CFDS® – Chartered Financial Data Scientist

Introduction to Python

Prof. Dr. Natalie Packham

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5 Model validation and measures of fit

- In Data Science, there is no one single statistical method that performs *best* across all data sets.
- It is an important -- and at times difficult -- task to select the appropriate method or model for a given data set.
- We therefore study a number of measures to assess the quality of fit, which in turn allows to compare methods and models.
- For a more in-depth treatment, see Chapters 2.2, 5.1 and 6.1.3 of

  James, Witten, Hastie, Tibshirani: An Introduction to Statistical Learning. Springer, 2013.

5.1 Mean-square error and overfitting

- A commonly used measure for assessing how well predictions match observed data is the **mean squared error (MSE)**, which you know e.g. from Ordinary Least Squares (OLS) in linear regression:

  $\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2,$

where $\hat{f}(x_i)$ is the prediction that the fitted method $\hat{f}$ gives for the i-th observation.

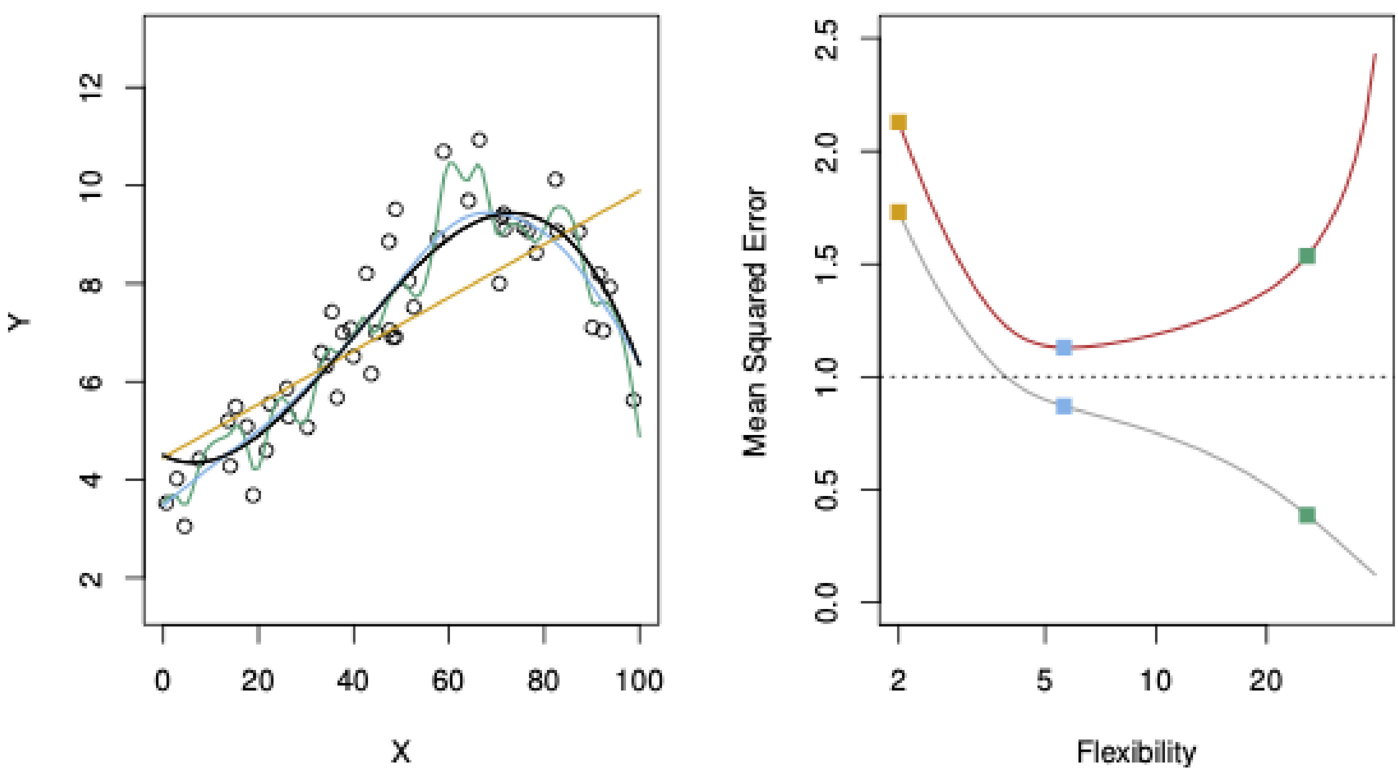
Training and tests MSE

- In Linear Regression (a statistics method), the whole data set is used for finding a linear function $\hat{f}$ that minimises the MSE.
