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# COMP6237 Data Mining
# Lecture 8: Nearest Neighbours

Zhiwu Huang

Zhiwu.Huang@soton.ac.uk

Lecturer (Assistant Professor) @ VLC of ECS

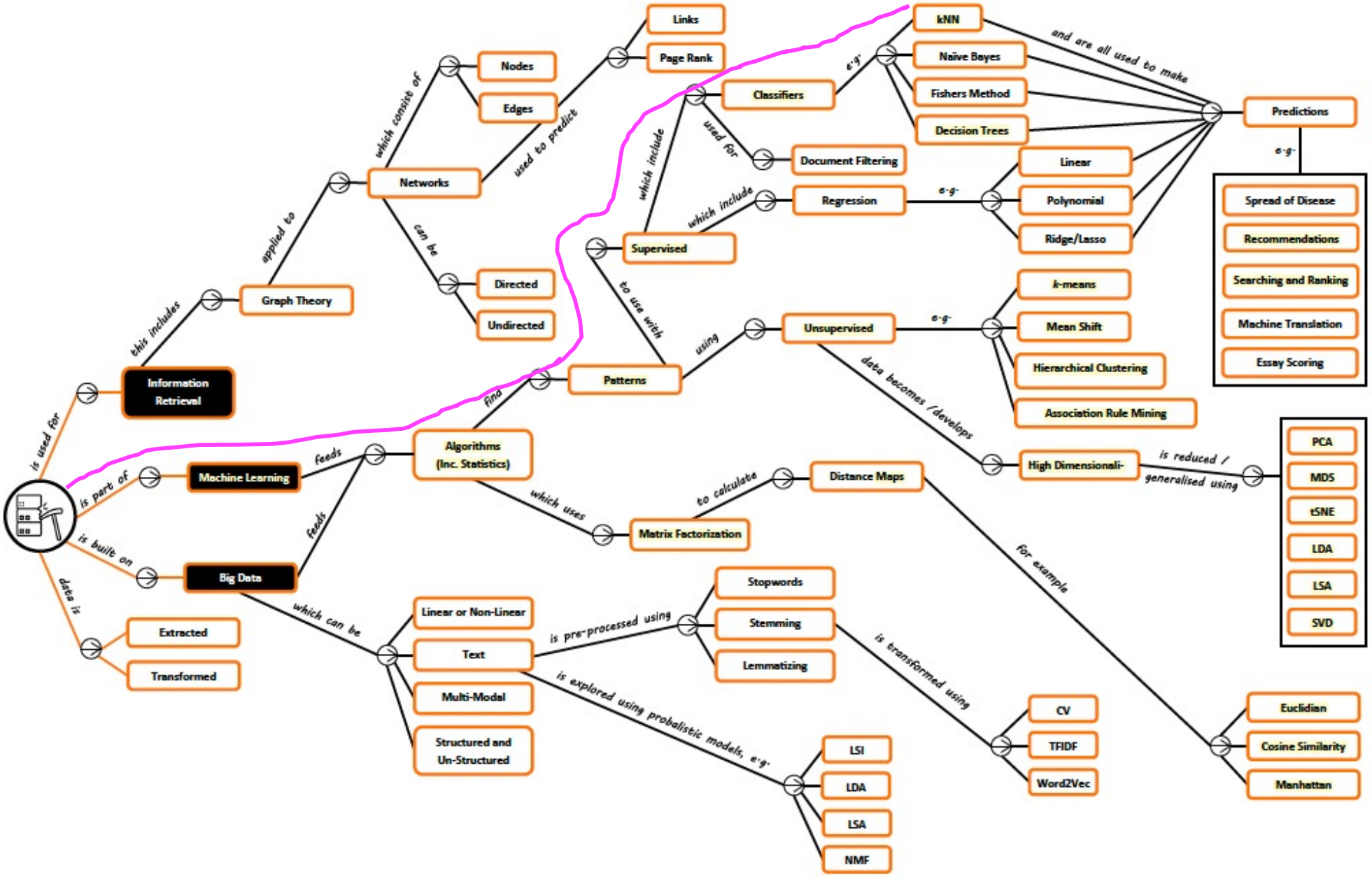
University of Southampton

Lecture slides available here:

http://comp6237.ecs.soton.ac.uk/zh.html

(Thanks to Prof. Jonathon Hare and Dr. Jo Grundy for providing the lecture materials used to develop the slides.)

# Nearest Neighbours – **Roadmap**



# Nearest Neighbours – **Textbook**

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**PART FOUR** CLASSIFICATION

The classification task is to predict the label or class for a given unlabeled point. Formally, a classifier is a model or function $M$ that predicts the class label $\hat{y}$ for a given input example $\mathbf{x}$, that is, $\hat{y} = M(\mathbf{x})$, where $\hat{y} \in \{c_1, c_2, \ldots, c_k\}$ and each $c_i$ is a class label (a categorical attribute value). Classification is a *supervised learning* approach,

- Data Mining and Machine Learning: Fundamental Concepts and Algorithms M. L. Zaki and W. Meira

## **4** Classification: Alternative Techniques

*The previous chapter introduced the classification problem and presented a technique known as the decision tree classifier. Issues such as model overfitting and model evaluation were also discussed. This chapter presents alternative techniques for building classification models—from simple techniques such as rule-based and nearest neighbor classifiers to more sophisticated techniques such as artificial neural networks, deep learning, support vector machines, and ensemble methods. Other practical issues such as the class imbalance and multiclass problems are also discussed at the end of the chapter.*

