

Machine Learning and Pervasive Computing

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Overview and Structure

- 22.10.2014 Organisation
- 22.10.3014 Introduction (Def.: Machine learning, Supervised/Unsupervised, Examples)
- 29.10.2014 Machine Learning Basics (Toolchain, Features, Metrics, Rule-based)
- 05.11.2014** A simple Supervised learning algorithm
- 12.11.2014 Excursion: Avoiding local optima with random search
- 19.11.2014 –
- 26.11.2014** Bayesian learner
- 03.12.2014 –
- 10.12.2014 Decision tree learner
- 17.12.2014** k-nearest neighbour
- 07.01.2015 Support Vector Machines
- 14.01.2015** Artificial Neural networks and Self Organizing Maps
- 21.01.2015 Hidden Markov models and Conditional random fields
- 28.01.2015** High dimensional data, Unsupervised learning
- 04.02.2015 Anomaly detection, Online learning, Recom. systems

Outline

Linear regression

Least squares estimation

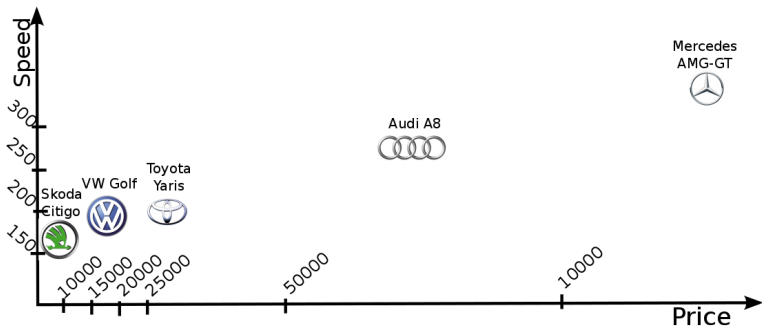
Polynomial regression

Multivariable linear regression

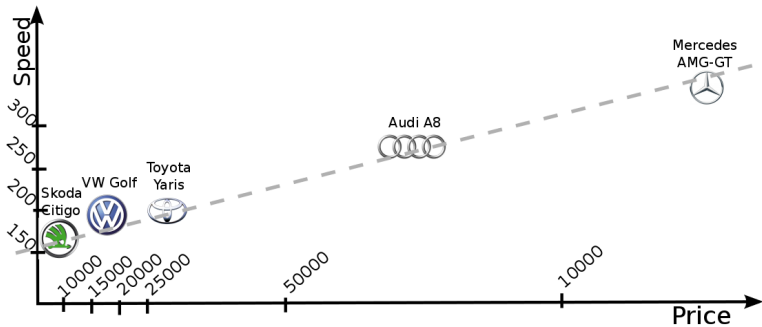
Multivariate linear regression

Logistic regression

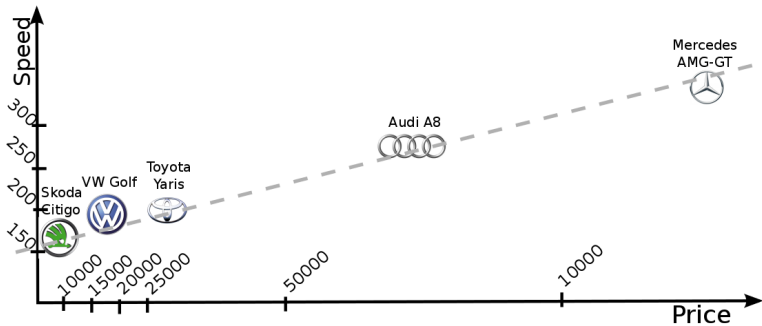
Linear regression



Linear regression

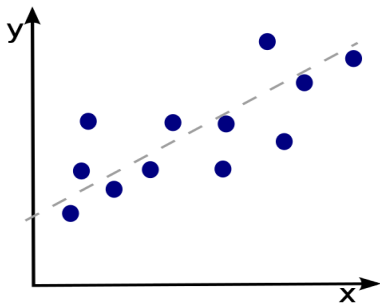


