Artificial Learning Models

Lecture 2 : Linear Regression

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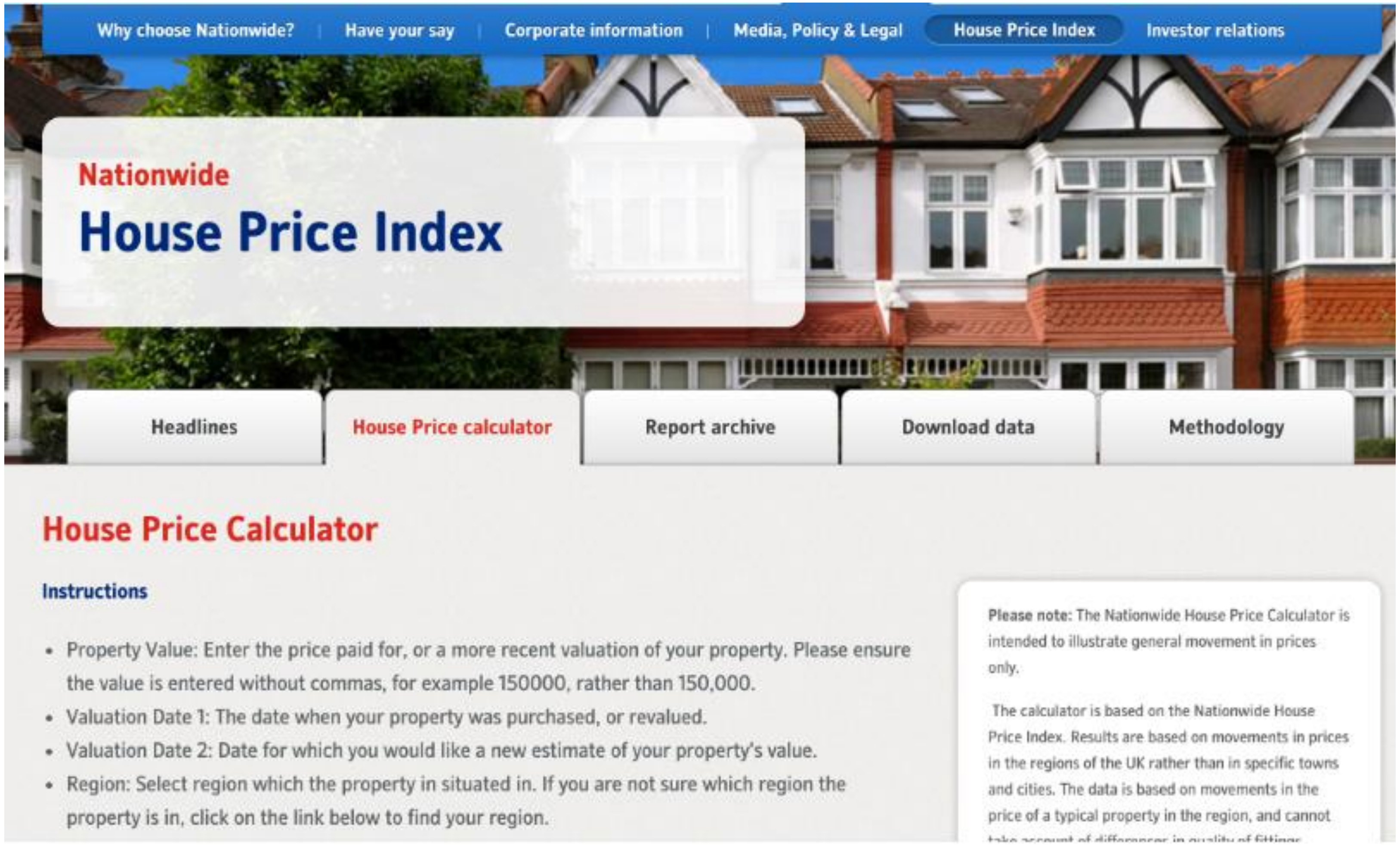
Agenda

Problems for Today

- How many views/subscribers can I get on my Youtube channel ?

Problems for Today

- Goal: Predict the price of the house



What do all these problems have in common?

