Aalto University
School of Electrical Engineering

CS-C3240 – Machine Learning D

Round 2: Regression

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Version 1.4, September 9, 2022

Outline

Regression

Least squares estimation

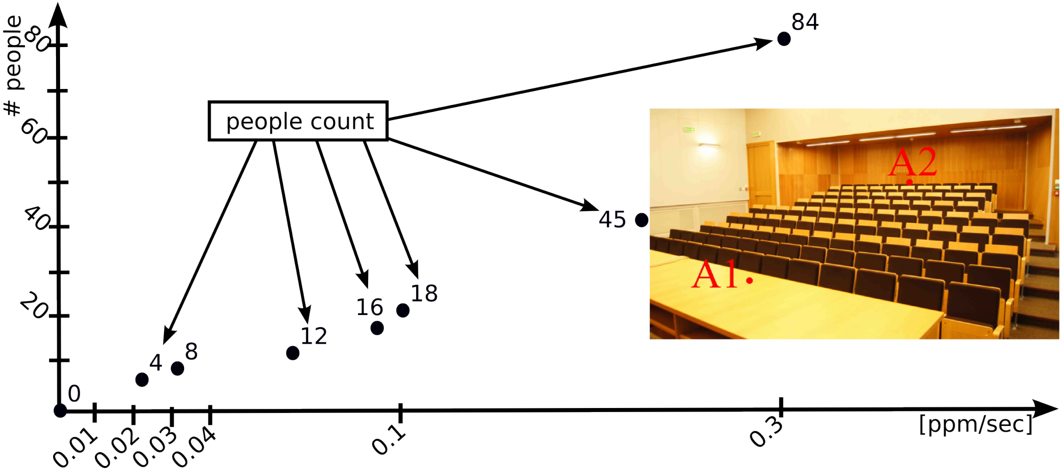
Polynomial regression

Multivariable linear regression

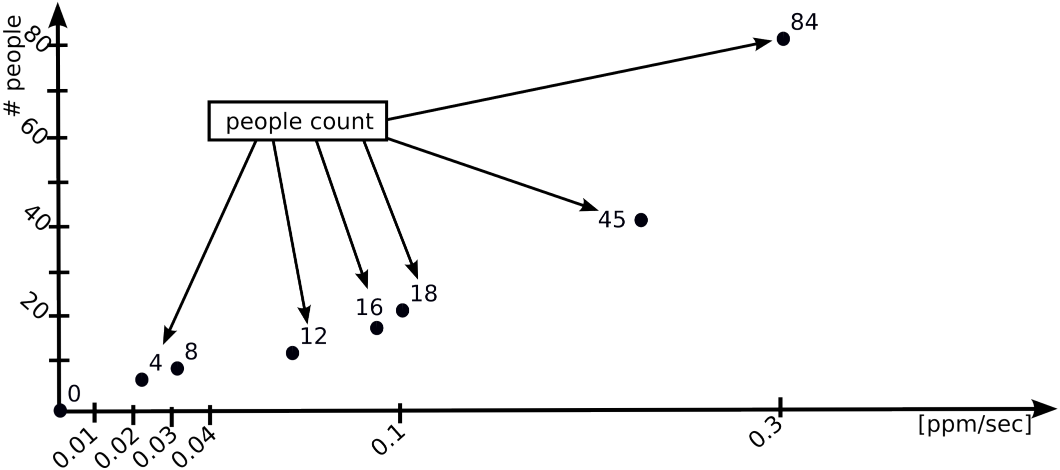
Multivariate linear regression

Logistic regression

Linear regression



Linear regression



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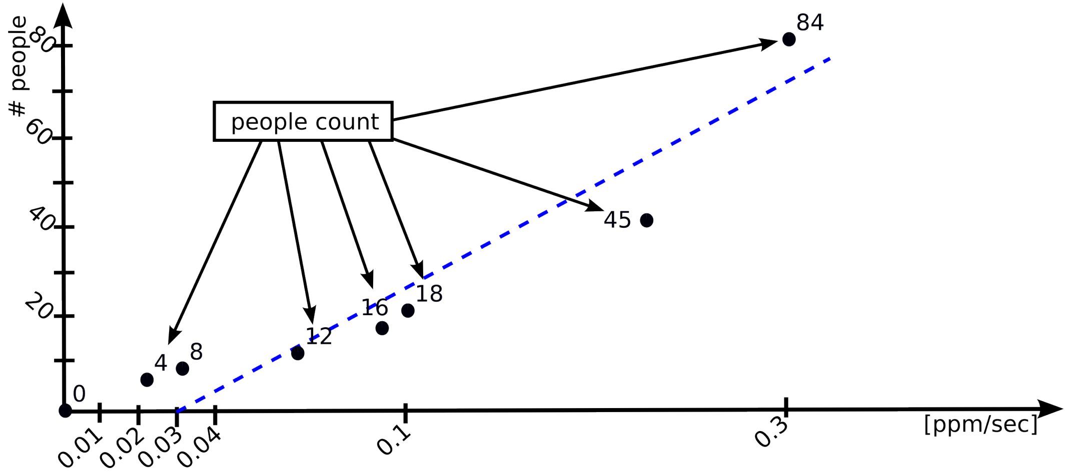

