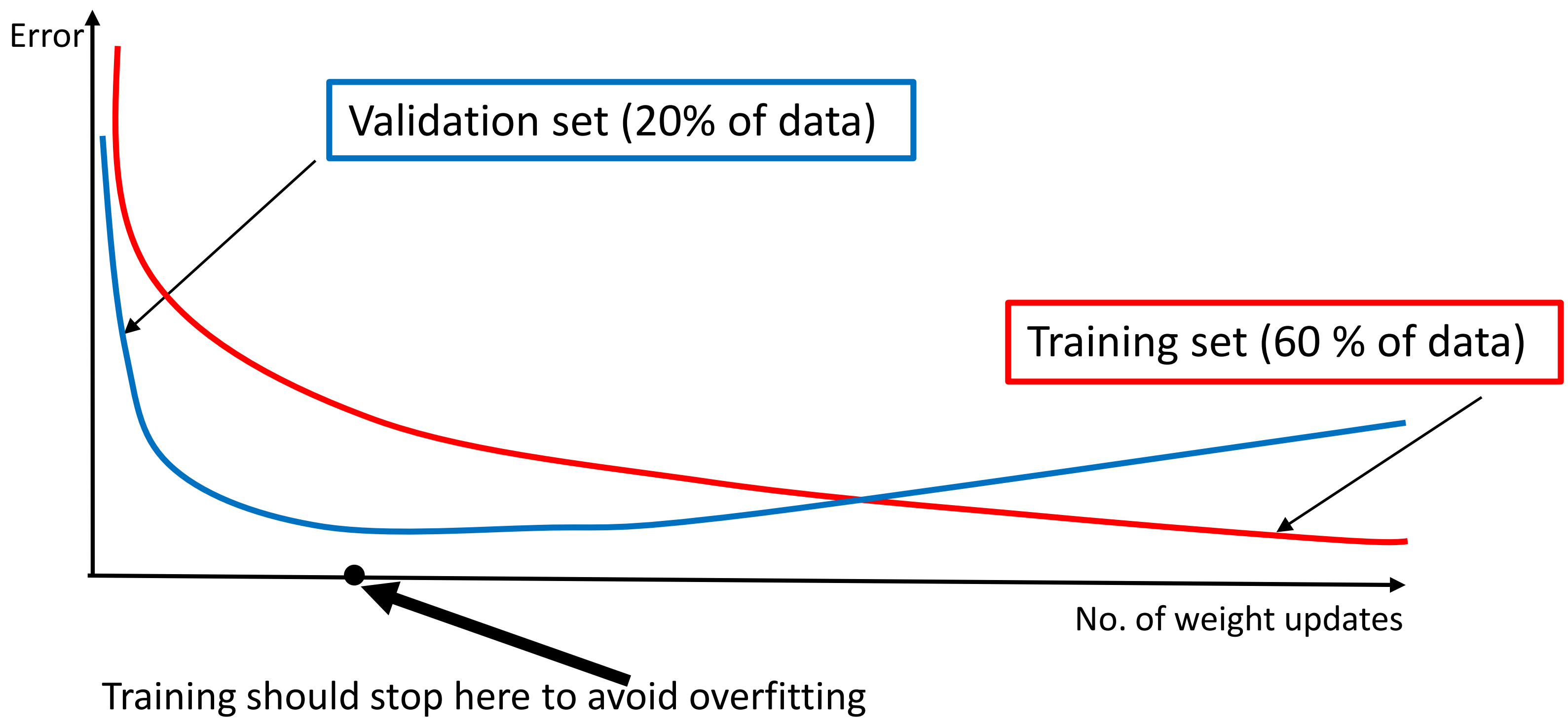
Set of functions that can be represented by feedforward networks:

- Boolean function:
  - every Boolean function can be represented exactly by some two layers of units.
  - The number of hidden units needed may be equal to the number of network inputs in the worst case.
- Continuous function:
  - every bounded continuous function can be approximated with arbitrarily small error by a network with two layers of units.
  - Hidden layer with sigmoid units and output layer with linear units.

Remarks on the backpropagation algorithm

Generalization, overfitting and stopping criteria

- To improve generalization and reduce overfitting, it is recommended that the available data samples be split into three sets: training set, cross validation set and test set. For example: 60%, 20%, 20%.
- Network training is terminated when the network weights produce the lowest total error for the samples in the cross validation set.



References.

- Machine Learning, Tom M. Mitchell, McGraw-Hill International Editions, Chapter 4.
- Neural Networks, Simon Haykin, Prentice Hall, Chapter 4.
- Introduction to Artificial Neural Systems, Jacek M. Zurada, PWS Publishing Company, Chapter 4.