Model Selection and Prediction Accuracy

Eltecon Data Science Course by Emarsys

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Goal of the lesson

- Intro to the **theory of model selection**, model complexity and overfitting
- Understand the concept through real life examples
- Cover most commonly used **practical solutions** to the model selection problem
- Get some hands-on experience

Section 1

Model Selection in Theory

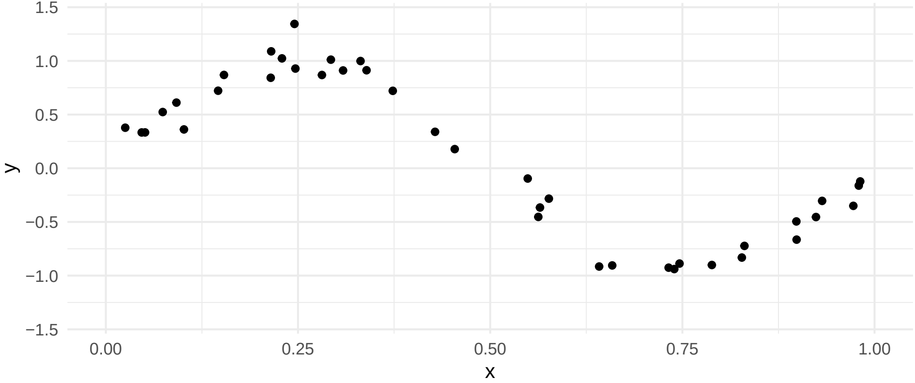
How to Select the Best Model

Goal: Good generalisation i.e.: best predictive performance on new data

What if I choose the one with the lowest error $(RMSE)/$ best fit (R^2)?

How to select the best type of model for our application?

How to Select the Best Model



The Loss Function

Common choice for regression problem is the **squared loss**:

$$L(f(x), y) = (f(x) - y)^2$$

Goal is to choose $f(x)$ that **minimises the expected loss**:

$$E[L(f)] = E[(f(x) - y)^2]$$

The Empirical Loss Minimiser

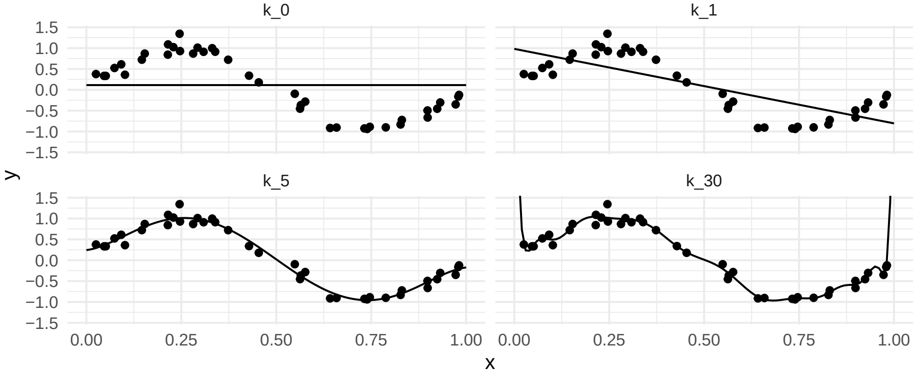
Assume you choose to approximate the relationship with a linear function with k variables (f_k).

The **empirical loss** of the fitted model:

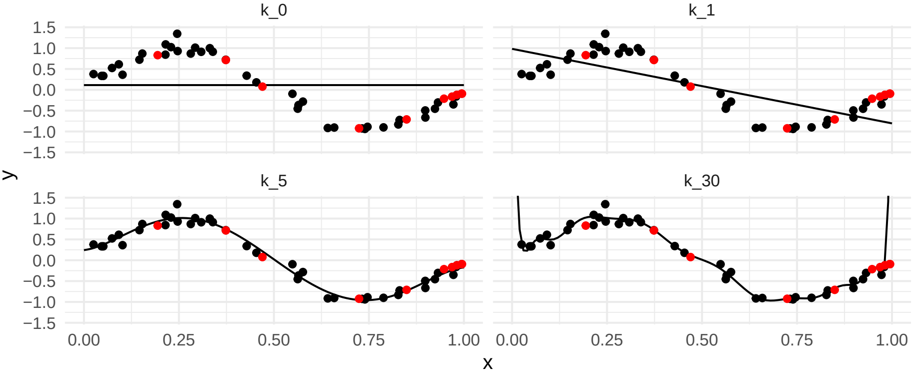
$$\hat{L}(f_k) = \frac{1}{n} \sum (f_k(x) - y)^2$$

Is this a good estimate of the expected loss of $f_k(x)$? Beware of overfitting!

