

dm24s1

Topic 02 : Motivating Example

Part 01 : Introduction to Classification

Preparation

Data Handling

Exploring Data

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Building Data 2

Building Models

Autumn Semester, 2024

Prediction

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

Clustering

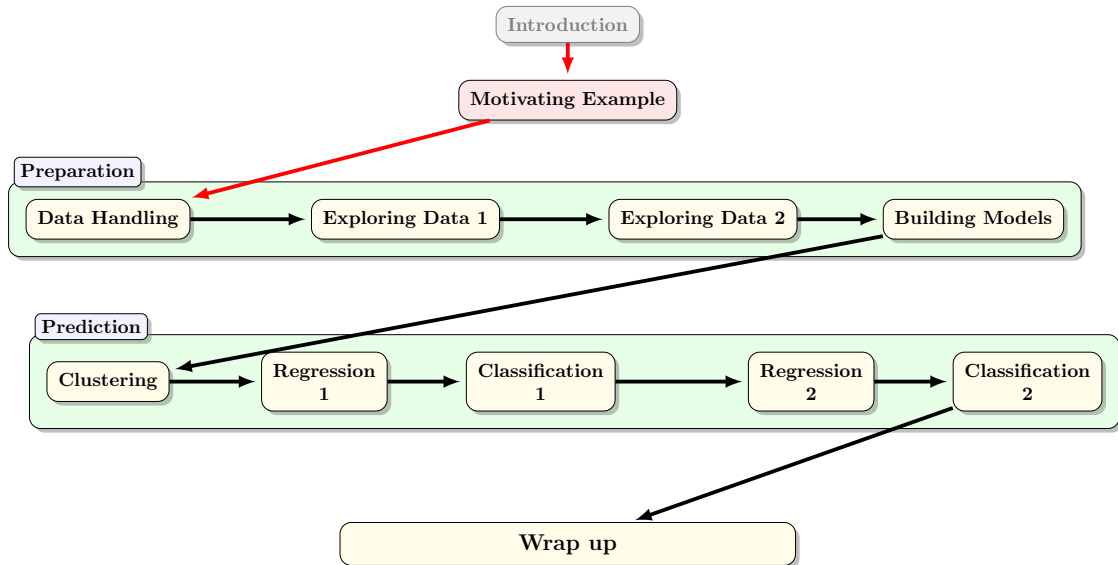
Regression
1

Classification
1

Regression
2

Classification
2

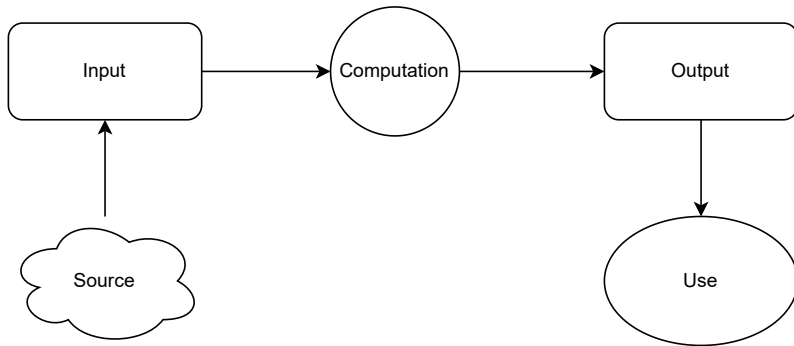
Wrap up



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1.1. Learning from data	4
1.2. Lazy vs Eager Learners	6
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What does it mean to learn from data?



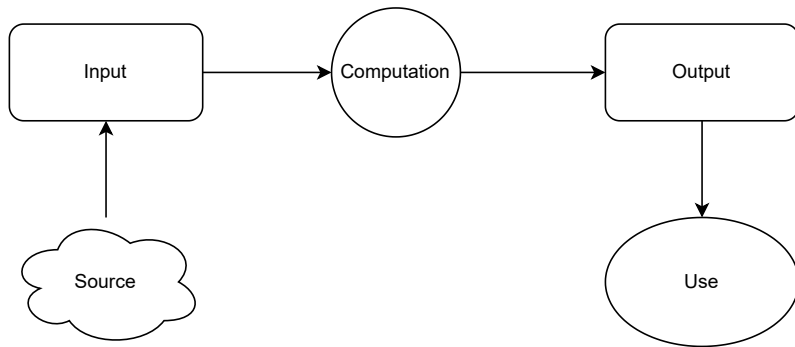
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- Explicit, detailed programming logic

