Numerical features

- ► Throughout this lecture we assume that all features are numerical, i.e. feature vectors belong to ℝⁿ.
- Most non-numerical features can be conveniently transformed to numerical ones.

For example:

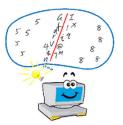
- \blacktriangleright Colors {blue, red, yellow} can be represented by {0,1,2} (or {-1,0,1}, ...)
- ► A black-and-white picture of x × y pixels can be encoded as a vector of xy numbers that capture the shades of gray of the pixels.

Basic Problems

We consider two basic problems:

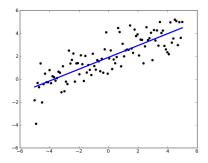
(Binary) classification

Our goal: Classify inputs into two categories.



 Function approximation (regression)

Our goal: Find a (hypothesized) functional dependency in data.



Binary classification in \mathbb{R}^n

- Assume
 - ▶ a set of instances $X \subseteq \mathbb{R}^n$,
 - an *unknown* categorization function $c : X \to \{0, 1\}$.
- Our goal:
 - Given a set *D* of training examples of the form $(\vec{x}, c(\vec{x}))$ where $\vec{x} \in X$,
 - ► construct a hypothesized categorization function h ∈ H that is consistent with c on the training examples, i.e.,

 $h(\vec{x}) = c(\vec{x})$ for all training examples $(\vec{x}, c(\vec{x})) \in D$

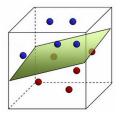
Comments:

- In practice, we often do not strictly demand h(x̄) = c(x̄) for all training examples (x̄, c(x̄)) ∈ D (often it is impossible)
- ▶ We are more interested in good generalization, that is how well *h* classifies new instances that do not belong to *D*.
 - Recall that we usually evaluate accuracy of the resulting hypothesized function h on a test set.

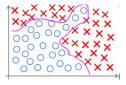
Hypothesis Spaces

We consider two kinds of hypothesis spaces:

Linear (affine) classifiers (this lecture)



 Classifiers based on combinations of linear and sigmoidal functions (classical neural networks) (next lecture)



Length and Scalar Product of Vectors

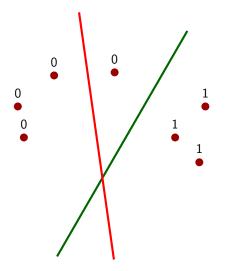
• We consider vectors $\vec{x} = (x_1, \dots, x_m) \in \mathbb{R}^m$.

- ► Typically, we use Euclidean metric on vectors: $|\vec{x}| = \sqrt{\sum_{i=1}^{m} x_i^2}$ The distance between two vectors (points) \vec{x}, \vec{y} is $|\vec{x} - \vec{y}|$.
- We use the scalar product x → y of vectors x = (x₁,...,x_m) and y = (y₁,...,y_m) defined by

$$\vec{x} \cdot \vec{y} = \sum_{i=1}^{m} x_i y_i$$

- Recall that x · y = |x||y| cos θ where θ is the angle between x and y. That is x · y is the length of the projection of y on x multiplied by |x|.
- Note that $\vec{x} \cdot \vec{x} = |\vec{x}|^2$

Linear classifier - example



- classification in plane using a linear classifier
- if a point is incorrectly classified, the learning algorithm turns the line (hyperplane) to improve the classification.

Linear Classifier

A *linear classifier* $h[\vec{w}]$ is determined by a vector of *weights* $\vec{w} = (w_0, w_1, \dots, w_n) \in \mathbb{R}^{n+1}$ as follows:

Given $\vec{x} = (x_1, \ldots, x_n) \in X \subseteq \mathbb{R}^n$,

$$h[\vec{w}](\vec{x}) := \begin{cases} 1 & w_0 + \sum_{i=1}^n w_i \cdot x_i \ge 0\\ 0 & w_0 + \sum_{i=1}^n w_i \cdot x_i < 0 \end{cases}$$

More succinctly:

$$h(\vec{x}) = sgn\left(w_0 + \sum_{i=1}^n w_i \cdot x_i\right) \qquad \text{where} \qquad sgn(y) = \begin{cases} 1 & y \ge 0\\ 0 & y < 0 \end{cases}$$