- In Data Science (i.e., statistical learning, machine learning, artificial intelligence), it is common to split the data set into a **training data set** and a **test data set**.
- This reflects that we do not really care how well a method works on the training data, but rather we are interested in the accuracy of the prediction when applying the method to previously unseen data (the test data).
- In other words, first we fit the training data $\{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}$to obtain the estimate $\hat{f}$, e.g. by minimising the MSE on the training data.
- Then we calculate the MSE on the test data, which are data points $\{(x_0, y_0)\}$ that were not used to training the method.
- We want to choose the method that gives the lowest *test MSE*.

Remarks

- Sometimes an additional **validation data set** is added to allow for tuning parameters such as the number of hidden units in a neural network.
- In econometrics, instead of the terminology training and test data set, we speak of **in-sample** and **out-of-sample testing**.

Training and test MSE



Source: James et al.: An Introduction to Statistical Learning. Springer, 2013.

Left:

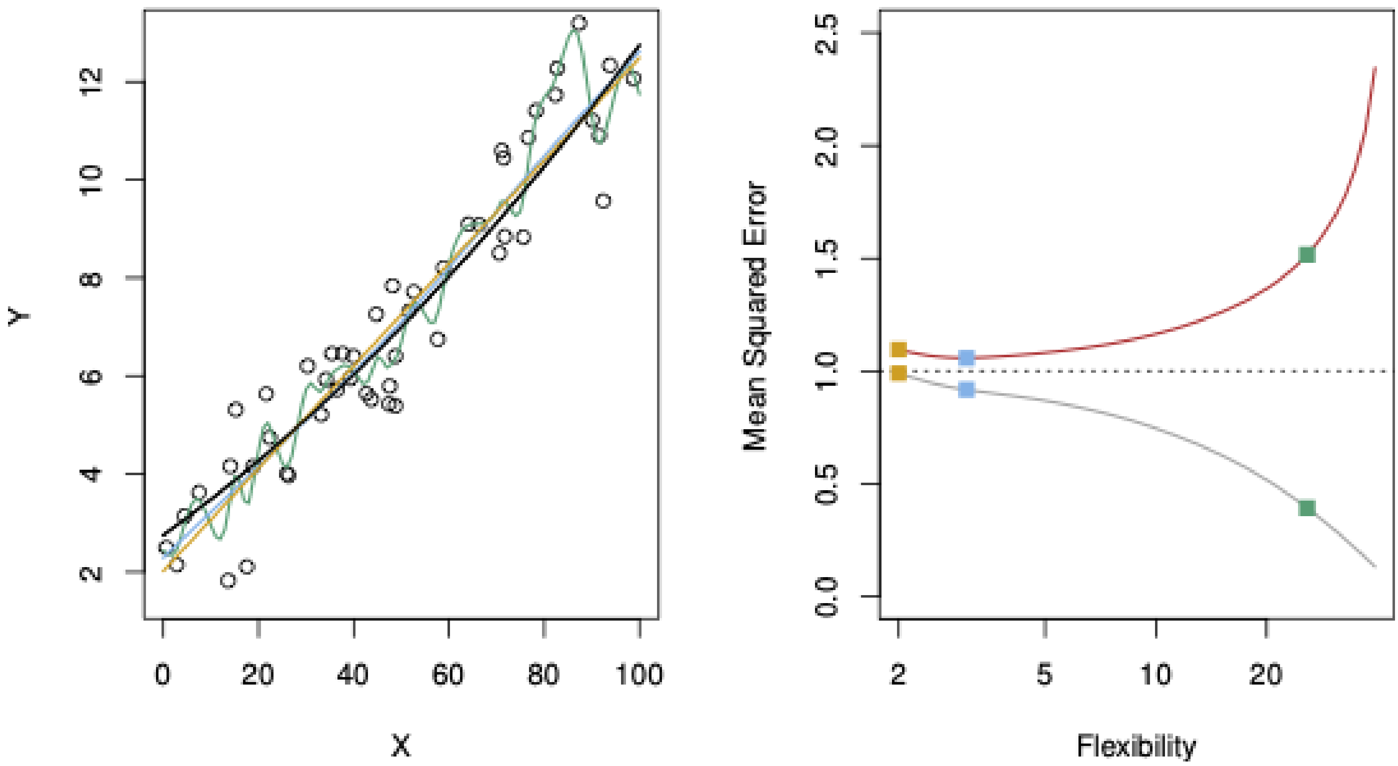
- **Test data**, simulated from f (black smooth line) are shown as black dots.
- Estimates of f:
  - linear regression line (orange)
  - smoothing spline I (blue)
  - smoothing spline II (green)

Right:

- Training MSE (grey)
- Test MSE (red)
- Flexibility denotes the complexity of the models (e.g. number of parameters)

Training and test MSE

- The green smoothing spline will have the smallest MSE on the training data set.
- It does not perform well, however, when **extrapolating** to the test data set.
- This effect is called **overfitting**.
- **Overfitting** refers to choosing a model that fails to capture the *general* effects due to a too many *degrees of freedom*.
- In other words, a less flexible model performs better on the test data than a more flexible model.
- A second example is shown on the next slide.



Source: James et al.: An Introduction to Statistical Learning. Springer, 2013.

5.2 The classification setting

- The measure MSE applies in a regression setting.

- In a classification setting, we seek to estimate f on the basis of training observations $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$, where $y_1, \ldots, y_n$ are qualitative.
- Here, the training **error rate**, which denotes the proportion of mistakes when applying the $\hat{f}$ to the training observations is a measure of **accuracy**:

  $$\frac{1}{n}\sum_{i=1}^{n} \mathbf{1}_{y_i \neq \hat{y}_i},$$

  where $\mathbf{1}_A$ is an *indicator function* taking value 1 if A is true and 0 otherwise.
- The **test error rate** is giving as the error rate from applying $\hat{f}$ to the test data set.

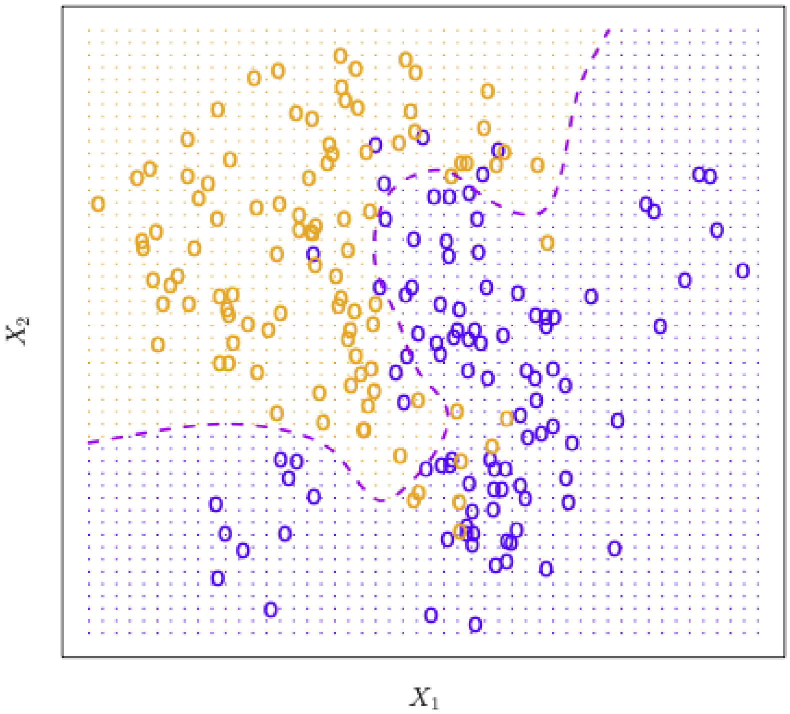
The Bayes classifier

- The test error rate is minimised, on average, by the **Bayes classifier** which assigns each observation to the most likely class given its predictor value, i.e., for an observation x_k, and classes $1, \ldots, j$, it determines the conditional probabilities

  $$\mathbb{P}(Y = 1|X = x_k), \ldots, \mathbb{P}(Y = J|X = x_k)$$

  and assigns the class, for which the conditional probability is highest.

The Bayes classifier



Source: James et al.: An Introduction to Statistical Learning. Springer, 2013.

- Two-dimensional predictors X_1 and X_2 and two classes (blue, orange).
- Dashed line is the Bayes decision boundary.

5.3 Choosing the optimal model

AIC, BIC, Adjusted R^2

- If the optimal model is chosen based on the training data set, then measures such as MSE or R^2 might be misleading.
- This is the case for example in a standard regression setting, where we do not differentiate between training and test data sets.
- In a regression setting, the R^2 will always improve if more independent variables are added.
- There are a number of techniques for *adjusting* the training error according to model size (e.g. different number of independent variables).
- These can be used to select amongst models of different size.
- Typical measures are:
  - Akaike information criterion (AIC)
  - Bayesian information criterion (BIC)
  - adjusted R^2

AIC, BIC, Adjusted R^2

- Consider the problem of finding the appropriate predictors (independent variables) in a regression model.
- Should you include all variables? Or just a subset of the variables?
- Define the *residual sum of squares (RSS)* as

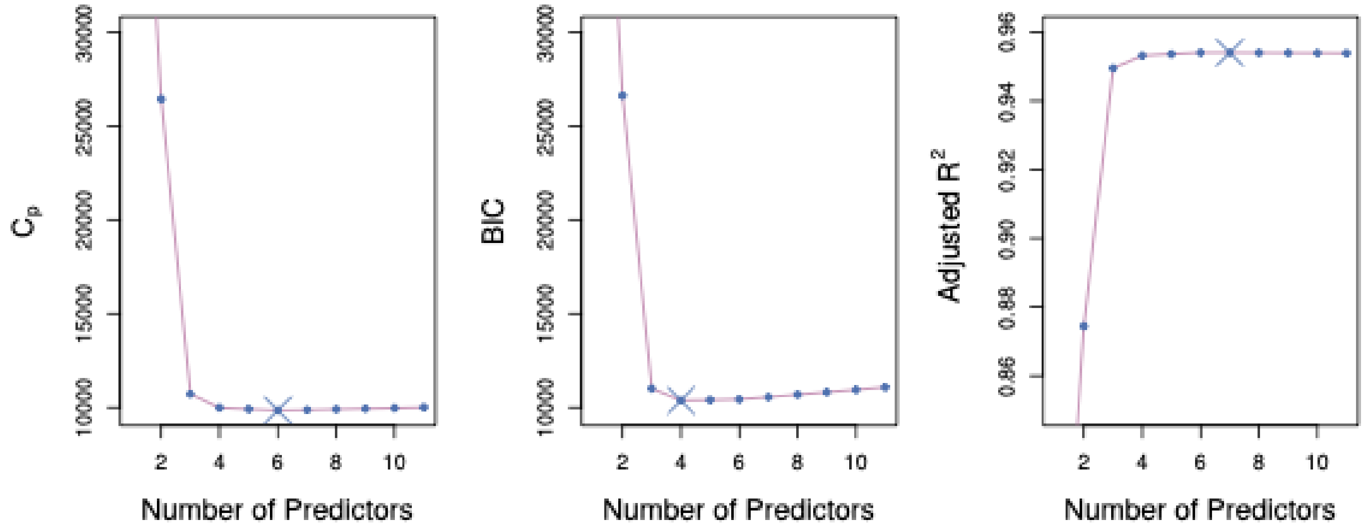
  $$\mathrm{RSS} = \epsilon_1^2 + \epsilon_2^2 + \cdots + \epsilon_n^2 = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \cdots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2,$$

  where $\hat{\beta}_i$ and x_k may be vectors.

AIC, BIC, Adjusted R^2

- Then, the measures above are defined as
  - $\mathrm{AIC} = \frac{1}{n\hat{\sigma}^2}(\mathrm{RSS} + 2d\hat{\sigma}^2)$;
  - $\mathrm{BIC} = \frac{1}{n}(\mathrm{RSS} + \ln(n)d\hat{\sigma}^2)$;
  - $\text{Adjusted } R^2 = 1 - \dfrac{\mathrm{RSS}/(n-d-1)}{\mathrm{TSS}/(n-1)}$, with $\mathrm{TSS} = \sum(y_i - \bar{y})^2$ the _total sum of squares of the response.
- A further measure, which in OLS regression yields an equivalent model choice as AIC is:
  - $C_p = \frac{1}{n}(\mathrm{RSS} + 2d\hat{\sigma}^2)$, with $\hat{\sigma}^2$ an estimate of the error variance and d the dimension of x_k.
- All measures have in common that they place a penalty on a more complex model, measured by the number of explanatory variables d.
- Each measure has a theoretical justification; this is beyond the scope of the course, however.

AIC, BIC, Adjusted R^2



Source: James et al.: An Introduction to Statistical Learning. Springer, 2013.

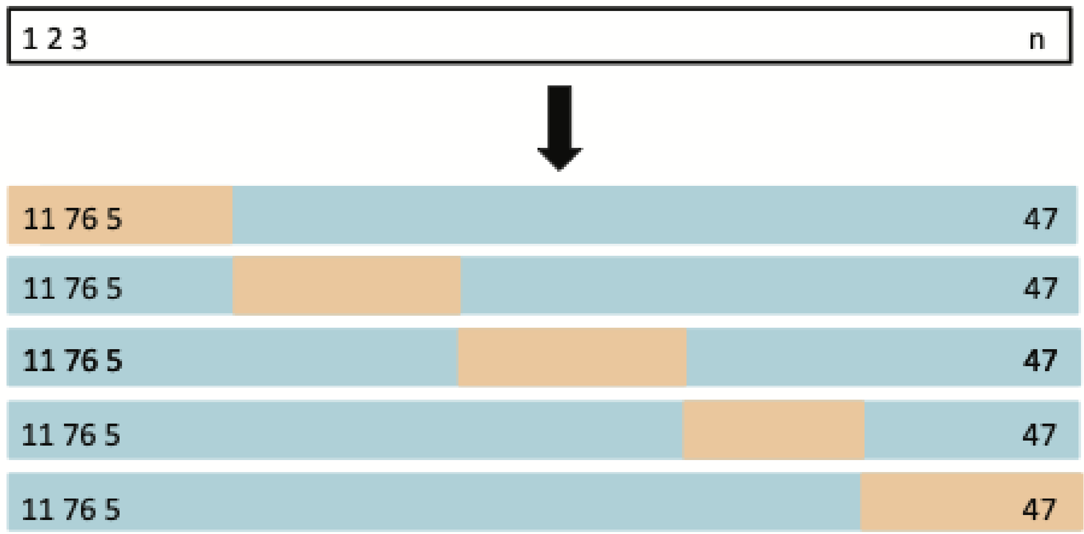
- Estimates of C_p (proportional to AIC), BIC and Adjusted R^2 for a data set of credit card defaults with predictors such as age, income, marital status, etc.
- A lower C_p and BIC indicate a superior model; likewise a higher Adjusted R^2.

5.4 Cross-validation

- **Cross validation (CV)** refers to several methods of building the test and training data sets.
- In k-fold CV, the data set is randomly divided in k groups or *folds* of approximately equal size.
- In k iterations, each first fold is treated as the test or validation data set, while the $k-1$ other folds are taken as the training data.
- In this way, k MSE's of the test error are estimated and the k-fold CV estimate is given by

$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k}\mathrm{MSE}_i.$$

Cross-validation



Source: James et al.: An Introduction to Statistical Learning. Springer, 2013.

- A schematic display of 5-fold CV.
- A set of n observations is randomly split into five non-overlapping groups.
- Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue).
- The test error is estimated by averaging the five resulting MSE estimates.