Linear regression



$$h(x) = w_0 + w_1x$$

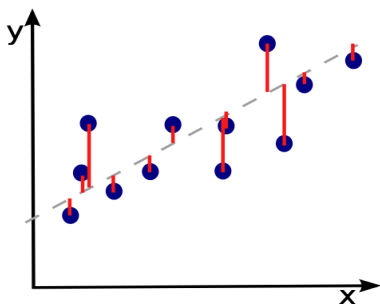
Linear regression



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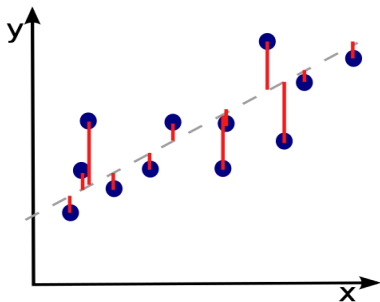
How to choose the parameter w_0 and w_1 ?

Linear regression



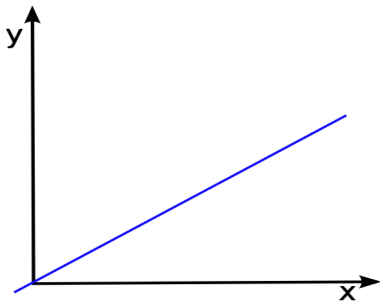
$$h(x) = w_0 + w_1x$$

Cost function to estimate the quality of the current solution
(Gradient descent).



$$h(x) = w_0 + w_1x$$
$$\text{minimize } E[w_0, w_1] = \frac{1}{2n} \sum_{i=1}^n (h(x_i) - y_i)^2$$

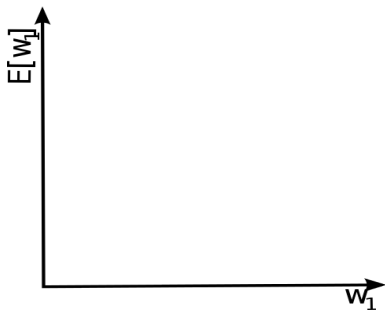
Gradient descent cost function – intuition



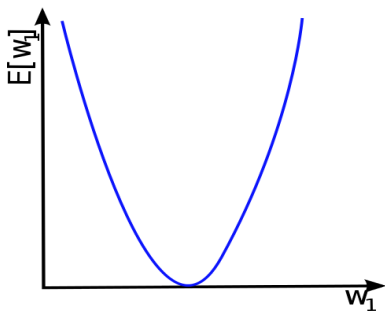
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For fixed w_1 this is a function of x
(additive constant w_0 ignored in this figure)

Gradient descent cost function – intuition



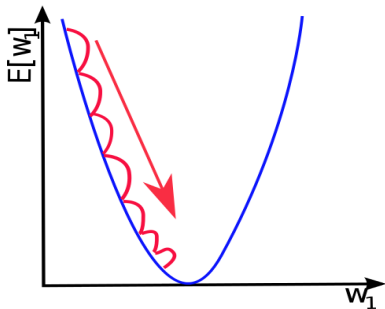
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(additive constant w_0 ignored in this figure)

Gradient descent cost function – Gradient descent



$$\text{minimize } E[w_0, w_1] = \frac{1}{2n} \sum_{i=1}^n (h(x_i) - y_i)^2$$

$$\text{E.g.: } w_1 = w_1 - \delta \cdot \frac{\partial}{\partial w_1} E[w_0, w_1]$$

