VICTORIA UNIVERSITY OF WELLINGTON
Te Whare Wananga o te Upoko o te Ika a Maui

School of Engineering and Computer Science

COMP 307 — Lecture 05

Machine Learning 2

3-K Techniques: K-Nearest Neighbour, K-fold Cross Validation and K-Means Clustering

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Outline

- Nearest neighbour method
  - Basic nearest neighbour method
  - K-Neighbour method
  - Distance measure/Similarity measure
- K-fold cross validation
  - Leave-one out cross validation
  - k-fold cross validation vs validation set
- K-means clustering
  - r binary classification

Dataset (Classification)

Iris Dataset:

- 150 examples/ instances/ observations/objects
  - Each instance is represented as a *feature vector* and a desired/target *class label*
- 3 classes: Iris-Setosa, Iris-Versicolor, Iris-Virginica
- 4 features/variables/attributes:
  - sepal length in cm
  - sepal width in cm
  - petal length in cm
  - petal width in cm

```
@Iris:
5.1,3.5,1.4,0.2,  Iris-setosa
4.9,3.0,1.4,0.2,  Iris-setosa
4.7,3.2,1.3,0.2,  Iris-setosa
4.6,3.1,1.5,0.2,  Iris-setosa
5.0,3.6,1.4,0.2,  Iris-setosa
.
.
7.0,3.2,4.7,1.4,  Iris-versicolor
6.4,3.2,4.5,1.5,  Iris-versicolor
6.9,3.1,4.9,1.5,  Iris-versicolor
5.5,2.3,4.0,1.3,  Iris-versicolor
6.5,2.8,4.6,1.5,  Iris-versicolor
.
.
6.3,3.3,6.0,2.5,  Iris-virginica
5.8,2.7,5.1,1.9,  Iris-virginica
7.1,3.0,5.9,2.1,  Iris-virginica
6.3,2.9,5.6,1.8,  Iris-virginica
.
.
```

Nearest Neighbour

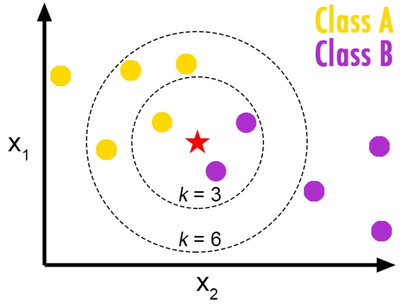
- Given a training set with a number of instances
- Nearest neighbour method
  - Each unseen instance (in the test set) is compared with all the instances in the training set
  - Find the "nearest neighbour" (instance) from the training set
  - the unseen instance is classified as the class of the nearest neighbour

```
@Iris:
5.1,3.5,1.4,0.2, Iris-setosa
4.9,3.0,1.4,0.2, Iris-setosa
.
.
7.0,3.2,4.7,1.4, Iris-versicolor
6.4,3.2,4.5,1.5, Iris-versicolor

6.3,3.3,6.0,2.5, Iris-virginica
5.8,2.7,5.1,1.9, Iris-virginica
```

K-Nearest Neighbour

- K-Nearest Neighbour method:
  - Similar to the nearest neighbour method
  - But find k *nearest* instances from the training set
  - Then choose the majority class as the class label of the unseen instance
- But how to find the nearest neighbours?



Nearest Neighbour — Distance Measures

- Given two feature vectors with numeric values

$$A = (a_1, a_2, ..., a_n) \text{ and } B = (b_1, b_2, ..., b_n)$$

- Use the *distance measure*:

$$d = \sqrt{\sum_{i=1}^{n} \frac{(a_i - b_i)^2}{R_i^2}} = \sqrt{\frac{(a_1 - b_1)^2}{R_1^2} + \frac{(a_2 - b_2)^2}{R_2^2} + ... + \frac{(a_n - b_n)^2}{R_n^2}}$$

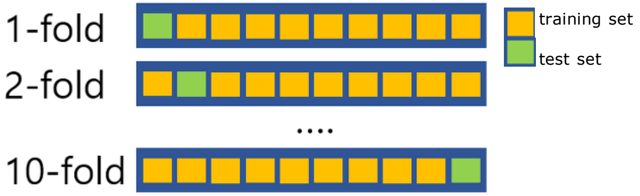
- ***Ri*** is the *range* of the *i*th component
- The (k-)nearest neighbour method is simple, easy to use, and can achieve good results in many cases
- What problem can you find?
  - Does this method explicitly learn a classifier? If yes, what is it?
  - Efficient?