Learned Computation

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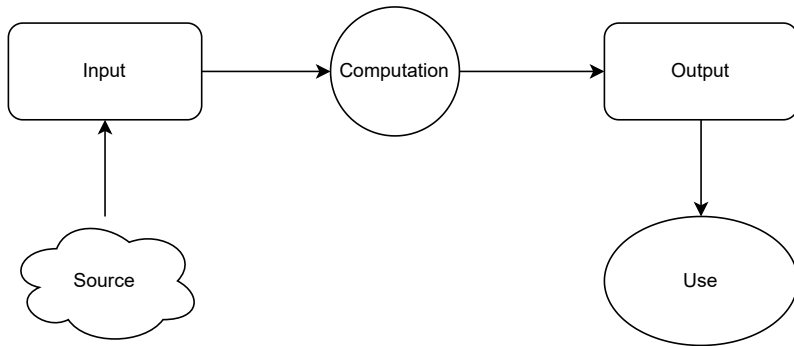
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- Less brittle, but harder to test

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Programmed Computation

- Explicit, detailed programming logic
- Handle edge cases, messy data
- Software engineering - unit testing, etc.

Learned Computation

- Implicit, learning from examples
- Less brittle, but harder to test
- New paradigms - iterative model building

Machine learning pros and cons

Benefits

- Less programming effort
- Subtle rules are inferred
- One algorithm works for a range of problems
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Challenges

- Need (lots of) data for training
- Training data (sample) needs to represent population
- Algorithms have many configuration settings
- Need to understand and validate
- Prediction error needs to be minimised

Lazy vs Eager Learners

Lazy learner

Stores training data (or only minor processing) and uses local approximation to predict a value from test data.

Eager learner

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

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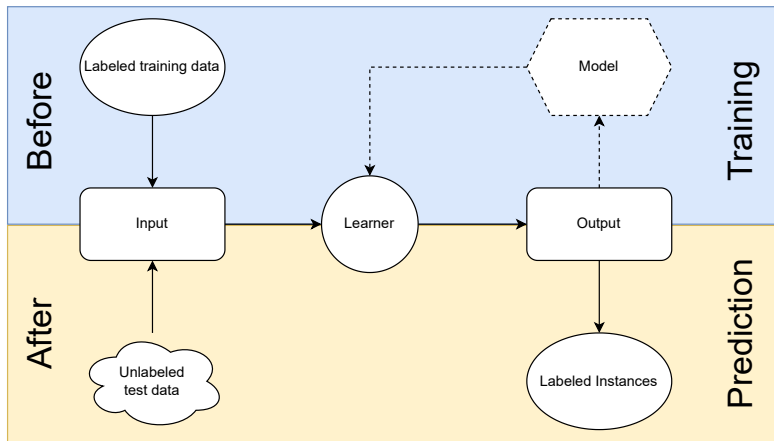
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- Some *classifiers* generate class membership probabilities en route to predicting class membership (of the most likely class), so the predicted class can be defined by a set of numbers rather than a simple label.
- There are many classification algorithms!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

Classification Overview



Today's classifier is a lazy learner and so uses local approximation, not a model

Example Applications

➤ In 5 minutes, identify 3 possible applications for classification

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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?

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- 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



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- ⑥ function L that applies this representative label to the incoming instance



K-Nearest Neighbours: Practical Considerations

Implementation

- ❶ The training set needs to be stored in a format (such as a `pandas` dataframe) that is ready for both searching and computation

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Conceptually this is a very simple algorithm. It can be tweaked by varying k and D (or, very rarely, A).

