Regression extensions

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Lecture 33

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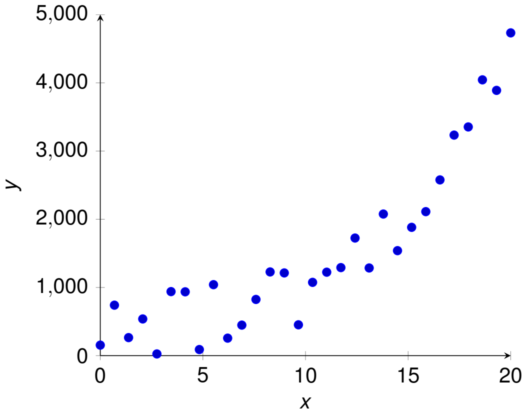
Polynomial regression

What if our data looks like this?



Polynomial regression

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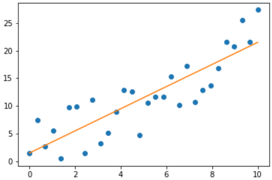

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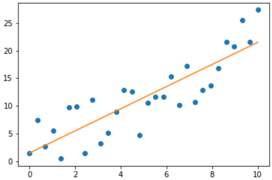

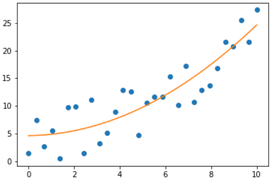

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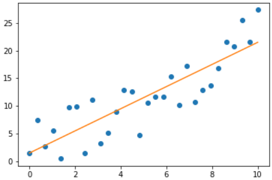

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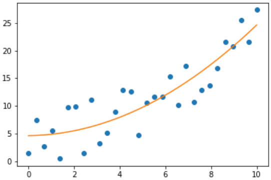

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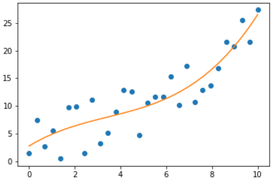

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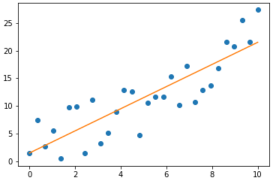

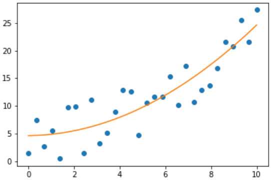

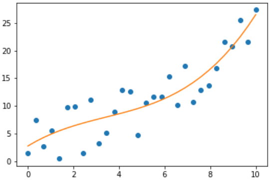

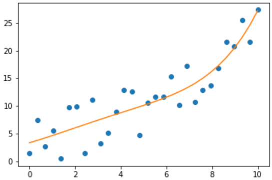

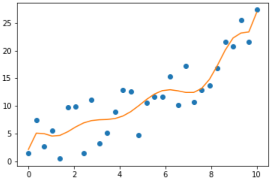

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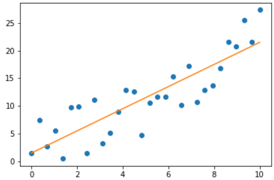
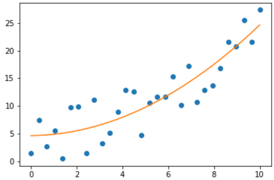
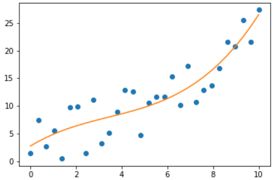
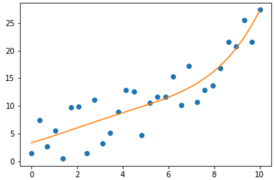
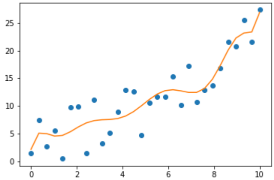
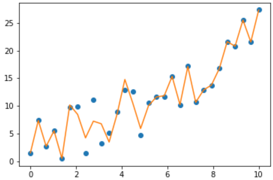

Appropriate model selection

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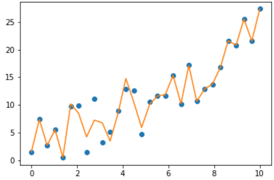
Overfitting



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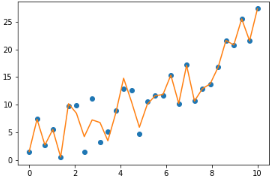

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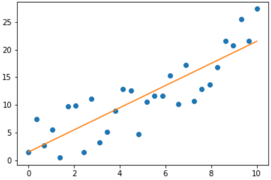

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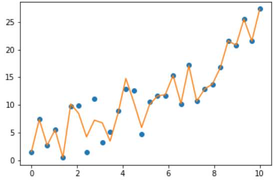

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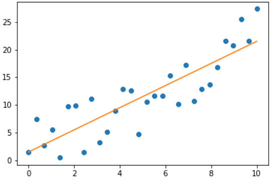

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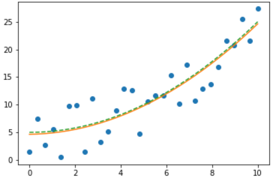

Polynomial regression: a small example

How to fit data points with a line of the form:

$$y = \beta_0 + \beta_1 x + \beta_{11} x_1^2?$$

Pretty simple idea!