Iterative approximation of w_1

Outline

Linear regression

Least squares estimation

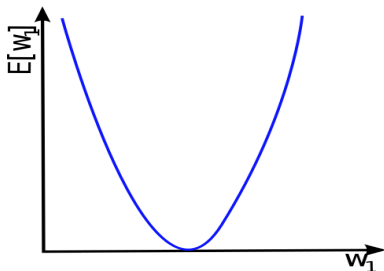
Polynomial regression

Multivariable linear regression

Multivariate linear regression

Logistic regression

Least squares estimation



Given an error function

$$E[w_0, w_1] = \sum_{i=1}^n (y_i - (w_0 + w_1 x))^2$$

we can minimize the error by requiring

$$\frac{\partial E}{\partial w_0} = 0, \frac{\partial E}{\partial w_1} = 0$$

Least squares estimation

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$$E[w_0, w_1] = \sum_{i=1}^n (y_i - (w_0 + w_1 x_i))^2$$

we can minimize the error by requiring

$$\frac{\partial E}{\partial w_0} = 0, \frac{\partial E}{\partial w_1} = 0$$

Differentiation yields

$$\begin{aligned} \frac{\partial E}{\partial w_0} &= \sum_{i=1}^n 2(y_i - (w_1 x_i + w_0)) \cdot 1 \\ \frac{\partial E}{\partial w_1} &= \sum_{i=1}^n 2(y_i - (w_1 x_i + w_0)) \cdot (-x_i) \end{aligned}$$

Least squares estimation

$$\frac{\partial E}{\partial w_0} = \sum_{i=1}^n 2(y_i - (w_1 x_i + w_0)) \cdot 1$$
$$\frac{\partial E}{\partial w_1} = \sum_{i=1}^n 2(y_i - (w_1 x_i + w_0)) \cdot (-x_i)$$

Setting

$$\frac{\partial E}{\partial w_0} = \frac{\partial E}{\partial w_1} = 0$$

will lead to

$$\sum_{i=1}^n (y_i - (w_1 x_i + w_0)) \cdot x_i = 0$$
$$\sum_{i=1}^n (y_i - (w_1 x_i + w_0)) = 0$$

Least squares estimation

$$\sum_{i=1}^n (y_i - (w_1 x_i + w_0)) \cdot x_i = 0$$

$$\sum_{i=1}^n (y_i - (w_1 x_i + w_0)) = 0$$

rewrite as

$$\left(\sum_{i=1}^n x_i^2 \right) w_1 + \left(\sum_{i=1}^n x_i \right) w_0 = \sum_{i=1}^n x_i y_i$$

$$\left(\sum_{i=1}^n x_i \right) w_1 + \left(\sum_{i=1}^n 1 \right) w_0 = \sum_{i=1}^n y_i$$

Least squares estimation

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Consequently, values of w_0 and w_1 that minimize the error satisfy

$$\begin{pmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{pmatrix} \begin{pmatrix} w_1 \\ w_0 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{pmatrix}$$

Least squares estimation

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for an invertible matrix this implies

$$\begin{pmatrix} w_1 \\ w_0 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i \\ \sum_{i=1}^n x_i & \sum_{i=1}^n 1 \end{pmatrix}^{-1} \begin{pmatrix} \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n y_i \end{pmatrix}$$

By solving this linear equation system, optimal values of w_0 and w_1 can be determined.

Least squares estimation

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By solving this linear equation system, optimal values of w_0 and w_1 can be determined.

However, for least squares to be applicable, it is necessary that the matrix is invertible.

Outline

Linear regression

Least squares estimation

Polynomial regression

Multivariable linear regression

Multivariate linear regression

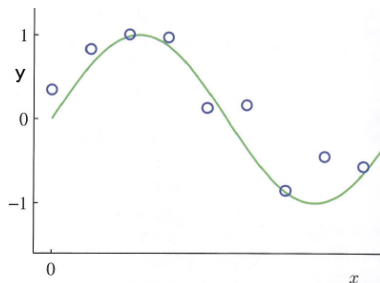
Logistic regression

Polynomial regression (Polynomial curve fitting)