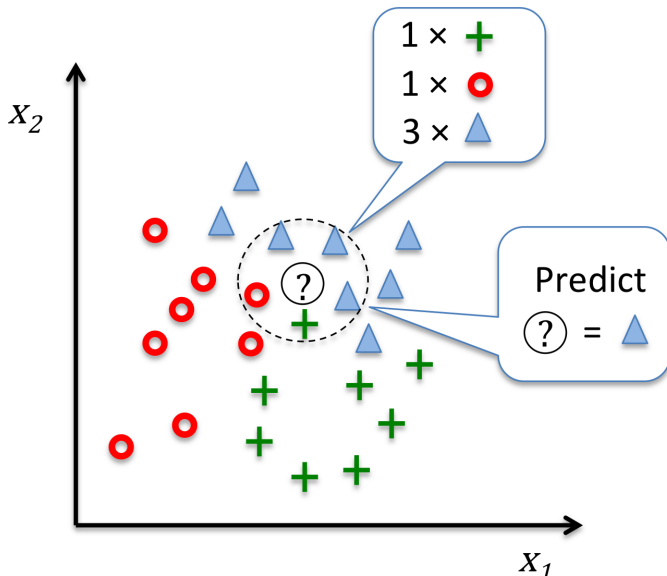
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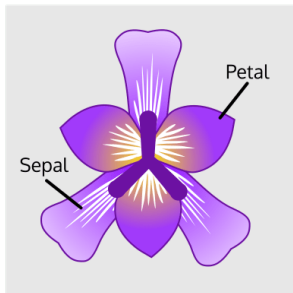
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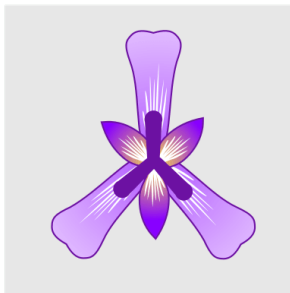
K-Nearest Neighbours: Example prediction



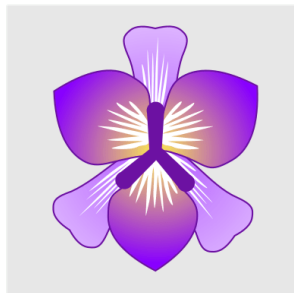
Classifying iris species



Iris Versicolor



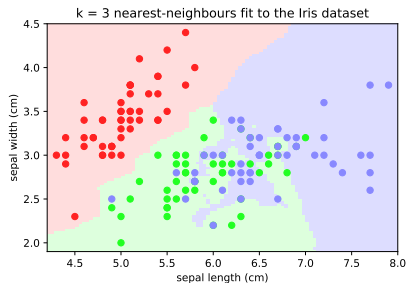
Iris Setosa



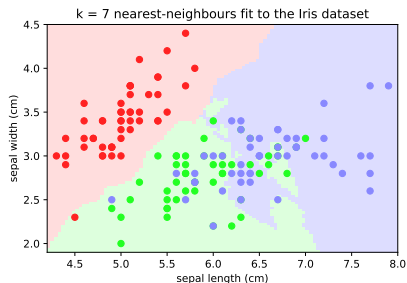
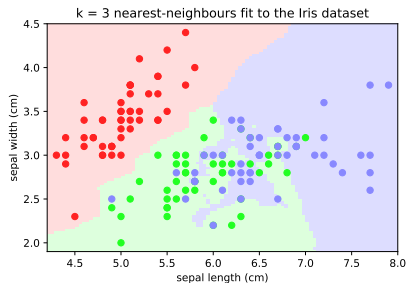
Iris Virginica

Given measurements of sepal and petal lengths and widths, can we distinguish between the 3 species?

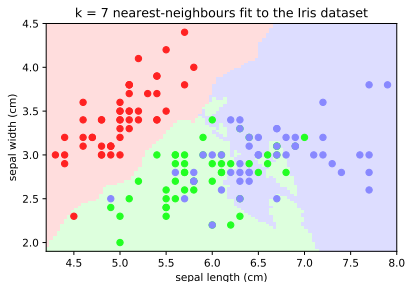
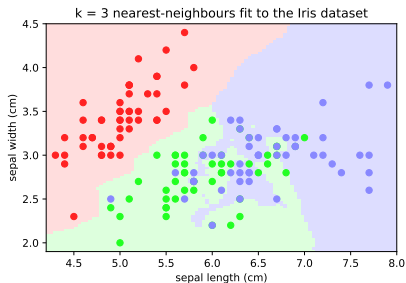
K-Nearest Neighbours: Iris SW-SL