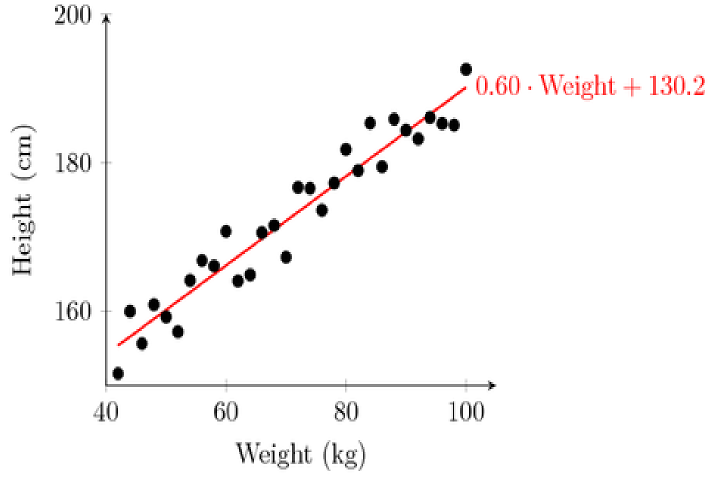
- Continuous outputs
- Predicting continuous outputs is called regression

Linear regression :

- Continuous outputs
- Simple model (linear)

What is Linear Regression ?

- Used to predict the relationship between two variables.
- Fit a line to a data set of observations
  - It assumes a linear relationship between the independent variable and the dependent variable
- Use this line to predict unobserved values
- Key Questions: How to determine this line ?
  - How do we parametrize the model?
  - What loss (objective) function should we use to judge the fit?
  - How do we optimize fit to unseen test data (generalization)?



Regression

- Simple Linear Regression
- Multiple Linear Regression
- Polynomial Regression

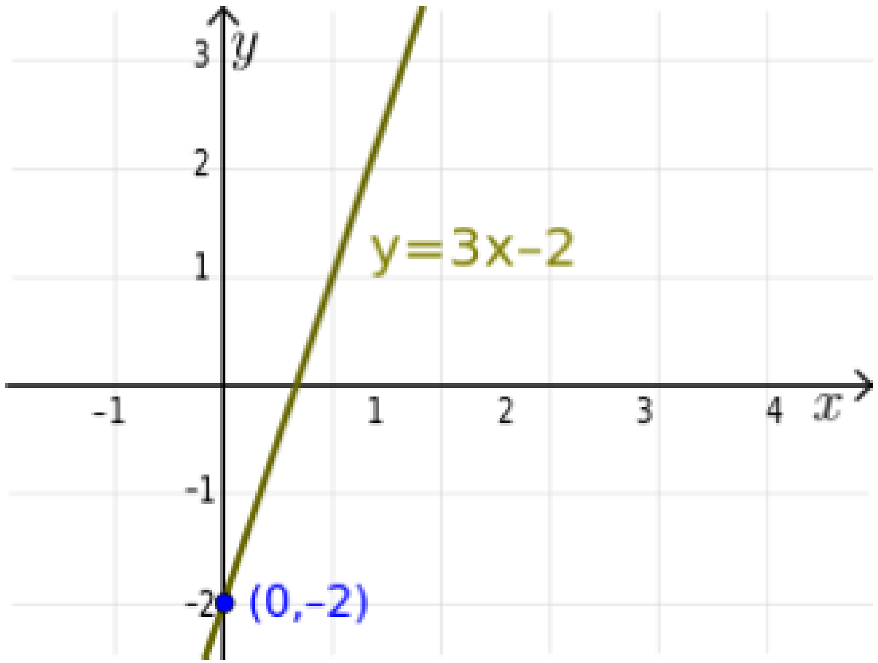
Simple Linear Regression

- One independent variable and one dependent variable.
- The model estimates the slope and intercept of the line of best fit
  - The relationship between the variables.
- If there is a single input variable **X**(independent variable), such linear regression is called ***simple linear regression***

Simple Linear Regression

How does it work?

- Using a Cost function (To be minimized)
- Linear model : $\hat{y} = \phi(x) = w_1 . x + w_0$
- The slope w_1 is the correlation between the two variables times the standard deviation in Y, all divided by the standard deviation in X.
- The intercept w_0 is the mean of Y minus the slope times the mean of X
- But Python will do all that for you.



Cost Function for Linear Regression

- Helps to find the optimal values of the slope and the intercept
- Provids the fit line for the data points
- Commonly used cost functions:
  - **Mean Squared Error (MSE):** average of squared error that occurred between the $\mathbf{y_{predicted}}$ and $\mathbf{y_i}$.

$$MSE = \ell(w) = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y_i})^2 = \frac{1}{N}\sum_{i=1}^{N}\big(y_i - (w_1.x + w_0)\big)^2$$

  - **Least Squared Error LSE**

$$LSE = \ell(w) = \sum_{i=1}^{N}(y_i - \hat{y_i})^2 = \frac{1}{N}\sum_{i=1}^{N}\big(y_i - (w_1.x + w_0)\big)^2$$

- **Goal:** find the best values of w_0 and w_1 that minimizes the cost function

How do we obtain $\mathrm{w} = (w_0, w_1)$?

Obtain w_0 and w_1

- Optimizing across training set
  - Gradient descent

- Analytical solution (in some cases)
  - in the case of linear least-squares regression

- How?

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

Evaluation Metrics for Linear Regression

- Evaluation metrics used to assess the strength of any linear regression model
- Measure of how well the observed outputs are being generated by the model.
- The most used metrics are:
  - Coefficient of Determination or R-Squared (R2)
  - Root Mean Squared Error (RSME) and Residual Standard Error (RSE)

R-squared

- It anges between 0 and 1
- The higher the value of R-squared, the better the model fits the data.
  - 0 is bad (none of the variance is captured),
  - 1 is good (all of the variance is captured).

$$R^2 = 1 - (RSS/TSS)$$

$$RSS = \sum_{i=1}^{n}(y_i - b_0 - b_1 x_i)^2 \qquad TSS = \sum (y_i - \bar{y}_i)^2$$

RSS : Residual sum of Squares, **TSS :** Total Sum of Squares

$\bar{y}_i$ is the mean of the sample data points.

Root Mean Squared Error

- It specifies how close the observed data points are to the predicted values.
- Mathematically

$$RMSE = \sqrt{\frac{RSS}{n}} = \sqrt{\sum_{i=1}^{n}\left(y_i^{Actual} - y_i^{Predicted}\right)^2 / n}$$

- R-squared is a better measure than RSME.

Multiple Regression

Multiple Regression

- What if more than one variable influences the one you're interested in?
- Example: predicting a price for a car based on its many attributes (body style, color, number of seats, …)
- Technique to understand the relationship between a *single* dependent variable and *multiple* independent variables.

$$Y = w_0 + w_1X_1 + w_2X_2 + \ldots + w_pX_p = W^T X$$

Still uses least squares

- We just end up with coefficients for each factor.
  - For example, $price$=α+β1.mileage + β2.age + β3.doors
  - These coefficients imply how important each factor is (if the data is all normalized!)
- Can still measure fit with r-squared
- Need to assume the different factors are not themselves dependent on each other.

What if our linear model is not good? How can we create a more complicated model?

- How do we know that a linear regression model is the best choice?
- What other types of regression are there?
  - There are many other types.
  - The linear model is by far the simplest, but it is not the only choice.

Nonlinear Regression

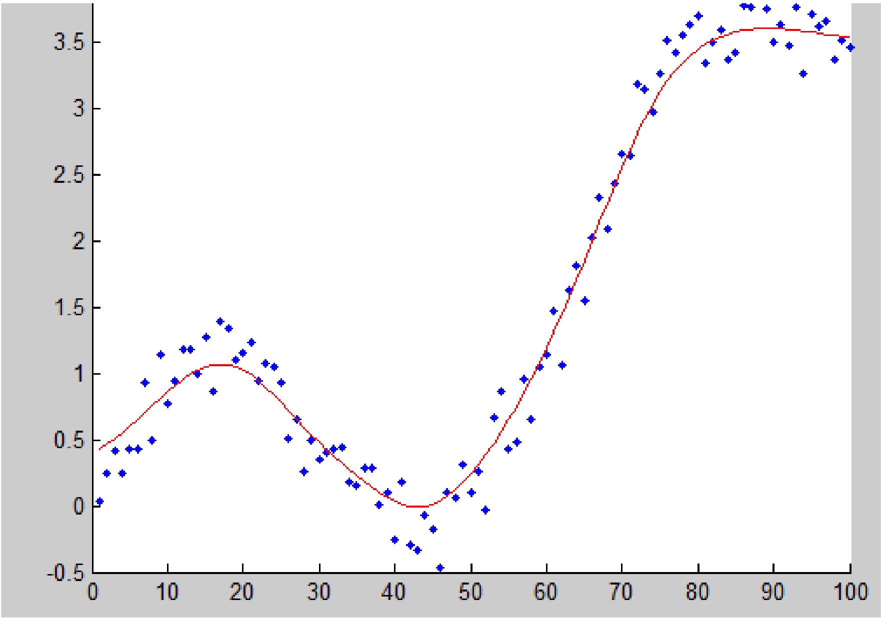
- Nonlinear Regression (Polynomial regression):
  - Quadratic regression: $\hat{y} = ax^2 + bx + c$.
  - Cubic regression: $\hat{y} = ax^3 + bx^2 + cx + d$.
  - Quartic regression: $\hat{y} = ax^4 + bx^3 + cx^2 + dx + e$
- Other Nonlinear Regression (Not polynomial)
  - Logarithmic regression: $\hat{y} = a + b\ln(x)$.
  - Exponential regression: $\hat{y} = ab^x$
  - Power regression: $\hat{y} = ax^b$
  - Logistic regression: $\hat{y} = \frac{c}{1+ae^{-bx}}$
  - …

Polynomial Regression

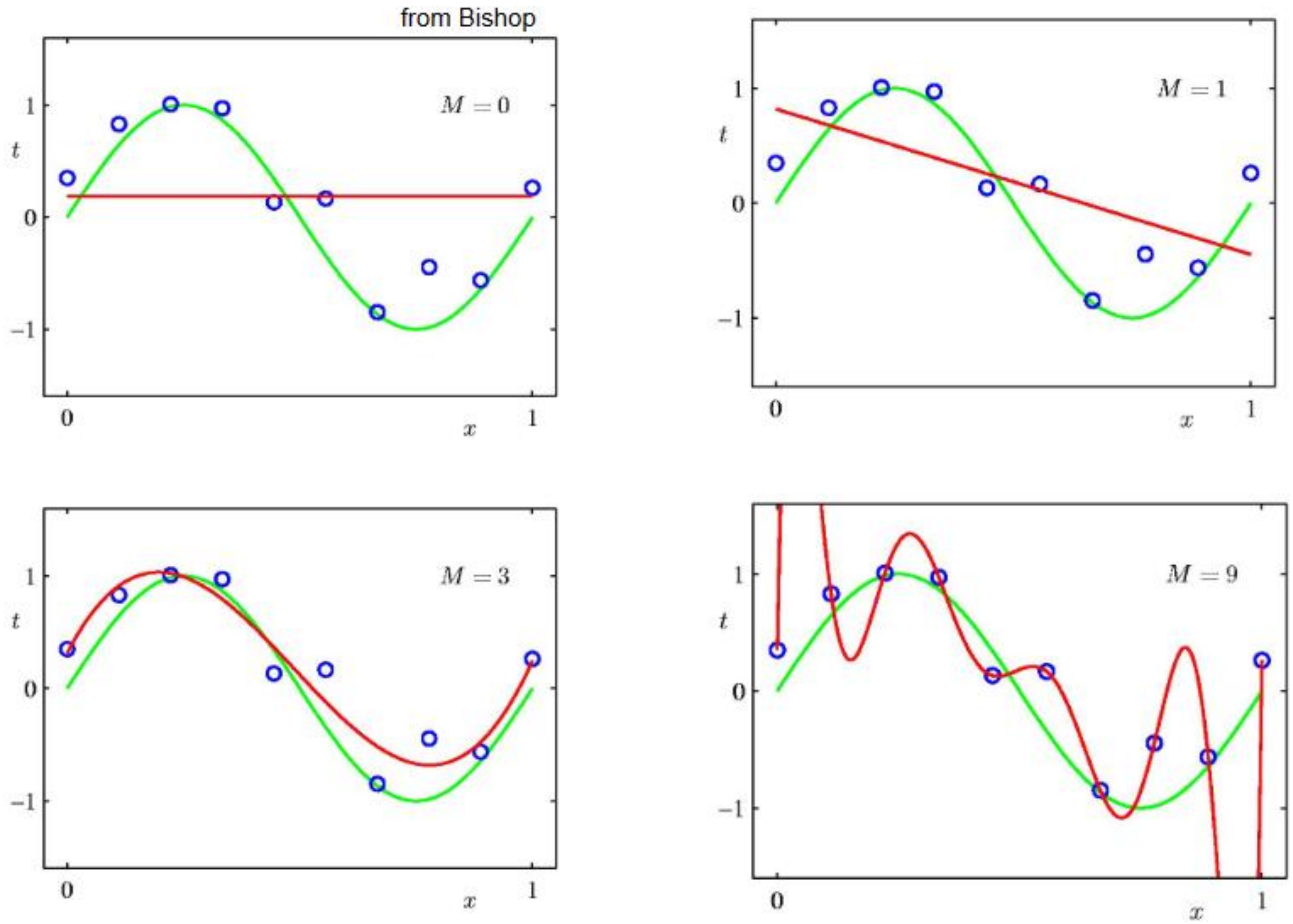
Why limit ourselves to straight lines?

- Not all relationships are linear.
- Linear formula: y = mx + b
  - This is a "first order" or "first degree" polynomial, as the power of x is 1
- Second order polynomial: $y=ax^2+bx+c$
- Third order: $y=ax^3+bx^2+cx+d$
- Higher orders produce more complex curves.

$$y(x, \mathbf{w}) = w_0 + \sum_{j=1}^{M} w_j x^j$$



Which Fit is Best?

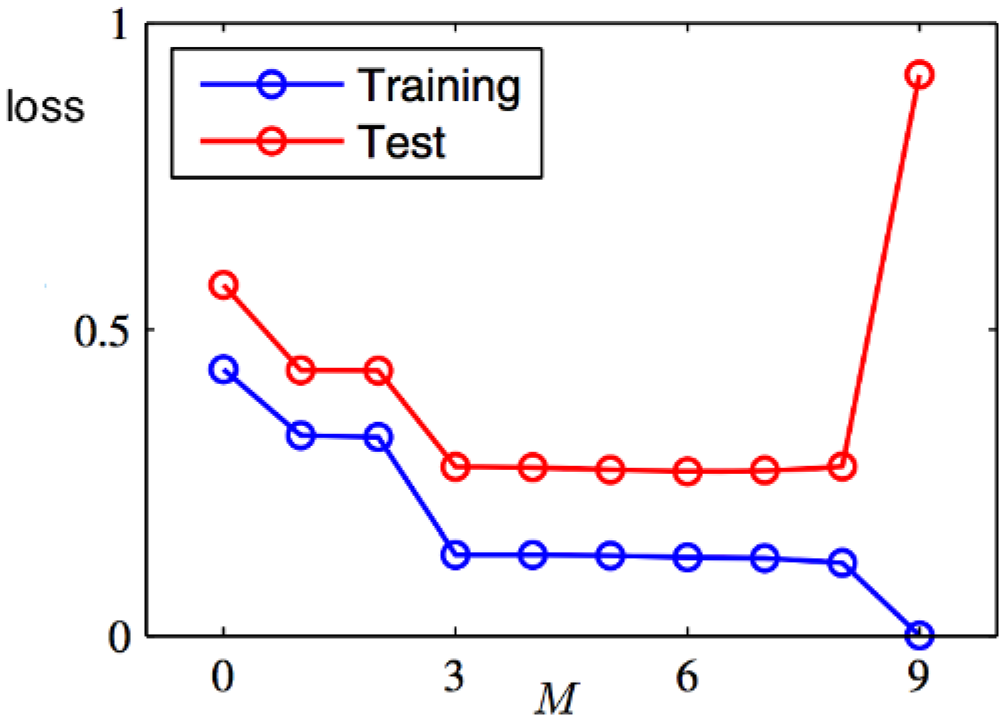


Beware overfitting

- Don't use more degrees than you need
- Visualize your data first to see how complex of a curve there might really be
- Visualize the fit is your curve going out of its way to accommodate outliers?
- A high r squared simply means your curve fits your training data well; but it may not be a good predictor.
- Later we'll talk about more principled ways to detect overfitting (train/test)

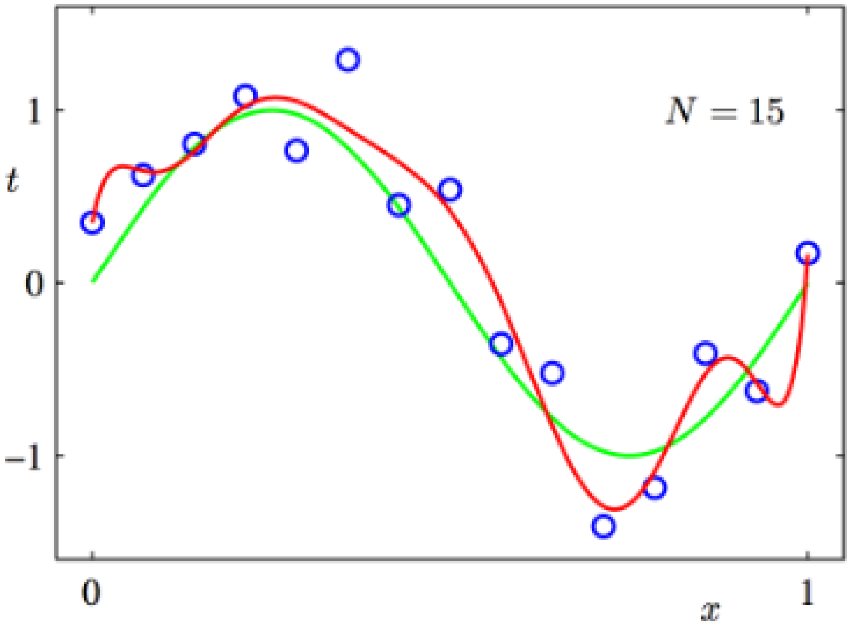
Generalization

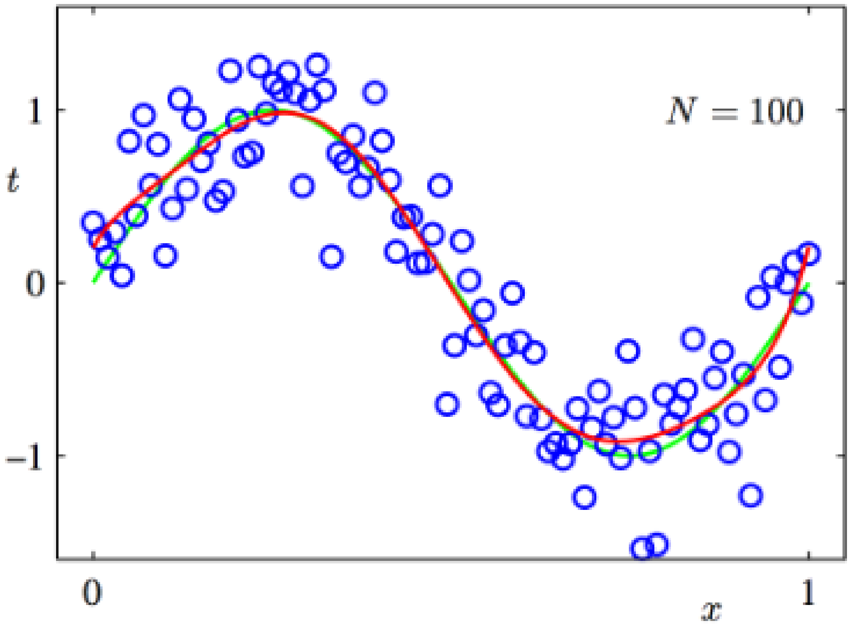
- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with M = 9 overfits the data (it models also noise)



Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with M = 9 overfits the data (it models also noise)
- Not a problem if we have lots of training examples





Outliers

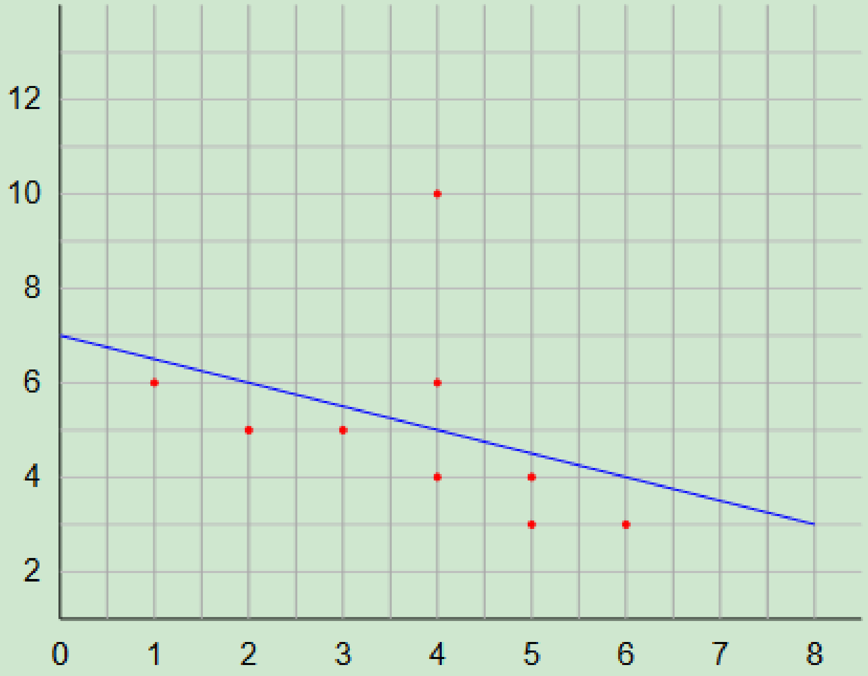
- Outlier
  - An outlier is a point with an unusually large residual (e.g., at least 2.5 standard deviations from the mean).
- Influential Point
  - An influential point is a point that exerts a inordinate influence on the regression line.
- An outlier may or may not be influential.
- An influential point may or may not be an outlier.

Example

- Consider the following data.

x	y
1	6
2	5
3	5
4	6
4	4
4	10
5	3
5	4
6	3

The scatterplot



Example

- The regression line is $\hat{y} = 7.0 - 0.5x$.

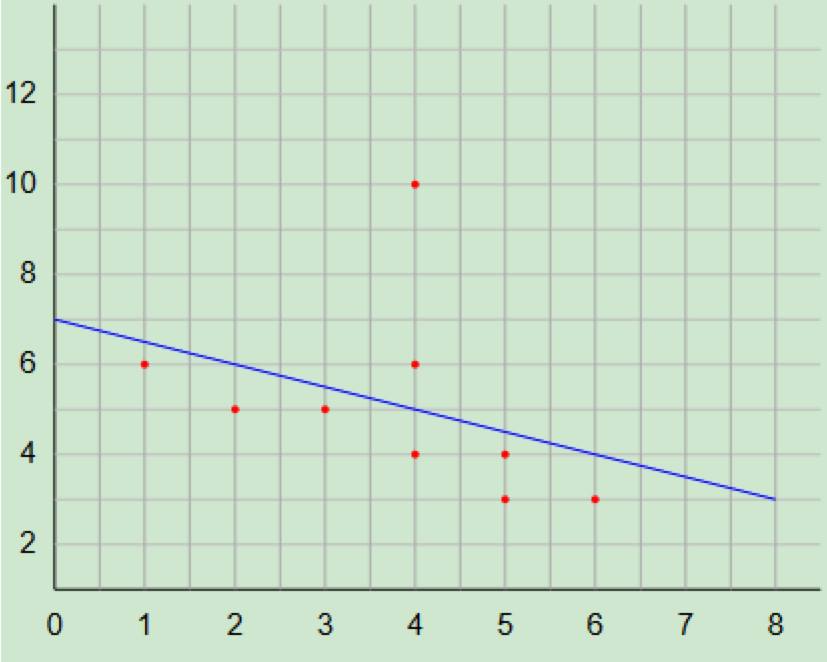
x	y	$\hat{y}$	$y - \hat{y}$
1	6	6.5	−0.5
2	5	6.0	−1.0
3	5	5.5	−0.5
4	6	5.0	1.0
4	4	5.0	−1.0
4	10	5.0	5.0
5	3	4.5	−1.5
5	4	4.5	−0.5
6	3	4.0	−1.0

- The mean residual is 0.0 (always) and the standard deviation of these residuals is 2.0.
- Thus, the residual 5.0 is 2.5 standard deviations above the mean, an outlier.
- But, is the point (4, 10) influential?
- Remove it and see what the effect is.

Example

Including the point (4, 10)

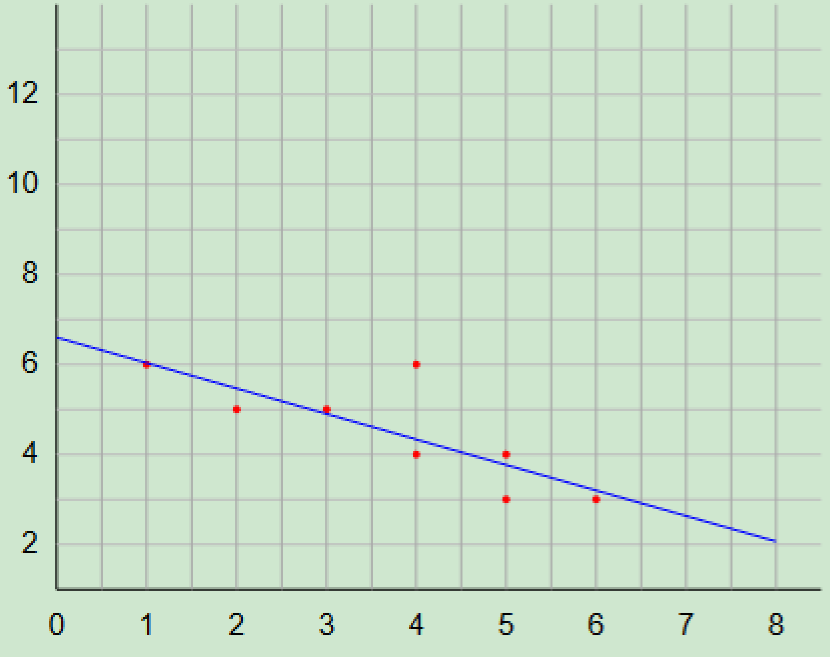
$\hat{y} = 7.0 - 0.5x.$



This is nearly the same as →

Excluding the point (4, 10)