Linear Classifier – Notation

Given $\vec{x} = (x_1, \ldots, x_n) \in \mathbb{R}^n$ we define an *augmented feature vector*

 $\widetilde{\mathbf{x}} = (x_0, x_1, \dots, x_n)$ where $x_0 = 1$

This makes the notation for the linear classifier more succinct:

 $h[\vec{w}](\vec{x}) = sgn(\vec{w}\cdot\widetilde{\mathbf{x}})$

Perceptron Learning

Given a training set

 $D = \{ (\vec{x}_1, c(\vec{x}_1)), (\vec{x}_2, c(\vec{x}_2)), \dots, (\vec{x}_p, c(\vec{x}_p)) \}$ Here $\vec{x}_k = (x_{k1} \dots, x_{kn}) \in X \subseteq \mathbb{R}^n$ and $c(\vec{x}_k) \in \{0, 1\}$. We write c_k instead of $c(\vec{x}_k)$. Note that $\widetilde{x}_k = (x_{k0}, x_{k1} \dots, x_{kn})$ where $x_{k0} = 1$.

► A weight vector $\vec{w} \in \mathbb{R}^{n+1}$ is consistent with *D* if $h[\vec{w}](\vec{x}_k) = sgn(\vec{w} \cdot \widetilde{\mathbf{x}}_k) = c_k$ for all k = 1, ..., p

D is **linearly separable** if there is a vector $\vec{w} \in \mathbb{R}^{n+1}$ which is consistent with *D*.

• Our goal is to find a consistent \vec{w} assuming that D is linearly separable.

Perceptron – Learning Algorithm

Online learning algorithm:

Idea: Cyclically go through the training examples in D and adapt weights. Whenever an example is incorrectly classified, turn the hyperplane so that the example is closer to it's correct half-space.

Compute a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$

\$\vec{w}^{(0)}\$ is randomly initialized close to \$\vec{0} = (0,...,0\$)\$
\$\ln (t+1)\$-th step, \$\vec{w}^{(t+1)}\$ is computed as follows:
\$\vec{w}^{(t+1)}\$ = \$\vec{w}^{(t)}\$ − \$\varepsilon\$ · \$\left(h[\vec{w}^{(t)}](\vec{x}_k) - c_k\$\right)\$ · \$\vec{x}_k\$
\$\vec{w}^{(t)}\$ − \$\varepsilon\$ · \$\left(sgn(\vec{w}^{(t)} · \$\vec{x}_k\$\right)\$ − \$c_k\$\right)\$ · \$\vec{x}_k\$
Here \$k = (t\$ mod \$p\$) + 1\$, i.e. the examples are considered cyclically, and \$0 < \varepsilon\$ ≤ 1 is a learning speed.

Věta (Rosenblatt)

If D is linearly separable, then there is t^* such that $\vec{w}^{(t^*)}$ is consistent with D.

Example

Training set:

$$D = \{((2,-1),1),((2,1),1),((1,3),0)\}$$
 That is

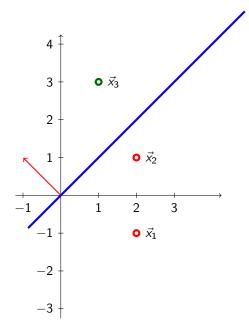
$$\begin{array}{rcl} \vec{x_1} &=& (2,-1) & & & \widetilde{x_1} &=& (1,2,-1) \\ \vec{x_2} &=& (2,1) & & & & \widetilde{x_2} &=& (1,2,1) \\ \vec{x_3} &=& (1,3) & & & & & \widetilde{x_3} &=& (1,1,3) \\ \end{array}$$

$$c_1 = 1$$

 $c_2 = 1$
 $c_3 = 0$

Assume that the initial vector $\vec{w}^{(0)}$ is $\vec{w}^{(0)} = (0, -1, 1)$. Consider $\varepsilon = 1$.

Example: Separating by $\vec{w}^{(0)}$



Denoting $\vec{w}^{(0)} =$ $(w_0, w_1, w_2) = (0, -1, 1)$ the blue separating line is given by $w_0 + w_1x_1 + w_2x_2 = 0$.

The red vector normal to the blue line is (w_1, w_2) .