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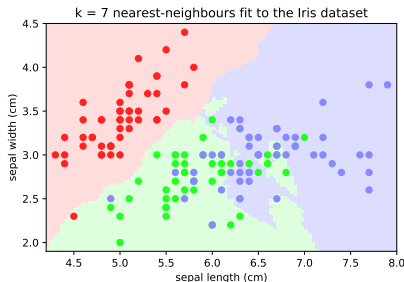
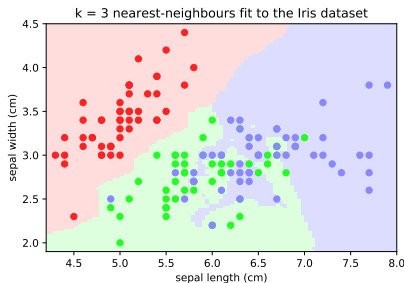


K-Nearest Neighbours: Iris SW-SL



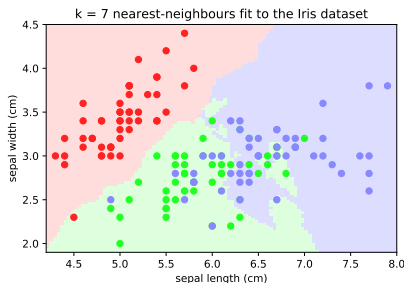
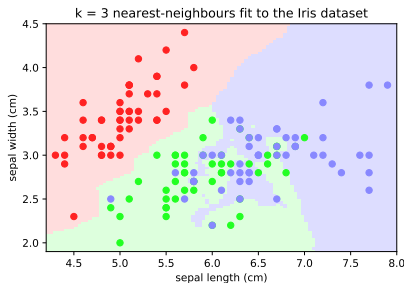
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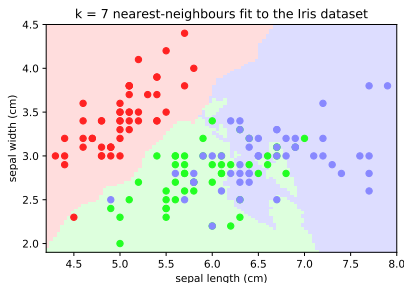
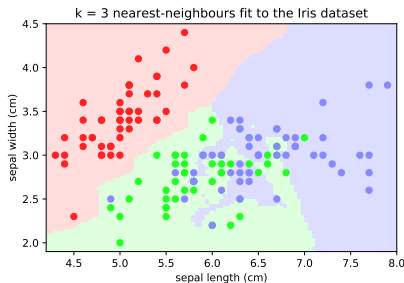
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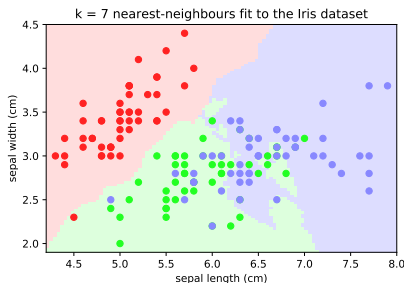
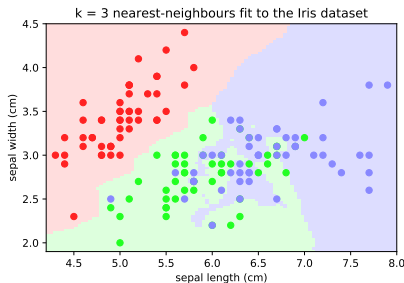
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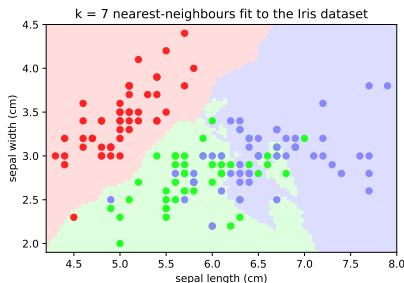
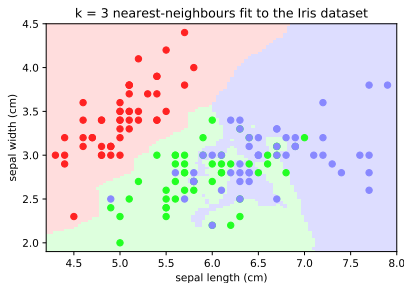
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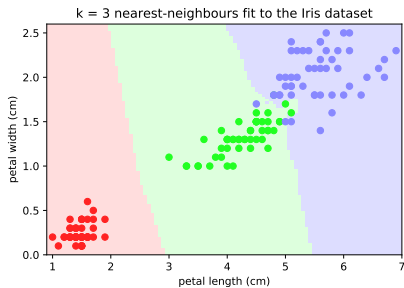
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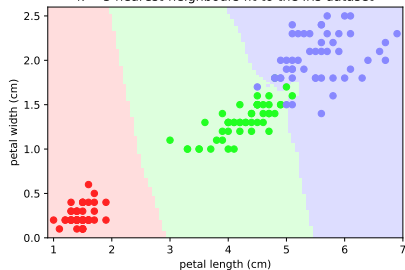
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- $k = 7$ has lower variance, pays less attention to “outliers”, so region boundaries are smoother