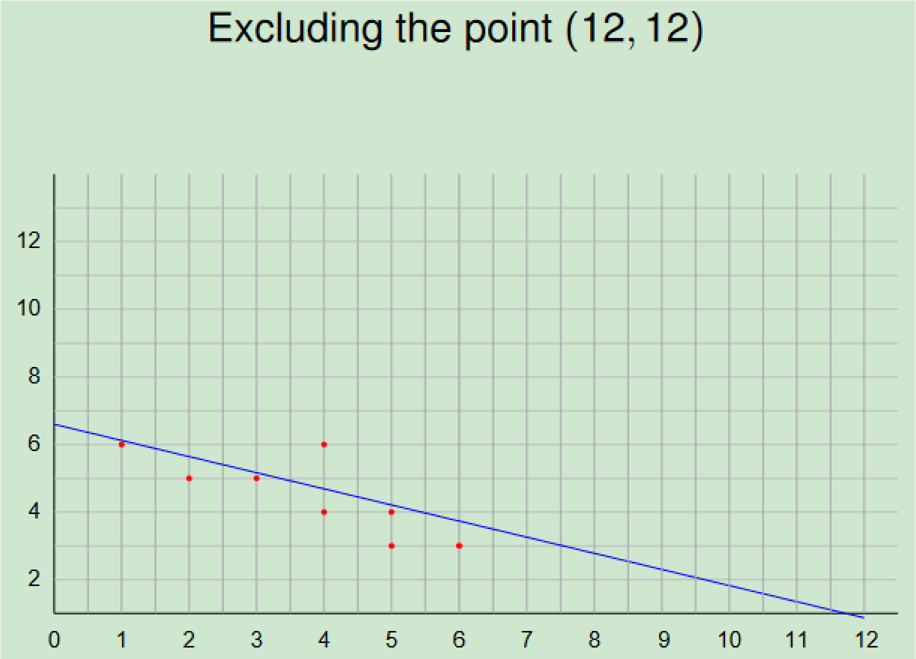
$\hat{y} = 6.615 - 0.564x.$



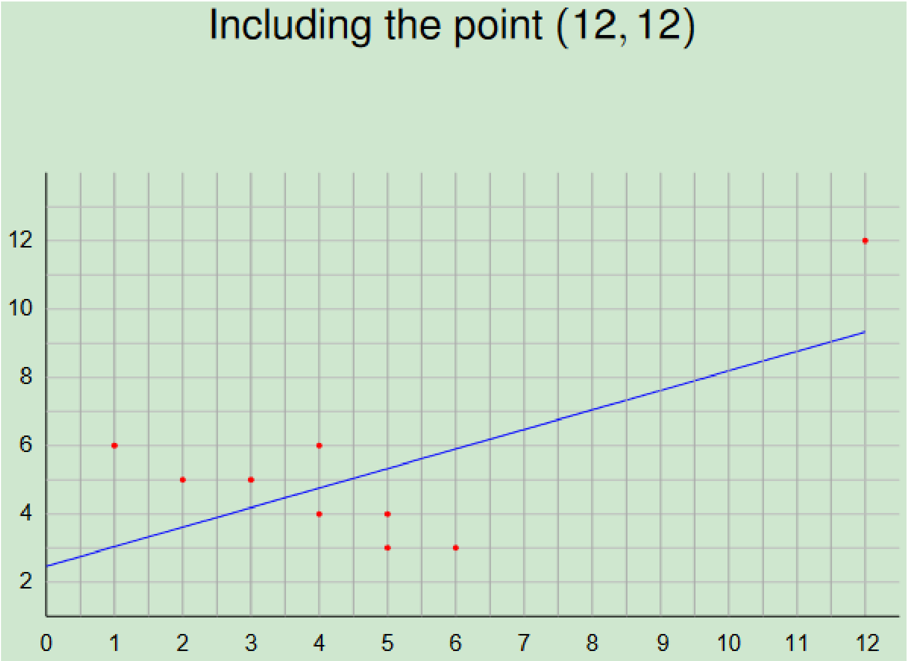
Example

- Now change the point (4, 10) to the point (12, 12).

x	y
1	6
2	5
3	5
4	6
4	4
5	3
5	4
6	3
12	12



$$\hat{y} = 6.615 - 0.564x$$



$$\hat{y} = 2.767 + 0.55x.$$