The Empirical Loss Minimiser



The Empirical Loss Minimiser



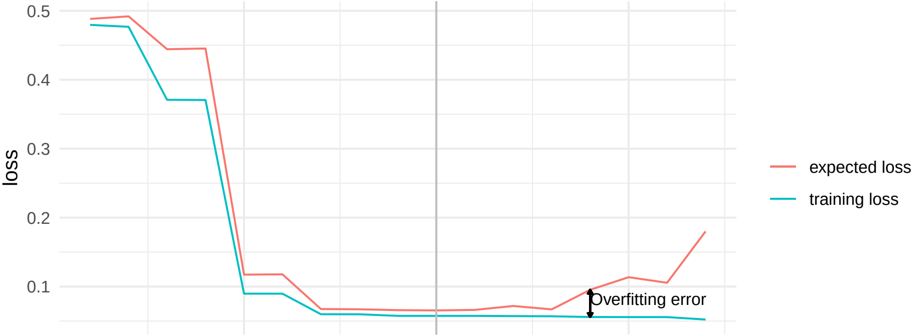
What is overfitting

Among a set of possible models we choose one that is too complex and has poor generalisation properties.

Why? Because we have an incorrect estimate of its expected loss.

Overfitting error:

$$E[L(f_k)] - \hat{L}(f_k)$$



Model Complexity in Practice

- "Classic" variable selection: Which explanatory variables should I include?
- Functional form selection: In what form should I include my variables?
- Tree models: How complex tree structure should I allow?
- Deep learning: How complex neural network should I train?

Model Complexity in Practice

Take the bike rental example from last time.

How should we incorporate the information on the time of the day?

1. include “hour” variable as it is
2. create a dummy variable for each value of hour
3. include “hour” as a third degree polynomial
4. include a dummy variable for morning/afternoon

Task: Order the listed options by model complexity. Share your results in Socrative!

Section 2

Model Selection in Practice

Model Selection in Practice

Find the ideal level of **model complexity** within a given model type (e.g.: choose k for linear regression) for a **given set of data**.

Note that we have two conflicting goals:

- have a larger set of models to choose from in order to find the best among all possible models → increase complexity
- have a realistic estimate of the models' preformance so we find the best model out of the set of models we consider → decrease complexity

Train vs. Test Error

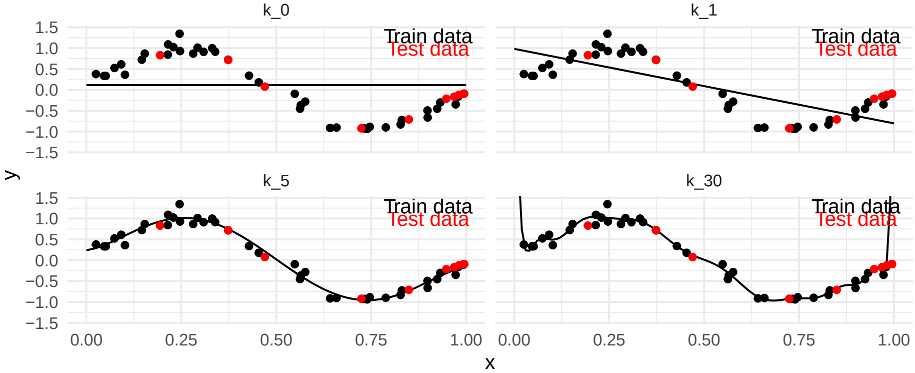
Idea: have an independent sample to estimate the performance of the fitted model

Training set: N observations of labeled data used to tune the parameters of the model (e.g.: estimate coefficients of linear regression)

Validation set/Test set: M observations of labeled data used to estimate the performance of the fitted model and possibly optimize model complexity and/or choose between different types of models

Watch out for use-cases where random assignment does not work!

Train vs. Test Error



Train vs. Test Error

$$RMSE = \sqrt{\frac{1}{n}\sum(\hat{f}(x) - y)^2}$$

	train RMSE	test RMSE
pred0	0.71	0.54
pred1	0.45	0.51
pred5	0.11	**0.08**
pred30	**0.09**	1.49

SMS Spam Prediction Dataset

- Source: Kaggle
- Goal: Predict if SMS was a spam using text of the SMS

Pre-cleaned the data (removed stopwords, special characters etc.) and created word count variables: **spam_clean.csv**

is_spam	message	nchar	nwords
0	Go until jurong point, crazy.. Available only in bugis n great world la e buffet... Cine there got amore wat...	111	12
0	Ok lar... Joking wif u oni...	29	4
1	Free entry in 2 a wkly comp to win FA Cup final tkts 21st May 2005. Text FA to 87121 to receive entry question(std txt rate)T&C's apply 08452810075over18's	155	20
0	U dun say so early hor... U c already then say...	49	6
0	Nah I don't think he goes to usf, he lives around here though	61	8
1	FreeMsg Hey there darling it's been 3 week's now and no word back! I'd like some fun you up for it still? Tb ok! XxX std chgs to send, å£1.50 to rcv	148	16

plus top 400 most frequent words.

SMS Spam Prediction

Let's see some prediction models! **spam_pred_train_test.R**

Practice Time

- Task: estimate at least two more models with different complexity, compute their train and test accuracy and conclude which one to use to spot spam messages!
- Share your results in Socrative!
- You have 20 minutes - feel free to take a break if needed.

Train vs. Test Error

Advantages:

- Simple approach

Disadvantages:

- Loss of valuable training data
- Small validation set gives noisy estimate of predictive performance

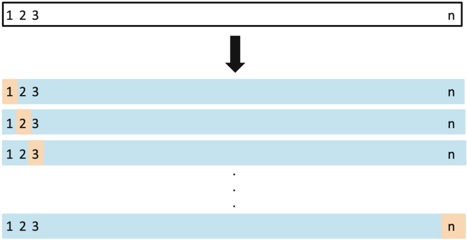
Overfitting to the validation set??? Possible!

One may want to set aside a third set of data to assess the performance of the final model.

Cross validation

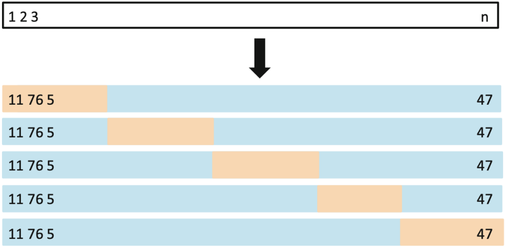
Idea: Instead of having a single validation set split the data multiple times to estimate the performance of the fitted model

Leave-one-out: split tha data N times, always leave one observation out for testing



Cross validation

K-fold: split the data into *k* sub-samples of equal size and leave one out for testing



How to choose k? Larger k results in larger variance in the error estimation but provides nearly unbiased estimate of the performance of the fitted model. ($k = 5$ is a common choice)

Cross validation

$$CV_k = \sqrt{\frac{1}{k}\sum MSE_i}$$

	train RMSE	test RMSE	CV RMSE
pred0	0.71	0.54	0.68
pred1	0.45	0.51	0.47
pred5	0.11	**0.08**	**0.12**
pred30	**0.09**	1.49	0.96

SMS Spam Prediction

Let's do cross-validation for our spam prediction models! **spam_pred_cv.R**

Practice Time

- Task: Compute leave-one-out CV accuracy for all models you fitted in the previous exercise and compare their performance!
- Share your results in Socrative!
- You have 20 minutes - feel free to take a break if needed.

Cross validation

Advantages:

- utilizes all the data
- suitable for parameter tuning
- can decrease variance of the error estimation

Disadvantages:

- computationally expensive

Homework

- Take a deeper look at the spam dataset and extract at least two more variables from the message text that you think could help the prediction. Describe your new variables.
- Include the new variables in your model and evaluate the model performance using CV.
- Summarise your results in a few sentence.

Resources

- Bishop, Christopher: Pattern Recognition and Machine Learning
- Gareth J., Witten D., Hastie T. and Tibshirani R.: An Introduction to Statistical Learning