K-Nearest Neighbours: Iris PW-PL

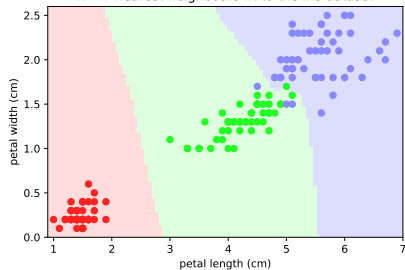


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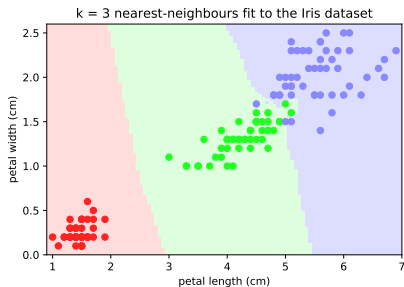
k = 3 nearest-neighbours fit to the Iris dataset



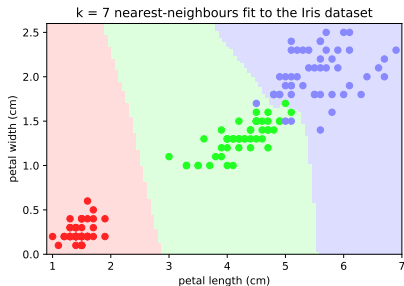
k = 7 nearest-neighbours fit to the Iris dataset



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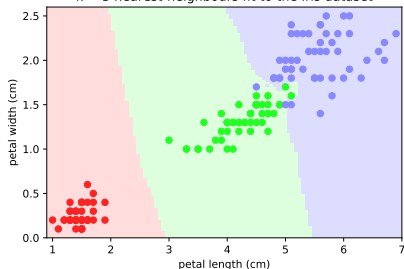


- As can be seen, the Petal-Width \times Petal-Length combination separates Iris species better

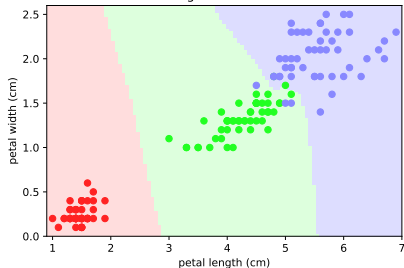


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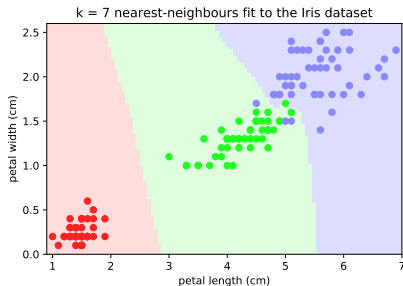
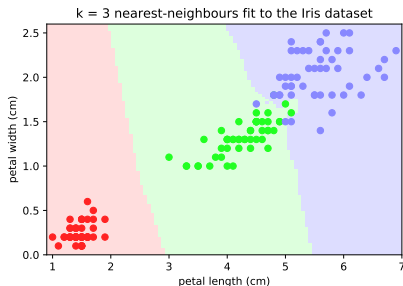


k = 7 nearest-neighbours fit to the Iris dataset



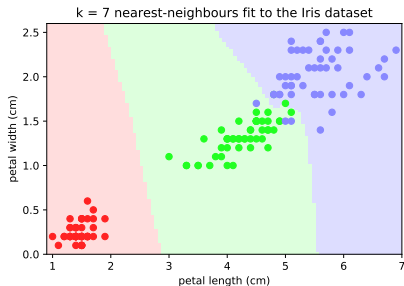
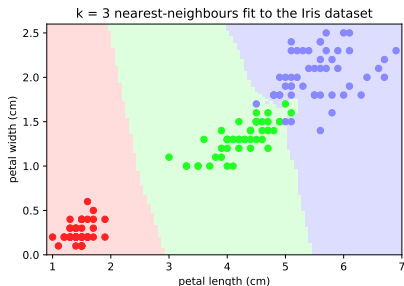
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K-Nearest Neighbours: Iris PW-PL



