BSc - Data Mining1

Topic 02 : Motivating Example

Part 02 : Introduction to Classification

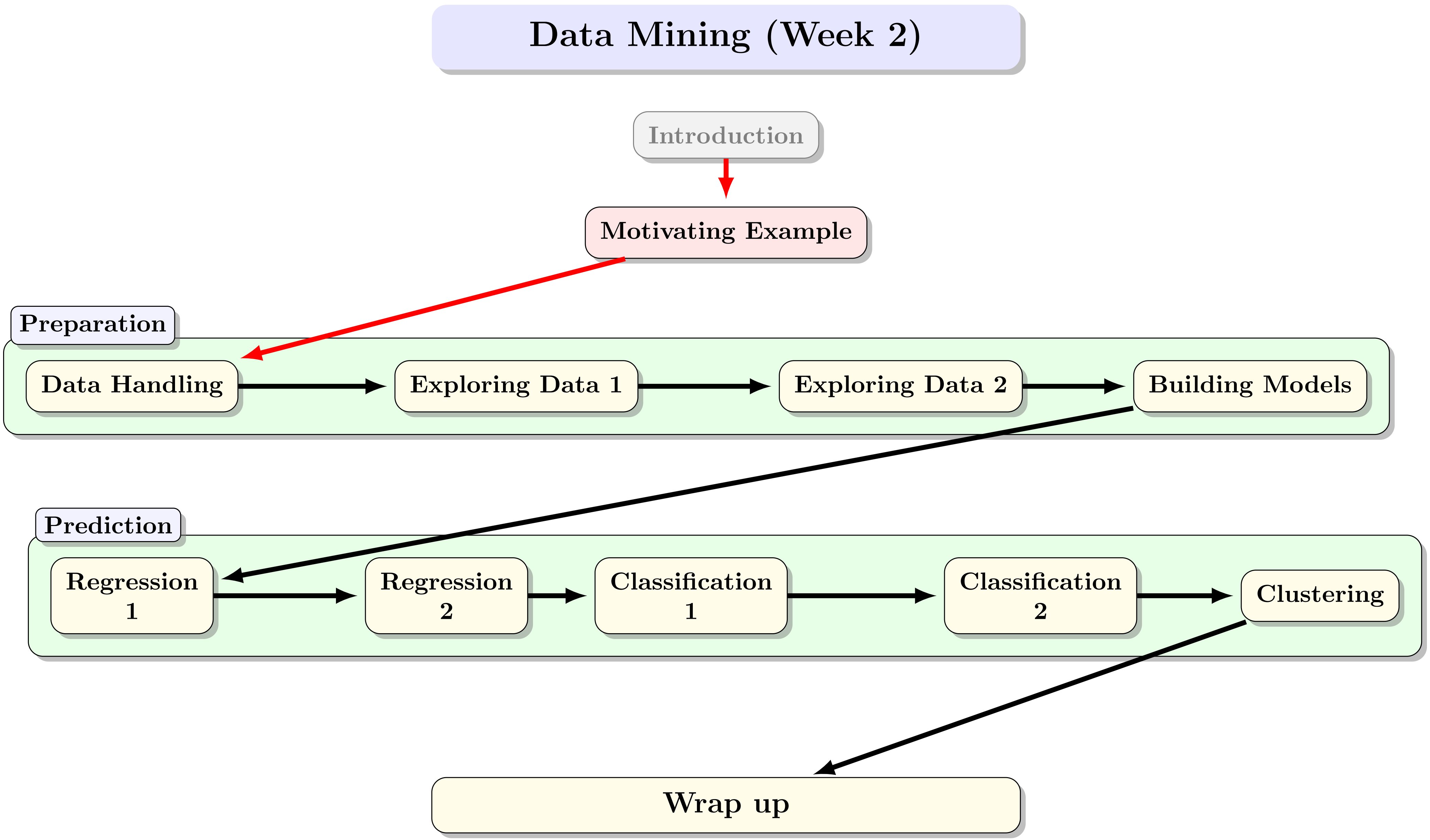
Dr Bernard Butler
Department of Computing and Mathematics, WIT.
(bernard.butler@setu.ie)

Autumn Semester, 2022

Outline

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

Wrap up



Data Mining (Week 2)
Introduction
Motivating Example
Preparation
Data Handling
Exploring Data 1
Exploring Data 2
Building Models
Prediction
Regression 1
Regression 2
Classification 1
Classification 2
Clustering
Wrap up

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.