Example

A curve shall be approximated by a machine learning approach

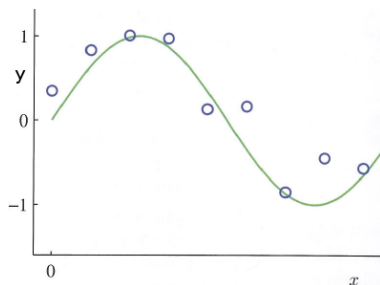
Sample points are created for the function $\sin(2\pi x) + \mathcal{N}$ where \mathcal{N} is a random noise value



Polynomial curve fitting

We will try to fit the data points into a polynomial function:

$$h(x, \vec{w}) = w_0 + w_1x + w_2x^2 + \cdots + w_Mx^M = \sum_{j=0}^M w_jx^j$$



Polynomial curve fitting

We will try to fit the data points into a polynomial function:

$$h(x, \vec{w}) = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j$$

This can be obtained by minimising an **error function** that measures the misfit between $h(x, \vec{w})$ and the training data set:

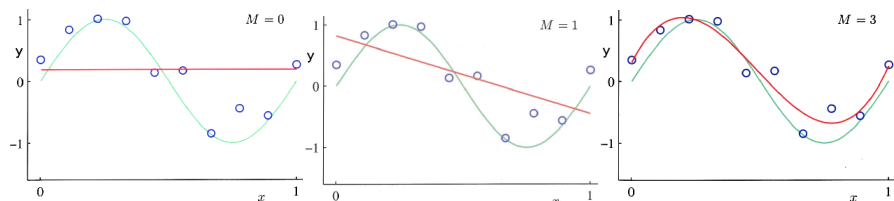
$$E(\vec{w}) = \frac{1}{2} \sum_{i=1}^N [h(x_i, \vec{w}) - y_i]^2$$

$E(\vec{w})$ is non-negative and zero if and only if all points are covered by the function

Polynomial curve fitting

One problem is the right choice of the dimension M

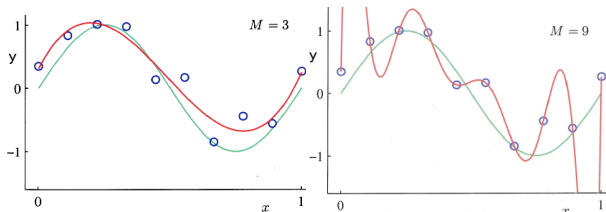
When M is too small, the approximation accuracy might be bad



Polynomial curve fitting

However, when M becomes too big, the resulting polynomial will cross all points exactly

When M reaches the count of samples in the training data set, it is always possible to create a polynomial of order M that contains all values in the data set exactly.



Polynomial curve fitting

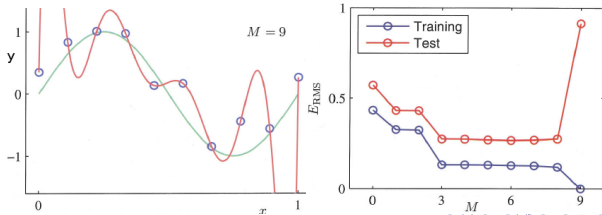
This event is called **overfitting**

The polynomial is now trained too well to the training data

It will therefore perform badly on another sample of test data for the same phenomenon

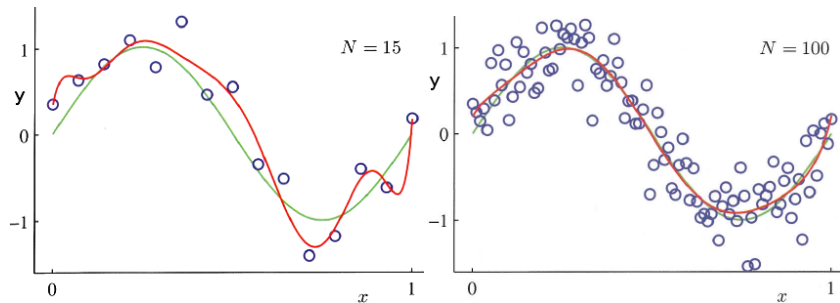
We visualise it by the Root of the Mean Square (RMS) of $E(\vec{w})$

$$E_{RMS} = \sqrt{\frac{2E(\vec{w})}{N}}$$



Polynomial curve fitting

With increasing number of data points, the problem of overfitting becomes less severe for a given value of M



