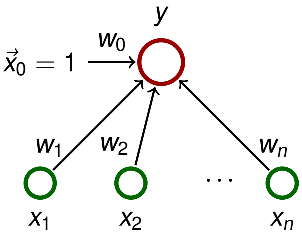
ADALINE

Architecture:



$\vec{w} = (w_0, w_1, \ldots, w_n)$ and $\vec{x} = (x_0, x_1, \ldots, x_n)$ where $x_0 = 1$.

Activity:

- inner potential: $\xi = w_0 + \sum_{i=1}^{n} w_i x_i = \sum_{i=0}^{n} w_i x_i = \vec{w} \cdot \vec{x}$
- activation function: $\sigma(\xi) = \xi$
- network function: $y[\vec{w}](\vec{x}) = \sigma(\xi) = \vec{w} \cdot \vec{x}$

ADALINE

Learning:

- Given a **training set**

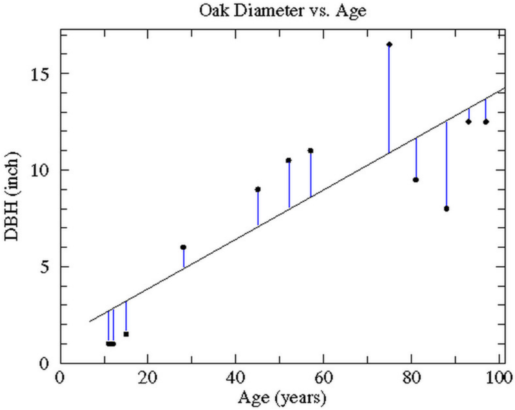
$$\mathcal{T} = \left\{ \left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \ldots, \left(\vec{x}_p, d_p\right) \right\}$$

Here $\vec{x}_k = (x_{k0}, x_{k1} \ldots, x_{kn}) \in \mathbb{R}^{n+1}$, $x_{k0} = 1$, is the k-th input, and $d_k \in \mathbb{R}$ is the expected output.

Intuition: The network is supposed to compute an affine approximation of the function (some of) whose values are given in the training set.

Oaks in Wisconsin

Age (years)	*DBH* (inch)
97	12.5
93	12.5
88	8.0
81	9.5
75	16.5
57	11.0
52	10.5
45	9.0
28	6.0
15	1.5
12	1.0
11	1.0



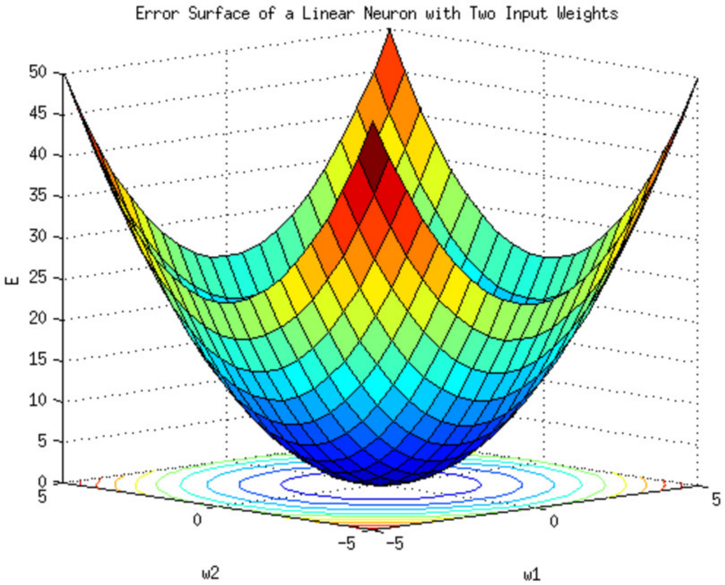
ADALINE

- **Error function:**

$$E(\vec{w}) = \frac{1}{2}\sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right)^2 = \frac{1}{2}\sum_{k=1}^{p}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2$$

- The goal is to find $\vec{w}$ which minimizes $E(\vec{w})$.

Error function



Gradient of the error function

Consider **gradient** of the error function:

$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w}) \right)$$

Intuition: $\nabla E(\vec{w})$ is a vector in the **weight space** which points in the direction of the *steepest ascent* of the error function.