The points on the side of (w_1, w_2) are assigned 1 by the classifier, the others zero. (In this case $\vec{x_3}$ is assigned one and $\vec{x_1}, \vec{x_2}$ are assigned zero, all of this is inconsistent with $c_1 = 1, c_2 = 1, c_3 = 0.$)

Example: $\vec{w}^{(1)}$

We have

$$\vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 = (0, -1, 1) \cdot (1, 2, -1) = 0 - 2 - 1 = -3$$

thus

$$sgn\left(ec{w}^{(0)}\cdot\widetilde{x}_{1}
ight)=0$$

and thus

$$sgn\left(ec{w}^{(0)}\cdot\widetilde{\mathtt{x}}_{1}
ight)-c_{1}=0-1=-1$$

(This means that $\vec{x_1}$ is not well classified, and $\vec{w}^{(0)}$ is not consistent with D.) Hence,

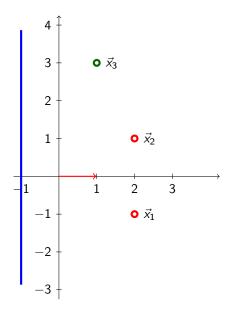
$$\vec{w}^{(1)} = \vec{w}^{(0)} - \left(sgn\left(\vec{w}^{(0)} \cdot \tilde{\mathbf{x}}_1 \right) - c_1 \right) \cdot \tilde{\mathbf{x}}_1$$

$$= \vec{w}^{(0)} + \tilde{\mathbf{x}}_1$$

$$= (0, -1, 1) + (1, 2, -1)$$

$$= (1, 1, 0)$$

Example



Example: Separating by $\vec{w}^{(1)}$

We have

$$\vec{w}^{(1)} \cdot \widetilde{x}_2 = (1, 1, 0) \cdot (1, 2, 1) = 1 + 2 = 3$$

thus

$$\textit{sgn}\left(ec{w}^{(1)}\cdot\widetilde{{\sf x}}_{2}
ight)=1$$

and thus

$$sgn\left(ec{w}^{(1)}\cdot\widetilde{\mathbf{x}}_{2}
ight)-c_{2}=1-1=0$$

(This means that \vec{x}_2 *is* currently well classified by $\vec{w}^{(1)}$. However, as we will see, \vec{x}_3 is not well classified.) Hence.

$$\vec{w}^{(2)} = \vec{w}^{(1)} = (1, 1, 0)$$

Example: $\vec{w}^{(3)}$

We have

$$\vec{w}^{(2)} \cdot \widetilde{\mathbf{x}}_3 = (1, 1, 0) \cdot (1, 1, 3) = 1 + 1 = 2$$

thus

$$sgn\left(ec{w}^{(2)}\cdot\widetilde{{\sf x}}_3
ight)=1$$

and thus

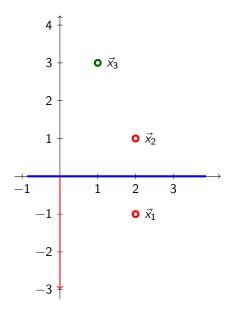
$$sgn\left(\vec{w}^{(2)}\cdot\widetilde{\mathbf{x}}_3\right)-c_3=1-0=1$$

(This means that \vec{x}_3 is not well classified, and $\vec{w}^{(2)}$ is not consistent with D.) Hence,

$$\vec{w}^{(3)} = \vec{w}^{(2)} - \left(sgn\left(\vec{w}^{(2)} \cdot \tilde{\mathbf{x}}_{3}\right) - c_{3}\right) \cdot \tilde{\mathbf{x}}_{3}$$

= $\vec{w}^{(2)} - \tilde{\mathbf{x}}_{3}$
= $(1, 1, 0) - (1, 1, 3)$
= $(0, 0, -3)$