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

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 $D : d(x_i, x_j) : \mathbb{R}^{p \times p} \rightarrow \mathbb{R}$ 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

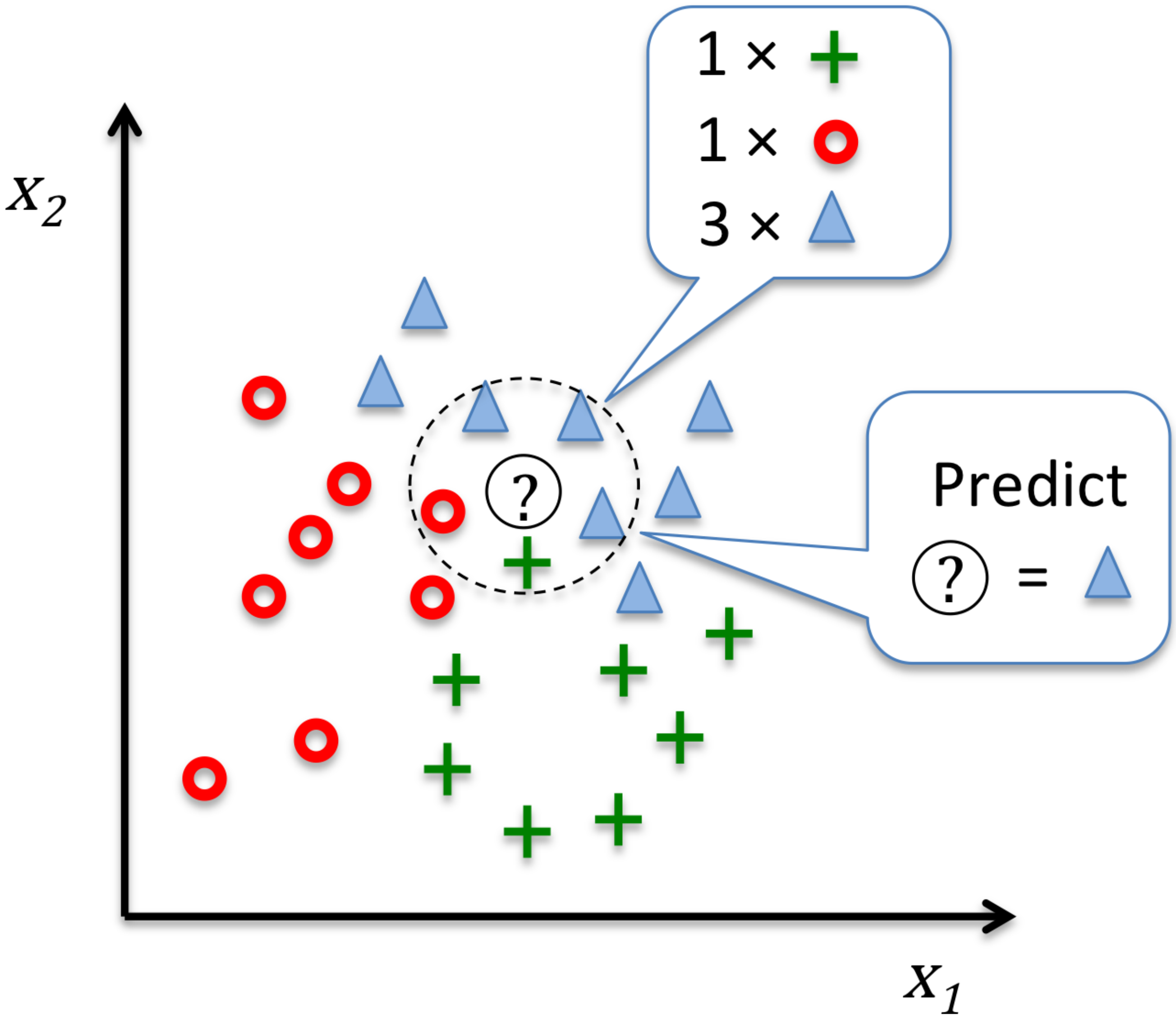
K-Nearest Neighbours: Practical Considerations