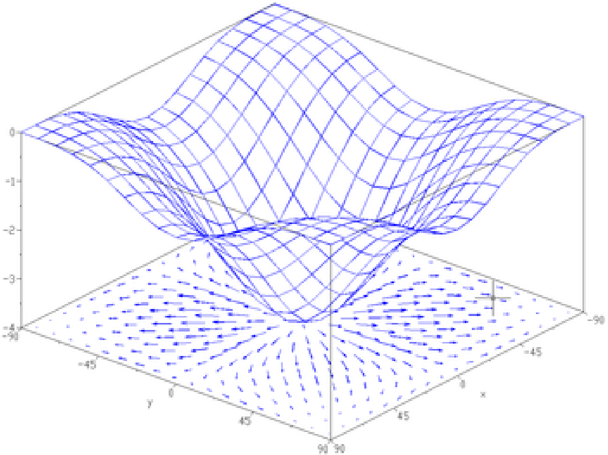
Note that the vectors $\vec{x}_k$ are just parameters of the function E, and are thus fixed!

Fact

If $\nabla E(\vec{w}) = \vec{0} = (0, \ldots, 0)$, *then* $\vec{w}$ *is a global minimum of* E.

For ADALINE, the error function $E(\vec{w})$ is a convex paraboloid and thus has the unique global minimum.

Gradient - illustration



Caution! This picture just illustrates the notion of gradient ... it is not the convex paraboloid $E(\vec{w})$!

Gradient of the error function (ADALINE)

$$\begin{aligned}
\frac{\partial E}{\partial w_\ell}(\vec{w}) &= \frac{1}{2}\sum_{k=1}^{p} \frac{\delta E}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)^2 \\
&= \frac{1}{2}\sum_{k=1}^{p} 2\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)\frac{\delta E}{\delta w_\ell}\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right) \\
&= \frac{1}{2}\sum_{k=1}^{p} 2\left(\sum_{i=0}^{n} w_i x_{ki} - d_k\right)\left(\sum_{i=0}^{n}\left(\frac{\delta E}{\delta w_\ell} w_i x_{ki}\right) - \frac{\delta E}{\delta w_\ell} d_k\right) \\
&= \sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right) x_{k\ell}
\end{aligned}$$

Thus

$$\nabla E(\vec{w}) = \left(\frac{\partial E}{\partial w_0}(\vec{w}), \ldots, \frac{\partial E}{\partial w_n}(\vec{w})\right) = \sum_{k=1}^{p}\left(\vec{w}\cdot\vec{x}_k - d_k\right)\vec{x}_k$$

ADALINE - learning

Batch algorithm (gradient descent):

Idea: In every step "move" the weights in the direction *opposite* to the gradient.

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$, weights $\vec{w}^{(t+1)}$ are computed as follows:

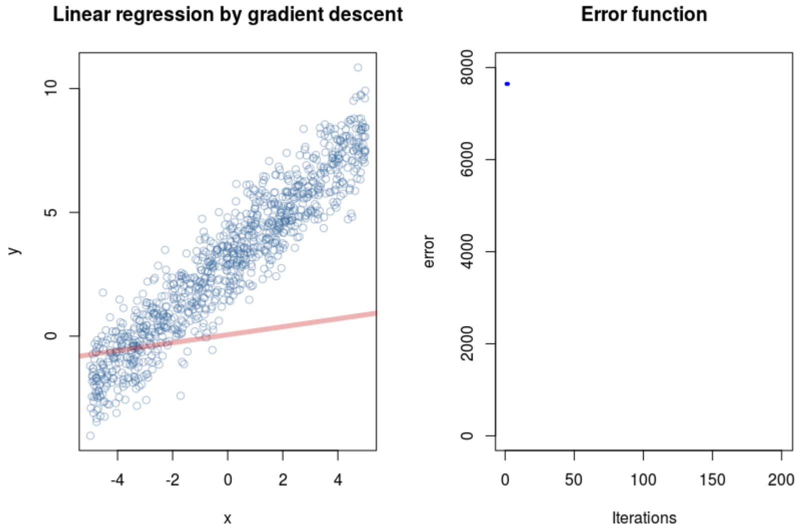
$$\begin{aligned} \vec{w}^{(t+1)} &= \vec{w}^{(t)} - \varepsilon \cdot \nabla E(\vec{w}^{(t)}) \\ &= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k \right) \cdot \vec{x}_k \end{aligned}$$

Here $k = (t \mod p) + 1$ and $0 < \varepsilon \leq 1$ is a *learning rate*.

Proposition

For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (componentwise) to the global minimum of E (i.e. to the vector $\vec{w}$ satisfying $\nabla E(\vec{w}) = \vec{0}$).