Polynomial curve fitting

One solution to cope with **overfitting** is **regularisation**

A penalty term is added to the error function

This term discourages the coefficients of \vec{w} from reaching large values

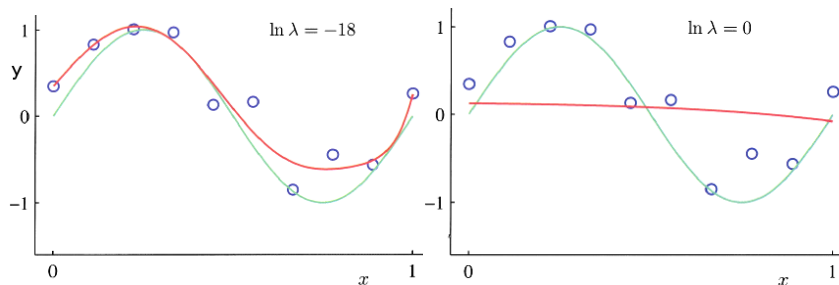
$$\bar{E}(\vec{w}) = \frac{1}{2} \sum_{i=1}^N [h(x_i, \vec{w}) - y_i]^2 + \frac{\lambda}{2} \|\vec{w}\|^2$$

with

$$\|\vec{w}\|^2 = \vec{w}^T \vec{w} = w_0^2 + w_1^2 + \dots + w_M^2$$

Polynomial curve fitting

Depending on the value of λ , overfitting is controlled



$$\bar{E}(\vec{w}) = \frac{1}{2} \sum_{i=1}^N [h(x_i, \vec{w}) - y_i]^2 + \frac{\lambda}{2} \|\vec{w}\|^2$$

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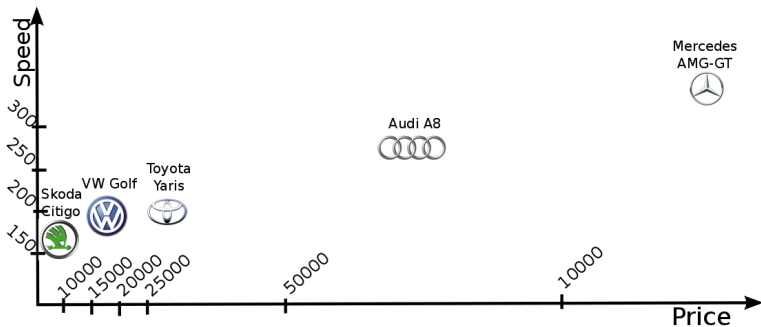
In multivariable linear regression problems we assume that multiple regression variables (features) apply.

Multivariable linear regression

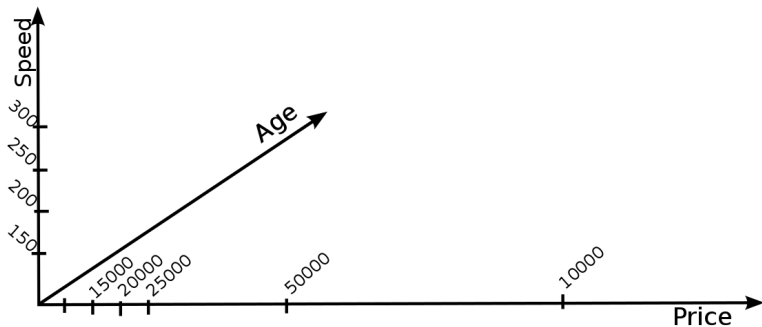
In multivariable linear regression problems we assume that multiple regression variables (features) apply.