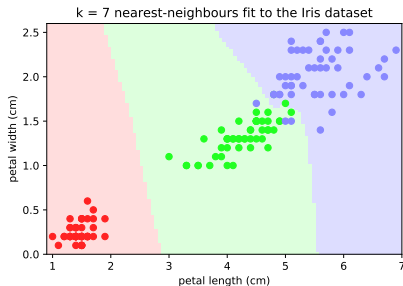
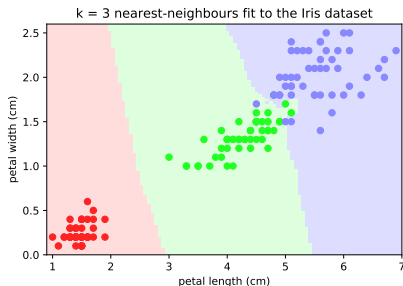
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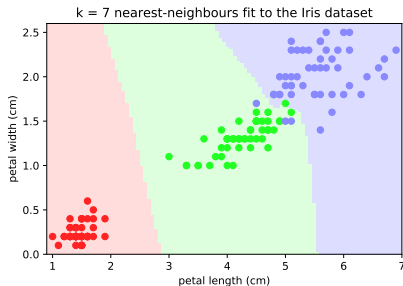
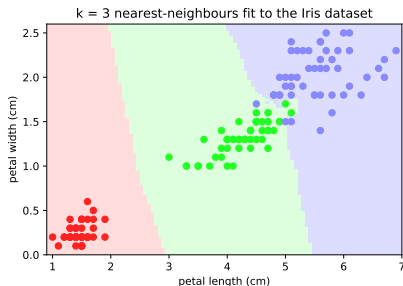
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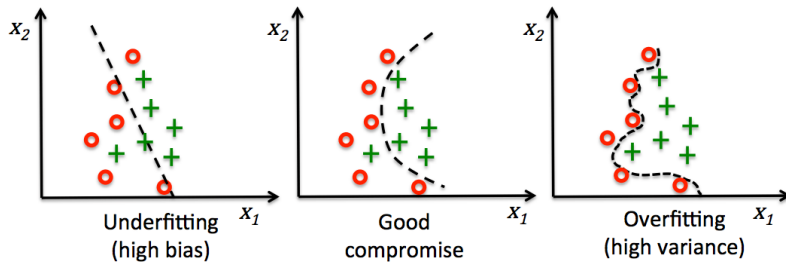
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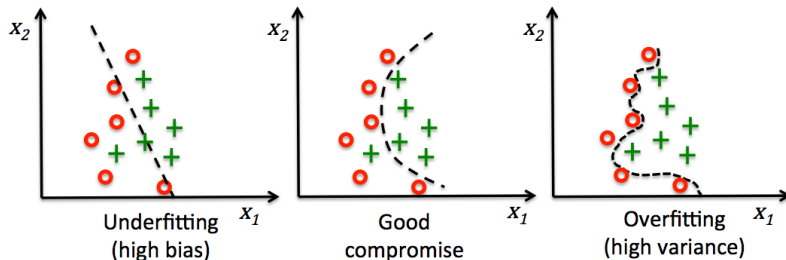


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- The size of k does have some effect, but not as dramatically as the more difficult SW-SL combination
- The distance function D depends on the number of dimensions p
- If the regions are well separated, as here, adding more dimensions rarely helps
- Over- and under-fitting is largely down to the choice of k