ADALINE – Animation



Linear regression by gradient descent

Error function

ADALINE - learning

Online algorithm (Delta-rule, Widrow-Hoff rule):

- weights in $\vec{w}^{(0)}$ initialized randomly close to 0
- in the step $t+1$, weights $\vec{w}^{(t+1)}$ are computed as follows:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \left(\vec{w}^{(t)} \cdot \vec{x}_k - d_k\right) \cdot \vec{x}_k$$

Here $k = t \mod p + 1$ and $0 < \varepsilon(t) \leq 1$ is a learning rate in the step $t+1$.

Note that the algorithm does not work with the complete gradient but only with its part determined by the currently considered training example.

Theorem (Widrow & Hoff)

If $\varepsilon(t) = \frac{1}{t}$, then $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges to the global minimum of E.

ADALINE - classification

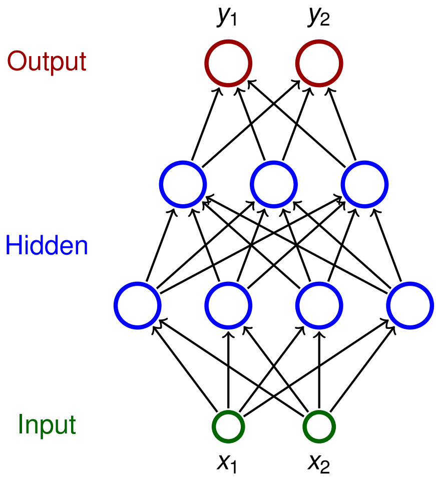
How to use the ADALINE for classification?

- The training set is

$$\mathcal{T} = \left\{ \left(\vec{x}_1, d_1\right), \left(\vec{x}_2, d_2\right), \ldots, \left(\vec{x}_p, d_p\right) \right\}$$

  kde $\vec{x}_k = (x_{k0}, x_{k1}, \ldots, x_{kn}) \in \mathbb{R}^{n+1}$ a $d_k \in \{1, -1\}$.
  Here d_k determines a class.
- Train the network using the ADALINE algorithm.
- We may expect the following:
  - if $d_k = 1$, then $\vec{w} \cdot \vec{x}_k \geq 0$
  - if $d_k = -1$, then $\vec{w} \cdot \vec{x}_k < 0$
- This does not have to be always true but if the training set is reasonably linearly separable, then the algorithm typically gives satisfactory results.

Architecture – Multilayer Perceptron (MLP)



- Neurons partitioned into **layers**; one input layer, one output layer, possibly several hidden layers
- layers numbered from 0; the input layer has number 0
  - E.g. three-layer network has two hidden layers and one output layer
- Neurons in the i-th layer are connected with all neurons in the $i+1$-st layer
- Architecture of a MLP is typically described by numbers of neurons in individual layers (e.g. 2-4-3-2)

MLP – architecture

Notation:

- Denote
  - X a set of *input* neurons
  - Y a set of *output* neurons
  - Z a set of *all* neurons ($X, Y \subseteq Z$)
- individual neurons denoted by indices i, j etc.
  - ξ_j is the inner potential of the neuron j *after the computation stops*
  - y_j is the output of the neuron j *after the computation stops*

  (define $y_0 = 1$ is the value of the formal unit input)
- w_{ji} is the weight of the connection **from** i **to** j

  (in particular, w_{j0} is the weight of the connection from the formal unit input, i.e. $w_{j0} = -b_j$ where b_j is the bias of the neuron j)
- $j_{\leftarrow}$ is a set of all i such that j is adjacent from i
  (i.e. there is an arc **to** j from i)
- $j^{\rightarrow}$ is a set of all i such that j is adjacent to i
  (i.e. there is an arc **from** j to i)

MLP – activity

Activity:

- inner potential of neuron j:

$$\xi_j = \sum_{i \in j_{\leftarrow}} w_{ji} y_i$$

- activation function σ_j for neuron j (arbitrary differentiable)
  [e.g. logistic sigmoid $\sigma_j(\xi) = \frac{1}{1+e^{-\lambda_j \xi}}$]
- State of non-input neuron $j \in Z \setminus X$ after the computation stops:

$$y_j = \sigma_j(\xi_j)$$

  (y_j depends on the configuration $\vec{w}$ and the input $\vec{x}$, so we sometimes write $y_j(\vec{w}, \vec{x})$)
- The network computes a function $\mathbb{R}^{|X|}$ do $\mathbb{R}^{|Y|}$. Layer-wise computation: First, all input neurons are assigned values of the input. In the ℓ-th step, all neurons of the ℓ-th layer are evaluated.