$$h(x_{j1}, \dots, x_{jm}) = \sum_{i=0}^m w_i x_{ji}$$
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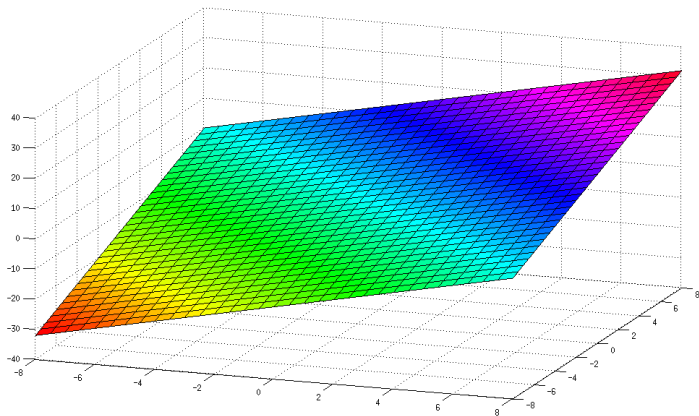
Multivariable linear regression



Multivariable linear regression



Multivariable linear regression



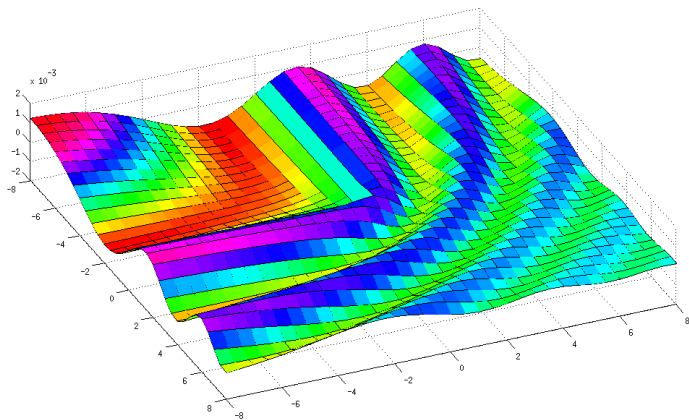
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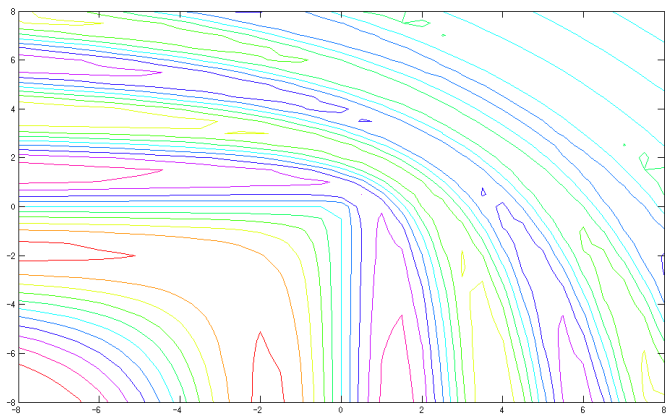
$$\text{E.g.: } w_i = w_i - \delta \cdot \frac{\partial}{\partial w_i} E[W]$$

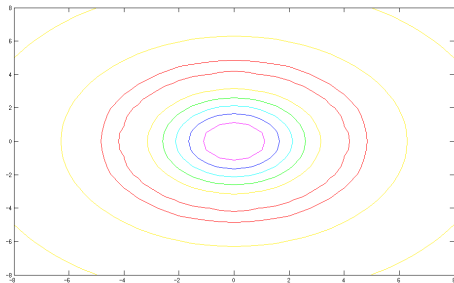
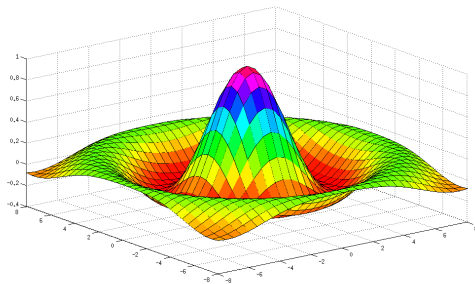
w_i are optimised together over several iterations

Local optima



Local optima – contour plot





Outline

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Multivariate linear regression

Logistic regression

Multivariate linear regression

Multivariate linear regression describes a regression problem with multiple classes.

