University of Exeter

Intro to Machine Learning

Part 2 - Model selection and evaluation

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- **Slides: model selection and evaluation**

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- Tutorial: machine learning pipeline task

Session 3

- Continue with machine learning pipeline task
- Tutorial: unsupervised learning

How do we get the best possible model performance?

- Model selection – select appropriate model
- Model validation – assess generalisability & prevent overfitting
- Model evaluation – assess model performance

We are going to discuss these three things.

Model selection

- There are different types of machine learning problem
- These will influence what models are appropriate to select
- Hence, first stage of machine learning task is to explore your data

The “no free lunch theorem”: Wolpert and Macready

- Applied to machine learning: no single best algorithm for predictive modeling problems, i.e. classification and regression.
- Means you cannot blindly take a “good” algorithm, and expect it to perform well on a new problem.

Model selection - a warning

- Libraries with consistent APIs, such as scikit-learn, make it trivially easy to select different machine learning algorithms, and apply them.
- This can be dangerous: it is possible to select a model that is not appropriate for your use case, or that does not make mathematical or physical sense.
- Similarly, when tuning parameters, these should also be assessed in a similar way.

Model evaluation

- Assess how well the model performs
- Metrics such as:
    - Accuracy (classification)
    - Precision, recall, f1-score (classification)
    - MSE/RMSE (regression)
- Usually assessed on a test (an unseen) dataset
- How do we do this so we are not "marking our own homework?"

Model evaluation - train test split

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First thing we should always do is split our data

- Train set: the data we use for training our model - commonly 80%
- Test set: data we evaluate our model on/assess its performance on - 20%
- Should be before you perform serious investigation into the data!

Train data	Test data
Commonly 80%	20%

Train test split: bias

It is really common to hear about problems of bias in ML algorithms.

Bias can creep in at this stage!

- Your test set needs to be representative of the training data (and vice versa)
- Assessing bias in these splits will also require domain/problem knowledge!

- i.e. if your data is sorted by gender, dont take the last 20% as your test set
  - Because your train set could be mostly the other gender
- We can use scikit-learn to do lots of this for us.

Model validation: overfitting vs underfitting

Overfitting: learning the training features.

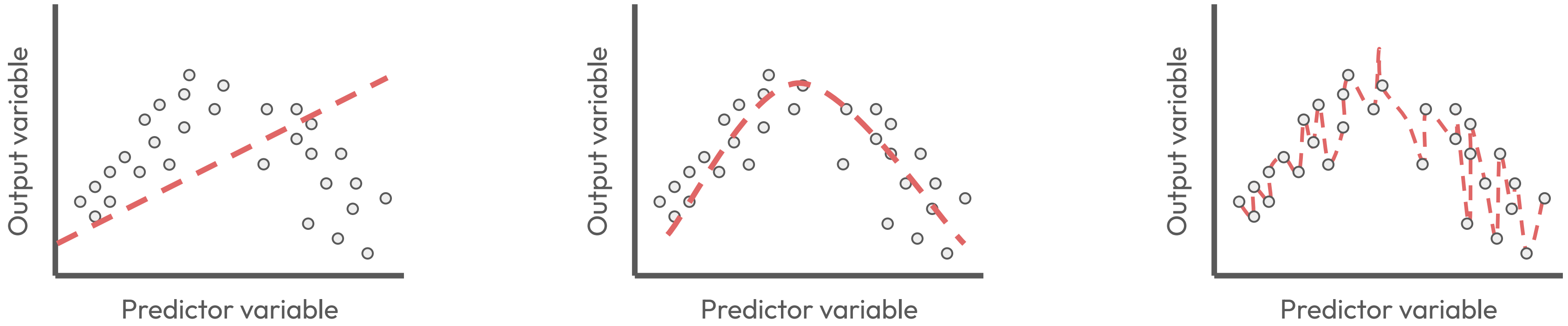
- Symptoms: high accuracy on train set, low accuracy on test set

Underfitting: model has not/cannot learnt the training features

- Symptoms: low accuracy on train AND test sets

Model validation: overfitting vs underfitting

This can be visualised with a polynomial with different degrees of freedom



Model is underfitting:

Poor accuracy, but not possible to learn the shape of the data

Model is fitting well:

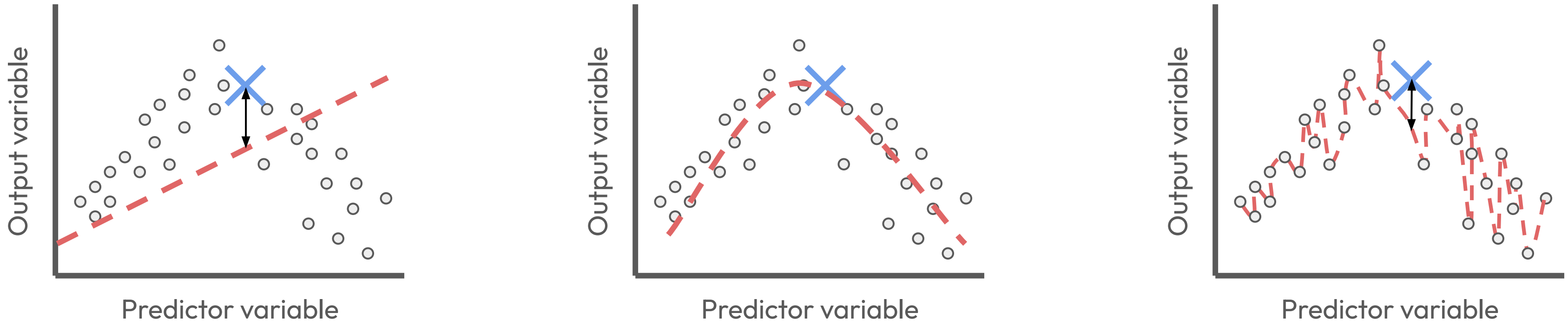
Good accuracy: general shape learnt well

Model is overfitting:

Perfect accuracy on this data. **So what is the problem?**

Model validation: overfitting vs underfitting

Lets add a new, unseen point. This could be from the test set.



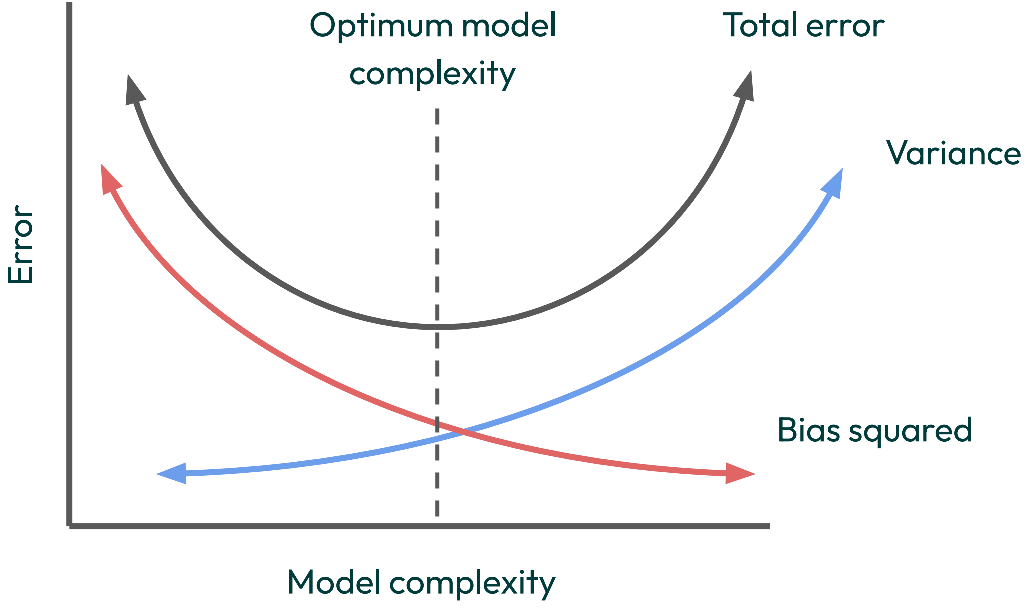
Model does not predict new point well

Model predicts new point well

Model does not predict new point well

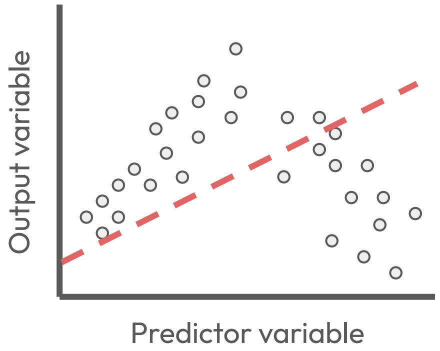
Model validation: bias variance tradeoff

Total error is a function of the bias and the variance

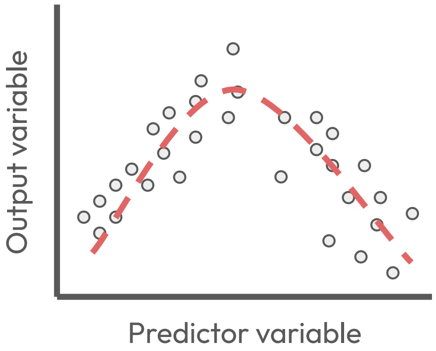


Model validation: bias variance tradeoff

Total error is a function of the bias and the variance

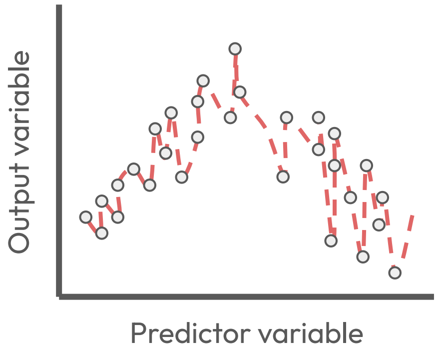


Low complexity, high bias, low variance



Optimal complexity, minimises error

Optimal balance of bias and variance



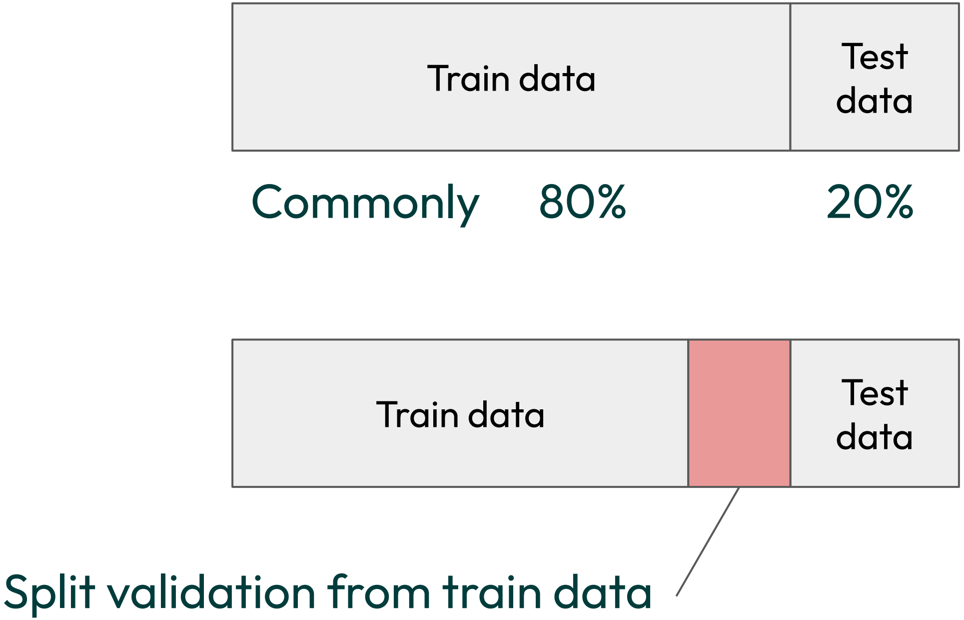
High complexity, low bias, high variance

Model validation: in summary

- A model that is generalisable makes accurate predictions on new, unseen data.
- Models that do not generalise well have not learned a true relationship between the input features, and the outcomes.
- A model that has been overfit is often not generalisable.

Better evaluation: validation holdout

During training, we can split our training set up into a train set and a validation set

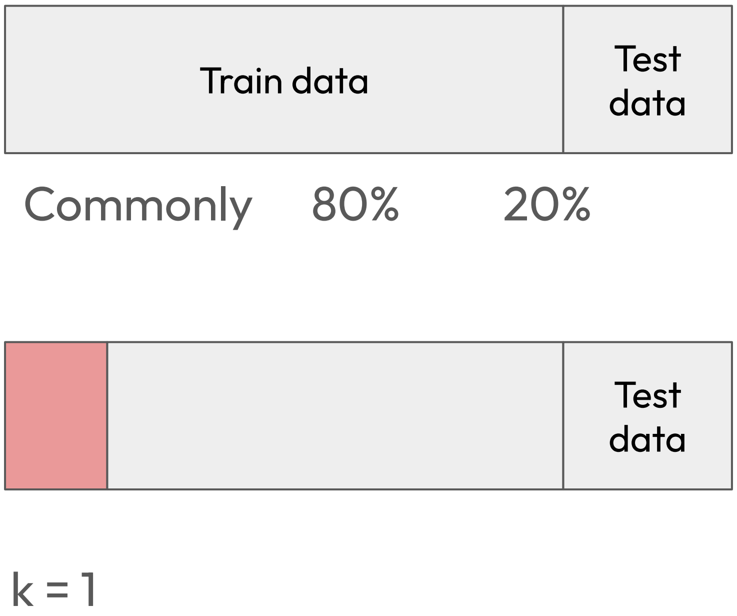


This is a good way of preventing overfitting.

Introduces a problem: reduces the size of our train set.

Better evaluation: validation holdout

We can do this k times: k-fold cross validation. Allows us to still use this validation data in training.



We assess the performance on each “fold”, helping to reduce change of overfitting

Better evaluation: validation holdout

We can do this k times: k-fold cross validation. Allows us to still use this validation data in training.

Commonly 80% 20%

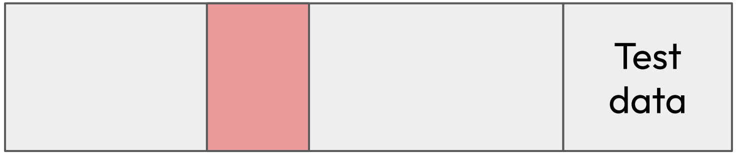
k = 2

We assess the performance on each "fold", helping to reduce change of overfitting

Better evaluation: validation holdout

We can do this k times: k-fold cross validation. Allows us to still use this validation data in training.

Commonly 80% 20%

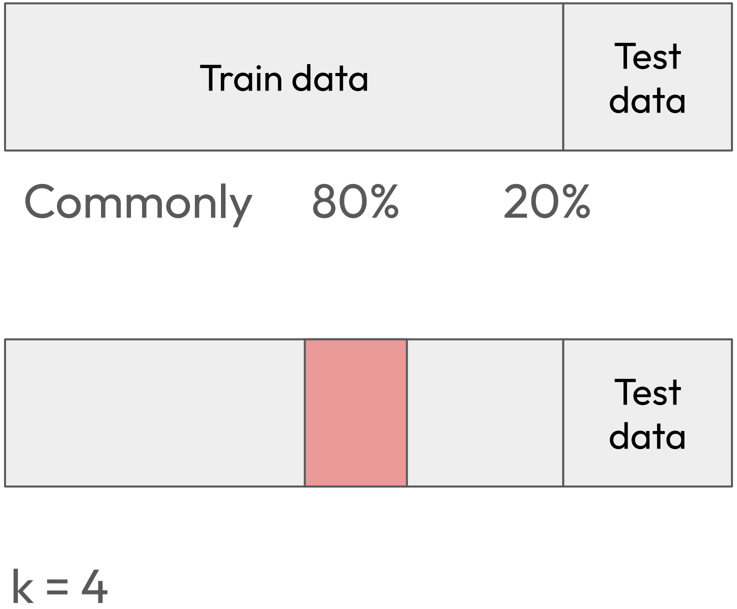


k = 3

We assess the performance on each “fold”, helping to reduce change of overfitting

Better evaluation: validation holdout

We can do this k times: k-fold cross validation. Allows us to still use this validation data in training.



We assess the performance on each "fold", helping to reduce change of overfitting