Model Selection and Prediction Accuracy

Eltecon Data Science Course by Emarsys

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November 13, 2019

Goal of the lesson

- Intro to the **theory of model selection**, model complexity, overfitting, etc.
- Cover some **practical solutions** to the model selection problem
- Implement cross-validation in `R`
- Get some hands-on experience with your own data

Section 1

Model Selection in Theory

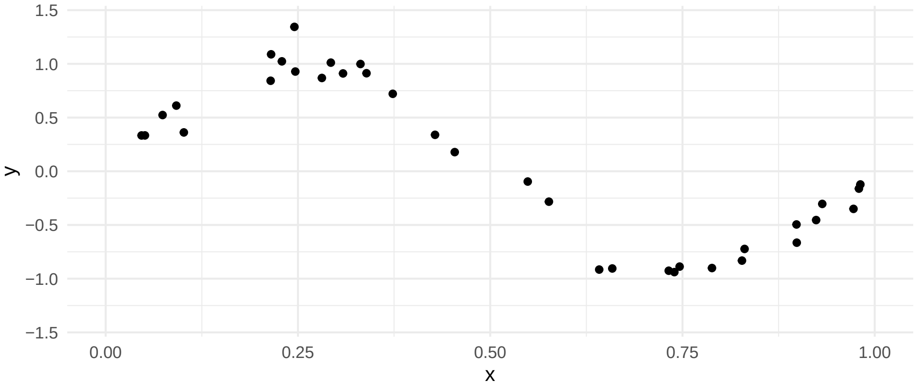
How to Select the Best Model

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

What if I choose the one with the lowest error (MSE)/ 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**:

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

On can show that the:

$$f^*(x) = argmin_{f(x)} E[L(f(x), y)] = E[y|x]$$

The Empirical Loss Minimiser

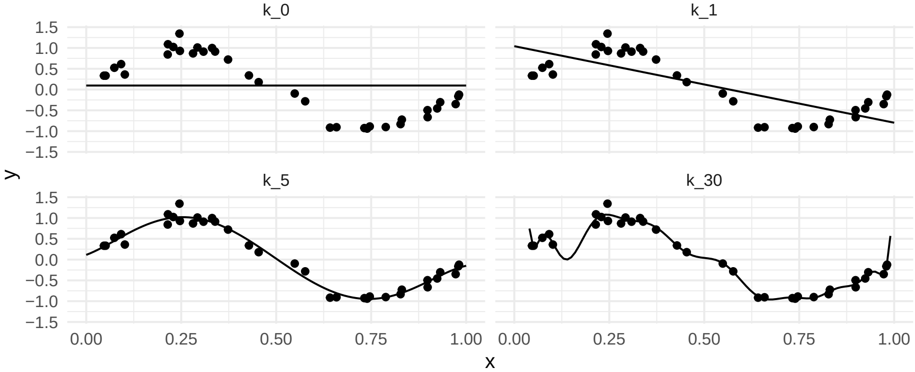
Assume you choose to approximate the relationship with a linear function with k variables.

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

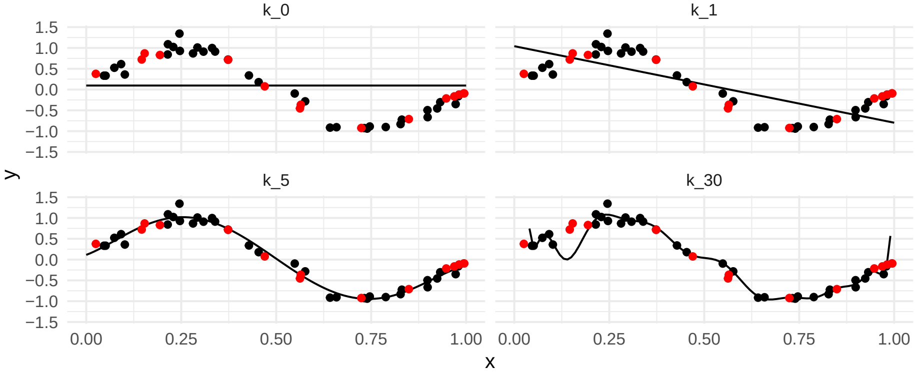
$$\hat{L}(f_k) = \frac{1}{n}\sum(f_k(x) - y)^2$$

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

The Empirical Loss Minimiser



The Empirical Loss Minimiser



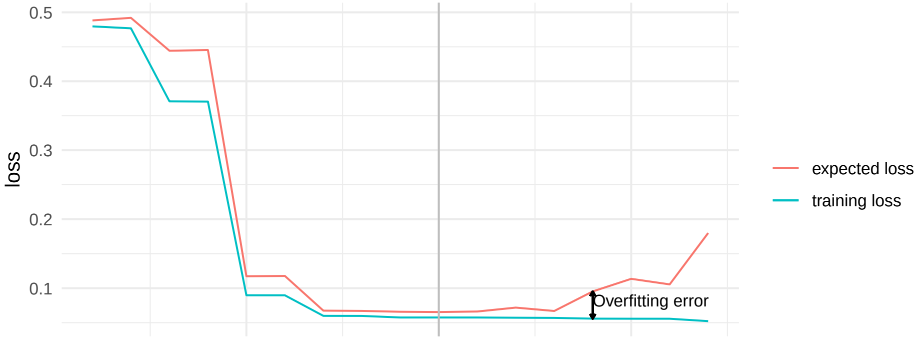
What is overfitting

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

How to avoid overfitting?

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**.

$$E[L(f_k)] - E[L(f^*)] = \underbrace{[E[L(f_k)] - E[L(f_k^*)]]}_{\text{estimation error}} + \underbrace{[E[L(f_k^*)] - E[L(f^*)]]}_{\text{approximation error}}$$

where f_k^* is the best estimator among models with complexity k.

Section 2

Model Selection in Practice

Train vs. Test Error

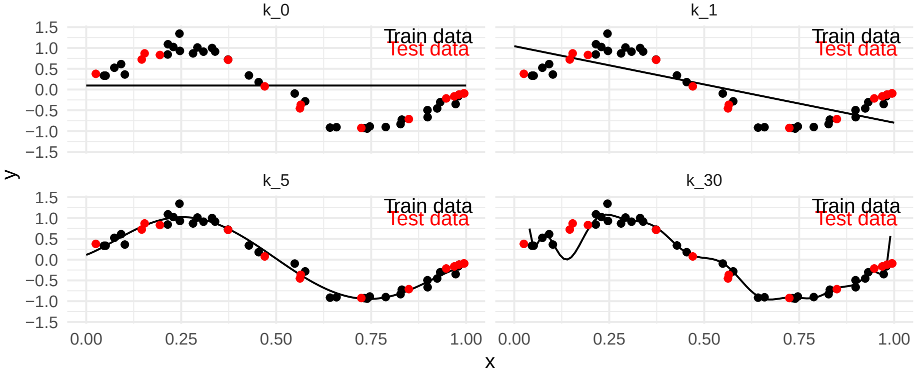
Idea: have an independent sample to estimate the performance of the fitted model

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 data used to 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

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

	train MSE	test MSE
pred0	0.54	0.30
pred1	0.21	0.22
pred5	0.01	0.01
pred30	0.01	1.32

Train vs. Test Error

Advantages:

- Simple approach

Disadvantages:

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

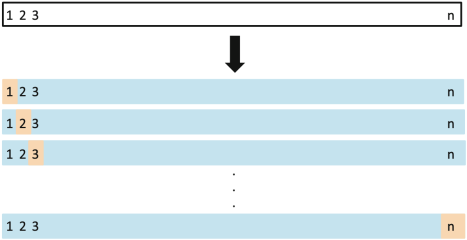
Overfitting to the validation set??? Possible!

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

Cross validation

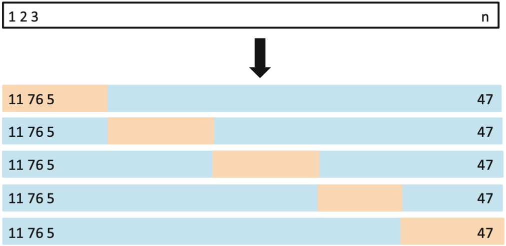
Idea: Instead of having a single validation set split the data multiple times to estimate the performance of the fitted model

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

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

	train MSE	test MSE	CV MSE
pred0	0.54	0.30	0.46
pred1	0.21	0.22	0.22
pred5	0.01	0.01	0.01
pred30	0.01	1.32	0.93

Cross validation

Advantages:

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

Disadvantages:

- computationally expensive

Information criteria

Idea: Penalize model complexity by adding a penalty term.

Definition:

- **BIC** (Bayesian approach):

$$-\ln(\hat{L}) + \frac{1}{2} k \ln(N)$$

- **AIC** (Information theory):

$$-2\ln(\hat{L}) + 2k$$

where k is the number of parameters, N is the number of data points and $\hat{L}$ is the maximal value of the likelihood function.

Information criteria

Advantages:

- No need to set aside data for validation
- No need to train models multiple times

Disadvantages:

- Rely on assumptions that are often invalid in practice
- In practice, they tend to favor overly simple models

Information criteria

	train MSE	test MSE	CV MSE	AIC	BIC
pred0	0.54	0.30	0.46	81.65	84.76
pred1	0.21	0.22	0.22	51.08	55.74
pred5	0.01	0.01	0.01	-40.79	-29.90
pred30	0.01	1.32	0.93	-42.63	-11.53

Regularisation

Idea: Add a **penalty term** to the error function to discourage the coefficients from reaching large values.

$$E(w) = E_D(w) + \lambda E_W(w)$$

where $E_D(w)$ is the **data-dependent error**, $E_W(w)$ **regularisation term** and λ is the **regularisation parameter** that controls the relative importance of these two terms.

Regularisation

Advantages:

- allows to train complex models on limited size data
- computationally cheap (not always true)

Disadvantages:

- not clear how to choose λ

More on ridge, LASSO, the Bias-Variance trade-off later…

Now your turn!

1. Either use your project data or find Something on Kaggle **DONE**
2. Find a good research/business question that involves prediction and write it down **DONE**
3. Answer your question using what we've learned previously and today
    a. Select a set of candidate models with different complexity (i.e.: different variable sets)
    b. Separate a validation set from your data
    c. Fit all the candidate regressions on the rest of your data
    d. Compare the fit of your models on the train and validation data
    e. Perform cross-validation of your models
    f. Try regularisation if it makes sense!
    g. Conclude on your models in terms of their prediction performance
    h. Finish @ Home!

Resources

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