MLP – learning

Learning:

- Given a **training set** $\mathcal{T}$ of the form

$$\left\{ \left(\vec{x}_k, \vec{d}_k\right) \;\middle|\; k = 1, \ldots, p \right\}$$

  Here, every $\vec{x}_k \in \mathbb{R}^{|X|}$ is an *input vector* end every $\vec{d}_k \in \mathbb{R}^{|Y|}$ is the desired network output. For every $j \in Y$, denote by d_{kj} the desired output of the neuron j for a given network input $\vec{x}_k$ (the vector $\vec{d}_k$ can be written as $\left(d_{kj}\right)_{j \in Y}$).

- **Error function:**

$$E(\vec{w}) = \sum_{k=1}^{p} E_k(\vec{w})$$

  where

$$E_k(\vec{w}) = \frac{1}{2} \sum_{j \in Y} \left(y_j(\vec{w}, \vec{x}_k) - d_{kj}\right)^2$$

MLP – learning algorithm

Batch algorithm (gradient descent):

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2 \ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

  $$w_{ji}^{(t+1)} = w_{ji}^{(t)} + \Delta w_{ji}^{(t)}$$

  where

  $$\Delta w_{ji}^{(t)} = -\varepsilon(t) \cdot \frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$$

  is a *weight update* of w_{ji} in step $t+1$ and $0 < \varepsilon(t) \leq 1$ is a *learning rate* in step $t+1$.

Note that $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t)})$ is a component of the gradient ∇E, i.e. the weight update can be written as $\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon(t) \cdot \nabla E(\vec{w}^{(t)})$.

MLP – error function gradient

For every w_{ji} we have

$$\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$$

where for every $k = 1, \ldots, p$ holds

$$\frac{\partial E_k}{\partial w_{ji}} = \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

and for every $j \in Z \smallsetminus X$ we get

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj} \qquad \text{for } j \in Y$$

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj} \qquad \text{for } j \in Z \smallsetminus (Y \cup X)$$

(Here all y_j are in fact $y_j(\vec{w}, \vec{x}_k)$).

MLP – error function gradient

- If $\sigma_j(\xi) = \frac{1}{1+e^{-\lambda_j \xi}}$ for all $j \in Z$, then

$$\sigma'_j(\xi_j) = \lambda_j y_j (1 - y_j)$$

and thus for all $j \in Z \setminus X$:

$$\frac{\partial E_k}{\partial y_j} = y_j - d_{kj} \qquad \text{for } j \in Y$$

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \lambda_r y_r (1 - y_r) \cdot w_{rj} \qquad \text{for } j \in Z \setminus (Y \cup X)$$

- If $\sigma_j(\xi) = a \cdot \tanh(b \cdot \xi_j)$ for all $j \in Z$, then

$$\sigma'_j(\xi_j) = \frac{b}{a}(a - y_j)(a + y_j)$$

MLP – computing the gradient

Compute $\frac{\partial E}{\partial w_{ji}} = \sum_{k=1}^{p} \frac{\partial E_k}{\partial w_{ji}}$ as follows:

Initialize $\mathcal{E}_{ji} := 0$
(By the end of the computation: $\mathcal{E}_{ji} = \frac{\partial E}{\partial w_{ji}}$)

For every $k = 1, \ldots, p$ do:

1. **forward pass:** compute $y_j = y_j(\vec{w}, \vec{x}_k)$ for all $j \in Z$
2. **backward pass:** compute $\frac{\partial E_k}{\partial y_j}$ for all $j \in Z$ using *backpropagation* (see the next slide!)
3. compute $\frac{\partial E_k}{\partial w_{ji}}$ for all w_{ji} using

$$\frac{\partial E_k}{\partial w_{ji}} := \frac{\partial E_k}{\partial y_j} \cdot \sigma_j'(\xi_j) \cdot y_i$$

4. $\mathcal{E}_{ji} := \mathcal{E}_{ji} + \frac{\partial E_k}{\partial w_{ji}}$

The resulting $\mathcal{E}_{ji}$ equals $\frac{\partial E}{\partial w_{ji}}$.