- First, create a “new” predictor variable x_2.
- Set it equal to x_1^2!
- Create matrix X based on x_1 and $x_2 = x_1^2$.
- Solve for $\hat{\beta} = \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_{11} \end{bmatrix} = \left(X^T X\right)^{-1} X^T y$.

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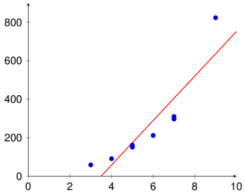
Example

Consider the following data:

x	y
7	310
3	59
5	153
5	162
4	91
6	212
7	297
5	151
9	823

We tried a linear regression and got the line:

$$y = 7.2404x - 2.2194.$$



Since it does not look great, we decide to try a second degree polynomial regression of the form: $y = \beta_0 + \beta_1 x + \beta_{11} x^2$.

Example solution

1. First, create a new column in the data: x^2.

x	x^2	y
7	49	310
3	9	59
5	25	153
5	25	162
4	16	91
6	36	212
7	49	297
5	25	151
9	81	823

2. Build X.

$$X = \begin{bmatrix} 1 & 7 & 49 \\ 1 & 3 & 9 \\ 1 & 5 & 25 \\ 1 & 5 & 25 \\ 1 & 4 & 16 \\ 1 & 6 & 36 \\ 1 & 7 & 49 \\ 1 & 5 & 25 \\ 1 & 9 & 81 \end{bmatrix}$$

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Example solution

3. Solve for $\hat{\beta}$:

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4. Plot $y = 437.74 - 190.47x_1 + 25.5x_1^2$:

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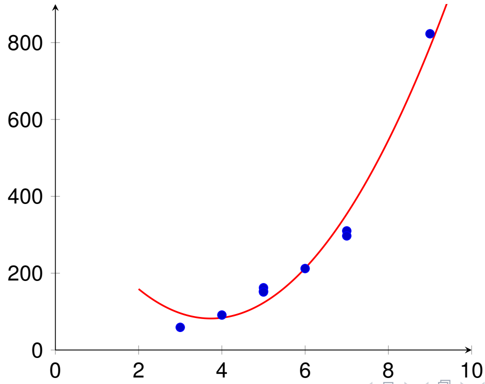

Other interactions

We can use that same logic for other, different variable interactions and functions. For example:

- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$
  - Introduce new variable $x_{12} = x_1 x_2$ and solve.
- $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{123} x_1 x_2 x_3$
  - Introduce new variable $x_{123} = x_1 x_2 x_3$ and solve.
- We can even do that with other nonlinear functions: for example $y = \beta_0 + \beta_1 x_1 + \beta_2 cos(x_1)$.
  - Introduce new variable $x_2 = cos(x_1)$ and solve.
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Model selection

Given k predictor variables, we saw that not all need to be significant. So, this begs the question: which variables should I include in my regression?

1. **All subsets selection.**
   - Consider all (2^k) possible combinations of variables.
   - Pick the model with highest R^2_{adj}.
2. **Backwards selection.**
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Validating a regression model

How can we validate our model?

- Split our data into two parts:
  - training data
  - testing data
- Common split is 80%-20% (in favor of training).
- Use the training data to create the regression.
- Use the testing data to test how well the regression is performing.
- Check the performance by calculating the MS_E:

$$MS_E = \frac{1}{n-2}\sum\left(y_i^{test} - \hat{y}_i^{test}\right)^2.$$

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- Split our data into K parts:
  - $K - 1$ parts with training data.
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- Output the best model amongst them.

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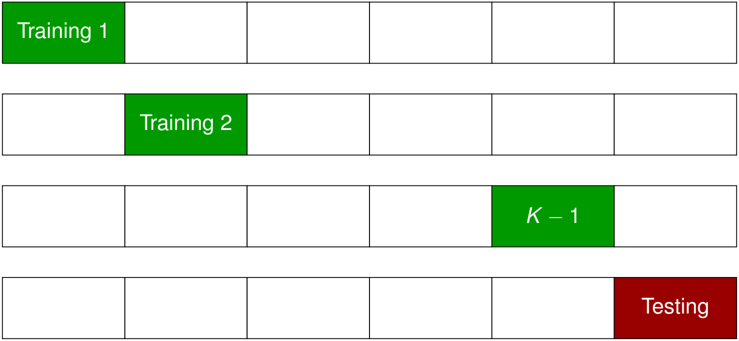

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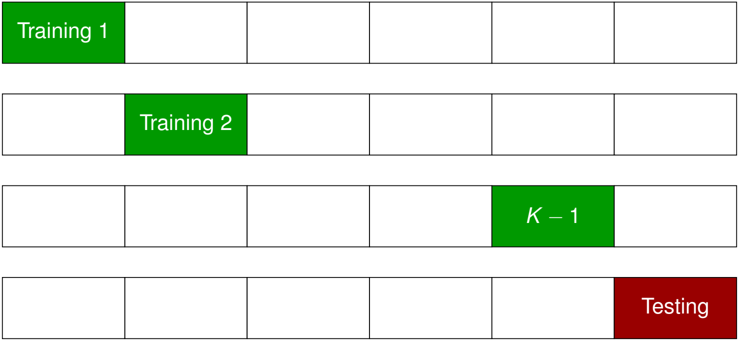

K-fold validation

- Split our data into K parts:
  - $K - 1$ parts with training data.
  - 1 part of testing data.
- Use the training data to create $K - 1$ models.
- Use the testing data to test how well **each of the regressions** are performing.
- Output the best model amongst them.