Example: Separating by $\vec{w}^{(3)}$



Example: $\vec{w}^{(4)}$

We have

$$\vec{w}^{(3)} \cdot \tilde{\mathbf{x}}_1 = (0, 0, -3) \cdot (1, 2, -1) = 3$$

thus

$$sgn\left(ec{w}^{(3)}\cdot\widetilde{{\sf x}}_{1}
ight)=1$$

and thus

$$sgn\left(ec{w}^{(3)}\cdot\widetilde{\mathbf{x}}_{1}
ight)-c_{1}=1-1=0$$

(This means that $\vec{x_1}$ is currently well classified by $\vec{w}^{(3)}$. However, as we will see, $\vec{x_2}$ is not.) Hence,

$$\vec{w}^{(4)} = \vec{w}^{(3)} = (0, 0, -3)$$

Example: $\vec{w}^{(5)}$

We have

$$\vec{w}^{(4)} \cdot \widetilde{x}_2 = (0, 0, -3) \cdot (1, 2, 1) = -3$$

thus

$$sgn\left(ec{w}^{(4)}\cdot\widetilde{\mathbf{x}}_{2}
ight)=0$$

and thus

$$sgn\left(ec{w}^{(4)}\cdot\widetilde{\mathbf{x}}_{2}
ight)-c_{2}=0-1=-1$$

(This means that \vec{x}_2 is not well classified, and $\vec{w}^{(4)}$ is not consistent with D.) Hence,

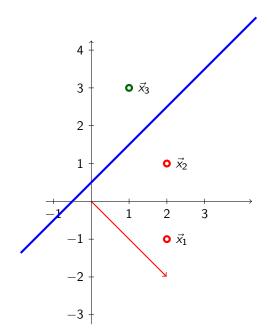
$$\vec{w}^{(5)} = \vec{w}^{(4)} - \left(sgn\left(\vec{w}^{(4)} \cdot \tilde{\mathbf{x}}_2 \right) - c_2 \right) \cdot \tilde{\mathbf{x}}_2$$

$$= \vec{w}^{(4)} + \tilde{\mathbf{x}}_2$$

$$= (0, 0, -3) + (1, 2, 1)$$

$$= (1, 2, -2)$$

Example: Separating by $\vec{w}^{(5)}$



Example: The result

The vector $\vec{w}^{(5)}$ is consistent with *D*:

$$sgn\left(\vec{w}^{(5)}\cdot\widetilde{x}_{1}\right) = sgn\left((1,2,-2)\cdot(1,2,-1)\right) = sgn(7) = 1 = c_{1}$$

$$sgn\left(\vec{w}^{(5)} \cdot \tilde{\mathbf{x}}_{2}\right) = sgn\left((1, 2, -2) \cdot (1, 2, 1)\right) = sgn(3) = 1 = c_{2}$$
$$sgn\left(\vec{w}^{(5)} \cdot \tilde{\mathbf{x}}_{3}\right) = sgn\left((1, 2, -2) \cdot (1, 1, 3)\right) = sgn(-3) = 0 = c_{3}$$

Perceptron – Learning Algorithm

Batch learning algorithm:

Compute a sequence of weight vectors $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \dots$

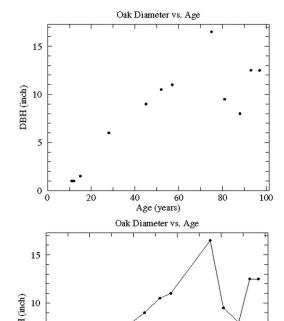
- $\vec{w}^{(0)}$ is randomly initialized close to $\vec{0} = (0, \dots, 0)$
- ▶ In (t + 1)-th step, $\vec{w}^{(t+1)}$ is computed as follows:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(h[\vec{w}^{(t)}](\vec{x}_{k}) - c_{k} \right) \cdot \widetilde{\mathbf{x}}_{k}$$
$$= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(sgn\left(\vec{w}^{(t)} \cdot \widetilde{\mathbf{x}}_{k}\right) - c_{k} \right) \cdot \widetilde{\mathbf{x}}_{k}$$

Here $k = (t \mod p) + 1$, i.e. the examples are considered cyclically, and $0 < \varepsilon \le 1$ is a learning speed.

Function Approximation – Oaks in Wisconsin

This example is from How to Lie with Statistics by Darrell Huff (1954)



Age (years)	<i>DBH</i> (inch)
97	12.5
93	12.5
00	0.0

Function Approximation

Assume

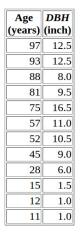
- a set $X \subseteq \mathbb{R}^n$ of instances,
- an *unknown* function $f: X \to \mathbb{R}$.
- Our goal:
 - Given a set *D* of training examples of the form $(\vec{x}, f(\vec{x}))$ where $\vec{x} \in X$,
 - construct a hypothesized function h ∈ H such that h(x) ≈ f(x) for all training examples (x, f(x)) ∈ D Here ≈ means that the values are somewhat close to each other w.r.t. an appropriate *error function E*.
- In what follows we use the *least squares* defined by

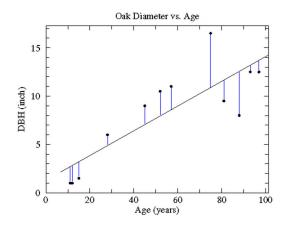
$$E = \frac{1}{2} \sum_{(\vec{x}, f(\vec{x})) \in D} (f(\vec{x}) - h(\vec{x}))^2$$

Our goal is to minimize E.

