BSc - Data Mining 1

Topic 02 : Motivating Example

Part 02 : Introduction to Classification

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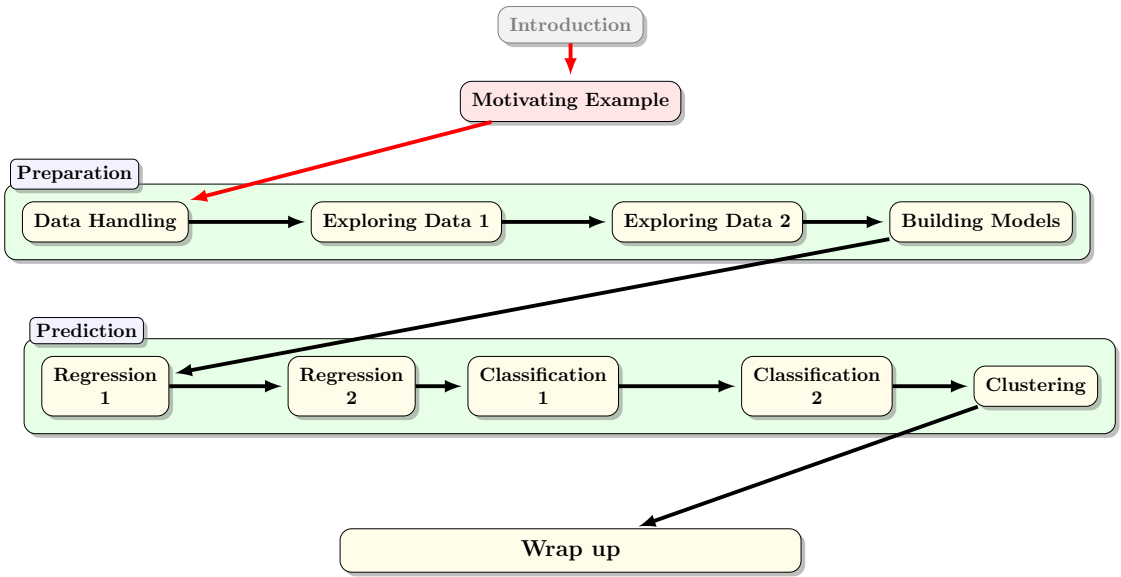
Outline

- How classification differs from regression
- Classification metrics
- Lazy vs Eager learners

Data Mining (Week 2)



Outline

Lazy vs Eager Learners

Lazy learner

Stores training data (or only minor processing) and uses this to compute prediction when given test data.

- Does not generalise until after training
- Does not produce a standalone model
- Training data must be kept for prediction
- Local approximations
- Often based on *search*
- If new data is just added to the training data, it can respond more easily to changing conditions

Eager learner

Builds a model from the train set, before receiving new data for prediction

- Training has an extra goal: to generalise from the data
- Training has an extra output: standalone model
- Training data can be discarded after use
- Local and/or global approximations
- Based on *computation*
- Models *drift* with time, so not suited to highly dynamic contexts, as it needs retraining

Usually an (eager) model requires much less memory than a (lazy) training set.

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Introduction to Classification

Definition 1 (Classification)

Classification aims to learn a function that takes attribute values and predicts a categorical/qualitative value, such as membership of a class, existence of an effect, etc.
The attributes can be categorical or numeric.
Classification is an example of *supervised learning* because it requires a training set of labeled observations.

- Some *classifiers* generate class membership probabilities en route to predicting class membership (of the most likely class), so the predicted class can be defined by a set of numbers rather than a simple label.
- There are many classification algorithms!
- We choose one of the simplest today, which works by *voting for the most likely label*.

Example Applications

In 5 minutes, identify 3 possible applications for classification

Outline

Motivation

Example 2 (Spam Detection)

A new email arrives. Is it spam? We have a large database of previous emails that have been labeled "Spam" or "Ham". Can we use this information *directly* to say whether the new email is spam or not?