K-fold Cross Validation

- Idea: chop the available data into K equal chunks
- For each chunk in turn:
  - Treat it as the *test* data set
  - Treat the rest K − 1 chunks as the *training* data set
  - The classifier trained/learned from the training set is applied to the test set
- The process is then repeated K times (the folds), with each of the K chunks used exactly once as the test data set.
- The K results from the folds can be then averaged (or otherwise combined) to produce a single estimation.
- Can be used for comparing two algorithms, or measure the performance of a particular algorithm when the data set is small.

10-fold Cross Validation

- Example: 150 instances for 10-fold cross validation
  - Splitting into 10 chunks 15, 15, 15, 15, 15, 15, 15, 15, 15, 15



Leave-one-out Cross Validation

- It is very similar to the K-fold cross-validation method
- Every time, it only uses *one instance* as the test data set
- The process needs to be repeated *m* times, where *m* is the total number of examples/instances in the entire data set

- K-fold cross validation (including leave-one-out cross validation) is ***NOT*** a machine learning or classification method or technique

- It is an *experimental design method* for setting up experiments for supervised learning tasks such as classification and regression

Validation Set vs Cross Validation

- Validation set (vs training set vs test set)
  - The validation set is a *data set*
  - Validation set is a separate data set from the training set and the test set.
  - Validation set is used for *monitoring* the training process but is not directly used for learning the classifier
  - the *validation set* is used for avoid *overfitting* or *overtraining*
  - Assume:
    - 100 examples – 50 vs 50
    - 40 vs 30 vs 30
- Cross Validation
  - Is a *experimental design method, NOT a data set*
  - In this method, there are only training sets and test sets
  - No validation set exists

Data Subset vs How to Use Data

K-Means Clustering

- Unlabelled data
- Expect to obtain good partitions for the instances using learning techniques.
- Need clustering techniques, unsupervised learning

- K-means clustering is a method of cluster analysis which aims to partition *m* instances into *k* clusters in which each instance belongs to the cluster with the nearest mean.

- Need some kind of distance measure such as Euclidean distance
- Need to *assume* the number of clusters

K-Means Clustering: Algorithm

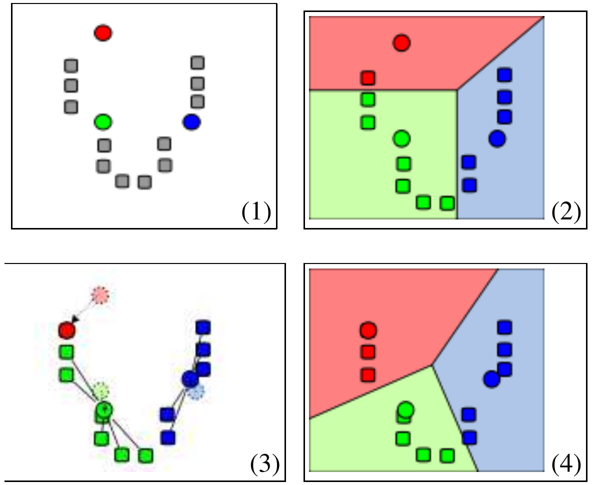
1. Set *k* initial "means" (in this case *k=3*) *randomly* from the data set (shown in color).

2. Create k clusters by associating every instance with the nearest mean based on a distance measure.

3. Replace the old means with the centroid of each of the k clusters (as the new means).

4. Repeat the above two steps until convergence (no change in each cluster center).

K-Means Clustering: An Example



K-means Algorithm Demo:
https://www.youtube.com/watch?v=zHbxbb2ye3E

Summary

- Nearest neighbour method for classification
  - K-Nearest neighbour method — classification method
  - Measures of comparing two feature vectors
- K-fold cross validation
  - experimental design method, NOT a learning method
  - validation set is a data set, NOT a method
- K-means method —- clustering method, NOT for classification

- Next Lecture: Decision tree learning for classification
- Suggested reading: Section 18.3 (both 2nd and 3rd editions) and online materials