The main reason is that this function has nice mathematical properties (as opposed e.g. to $\sum_{(\vec{x}, f(\vec{x})) \in D} |f(\vec{x}) - h(\vec{x})|$).

Least Squares – Oaks in Wisconsin





Linear Function Approximation

Given a set D of training examples:

$$D = \{ (\vec{x}_1, f(\vec{x}_1)), (\vec{x}_2, f(\vec{x}_2)), \dots, (\vec{x}_p, f(\vec{x}_p)) \}$$

Here $\vec{x}_k = (x_{k1} \dots, x_{kn}) \in \mathbb{R}^n$ and $f_k(\vec{x}) \in \mathbb{R}$. Recall that $\tilde{\mathbf{x}}_k = (x_{k0}, x_{k1} \dots, x_{kn})$.

Our goal: Find \vec{w} so that $h[\vec{w}](\vec{x}) = \vec{w} \cdot \vec{x}$ approximates the function f some of whose values are given by the training set.

Least Squares Error Function:

$$E(\vec{w}) = \frac{1}{2} \sum_{k=1}^{p} (\vec{w} \cdot \tilde{\mathbf{x}}_{k} - f_{k})^{2} = \frac{1}{2} \sum_{k=1}^{p} \left(\sum_{i=0}^{n} w_{i} x_{ki} - f_{k} \right)^{2}$$

Gradient of the Error Function

Consider the gradient of the error function:

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

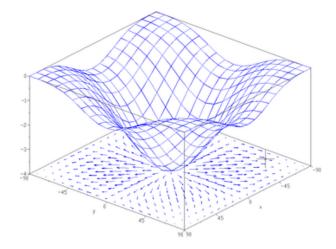
What is the gradient $\nabla E(\vec{w})$? It is a vector in \mathbb{R}^{n+1} which points in the direction of the steepest *ascent* of *E* (it's length corresponds to the steepness). Note that here the vectors $\tilde{\mathbf{x}}_k$ are *fixed* parameters of *E*!

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

This follows from the fact that E is a convex paraboloid that has a unique extreme which is a minimum.



Gradient - illustration



Function Approximation – Learning

Gradient Descent:

- Weights $\vec{w}^{(0)}$ are initialized randomly close to $\vec{0}$.
- ▶ In (t+1)-th step, $\vec{w}^{(t+1)}$ is computed as follows:

$$\vec{w}^{(t+1)} = \vec{w}^{(t)} - \varepsilon \cdot \nabla E(\vec{w}^{(t)})$$

$$= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(\vec{w}^{(t)} \cdot \widetilde{\mathbf{x}}_{k} - f_{k} \right) \cdot \widetilde{\mathbf{x}}_{k}$$

$$= \vec{w}^{(t)} - \varepsilon \cdot \sum_{k=1}^{p} \left(h[\vec{w}^{(t)}](\vec{x}_{k}) - f_{k} \right) \cdot \widetilde{\mathbf{x}}_{k}$$

Here $k = (t \mod p) + 1$ and $0 < \varepsilon \le 1$ is the learning speed.

Note that the algorithm is almost similar to the batch perceptron algorithm!

Tvrzení

For sufficiently small $\varepsilon > 0$ the sequence $\vec{w}^{(0)}, \vec{w}^{(1)}, \vec{w}^{(2)}, \ldots$ converges (component-wisely) to the global minimum of E.