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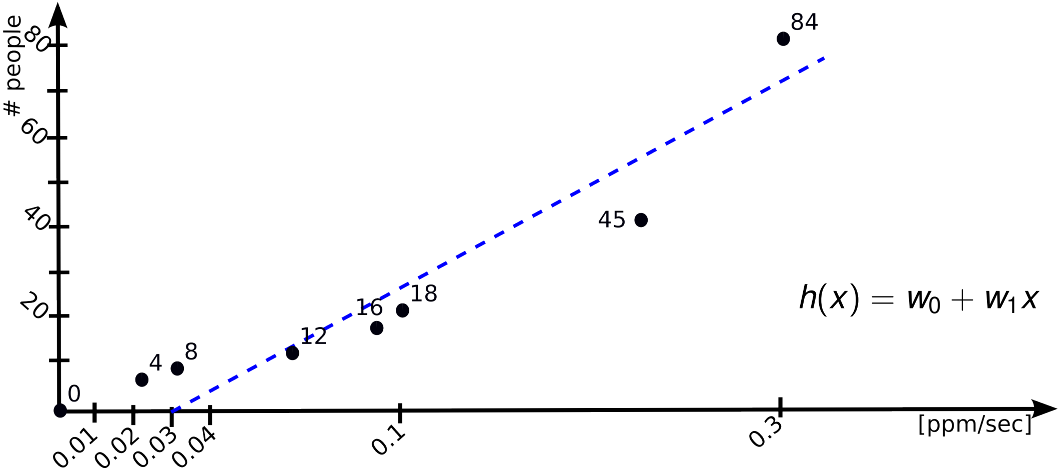

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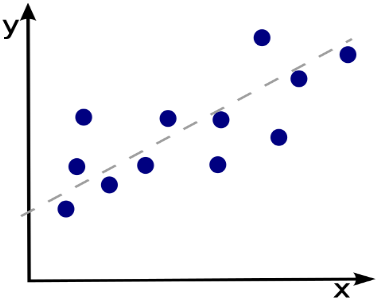
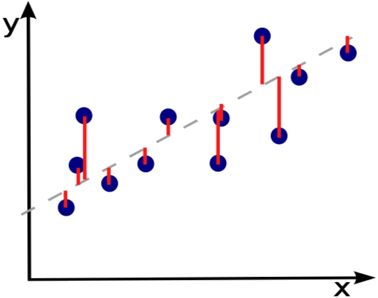


Objective function: $h(x) = w_0 + w_1 x$

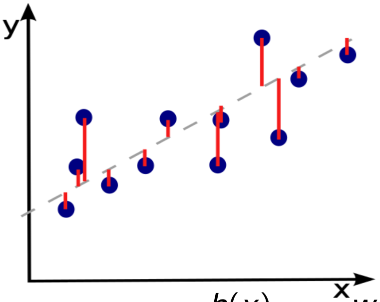
How to choose the parameter w_0 and w_1?

Linear regression



$$h(x) = w_0 + w_1 x$$

Linear regression

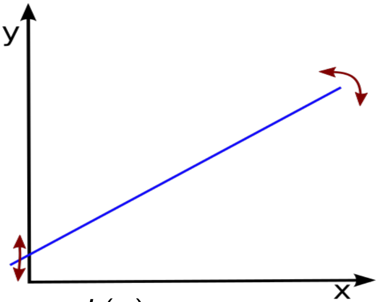


Some authors refer to the <u>Loss function</u> as *error function* or *cost function*. All these are synonyms.

$$
\begin{aligned}
h(x) &= w_0 + w_1 x \\
\text{minimize } E[w_0, w_1] = L[(X, Y), h(x)] &= \frac{1}{2n} \sum_{i=1}^{n} (h(x_i) - y_i)^2
\end{aligned}
$$

Loss function estimates quality of current solution (Gradient descent).

Gradient descent loss function – intuition



additive constant w_0 ignored in the following for simplicity

$$h(x) = w_0 + w_1 x$$

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

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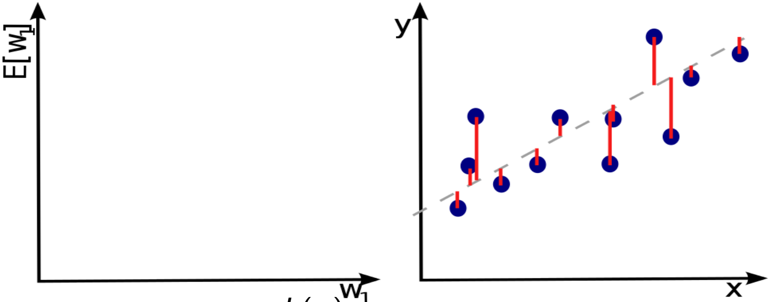

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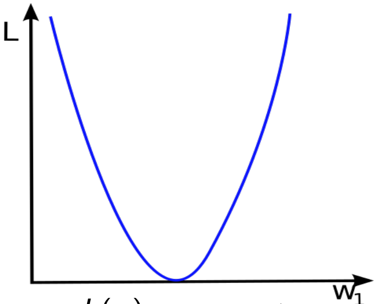

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Gradient descent loss function – intuition

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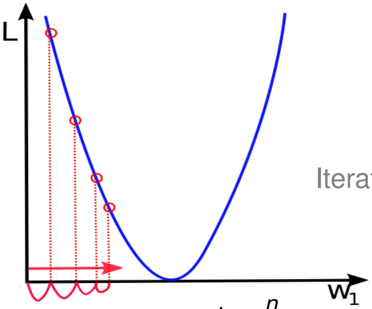
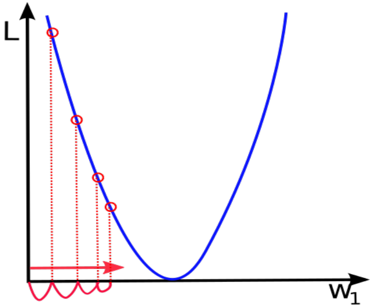


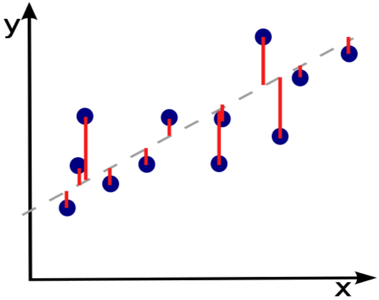
Iterative approximation of w_1

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

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

Gradient descent loss function





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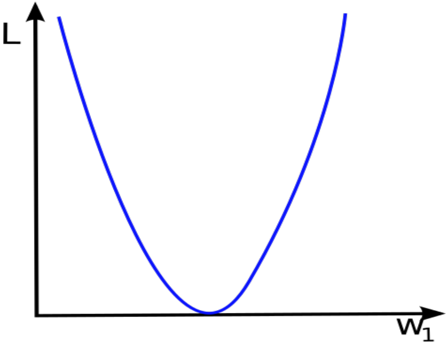
Least squares estimation

Given a loss function

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

we can minimize the error by requiring

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



Least squares estimation

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Differentiation yields

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

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

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

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

Setting

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

will lead to

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

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

Least squares estimation

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

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

rewrite as

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

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

Least squares estimation

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

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

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

Least squares estimation

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for an invertible matrix this implies

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

Solve this linear equation system to find optimal values for w_0 and w_1.

Least squares estimation

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Note: matrix must be invertible.

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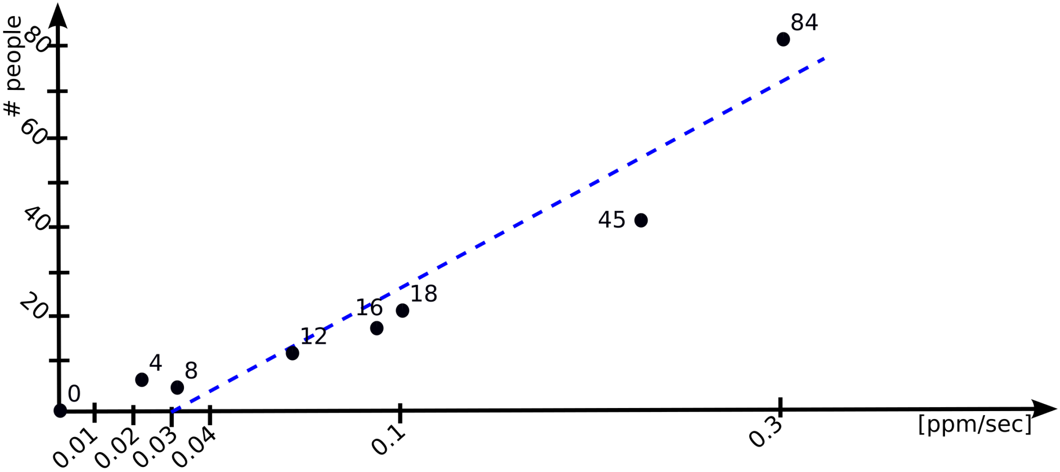
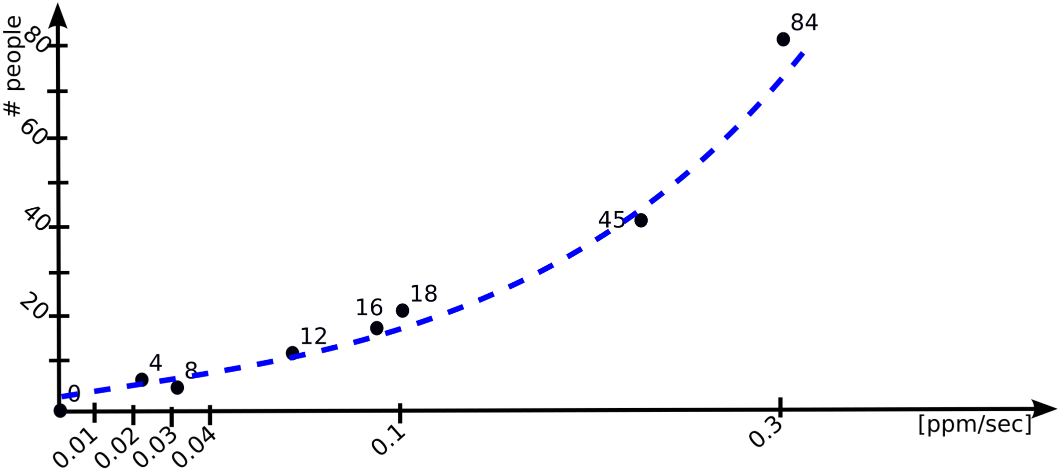


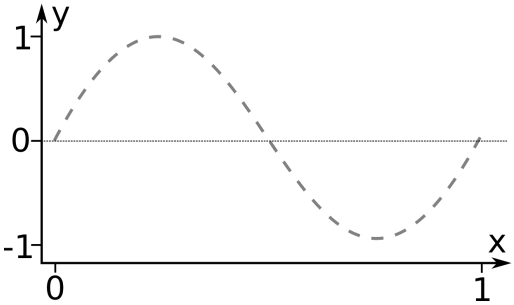
Polynomial regression



Polynomial regression (Polynomial curve fitting)

Example

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



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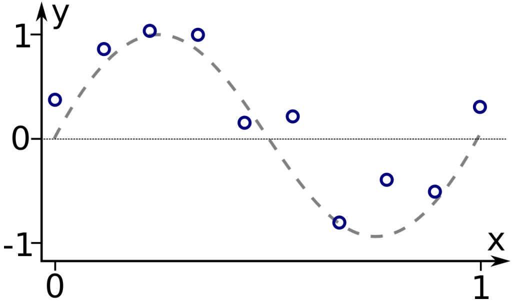

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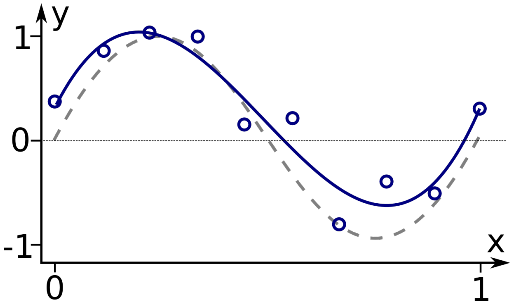
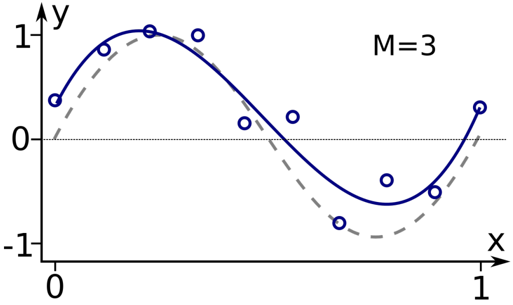


Polynomial curve fitting

We fit the data points into a polynomial function:

$$h(x, \vec{w}) = w_0 + w_1 x + w_2 x^2 + \cdots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$



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This can be obtained by minimising a loss function which measures the misfit between $h(x, \overrightarrow{w})$ and the training data set:

$$E(\overrightarrow{w}) = \frac{1}{2n} \sum_{i=1}^{n} \left[h(x_i, \overrightarrow{w}) - y_i \right]^2$$

$E(\overrightarrow{w}) \geq 0$; $E(\overrightarrow{w}) = 0$ IFF 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

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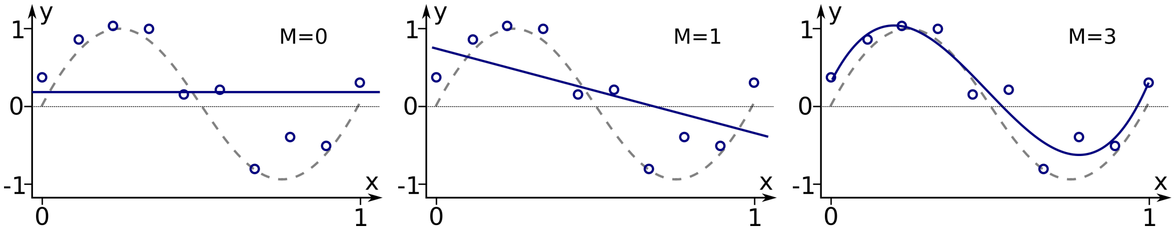
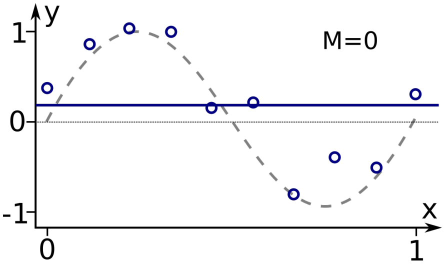
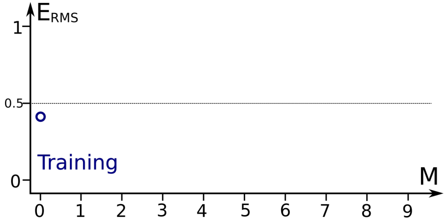


Polynomial curve fitting

Visualise error $E(\overrightarrow{w})$ wrt the data by Root of the Mean Squared (RMS)

$$E_{RMS} = \sqrt{\frac{2E(\overrightarrow{w})}{n}}$$





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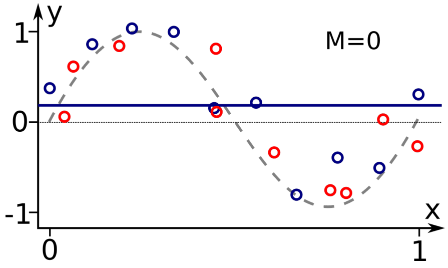

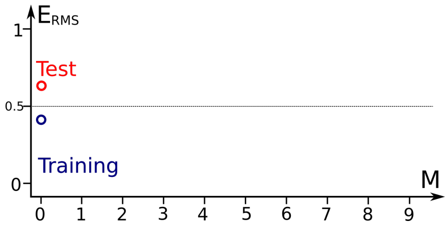

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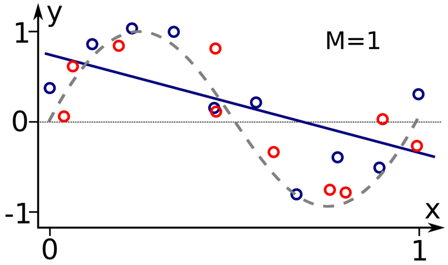

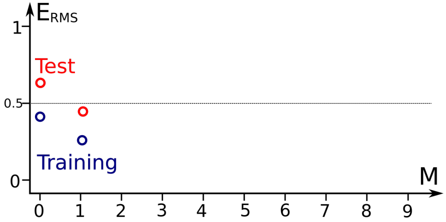

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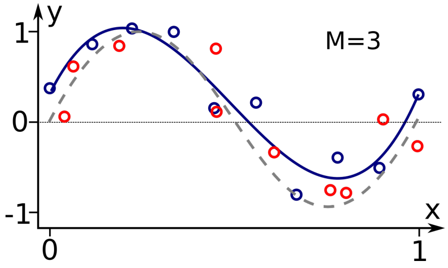

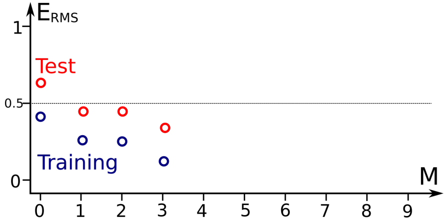

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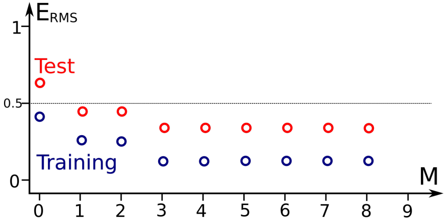

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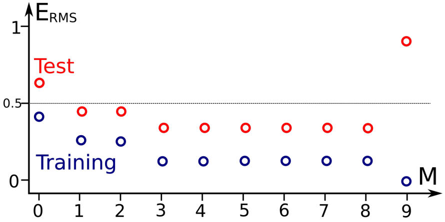

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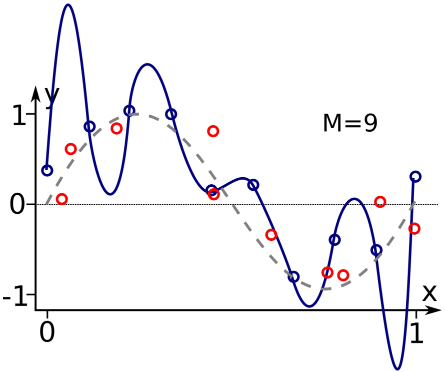
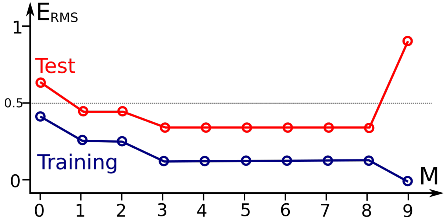


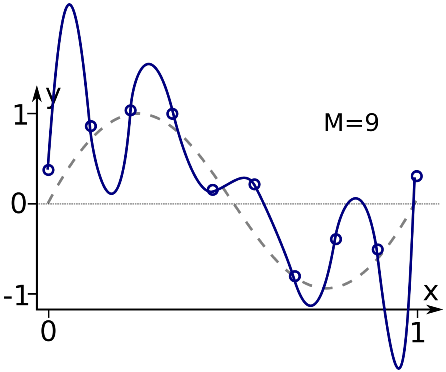


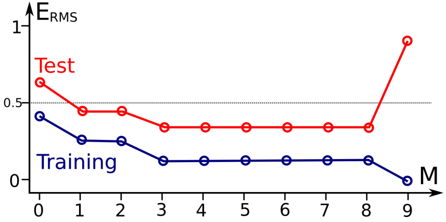
Polynomial curve fitting

This event is called overfitting

The polynomial is now trained too well to the training data

It performs badly on test data

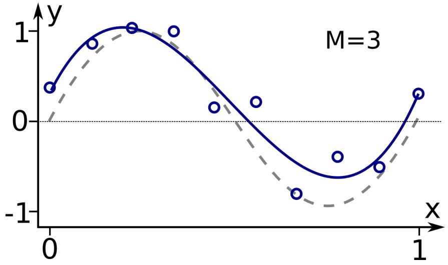


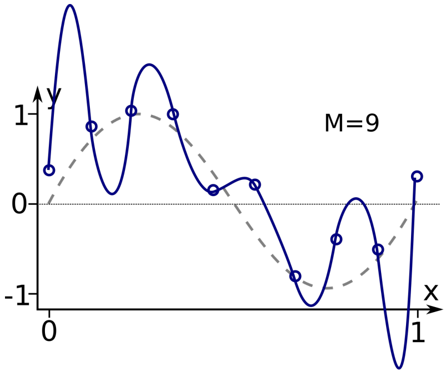


Polynomial curve fitting

When M becomes too big, the polynomial will cross all points exactly

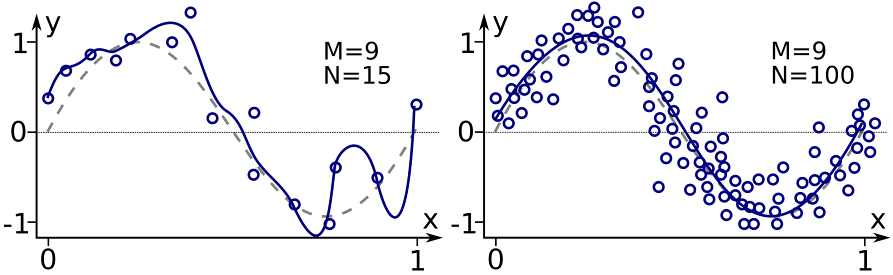
For $M = n$, it is always possible to create a polynomial of order M that contains all values in the data set.





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 loss function

This term discourages the coefficients $\overrightarrow{w}$ from reaching large values

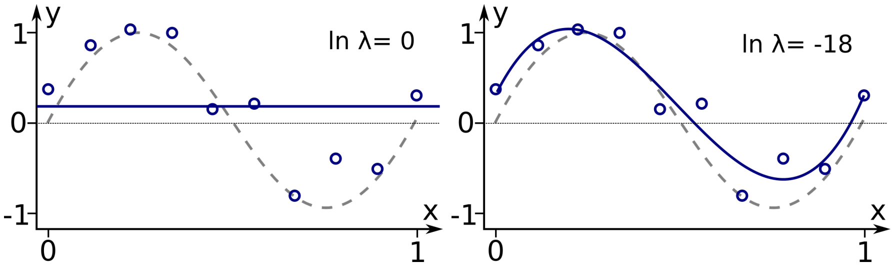
$$\overline{E}(\overrightarrow{w}) = \frac{1}{2n}\sum_{i=1}^{n}\left[h(x_i, \overrightarrow{w}) - y_i\right]^2 + \frac{\lambda}{2}||\overrightarrow{w}||^2$$

with

$$||\overrightarrow{w}||^2 = \overrightarrow{w}^T\overrightarrow{w} = w_0^2 + w_1^2 + \cdots + w_M^2$$

Polynomial curve fitting

Depending on the value of λ, overfitting is controlled



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TIME FOR A
SHORT BREAK, RIGHT?
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In multivariable linear regression problems we assume that multiple regression variables (features) apply.

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\begin{aligned}
h(x_{j1}, \ldots, x_{jm}) &= \sum_{i=0}^{m} w_i x_{ji} \\
\text{minimize } E[W] &= \frac{1}{2n} \sum_{j=1}^{n} \left(h(x_{j1}, \ldots, x_{jm}) - y_j \right)^2
\end{aligned}
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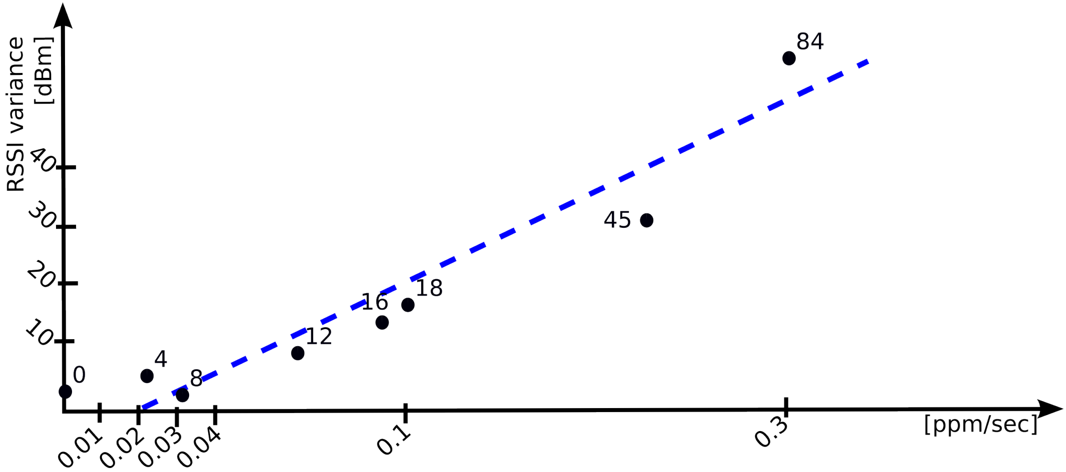
Multivariable linear regression



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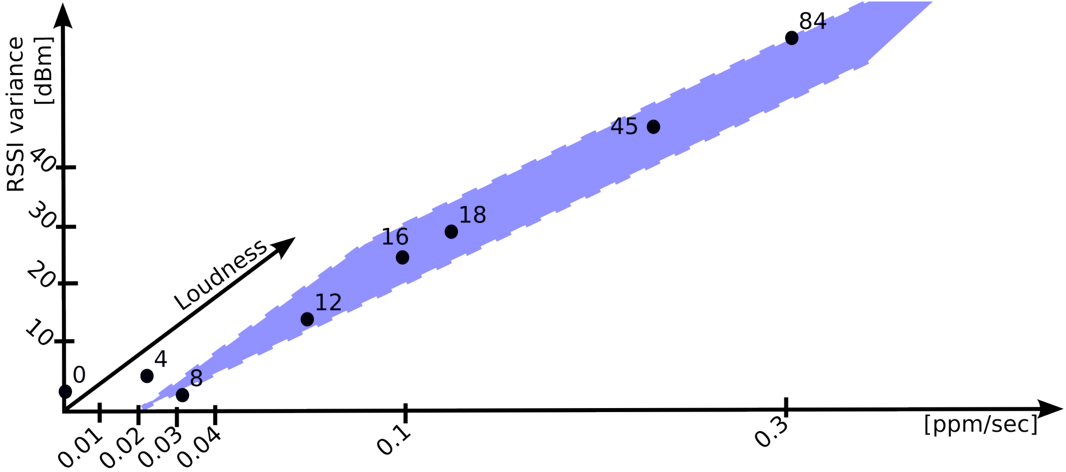

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\text{minimize } E[W] &= \frac{1}{2n} \sum_{j=1}^{n} \left(h(x_{j1}, \ldots, x_{jm}) - y_j \right)^2
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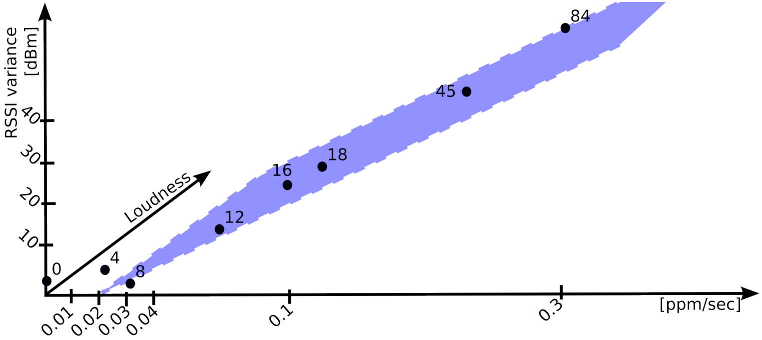
w_i &= w_i - \delta \cdot \frac{\partial}{\partial w_i} E[W]
\end{aligned}
$$

w_i are optimised together over several iterations

Outline

Multivariate linear regression

Multivariate linear regression describes a regression problem with multiple classes.



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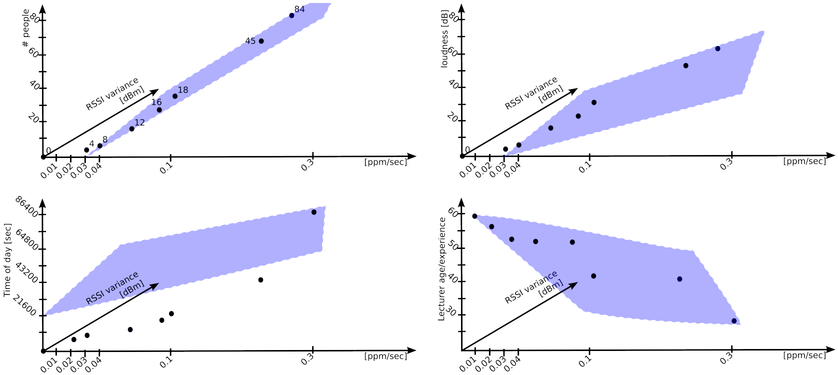

Multivariate linear regression

Regression model is extended to multiple responses: $Y_j = y_{j1}, \ldots, y_{jl}$

$$
\begin{aligned}
y_{j1} &= w_{01} + w_{11}x_{j1} + \cdots + w_{n1}x_{jn} \\
y_{j2} &= w_{02} + w_{12}x_{j1} + \cdots + w_{n2}x_{jn} \\
&\vdots \\
y_{jl} &= w_{0l} + w_{1l}x_{j1} + \cdots + w_{nl}x_{jn}
\end{aligned}
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Multivariate linear regression

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

$$
\begin{aligned}
y_{j1} &= w_{01} + w_{11}x_{j1} + \cdots + w_{n1}x_{jn} \\
y_{j2} &= w_{02} + w_{12}x_{j1} + \cdots + w_{n2}x_{jn} \\
\vdots & \qquad\qquad\quad \vdots \\
y_{jl} &= w_{0l} + w_{1l}x_{j1} + \cdots + w_{nl}x_{jn}
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Using least squares estimation 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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$$W_i = \left(X^T X\right)^{-1} X^T Y_{(i)}$$

and collecting all univariate estimates into a matrix

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

$Y_{(i)}$ 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 - Proof

To minimize $E(W)$, we can simply solve for where its gradient is zero: $\nabla_W E(W) = 0$.

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

Multivariable linear regression - Example (1/6)

Air Quality Sensor	RF Sensor	# People
210	3	400
160	3	330
240	3	370
140	2	230
300	4	500

1. The goal is to predict the number of people for air quality of 400 and RF activity level of 2.

Multivariable linear regression - Example (1/6)

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210	3	400
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1. The goal is to predict the number of people for air quality of 400 and RF activity level of 2.
2. First, we need to calculate w_0, w_1, and w_2 in $y = w_0 + w_1 x_1 + w_2 x_2$

Multivariable linear regression - Example (1/6)

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3. Using $W = (X^T X)^{-1} X^T y$

Multivariable linear regression - Example (2/6)

Air Quality Sensor	RF Sensor	# People
210	3	400
160	3	330
240	3	370
140	2	230
300	4	500

$$X = \begin{bmatrix} 1 & 210 & 3 \\ 1 & 160 & 3 \\ 1 & 240 & 3 \\ 1 & 140 & 2 \\ 1 & 300 & 4 \end{bmatrix} \quad y = \begin{bmatrix} 400 \\ 330 \\ 370 \\ 230 \\ 500 \end{bmatrix}$$

Multivariable linear regression - Example (3/6)

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 210 & 160 & 240 & 140 & 300 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 1 & 210 & 3 \\ 1 & 160 & 3 \\ 1 & 240 & 3 \\ 1 & 140 & 2 \\ 1 & 300 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 1050 & 15 \\ 1050 & 236900 & 3310 \\ 15 & 3310 & 47 \end{bmatrix}$$

Multivariable linear regression - Example (4/6)

$$(X^T X)^{-1} = \begin{bmatrix} 4.95 & 0.0083333333 & -2.1666666667 \\ 0.008333333333 & 0.00027777778 & -0.02222222222 \\ -2.1666666667 & -0.0222222222 & 2.27777777778 \end{bmatrix}$$

Multivariable linear regression - Example (5/6)

$$X^T y = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 210 & 160 & 240 & 140 & 300 \\ 3 & 3 & 3 & 2 & 4 \end{bmatrix} \begin{bmatrix} 400 \\ 330 \\ 370 \\ 230 \\ 500 \end{bmatrix} = \begin{bmatrix} 1730 \\ 386800 \\ 5460 \end{bmatrix}$$

Multivariable linear regression - Example (6/6)

$$(X^TX)^{-1}X^Ty = \begin{bmatrix} -43.166679742 \\ 0.52777864889 \\ 92.7777863278 \end{bmatrix}$$

$$\hat{y} = -43.166679742 + 0.52777864889 \times 400 + 92.7777863278 \times 4 = 539$$

Outline

Regression

Least squares estimation

Polynomial regression

Multivariable linear regression

Multivariate linear regression

Logistic regression

Logistic regression

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

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

Logistic regression

Nominal classes

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

Logistic regression

Nominal classes

Classes might be nominal in real-world problems

Weather: Sunny, rainy

Medical: positive diagnosis, negative diagnosis

Localisation: indoor, outdoor

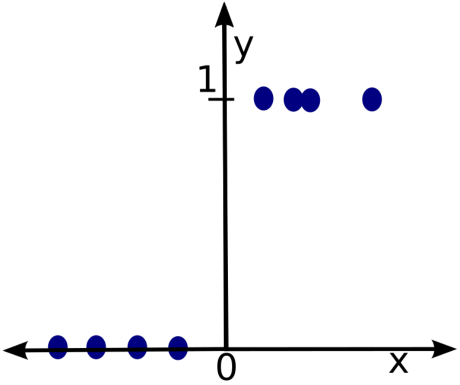
In such case, classification is binary: $y \in \{0, 1\}$

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

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

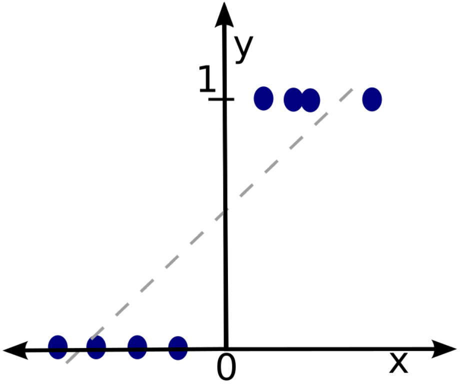
Logistic regression

Nominal classes



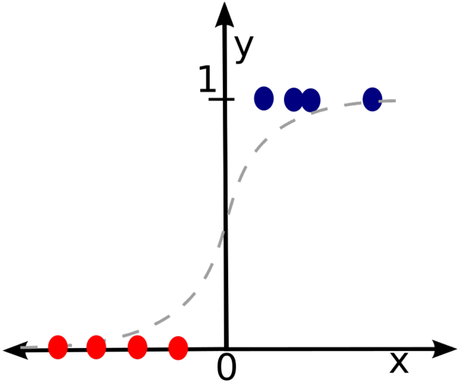
Logistic regression

Nominal classes



Logistic regression

Loss function



Logistic regression

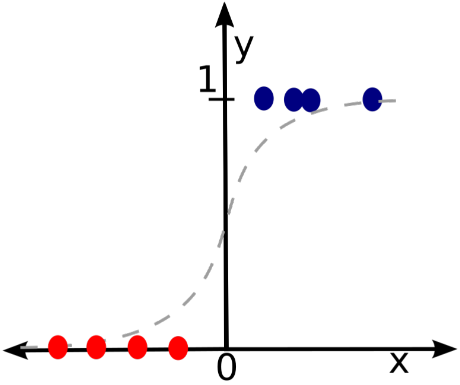
Loss function

Linear regression

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

Logistic regression

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



Logistic regression

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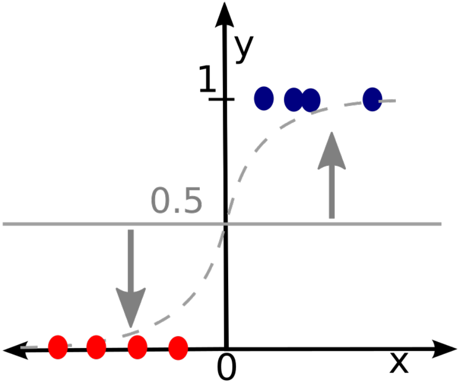
$$h(x) = \frac{1}{1+e^{-W^T x}}$$

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

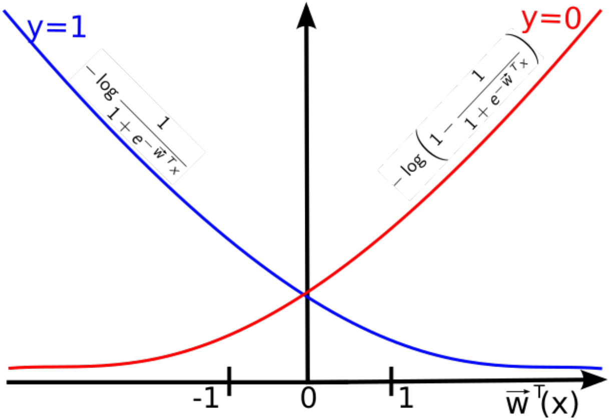


Logistic regression

Loss function

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

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

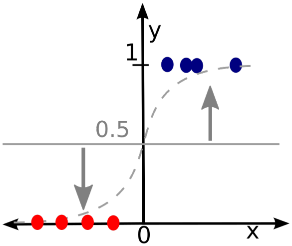


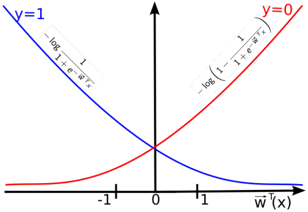
Logistic regression

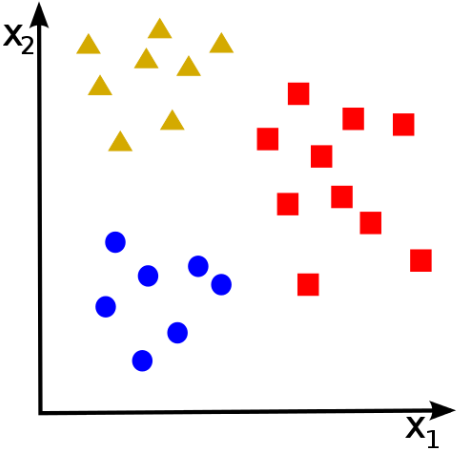
Multiclass classification

Multiple classes

Can we use logistic regression for problems with more than two classes?







Logistic regression

Multiclass classification

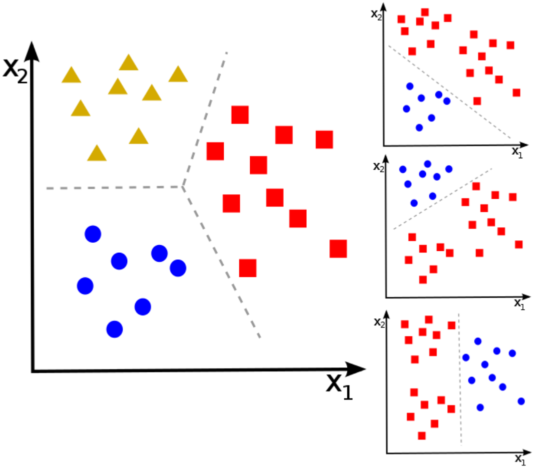
Multi-class: One-versus all:

Train classifiers for each class to obtain probability that x belongs to class i:

$$h_i(x) = P(y = i | \vec{x}, \vec{W})$$

then, choose

$$max_i \left(h_i(x) \right)$$



Questions?

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