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

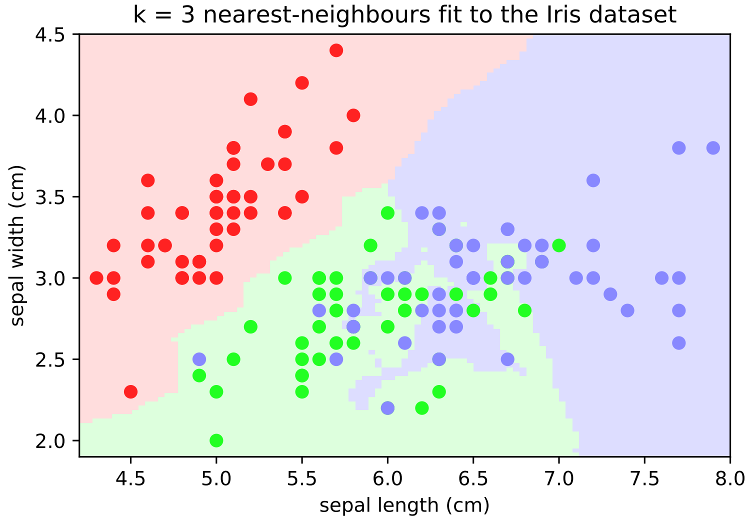
Conceptually this is a very simple algorithm. It can be tweaked by varying k and D (or, very rarely, A). Implementations exist in python (in `scikit-learn`).

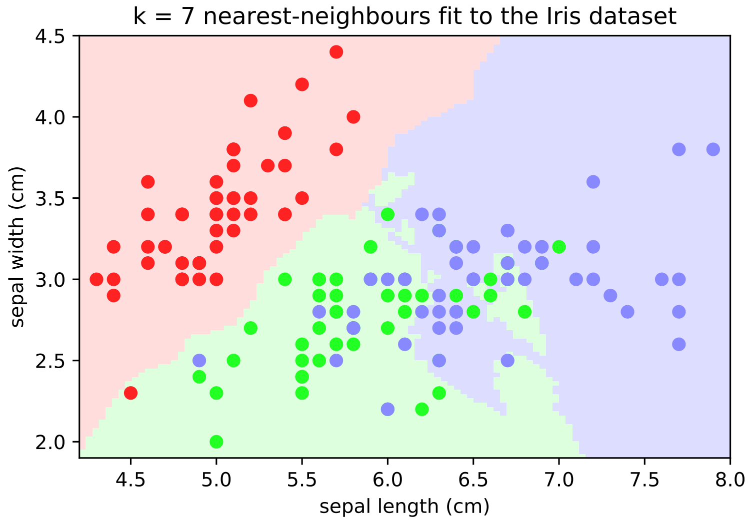
K-Nearest Neighbours: Example prediction