Finding the Minimum in Dimension One

Assume n = 1. Then the error function E is

$$E(w_0, w_1) = \frac{1}{2} \sum_{k=1}^{p} (w_0 + w_1 x_k - f_k)^2$$

Minimize E w.r.t. w_0 a w_1 :

$$\frac{\delta E}{\delta w_0} = 0 \quad \Leftrightarrow \quad w_0 = \bar{f} - w_1 \bar{x} \quad \Leftrightarrow \quad \bar{f} = w_0 + w_1 \bar{x}$$

where
$$\bar{x} = \frac{1}{p} \sum_{k=1}^{p} x_k$$
 a $\bar{f} = \frac{1}{p} \sum_{k=1}^{p} f_k$

$$\frac{\delta E}{\delta w_1} = 0 \quad \Leftrightarrow \quad w_1 = \frac{\frac{1}{p} \sum_{k=1}^{p} (f_k - \bar{f})(x_k - \bar{x})}{\frac{1}{p} \sum_{k=1}^{p} (x_k - \bar{x})^2}$$

i.e. $w_1 = cov(f, x) / var(x)$

Finding the Minimum in Arbitrary Dimension

Let A be a matrix $p \times (n+1)$ (p rows, n+1 columns) whose k-th row is the vector $\tilde{\mathbf{x}}_k$.

Let $\vec{f} = (f_1, \dots, f_p)^\top$ be the *column* vector formed by values of f in the training set.

Then

$$abla E(\vec{w}) = 0 \quad \Leftrightarrow \quad \vec{w} = (A^{\top}A)^{-1}A^{\top}\vec{f}$$

if $(A^{\top}A)^{-1}$ exists

(Then $(A^{\top}A)^{-1}A^{\top}$ is the so called Moore-Penrose pseudoinverse of A.)

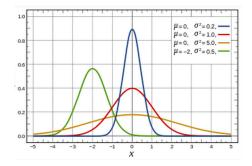
Normal Distribution – Reminder

Distribution of continuous random variables.

Density (one dimensional, that is over \mathbb{R}):

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} =: N[\mu,\sigma^2](x)$$

 μ is the expected value (the mean), σ^2 is the variance.



Maximum Likelihood vs Least Squares (Dim 1)

Fix a training set $D = \{(x_1, f_1), (x_2, f_2), \dots, (x_p, f_p)\}$ Assume that each f_k has been generated randomly by

 $f_k = (w_0 + w_1 \cdot x_k) + \epsilon_k$

Here

w₀, w₁ are unknown numbers

• ϵ_k are normally distributed with mean 0 and an unknown variance σ^2

Assume that $\epsilon_1, \ldots, \epsilon_p$ were generated **independently**.

Denote by $p(f_1, \ldots, f_p | w_0, w_1, \sigma^2)$ the probability density according to which the values f_1, \ldots, f_n were generated assuming fixed $w_0, w_1, \sigma^2, x_1, \ldots, x_p$.

(For interested: The independence and normality imply

$$p(f_1,\ldots,f_p \mid w_0,w_1,\sigma^2) = \prod_{k=1}^p N[w_0 + w_1x_k,\sigma^2](f_k)$$

where $N[w_0 + w_1 x_k, \sigma^2](f_k)$ is a normal distribution with the mean $w_0 + w_1 x_k$ and the variance σ^2 .)

Maximum Likelihood vs Least Squares

Our goal is to find (w_0, w_1) that maximizes the likelihood that the training set D with fixed values f_1, \ldots, f_n has been generated:

 $L(w_0, w_1, \sigma^2) := p(f_1, \ldots, f_p \mid w_0, w_1, \sigma^2)$

Věta

 (w_0, w_1) maximizes $L(w_0, w_1, \sigma^2)$ for arbitrary σ^2 iff (w_0, w_1) minimizes $E(w_0, w_1)$, i.e. the least squares error function.

Note that the maximizing/minimizing (w_0, w_1) does not depend on σ^2 .

Maximizing
$$\sigma^2$$
 satisfies $\sigma^2 = \frac{1}{p} \sum_{k=1}^{p} (f_k - w_0 - w_1 \cdot x_k)^2$.

Comments on Linear Models

- Linear models are parametric, i.e. they have a fixed form with a small number of parameters that need to be learned from data (as opposed e.g. to decision trees where the structure is not fixed in advance).
- Linear models are stable, i.e. small variations in the training data have only limited impact on the learned model. (tree models typically vary more with the training data).
- Linear models are less likely to overfit (low variance) the training data but sometimes tend to underfit (high bias).