Given each of the following

1. database of n instances $\{x_i\}$ with p attribute values per instance
2. distance function $D : d(x_i, x_j) : \mathbb{R}^{p \times p} \to \mathbb{R}$ where $d(x_i, x_j) > 0$ if $x_i \neq x_j$ and is zero otherwise
3. function S that searches for instances that "match" an incoming instance based on D
4. function R that identifies the k "nearest" (as defined by D) instances
5. function A that aggregates the "labels" of these k neighbours, yielding one representative value
6. function L that applies this representative label to the incoming instance

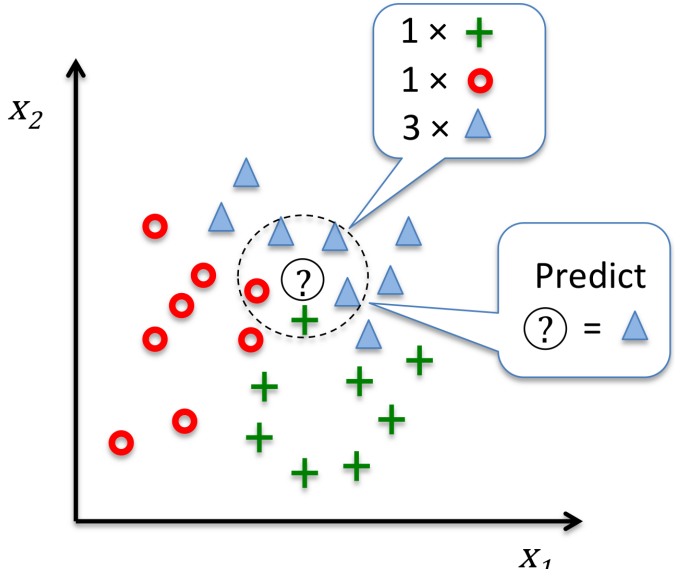
K-Nearest Neighbours: Practical Considerations

Implementation

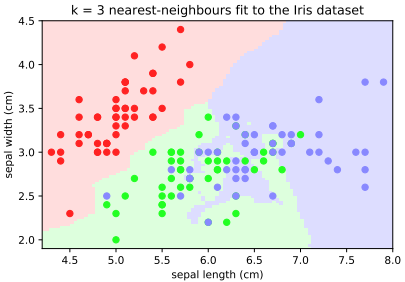
1. The training set needs to be stored in a format (such as a `pandas` dataframe) that is ready for both searching and computation
2. The distance function D needs to take account of all the relevant dimensions/attributes, possibly weighted
3. The search S and ranking R functions needs to work well together
4. The aggregation function A for k-nearest neighbours just takes the most frequent value (also known as the *mode*) of the k existing labels

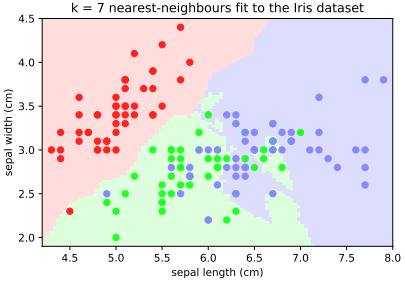
Conceptually this is a very simple algorithm. It can be tweaked by varying k and D (or, very rarely, A). Implementations exist in python (in `scikit-learn`).

K-Nearest Neighbours: Example prediction



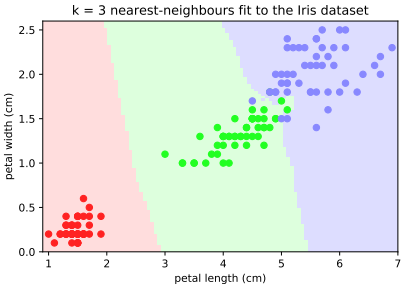
K-Nearest Neighbours: Iris SW-SL

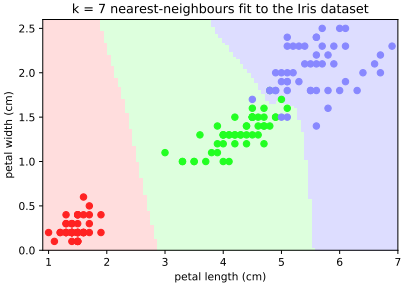




- The Iris dataset has 4 descriptive attributes, so there are 6 possible pairs
- Of these, the Sepal-Width $\times$ Sepal-Length combination is the least effective at distinguishing between the three species
- In this plot, *I. setosa* (red) is well separated from *I. versicolor* (green) and *I. virginica* (blue)
- However the boundary between *I. versicolor* (green) and *I. virginica* (blue) is unclear
- $k = 3$ has relatively low bias and (possibly) high variance
- $k = 7$ has lower variance, pays less attention to "outliers", so region boundaries are smoother

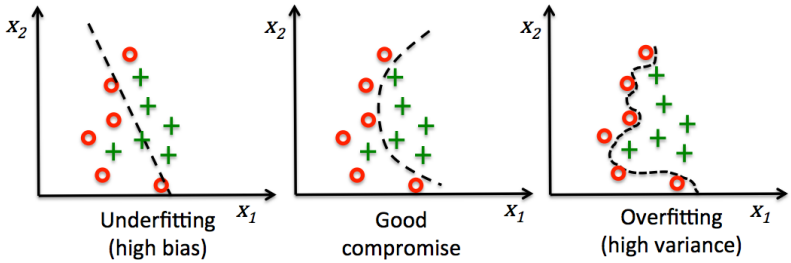
K-Nearest Neighbours: Iris PW-PL





- As can be seen, the Petal-Width $\times$ Petal-Length combination separates Iris species better
- There are still some difficulties distinguishing between *I. versicolor* (green) and *I. virginica* (blue).
- The size of k does have some effect, but not as dramatically as the more difficult SW-SL combination
- The distance function D depends on the number of dimensions p
- If the regions are well separated, as here, adding more dimensions rarely helps
- Over- and under-fitting is largely down to the choice of k

Sidebar: Classification over- and under-fitting



Generally, under-fitted models do not follow the training set closely enough, and so are likely to miss comparable features in the test set.

Over-fitted models do the opposite, pay too much attention to peculiarities of the training set. They "wiggle" too much!

Setting $k = 1$ ensures that all the training data is correctly labeled (by definition) but it rarely generalises well.

As k increases the boundary becomes smoother. Often that is what you need.

Sidebar: Classification result summary: Confusion Matrix

k = 1, training

		Actual		
		S	**V1**	**V2**
predicted	**S**	50	0	0
	V1	0	50	0
	V2	0	0	50

Note that each instance is assigned the correct label. There are no off-diagonal terms. **S** represents *I. setosa*, **V1** represents *I. versicolor* and **V2** represents *I. virginica*.

k = 3, training

		Actual		
		S	**V1**	**V2**
predicted	**S**	50	0	0
	V1	0	47	3
	V2	0	3	47

Note that each training instance of *I. setosa* is assigned the right label. However, of the 50 each of *I. versicolor* and *I. virginica*, 3 of each were incorrectly predicted to be the other.

k = 3, test

		Actual		
		S	**V1**	**V2**
predicted	**S**	10	0	0
	V1	0	7	3
	V2	0	0	10

Note that each test instance of *I. setosa* and *I. virginica* is assigned the right label. However, of the 10 predicted *I. versicolor* (from a stratified sample), 3 were actually *I. virginica*.

k-nearest neighbours works better with “small” dimension p but can scale well to “large” number of cases n. Unlike most other techniques, decision boundaries are implicit, not explicit.

k-nearest-neighbours in python

Python's `scikit-learn` libraries provide a general interface to model fitting that abstracts away most of the details.

Method (Identifying the Iris species)

```
# create the model
knn = neighbors.KNeighborsClassifier(n_neighbors=5)

# fit the model
knn.fit(X, y)

# What kind of iris has 3cm x 5cm sepal and 4cm x 2cm petal?
result = knn.predict([[3, 5, 4, 2],])

# it is a versicolor...
print(iris.target_names[result])

# class membership probabilities are [0. , 0.8, 0.2]
knn.predict_proba([[3, 5, 4, 2],])
```