Sidebar: Classification over- and under-fitting

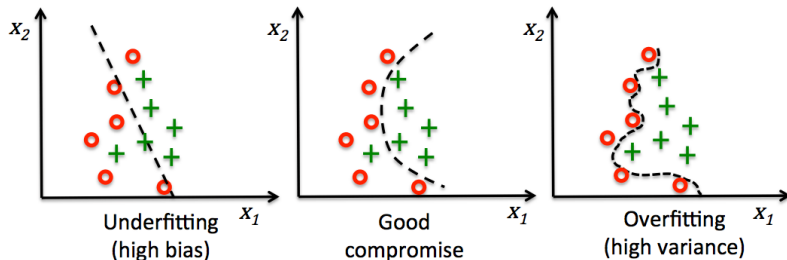


Sidebar: Classification over- and under-fitting



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

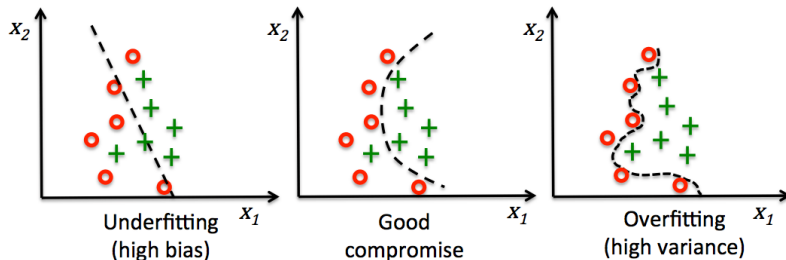
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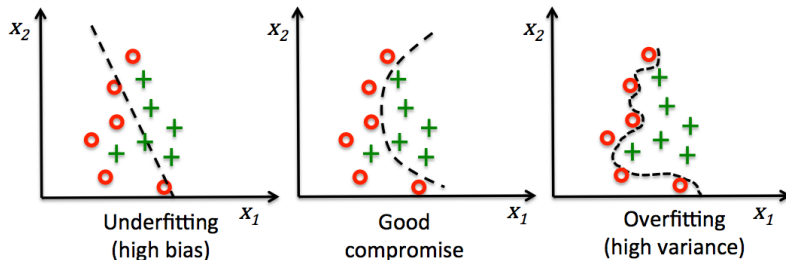


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Setting $k = 1$ ensures that all the training data is correctly labeled (by definition) but it rarely generalises well.

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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

k = 3, training

k = 3, test

Sidebar: Classification result summary: Confusion Matrix

k = 1, training

<i>predicted</i>		<i>Actual</i>		
		S	V1	V2
S		50	0	0
V1		0	50	0
V2		0	0	50

k = 3, training

<i>predicted</i>		<i>Actual</i>		
		S	V1	V2
S		50	0	0
V1		0	47	3
V2		0	3	47

k = 3, test

<i>predicted</i>		<i>Actual</i>		
		S	V1	V2
S		10	0	0
V1		0	7	3
V2		0	0	10

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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*.

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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)

```
1  # create the model
2  knn = neighbors.KNeighborsClassifier(n_neighbors=5)
3
4  # fit the model
5  knn.fit(X, y)
6
7  # What kind of iris has 3cm x 5cm sepal and 4cm x 2cm petal?
8  result = knn.predict([[3, 5, 4, 2],])
9
10 # it is a versicolor...
11 print(iris.target_names[result])
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13 # class membership probabilities are [0. , 0.8, 0.2]
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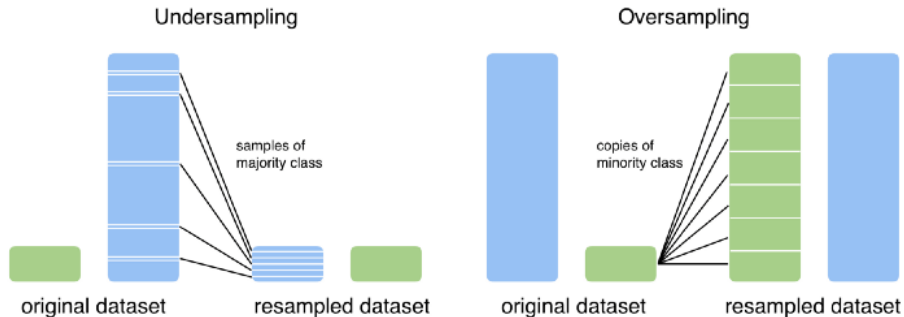
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Very few lines of code are needed!

How might things go wrong?



➤ K nearest neighbors is very sensitive to unbalanced data, so need to be careful!!

Outline

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- We can use such metrics to validate our classifier choice and search for optimal hyperparameters (*hyperparameter tuning*)