MLP – backpropagation

Compute $\frac{\partial E_k}{\partial y_j}$ for all $j \in Z$ as follows:

- if $j \in Y$, then $\frac{\partial E_k}{\partial y_j} = y_j - d_{kj}$
- if $j \in Z \setminus Y \cup X$, then assuming that j is in the ℓ-th layer and assuming that $\frac{\partial E_k}{\partial y_r}$ has already been computed for all neurons in the $\ell + 1$-st layer, compute

$$\frac{\partial E_k}{\partial y_j} = \sum_{r \in j^{\rightarrow}} \frac{\partial E_k}{\partial y_r} \cdot \sigma_r'(\xi_r) \cdot w_{rj}$$

(This works because all neurons of $r \in j^{\rightarrow}$ belong to the $\ell + 1$-st layer.)

Complexity of the batch algorithm

Computation of $\frac{\partial E}{\partial w_{ji}}(\vec{w}^{(t-1)})$ stops in time linear in the size of the network plus the size of the training set.

(assuming unit cost of operations including computation of $\sigma'_r(\xi_r)$ for given ξ_r)

Proof sketch: The algorithm does the following p times:

1. forward pass, i.e. computes $y_j(\vec{w}, \vec{x}_k)$
2. backpropagation, i.e. computes $\frac{\partial E_k}{\partial y_j}$
3. computes $\frac{\partial E_k}{\partial w_{ji}}$ and adds it to $\mathcal{E}_{ji}$ (a constant time operation in the unit cost framework)

The steps 1. - 3. take linear time.

Note that the speed of convergence of the gradient descent cannot be estimated ...

MLP – learning algorithm

Online algorithm:

The algorithm computes a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t = 0, 1, 2\ldots$), weights $\vec{w}^{(t+1)}$ are computed as follows:

$$w_{ji}^{(t+1)} = w_{ji}^{(t)} + \Delta w_{ji}^{(t)}$$

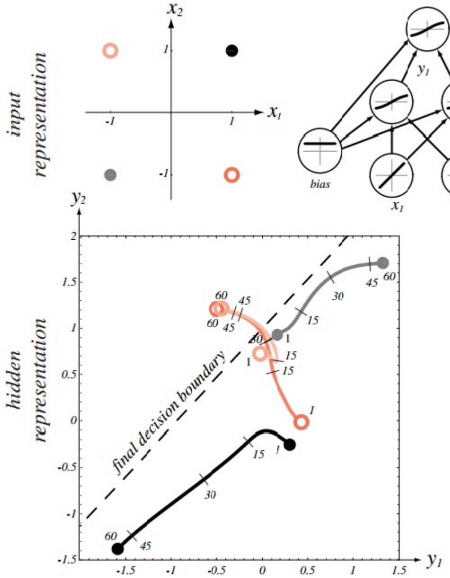
where

$$\Delta w_{ji}^{(t)} = -\varepsilon(t) \cdot \frac{\partial E_k}{\partial w_{ji}}(w_{ji}^{(t)})$$

is the *weight update* of w_{ji} in the step $t+1$ and $0 < \varepsilon(t) \leq 1$ is the *learning rate* in the step $t+1$.

There are other variants determined by selection of the training examples used for the error computation (more on this later).

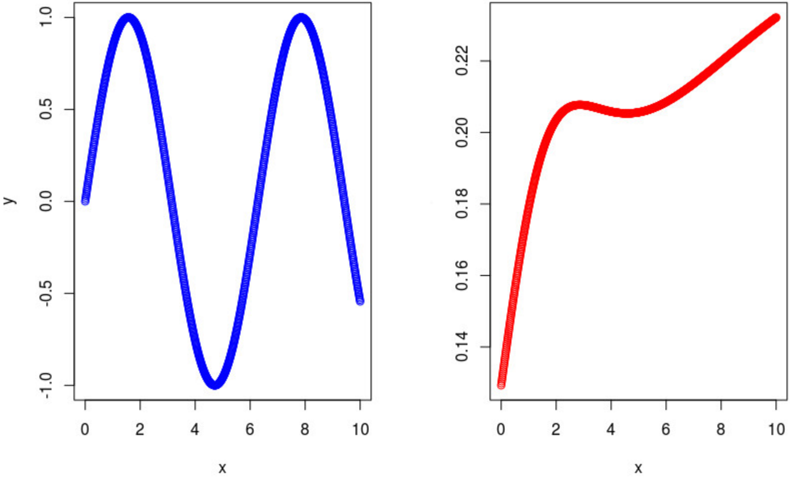
Illustration of the gradient descent – XOR



Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

Animation (sin(x)), network 1-5-1)

One iteration:



10 iterations: