COMS21202: Symbols, Patterns and Signals
Deterministic Data Models

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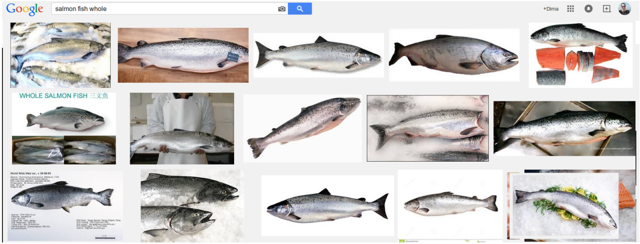
Data Modelling

- From Data to a Model



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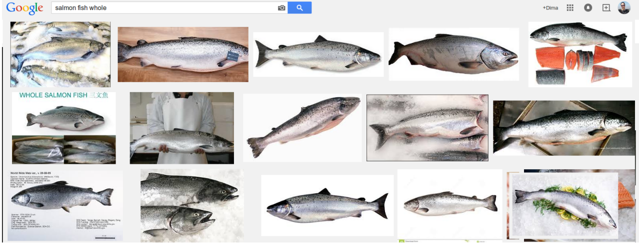

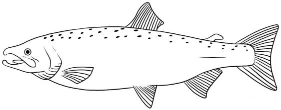

Data Modelling

- Models are descriptions of the data
- They encode our assumptions about the data
- Enabling us to:
  - design ‘optimal’ algorithms
  - compare and contrast methods
  - quantify performance
- A model is ‘more than’ the data - a ‘generalisation’ of the data

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- In some cases, we may approximate an underlying physical process as part of our model
- In others, this may be impossible and/or impractical
- Models only need to enable us to define a method to tackle the task at hand
- Performance of the method then depends on how well the model ‘maps’ the data onto the required solution
- choice of model is often dictated by practicality of method, as well as by our assumptions about the data

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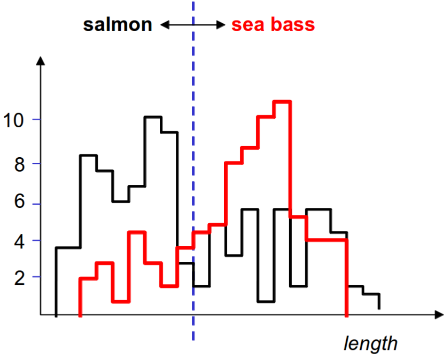
- Model selected here is a linear classifier



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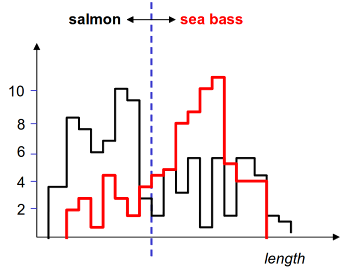

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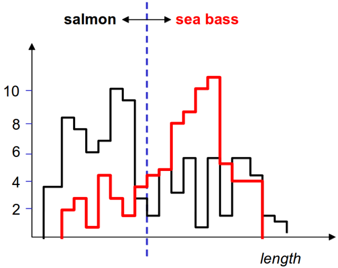

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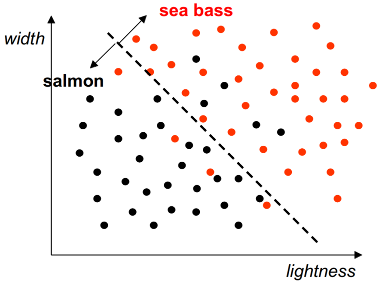

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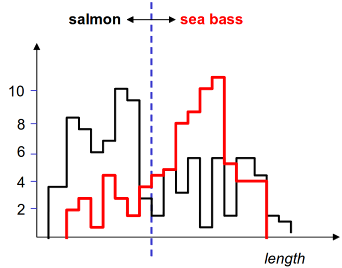

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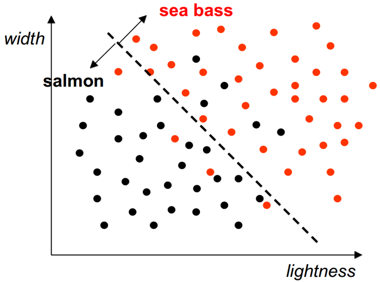

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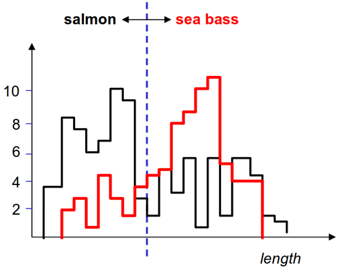
- or from training data by tuning or training the model



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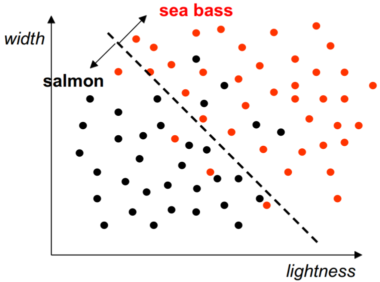

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- In fact trying *too hard* on training data leads to a damaging phenomenon called **overfitting**

Generalisation vs. Overfitting

Example

Imagine you are trying to prepare for *Symbols, Patterns and Signals* exam this June.

source: Flach (2012), Machine Learning

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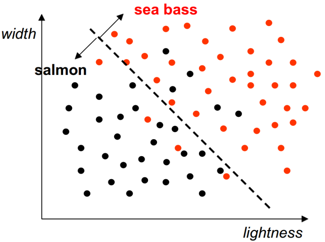

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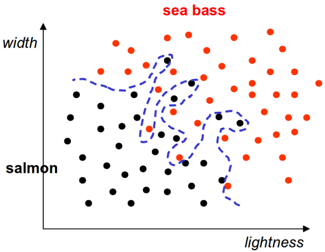

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Generalisation vs. Overfitting

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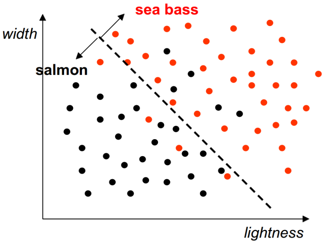

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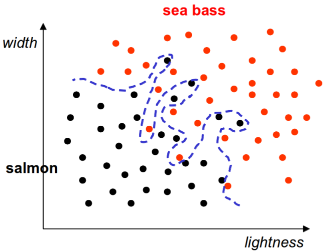

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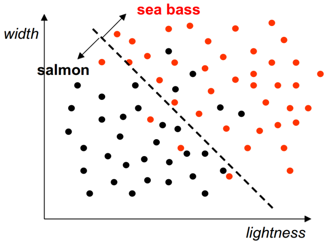
- **highly complex models** over-fit the training data



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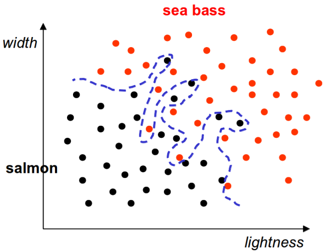

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- e.g. For the *fishy* model, prediction of whether the fish is salmon or sea bass is given, without an estimate of how good the prediction is
- Deterministic models do not encode the uncertainty in the data
- This is in contrast to probabilistic models (next lecture)

Deterministic Models

To build a deterministic model,

1. Understand the task
2. Hypothesise the model's type
3. Hypothesise the model's complexity
4. Tune/Train the model's parameters

Another Fish Problem

Data: a set of data points $D = \{(x_1, y_1), (x_2, y_2), \cdots, (x_N, y_N)\}$ where x_i is the length of fish i and y_i is the weight of fish i.

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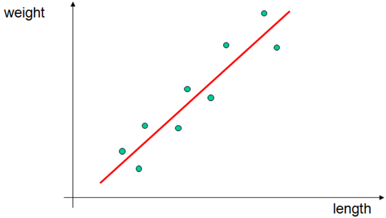
Model Parameters: model has two parameters a and b which should be estimated.

- a is the y-intercept
- b is the slope of the line

Determinist Model - Line Fitting

- Finding the linear model parameters amounts to finding the *best fitting line* given the data
- **criterion:** The best fitting line is that which minimises a distance measure from the points to the line

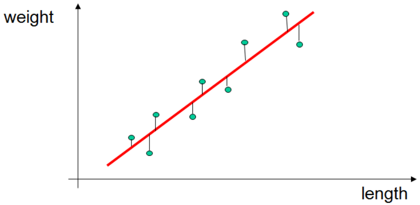


Determinist Model - Line Fitting

- Find a,b which minimises

$$R(a,b) = \sum_{i=1}^{N} (y_i - (a + bx_i))^2$$

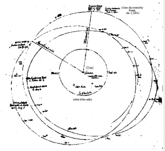
- This is known as the residual
- A method which gives a closed form solution is to minimise the sum of squared vertical offsets of the points from the line **Method of Least-Squares**



Least Squares Solution

Example

The Ceres Orbit of Gauss:



Sketch of the orbits of Ceres and Pallas (nachlaß Gauß, Handb. 4). Courtesy of Universitätsbibliothek Göttingen.

source: Leon (1994). Linear Algebra and its Applications

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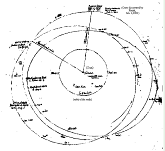

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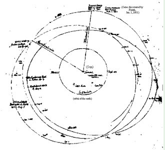

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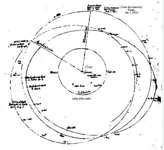

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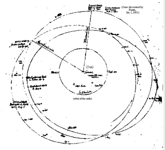

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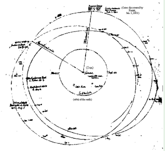

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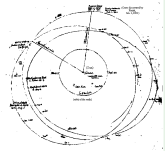

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Least Squares Solution

- A least squares problem is an overdetermined linear system of equations (i.e. number of equations $>>$ number of unknowns)
- Such systems are usually inconsistent

Least Squares Solution

Minimise residual by taking the partial derivatives, and setting them to zero (using chain rule)

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$$a_{LS} = \bar{y} - b_{LS}\bar{x}$$

$$b_{LS} = \frac{\sum_i x_i y_i - N\bar{x}\bar{y}}{\sum_i x_i^2 - N\bar{x}^2}$$

$\bar{x} \equiv$ mean of $\{x_i\}$

Least Squares Solution Example

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Find the best least squares fit by a linear function to the data

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$y = 1.8 + 2.9x$

Least Squares Solution - Outliers

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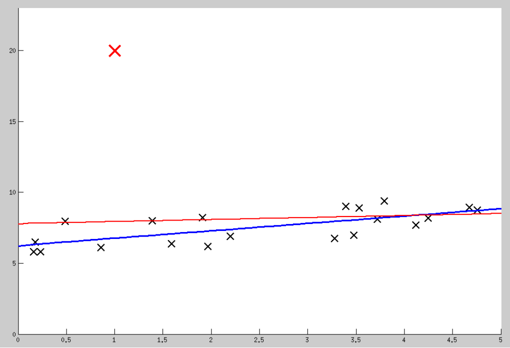

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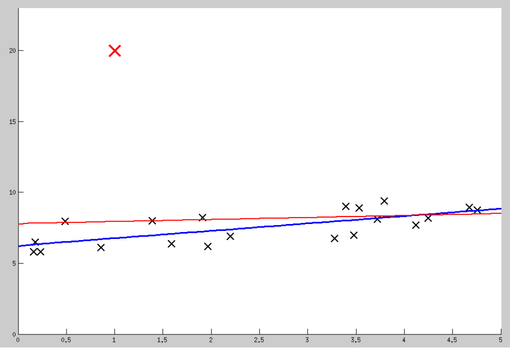
- Outliers can have disproportionate effects on parameter estimates when using least squares
- Because residual is defined in terms of squared differences
- 'Best line' moves closer to outliers



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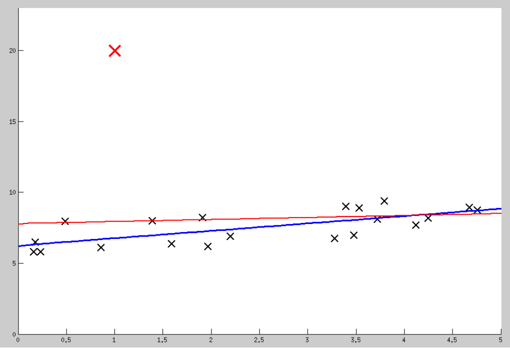

Least Squares Solution - matrix form

- Least squared solution can be defined using matrices and vectors
- Easier when dealing with variables

$$R(a,b) = \sum_i (y_i - (a + bx_i))^2 = \|\mathbf{y} - \mathbf{Xa}\|^2$$

where $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}$, $\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}$, $\mathbf{a} = \begin{bmatrix} a \\ b \end{bmatrix}$

$$\mathbf{y} - \mathbf{Xa} = \begin{bmatrix} y_1 - a - bx_1 \\ \vdots \\ y_N - a - bx_N \end{bmatrix}$$

Least Squares Solution - matrix form

- To solve least squares in matrix form, find $\mathbf{a}_{LS}$;

WARNING: This is not a derivation! It merely intends to give you intuition of the solution. For accurate understanding please refer to: this derivation - p8

Least Squares Solution - matrix form

- To solve least squares in matrix form, find $\mathbf{a}_{LS}$;

$$\|\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS}\|^2 = 0$$

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Least Squares Solution - matrix form

- To solve least squares in matrix form, find $\mathbf{a}_{LS}$;

$$\|\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS}\|^2 = 0$$ (minimise vector's length)

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Least Squares Solution - matrix form

- To solve least squares in matrix form, find $\mathbf{a}_{LS}$;

$$\|\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS}\|^2 = 0 \qquad \text{(minimise vector's length)}$$
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$$\mathbf{X}\,\mathbf{a}_{LS} = \mathbf{y} \qquad \text{(re-arrange)}$$

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$$\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\,\mathbf{X}^T\,\mathbf{y} \qquad \text{(matrix inverse)}$$

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Least Squares Solution - matrix form

- To solve least squares in matrix form, find $\mathbf{a}_{LS}$;

$$
\begin{aligned}
&\|\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS}\|^2 = 0 && \text{(minimise vector's length)}\\
&\mathbf{y} - \mathbf{X}\,\mathbf{a}_{LS} = 0 && \text{(optimal vector is of length 0)}\\
&\mathbf{X}\,\mathbf{a}_{LS} = \mathbf{y} && \text{(re-arrange)}\\
&\mathbf{X}^T\mathbf{X}\,\mathbf{a}_{LS} = \mathbf{X}^T\,\mathbf{y} && \text{(to get a square matrix)}\\
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\end{aligned}
$$

$$
\boxed{\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\,\mathbf{X}^T\,\mathbf{y}}
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Least Squares Solution Example - again

Example

Find the best least squares fit by a linear function to the data

x	-1	0	1	2
y	0	1	3	9

Least Squares Solution Example - again

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Least Squares Solution Example - again

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Find the best least squares fit by a linear function to the data

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$$y = 1.8 + 2.9x$$

K-D Least Squares - matrix form

- Matrix formulation allows least squares method to be easily extended to data points in higher dimensions

K-D Least Squares - matrix form

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- Consider set of points $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)\}$ where $\mathbf{x}_i$ has K dimensions

K-D Least Squares - matrix form

- Matrix formulation allows least squares method to be easily extended to data points in higher dimensions
- Consider set of points $D = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)\}$ where $\mathbf{x}_i$ has K dimensions
- For a model where y_i is linearly related to $\mathbf{x}_i$

$$y_i = a_0 + a_1 x_{i1} + a_2 x_{i2} + \cdots + a_K \ x_{iK} \tag{2}$$

K-D Least Squares - matrix form

- Solved in the same manner

,   ,

K-D Least Squares - matrix form

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$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \qquad ,$$

K-D Least Squares - matrix form

- Solved in the same manner

$$\mathbf{y}_{(N \times 1)} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \qquad ,$$

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K-D Least Squares - matrix form

- Solved in the same manner

$$\mathbf{y}_{(N\times 1)} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1K} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & \cdots & x_{NK} \end{bmatrix},$$

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$$R(\mathbf{a}) = \|\mathbf{y} - \mathbf{X}\mathbf{a}\|^2$$

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$$\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\,\mathbf{X}^T\,\mathbf{y}$$

where $(\mathbf{X}^T\mathbf{X})$ is a $(K+1)\times(K+1)$ square matrix

General Least Squares - matrix form

- Matrix formulation also allows least squares method to be extended to **polynomial fitting**
- For a polynomial of degree $p+1$

$$y_i = a_0 + a_1 x_i + a_2 x_i^2 + \cdots + a_p \, x_i^p$$

General Least Squares - matrix form

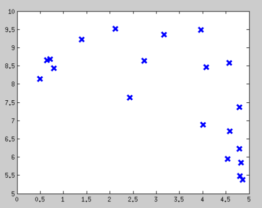
- Solved in the same manner

$$\mathbf{y}_{(N\times 1)} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \mathbf{X}_{(N\times(p+1))} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^p \\ 1 & x_2 & x_2^2 & \cdots & x_2^p \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^p \end{bmatrix}, \mathbf{a}_{((p+1)\times 1)} = \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_p \end{bmatrix}$$

$$\mathbf{a}_{LS} = (\mathbf{X}^T\mathbf{X})^{-1}\ \mathbf{X}^T\ \mathbf{y}$$

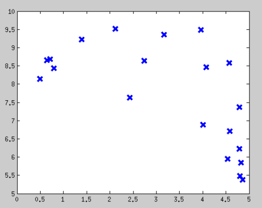
where $(\mathbf{X}^T\mathbf{X})$ is a $(p+1)\times(p+1)$ square matrix

Generalisation and Overfitting - again



Data

Generalisation and Overfitting - again



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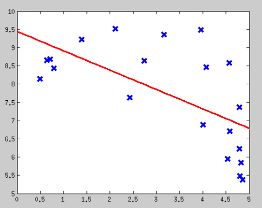
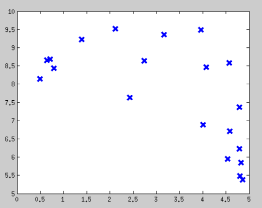


$p = 1$
Residual = 4.7557

Generalisation and Overfitting - again



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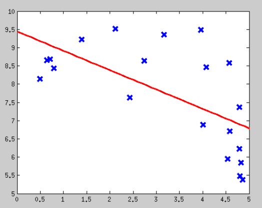

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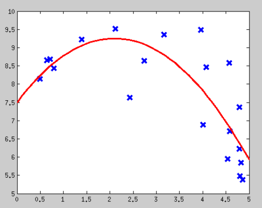

$p = 2$
Residual = 3.7405

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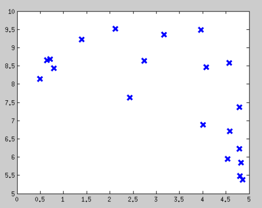
Generalisation and Overfitting - again



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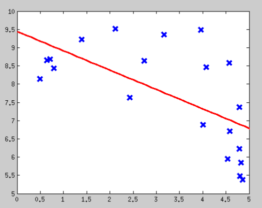

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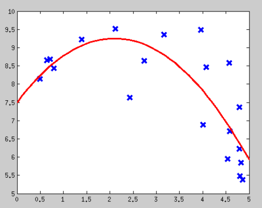

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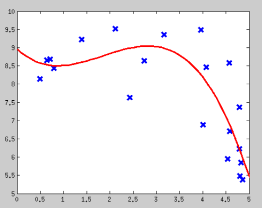
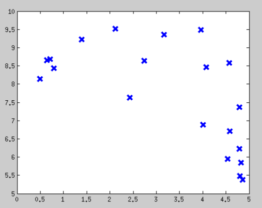


$p = 3$
Residual = 3.5744

Generalisation and Overfitting - again



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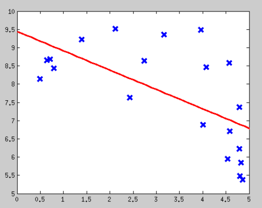
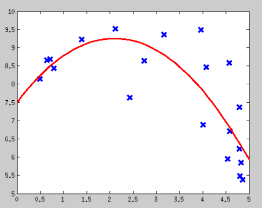
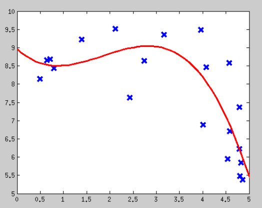


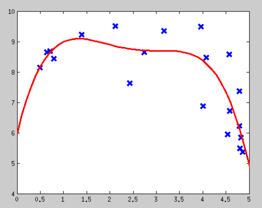
$p = 1$
Residual = 4.7557



$p = 2$
Residual = 3.7405



$p = 3$
Residual = 3.5744



$p = 4$
Residual = 3.4236

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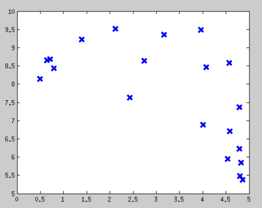
Generalisation and Overfitting - again



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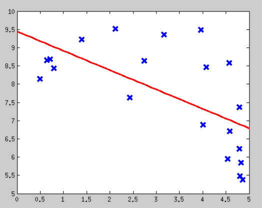
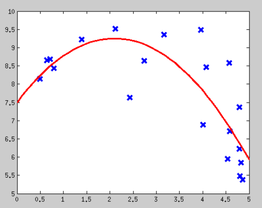
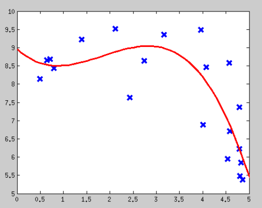


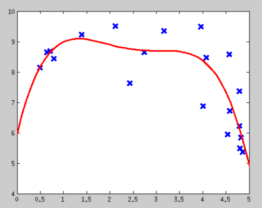
$p = 1$
Residual = 4.7557



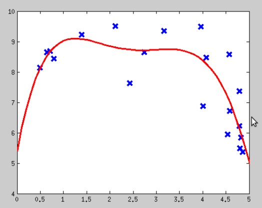
$p = 2$
Residual = 3.7405



$p = 3$
Residual = 3.5744



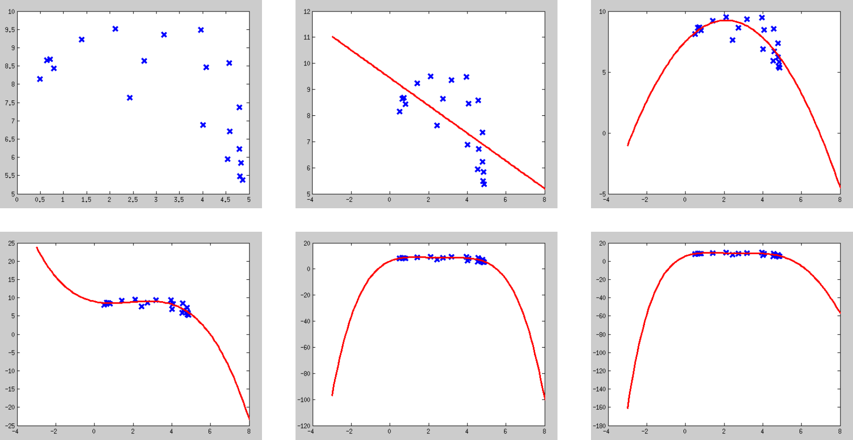
$p = 4$
Residual = 3.4236



$p = 5$
Residual = 3.4217

Generalisation and Overfitting - again

- Strong effect on how to generalise to future data



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Further Reading

- Linear Algebra and its applications
  Lay (2012)
  - Section 6.5
  - Section 6.6
  - Available online
    http://www.math.usu.edu/powell/pseudoinverses.pdf