Example e.g. from accelerometer data

Activities walking, standing, climbing/descending stairs, ...

Sentiment emotional states

Transportation mode office, riding tram, driving ...

Location Home, office, ...

Multivariate linear regression

Regression model is extended to multiple responses with respect to one class: $Y_j = y_{j1}, \dots, y_{jl}$

$$y_{j1} = w_{01} + w_{11}x_{j1} + \dots + w_{n1}x_{jn}$$

$$y_{j2} = w_{02} + w_{12}x_{j1} + \dots + w_{n2}x_{jn}$$

$$\vdots \qquad \qquad \qquad \vdots$$

$$y_{jl} = w_{0l} + w_{1l}x_{j1} + \dots + w_{nl}x_{jn}$$

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It is then possible to estimate the regression coefficients associated with y_{ji} using only the i -th row of the matrix.

Multivariate linear regression

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$$W_i = (X^T X)^{-1} X^T Y_{(i)}$$

and collecting all univariate estimates into a matrix

$$W = (X^T X)^{-1} X^T Y$$

$Y_{(i)}$ is the vector of n measurements of the i -th variable
 X^T denotes the transpose of X and X^{-1} its inverse

Multivariate linear regression

The least squares estimator for W minimizes the sums of squares elements on the diagonal of the residual sum of squares and crossproducts matrix $(Y - XW)^T(Y - XW)$

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Nominal classes

Classes might be nominal in real-world problems

Logistic regression

Nominal classes

Classes might be nominal in real-world problems

Weather Sunny, rainy

Medical positive diagnosis, negative diagnosis

Localisation indoor, outdoor

Logistic regression

Nominal classes

Classes might be nominal in real-world problems

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In such case, classification is binary: $y \in \{0, 1\}$

Logistic regression

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Linear regression: $h(x)$ can be smaller than 0 or greater than 1

Logistic regression

Nominal classes

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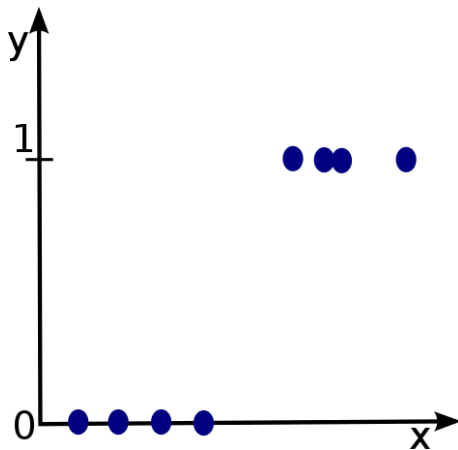
In such case, classification is binary: $y \in \{0, 1\}$