“Follow the crowd”: the new instance is labeled with a blue triangle

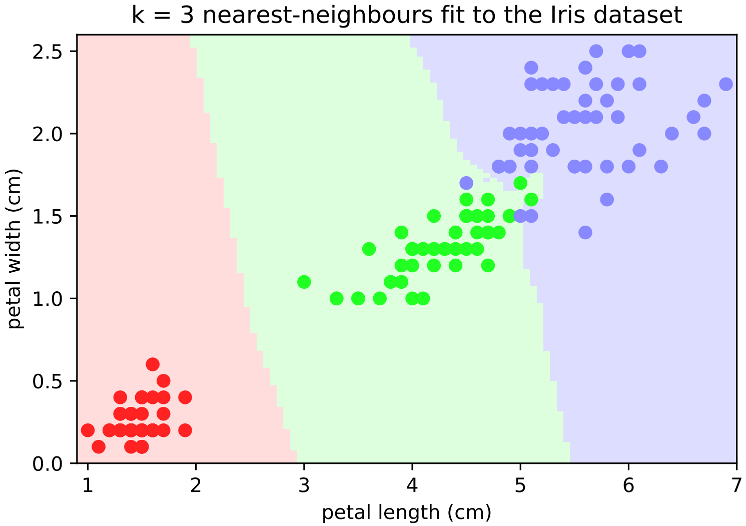
K-Nearest Neighbours: Iris SW-SL

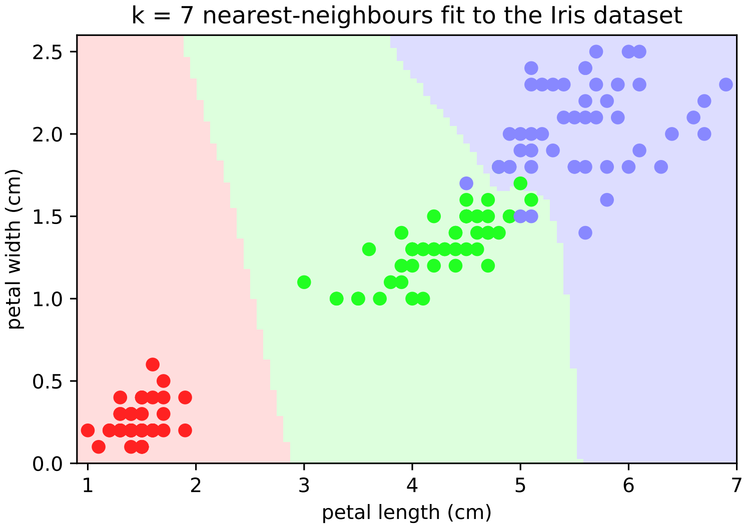




- The Iris dataset has 4 descriptive attributes, so there are 6 possible pairs
- Of these, the Sepal-Width $\times$ Sepal-Length combination is the least effective at distinguishing between the three species
- In this plot, *I. setosa* (red) is well separated from *I. versicolor* (green) and *I. virginica* (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

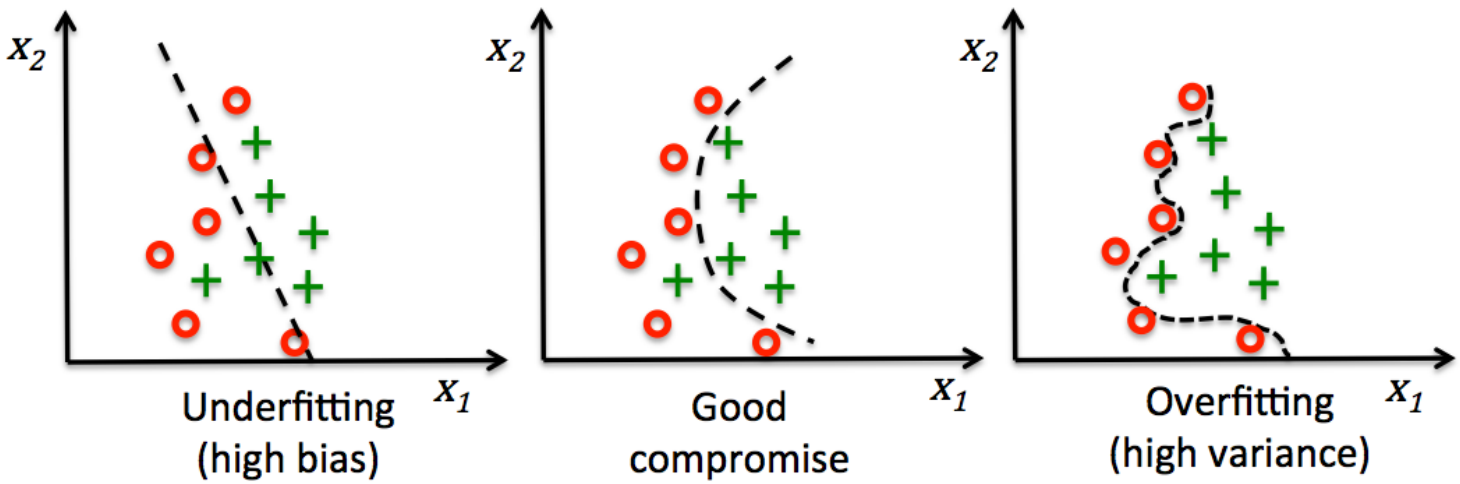
K-Nearest Neighbours: Iris PW-PL





- As can be seen, the Petal-Width × 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

predicted	Actual S	Actual V1	Actual V2
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

predicted	Actual S	Actual V1	Actual V2
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

predicted	Actual S	Actual V1	Actual V2
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)

```python
# 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],])
```