dm24s1

Topic 06 : Data Modelling

Part 01 : Data Modelling - Introduction

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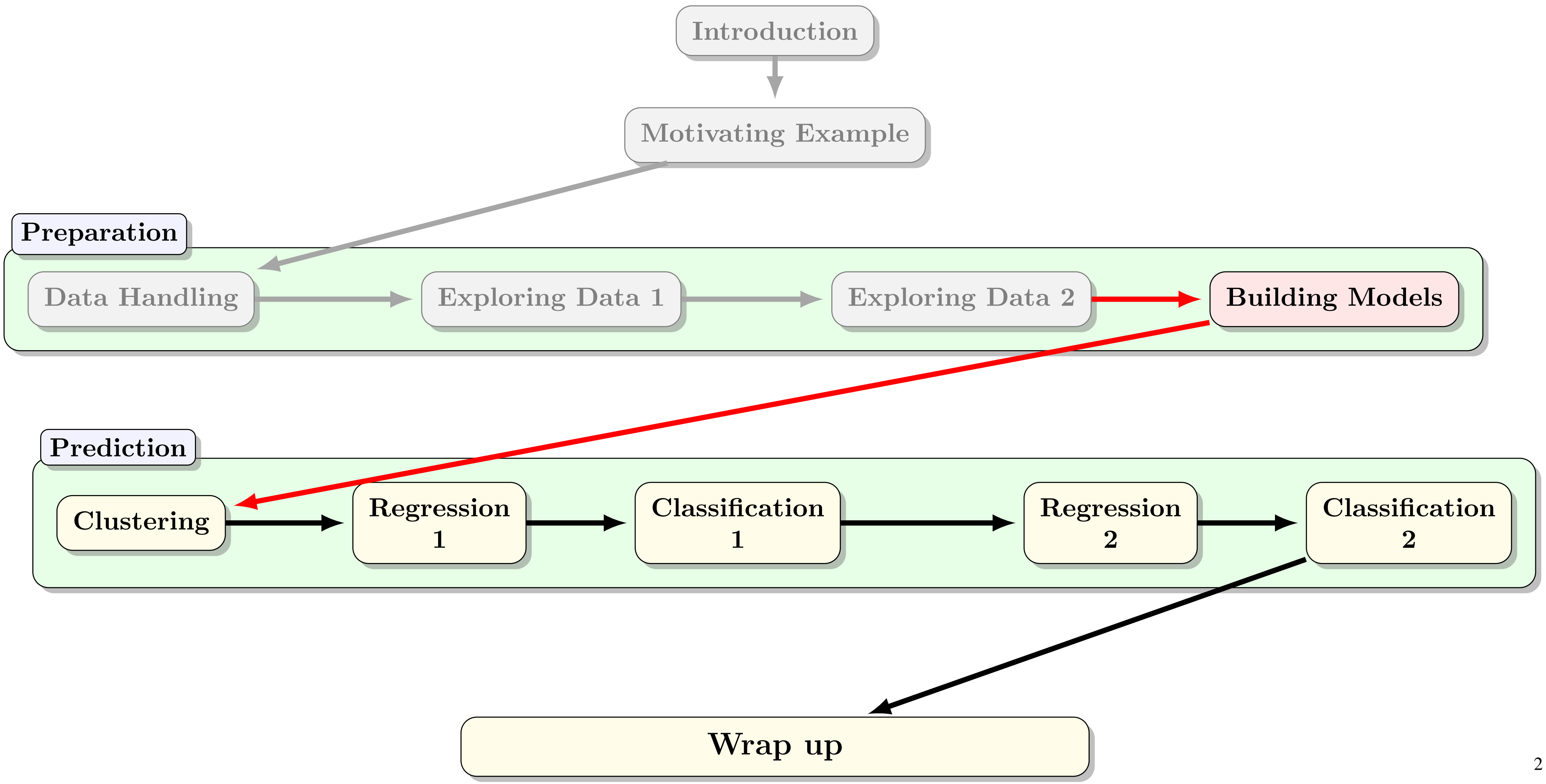
Outline

- Components of a machine learning problem
- Machine learning concepts and notation
- Bias vs variance
- Learning curves
- Regularisation

Wrap up

Data Mining (Week 6)



Three Components of a Machine Learning Problem

It is easy to get lost among the multitude of choices one needs to make when given data mining problem. A good decomposition is the following:

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search
Hyperplanes	Likelihood	Branch-and-bound
Naive Bayes	Posterior probability	Continuous optimization
Logistic regression	Information gain	Unconstrained
Decision trees	K-L divergence	Gradient descent
Sets of rules	Cost/Utility	Conjugate gradient
Propositional rules	Margin	Quasi-Newton methods
Logic programs		Constrained
Neural networks		Linear programming
Graphical models		Quadratic programming
Bayesian networks		
Conditional random fields		

A Few Useful Things to Know about Machine Learning, Domingos, 2012.

Three Components of a ML Problem — Representation

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search

Representation refers to formulating the problem as a machine learning problem — typically a classification problem, a regression problem or a clustering problem.

- How do we represent the input?
- What features to use?
- How do we learn additional features?
- With each type of problem, we have multiple subtypes:
  For example which classifier? a decision tree, a neural network, a support vector machine, etc.

Three Components of a ML Problem — Evaluation

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search

Evaluation refers to an objective function or a scoring function, to distinguish a good model from a bad model.

- For a classification problem, we need this function to know if a given classifier is good or bad. A typical function can be based on the number of errors made by the classifier on a test set, using precision and recall.
- For a regression problem, it could be the squared error, or likelihood. Do we include regularisation? etc

Three Components of a ML Problem — Optimisation

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search

Optimisation is concerned with searching among the models in the language for the highest scoring model.

- How do we search among all the alternatives?
- Can we use some greedy approaches, branch and bound approaches, gradient descent, linear programming or quadratic programming methods.

Data Modelling (aka Machine Learning)

As alternative to the three component (Representation / Evaluation / Optimisation) viewpoint we can think of a machine learning problem as

Definition 1 (Machine Learning)

Study of algorithms that improve their performance P at some task T with experience E.

Well defined learning task: $< P, T, E >$

- What metric should be used to measure performance?
- What cost function should be used?
- What is the cost of incorrect prediction?
- Computational cost?

- How complex is the task?
- Task type: classification, regression, ...
- Linear vs nonlinear?
- What family of functions should be used?

- How many historical observations are needed?
- How accurate/noisy is the data?
- Do we have missing values?
- Is the data representative?

Taxonomy of Machine Learning Models . . .

. . . by Intuition/Motivation

- Geometric models use intuitions from geometry such as separating (hyper-)planes, linear transformations and distance metrics.
- Probabilistic models view learning as a process of reducing uncertainty, modelled by means of probability distributions.
- Logical models are defined in terms of easily interpretable logical expressions.

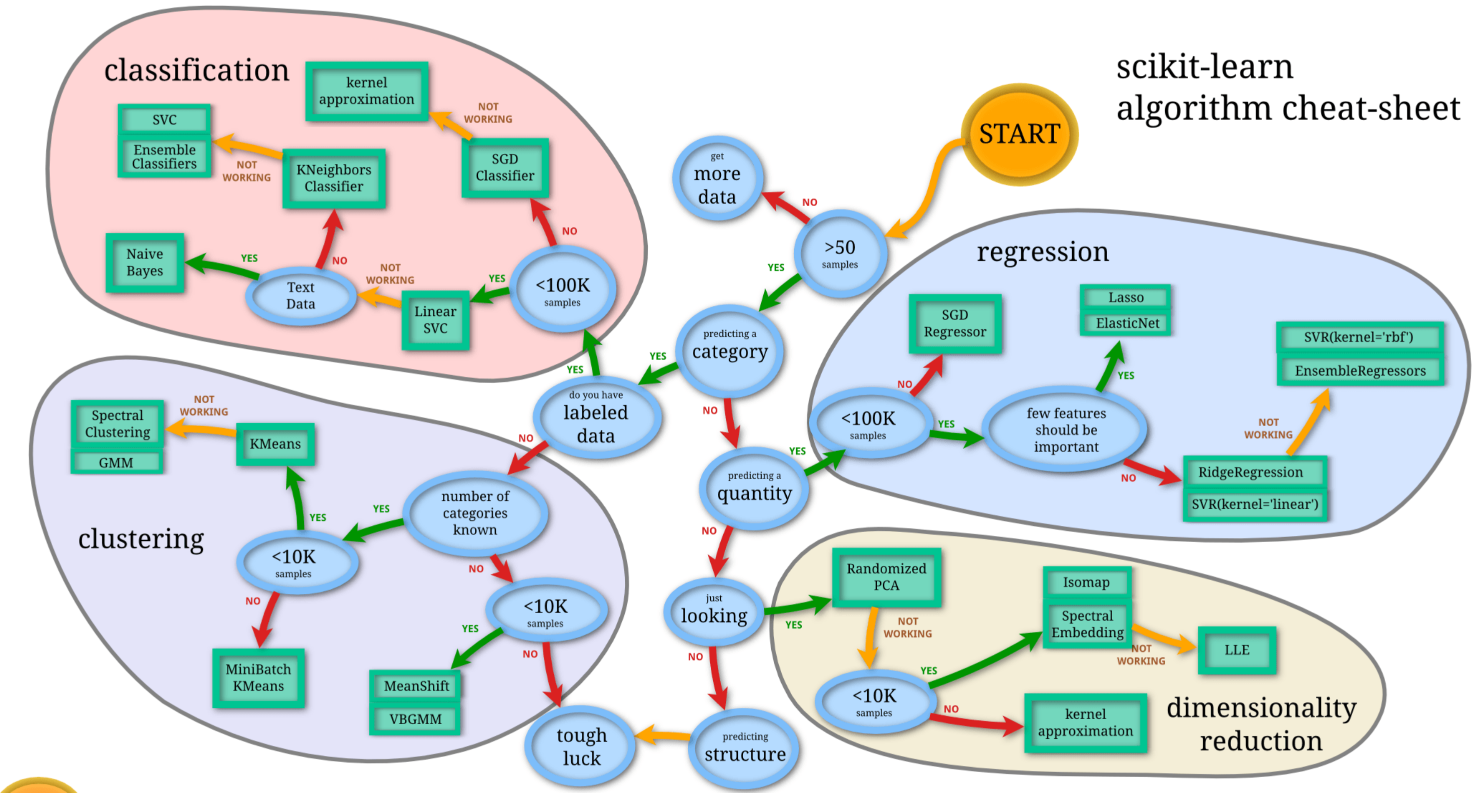
. . . by Algorithmic Properties

- Regression models predict a numeric output.
- Classification models predict a discrete class value.
- Neural networks learn based on a biological analogy
- Local models predict in the local region of a query instance.
- Tree-based models (recursively) partition the data to make predictions.
- Ensembles learn multiple models and combine their predictions.

. . . by Fixed/Variable Number of Parameters

- Parametric models have a fixed number of parameters.
- In non-parametric models the number of parameters grows with the amount of training data.

Aside: Scikit-learn Flowchart of Models (Shallow Learners)



Back

A neural network with more than one hidden layer is called a deep learner, all other learners are shallow learners.

Statistical Models vs Machine Learning Models

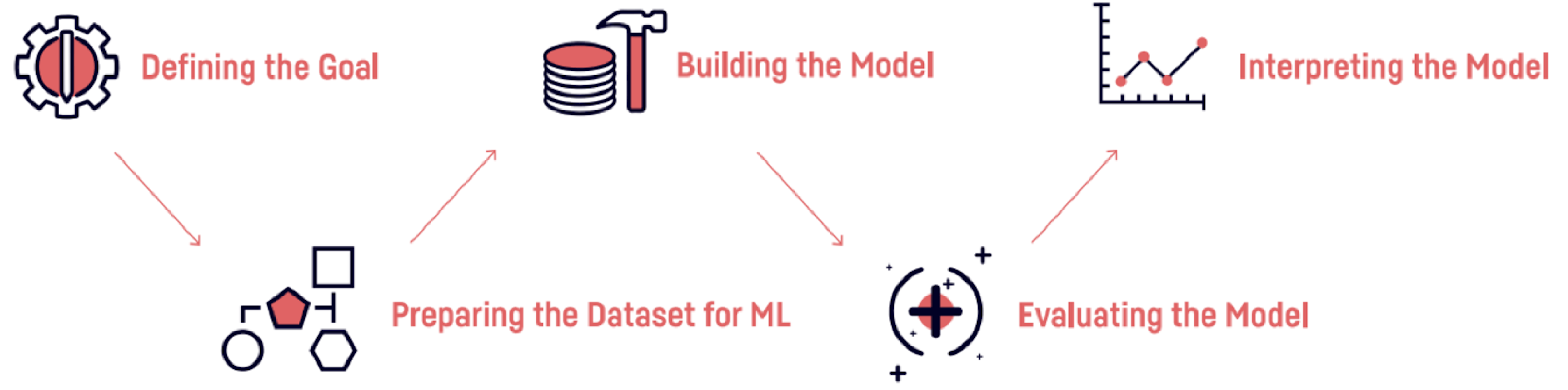
	Statistical Models	ML Models
Data	• Usually small (< 1000 observations) • Low dimension (< 10 variables) • Can have detailed understanding of data • Data is clean — human has looked at each data point	• Can be huge (million+ observations) • Large dimension (1000+, more for vision) • Too large for human to parse / understand • Data not clean — humans can't afford to understand/fix each point
Models	• Simple models — complexity limited by theory • Detailed/complex statistical assumptions re data • Model known, and data is carefully examined to verify assumptions.	• "No" upper limit on model complexity • Fewer statistical assumptions re data • Don't know right model? No problem! have multiple models and vote/weight results
Validation	• Evaluation based on theoretical estimates under stated statistical assumptions • Analysis of errors using theoretical distributions	• Empirical evaluation methods instead of theory — how well does it work on **unseen** data? • Don't calculate expected error, measure it from **unseen** data.

Statistics would be very different if it had been born after the computer instead of 100 years before

Splitting data into train+test(+validation) is vital

The Pipeline Metaphor

Model Building Pipeline



Source: Dataiku

Comments

- We saw the first two stages in previous weeks
- This week we look at the remaining stages
- Of course this pipeline is a simplification. In reality it is iterative.

What does a (supervised learning) model look like?

Definition 2 (Linear Model)

General form of linear model used in this module looks like

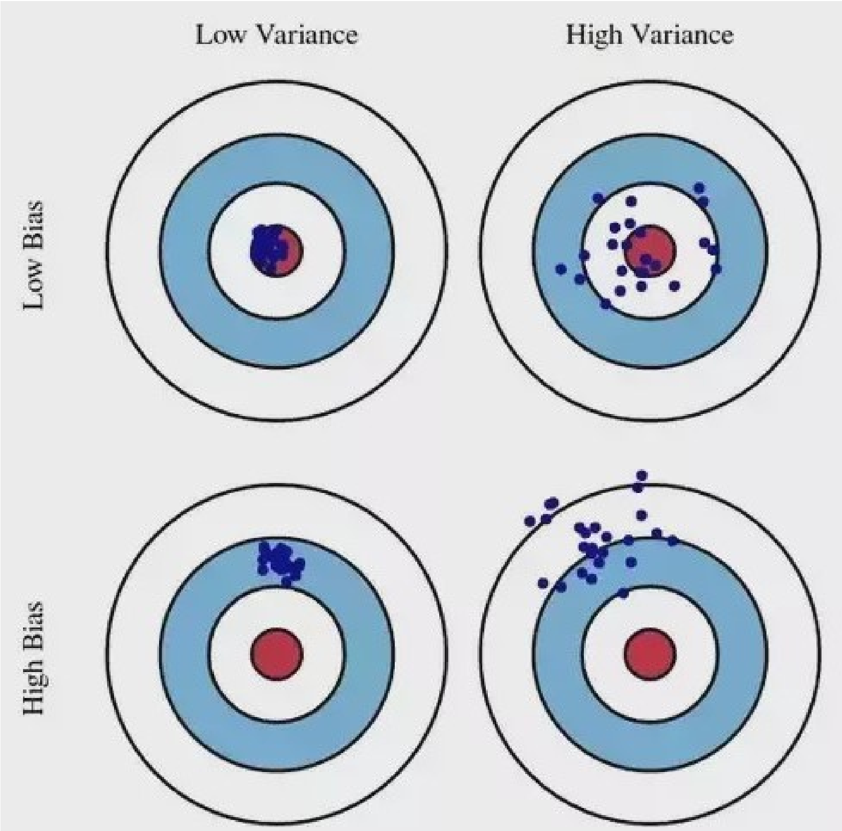
$$y_i \sim f_i^{(1)} + f_i^{(2)} + \ldots + f_i^{(\mathrm{n})}$$

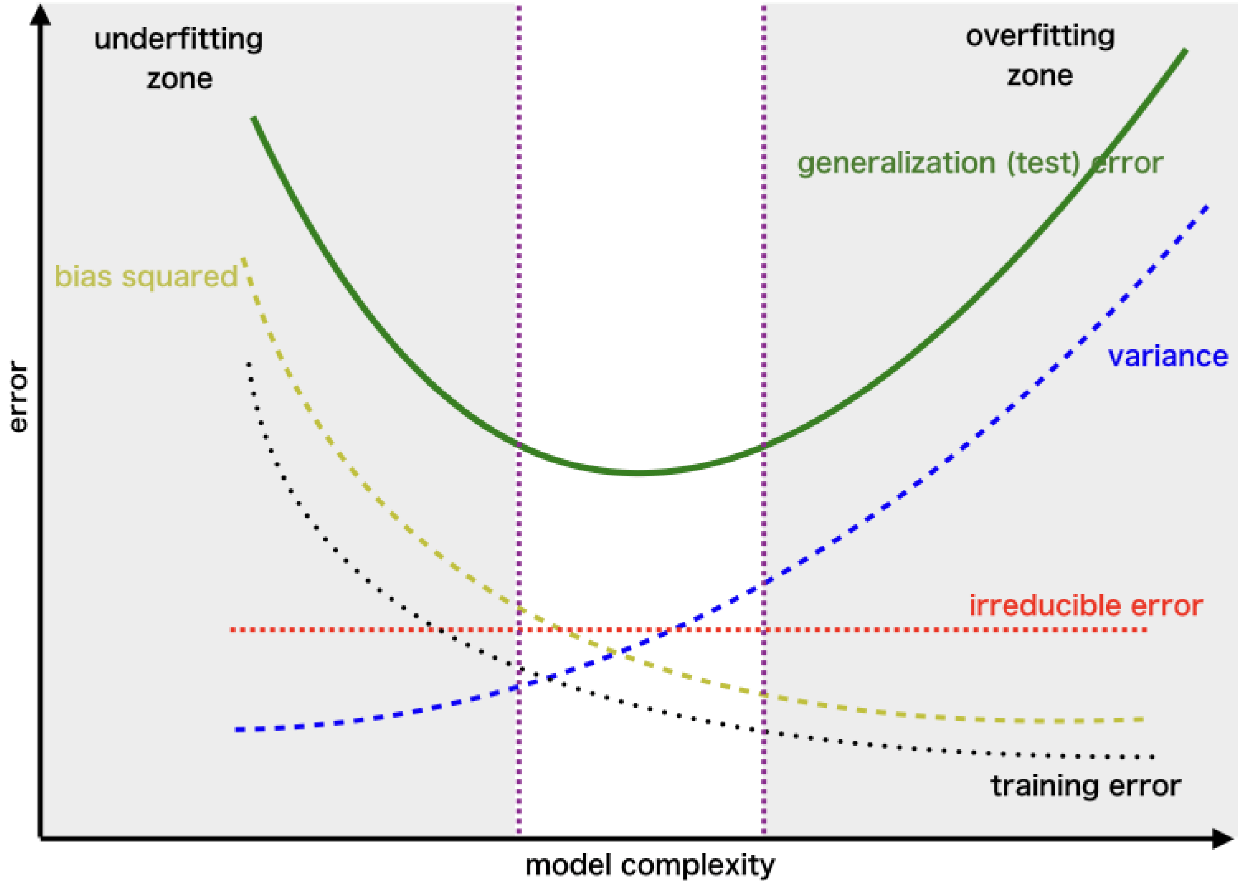
where y_i is the value of the response variable for observation i, and $f_i^{(\mathrm{j})}; j = 1, \ldots, n$ is the value of the j^{th} feature for that observation.
The model is linear in the sense that it can be turned into the following linear equation:

$$y_i = a_0 + a_1 f_i^{(1)} + a_2 f_i^{(2)} + \ldots + a_n f_i^{(\mathrm{n})} + \varepsilon_i$$

- Note that the features f can be nonlinear but the model parameters a must appear linearly.
- The goal of modelling is to find a so that the *prediction error* is a minimum.

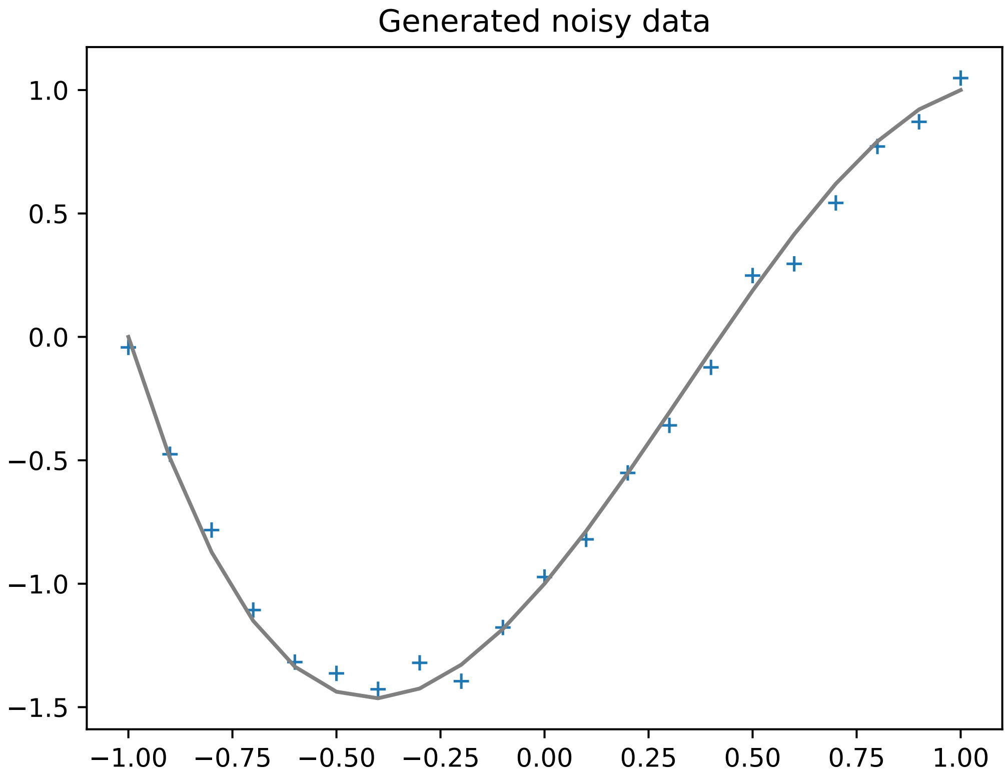
Bias-Variance and Total Error





Look for a that minimise the generalization error (estimated using the test set)

Example: Noisy data

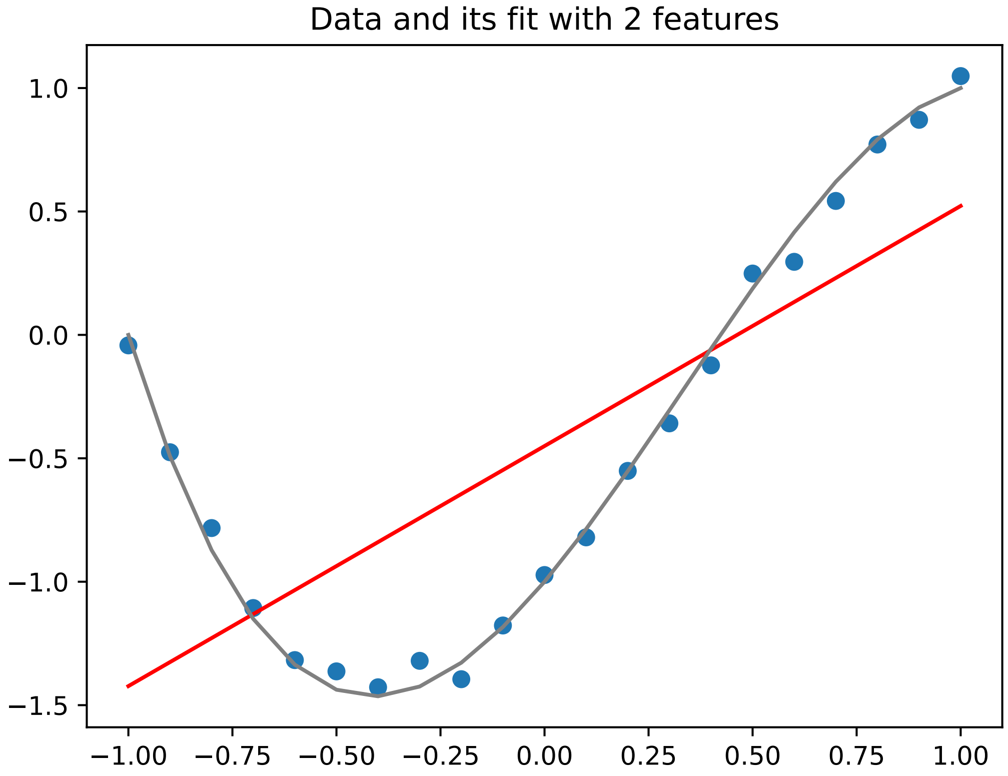


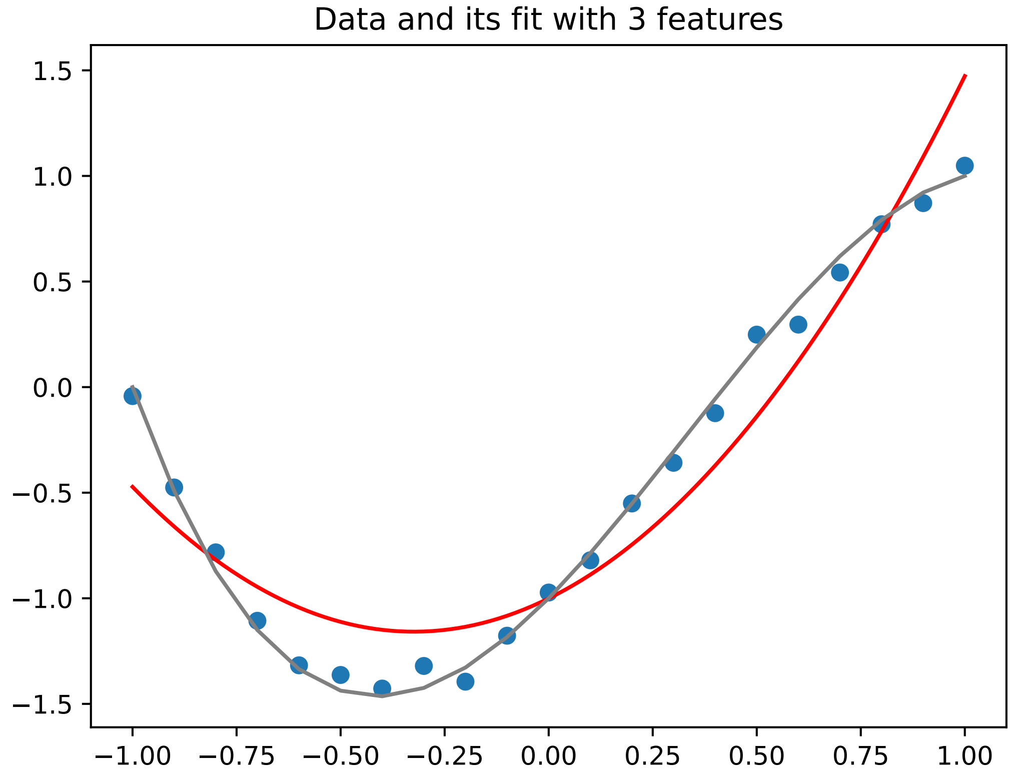
Comments

- Given data with some error (noise)
- Expected underlying model is indicated by the grey curve
- In the next slides we will compare different models, indicated by red curves
- The models have different numbers of *features*
- The values prediced by each model lie on the red curve
- The loss function is an estimate of how much the grey and red curves differ

Look for the number of features that minimise the loss function

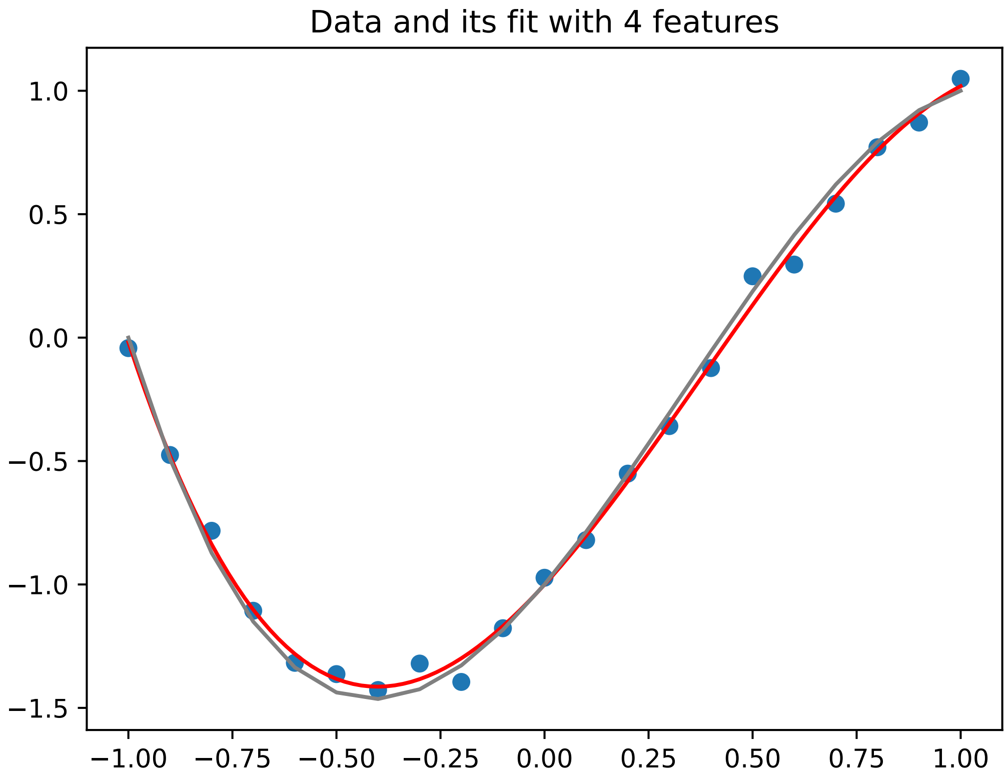
High Bias, Low variance

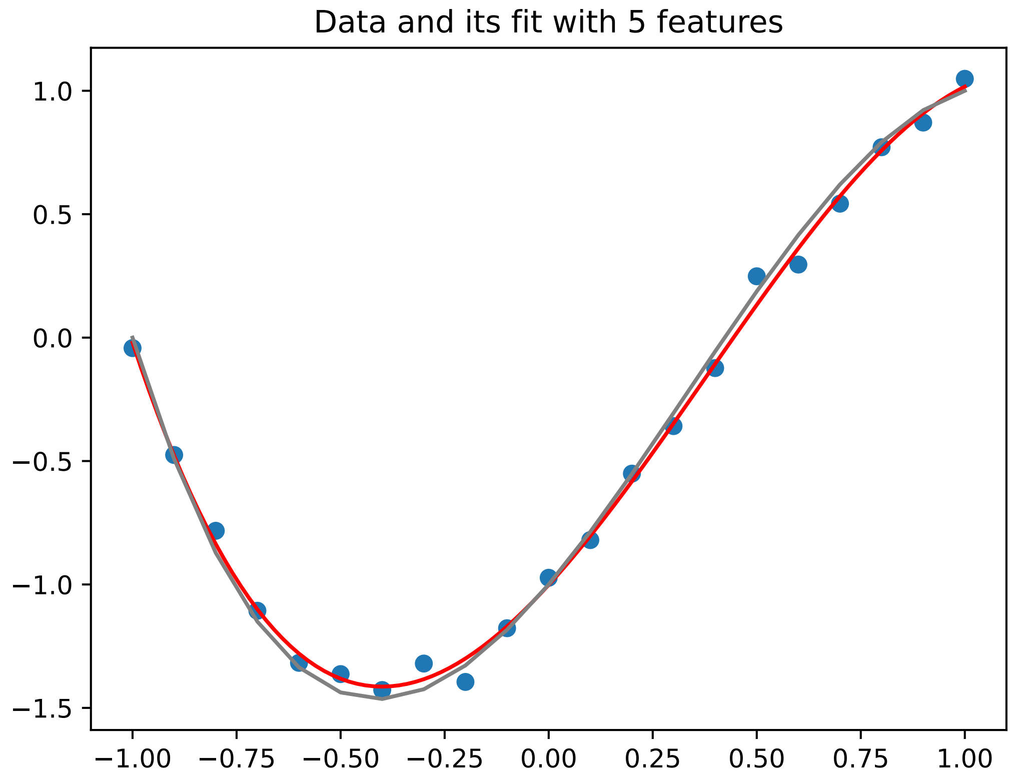




Need more features. . .

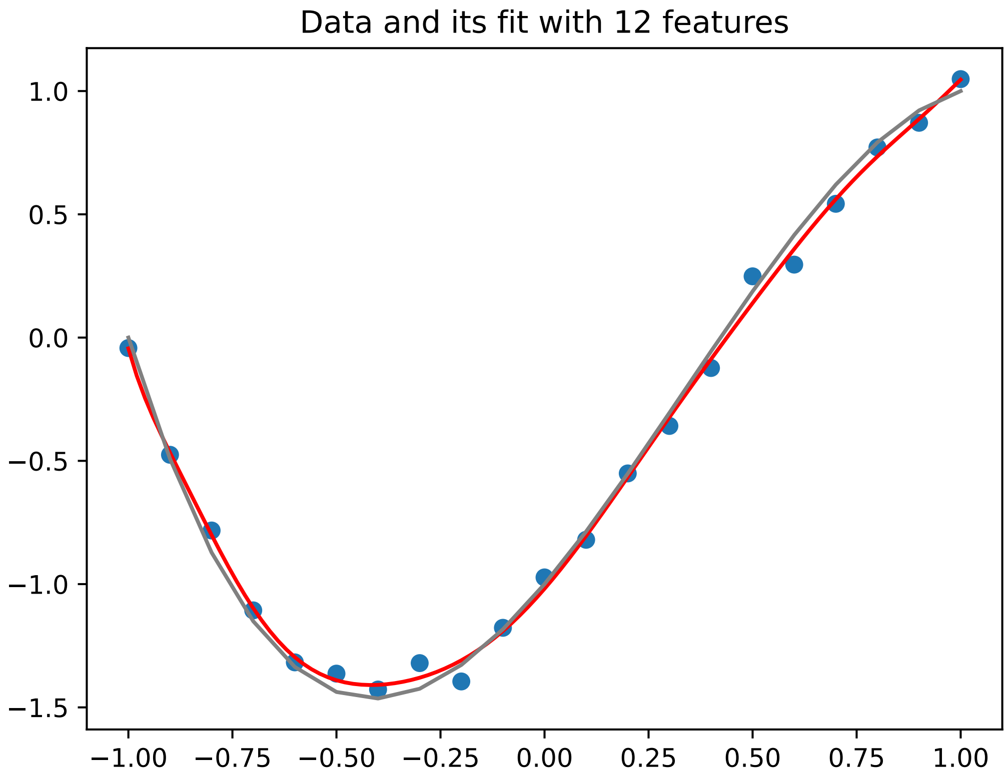
Low Bias, Low variance

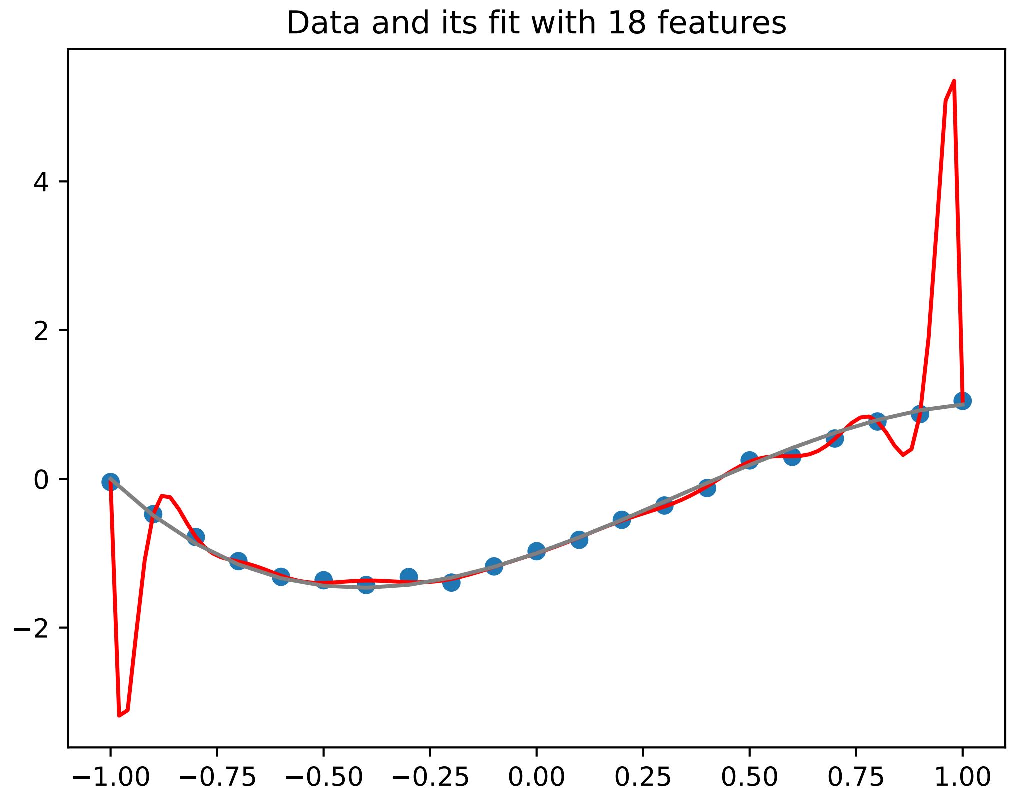




About the right number of features. . .

Low Bias, High variance





Too many features. . .

Example Model Types

Model	Applications	Concerns
Logistic Regression	X-ray classification	Regression with transformed variable
Fully connected networks	Classification	Classical ANN: choose encoding and size
Convolutional Neural Networks	Image processing	deep learning - choose segmentation
Recurrent Neural Networks	Voice recognition	ANN with feedback - how much?
Random Forest	Fraud Detection	Ensemble method - how many?
Reinforcement Learning	Learning by trial and error	Choose goal and penalties
Generative Models	Image creation	Choose parameters
K-means	Segmentation	Choose distance function and k
k-Nearest Neighbors	Recommendation systems	Choose distance function and k
Bayesian Classifiers	Spam and noise filtering	Deal with imbalances

Before you start. . .

Does a *pre-trained* model exist?

Transfer Learning

- Building a model from scratch is resource-intensive
- Open source data and model exist, particularly for deep learning (not in this nmodule)
- Most frameworks provide example models that can be used as a template
  - Select a similar model
  - Prune it (remove unnecessary terms)
  - Train using the pruned model as a starting point

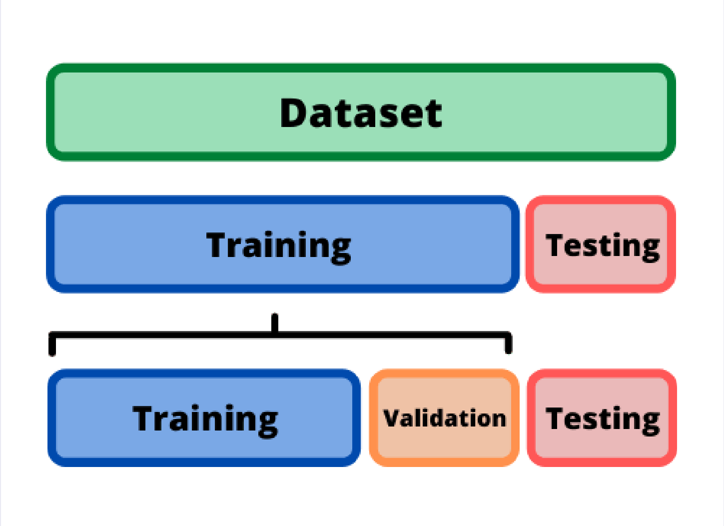
Training, test and valuation subsets: 3-way Holdout

Why Split?

Hold back some data to check how the model is doing.

- Training data is sample used to fit the model parameters.
- Test data is sample used to test the final model fitted to the training data.
- Validation data is sample used to test each interim model while tuning it.

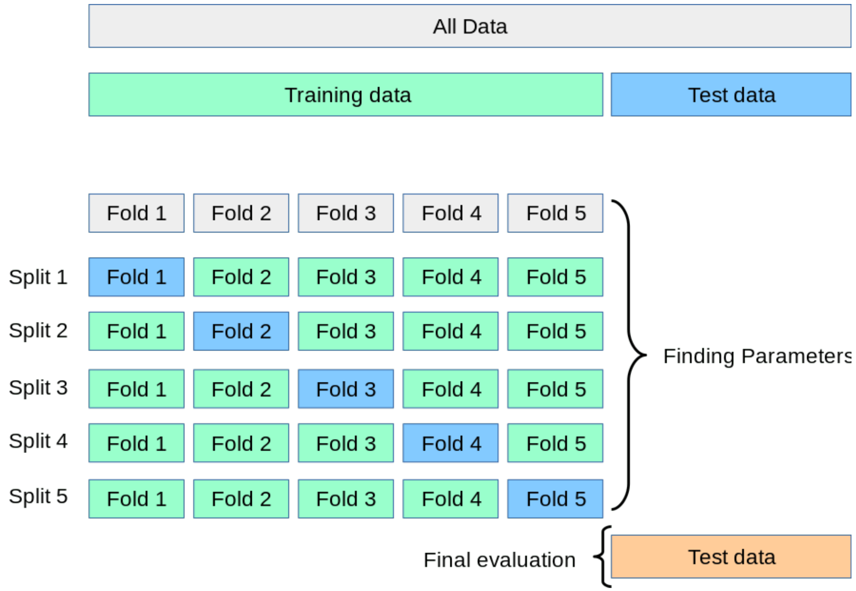
Typical Splits



sklearn example

```
from sklearn.model_selection import train_test_split
trainVal, test = train_test_split(df, test_size=0.2, seed=42)
train, validation = train_test_split(trainVal, test_size=0.1)
```

K-fold cross validation



Source: `https://scikit-learn.org/stable/modules/cross_validation.html`

sklearn example

```
from sklearn.model_selection import cross_val_score
# clf is some classifier, X and y are the features and target of the training set
scores = cross_val_score(clf, X, y, cv=5)
```

`scores` is a $k = 5$ element array, can be used to estimate the prediction error (or other score) while building a model

Featuring engineering 1: Scaling of numerical variables

Scaling - what it does

- If numeric features have different scales, e.g. [-0.005, -0.003] and [10000, 10001] some terms dominate, others are "lost"
- Better: transfer the scaling from the feature to the model parameter
- A min-max scaling is often a good choice:

$$\tilde{X} = \frac{X - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}}$$

- Note that X is in the range $[X_{\text{min}}, X_{\text{max}}]$ but $\tilde{X}$ is in the range $[0, 1]$.
- Other options include StandardScaler (subtract mean and divide by standard deviation) and a max-abs scaler (scales to [-1,1])

sklearn example

```python
from sklearn.preprocessing import MinMaxScaler
# df is a dataframe with numeric features
scaler = MinMaxScaler()
dfScaled = scaler.fit(df))
```

`dfScaled` can be used instead of `df` with the advantage that the fitted parameters are more accurate.

Feature Engineering 2: Choice of Features

- How many to include? Use metrics to decide. Will see some when considering regression and classification.
- How do we handle different feature types? Need to encode categorical variables.
- Can we derive new numeric features? Yes, $f' = \log(f)$ etc. is possible

Summary

- We have reviewed different types of models and considered their general form
- We looked at the goals of modelling: minimise predictive error
- We considered how feature engineering can help.
- In subsequent weeks we will put this theory into practice.

Resources

- **A Summary of the Basic Machine Learning Models**
  `towardsdatascience.com/a-summary-of-the-basic-machine-learning-models-e0a65627ecbe`

- **Train-Test Split for Evaluating Machine Learning Algorithms**
  `https://machinelearningmastery.com/train-test-split-for-evaluating-machine-learning-algorithms`
  This week I have focused on the theory rather than its (python) implementation. This is a nice article that covers the implementation side of things.

- **Cross-Validation: Estimator Evaluator**
  `medium.com/swlh/cross-validation-estimator-evaluator-897d28afb4ff`
  Nice article that covers cross-validation in a lot more detail — we will be using many of these variants in later weeks, especially k-fold stratified.