Linear regression: $h(x)$ can be smaller than 0 or greater than 1

Logistic regression: $0 \leq h(x) \leq 1$

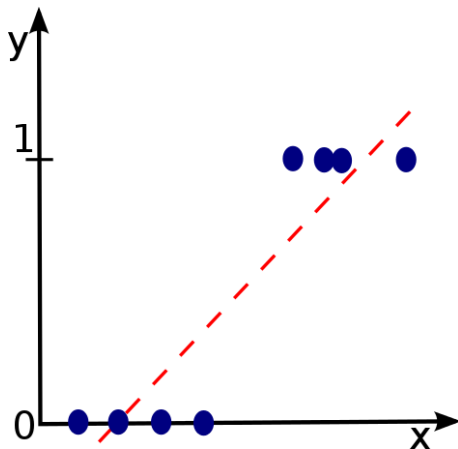
Logistic regression

Nominal classes



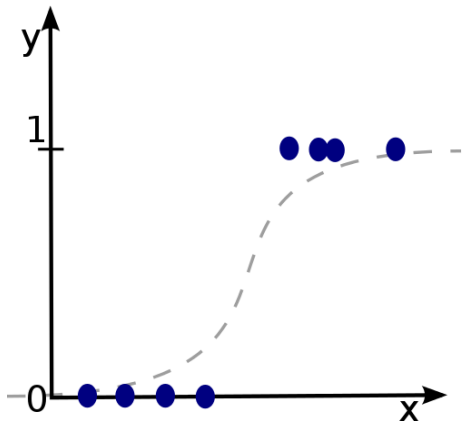
Logistic regression

Nominal classes



Logistic regression

Cost function



Logistic regression

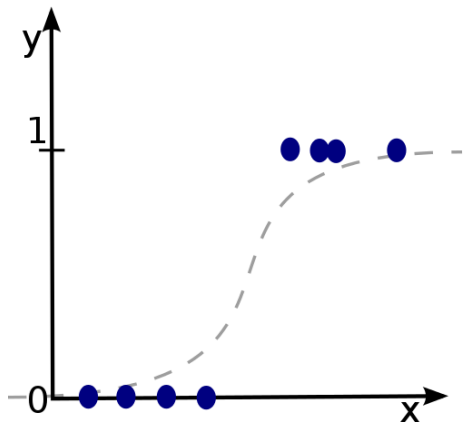
Cost function

Linear regression

$$h(x) = W^T x$$

Logistic regression

$$h(x) = \frac{1}{1 + e^{-W^T x}}$$



Logistic regression

Cost function

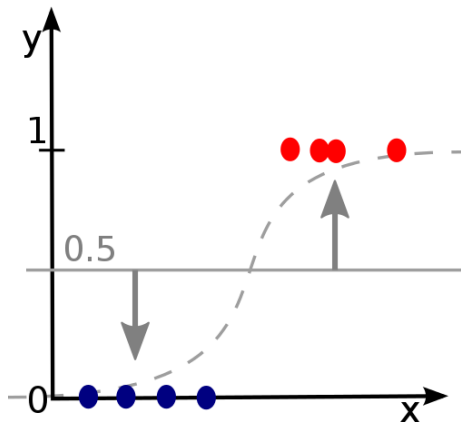
Linear regression

$$h(x) = W^T x$$

Logistic regression

$$h(x) = \frac{1}{1 + e^{-W^T x}}$$

$$y = \begin{cases} 1 & \text{if } h(x) \geq 0.5 \\ 0 & \text{else} \end{cases}$$

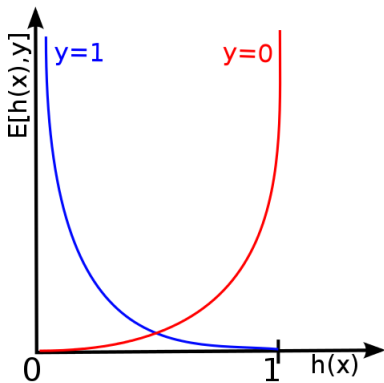


Logistic regression

Cost function

$$y = \begin{cases} 1 & \text{if } h(x) \geq 0.5 \\ 0 & \text{else} \end{cases}$$

$$E[h(x), y] = \begin{cases} -\log(h(x)) & \text{if } y = 1 \\ -\log(1 - h(x)) & \text{else} \end{cases}$$



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Questions?

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Literature

- C.M. Bishop: Pattern recognition and machine learning, Springer, 2007.
- R.O. Duda, P.E. Hart, D.G. Stork: Pattern Classification, Wiley, 2001.