- Introduction to Data Mining, *P. Tan et al*

# Nearest Neighbours – **Overview**




Assign class of unknown point based on **majority class** of *closest* ***K*** **neighbours** in feature space



Credit: Jon Hare

# Nearest Neighbours – Learning Outcomes

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- **LO1**: Demonstrate an understanding of the fundamentals of nearest neighbor classifiers, such as: (exam)
  - ❖ Understanding the k-NN algorithm, including key steps like distance calculations, voting, etc
  - ❖ Applying weighted k-NN and its use of weighted distance calculations
  - ❖ Employing K-D trees for efficient nearest neighbor search
  - ❖ Discussing advantages and disadvantages of k-NN models
- **LO2**: Implement the learned algorithms using K-NN methods (course work)

***Assessment hints: Multi-choice Questions (single answer: concepts, calculation etc)***

- *Textbook Exercises: textbooks (Programming + Mining)*
- *Other Exercises: https://www-users.cse.umn.edu/~kumar001/dmbook/sol.pdf*
- *ChatGPT or other AI-based techs*

# Nearest Neighbours – KNN Algorithm

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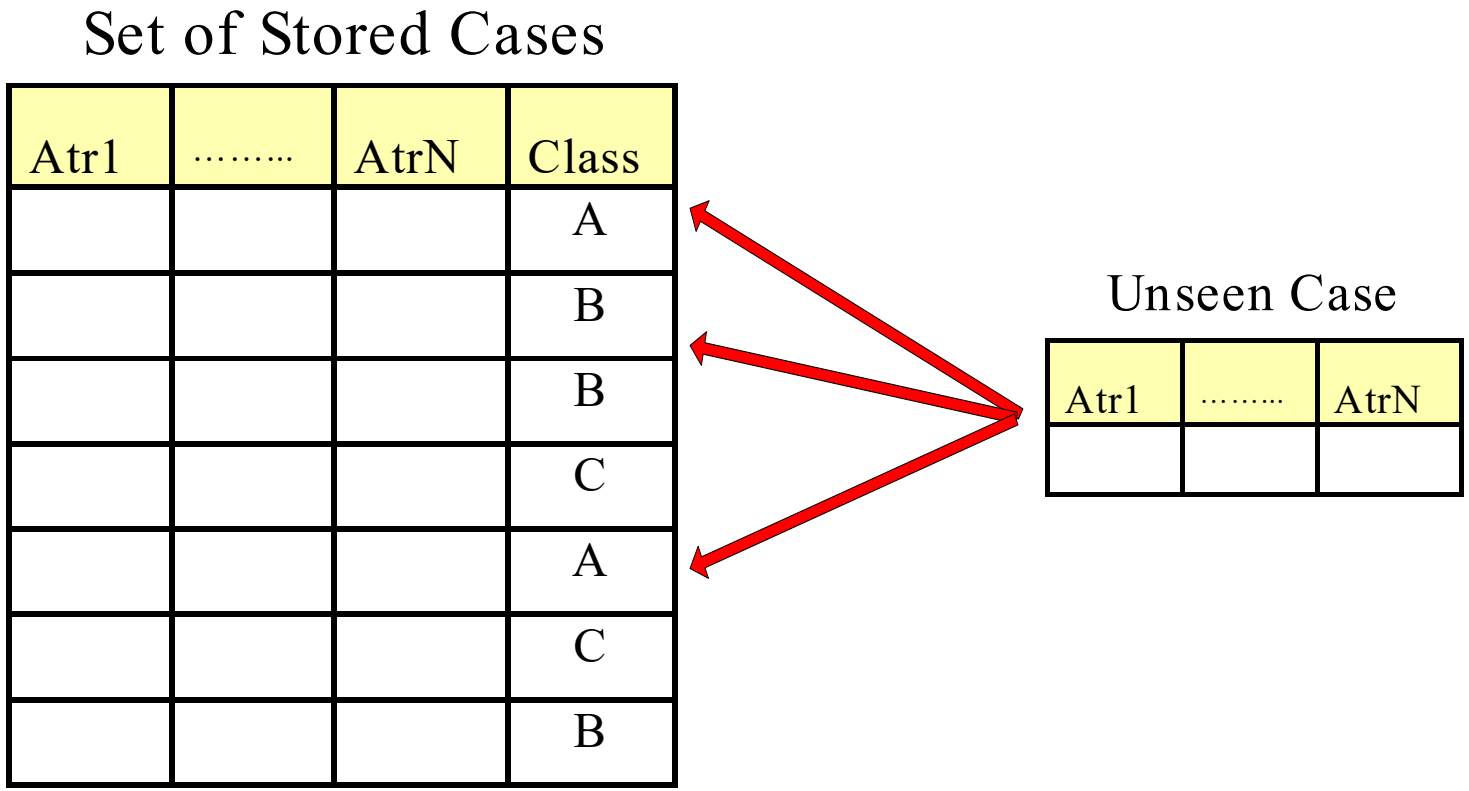
- Key idea: the majority of neighbors should share the same label
  - Use training records directly to predict the class label of test/unseen cases by considering their neighbor correlations
  - Store the training records without training explicit models



# Nearest Neighbours – KNN Algorithm

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- Uses k “closest” training points (nearest neighbors) for performing classification on test data
  - Properties include
    - Little or no prior knowledge about the distribution of the data
    - A simple algorithm that stores all available cases and classifies new cases based on a **similarity measure** (e.g., L2 distance and cosine similarity)
    - Computation merely happens on classification over test data
    - Lazy algorithm, as they don’t use training data to do any generalization

# Nearest Neighbours – KNN Algorithm

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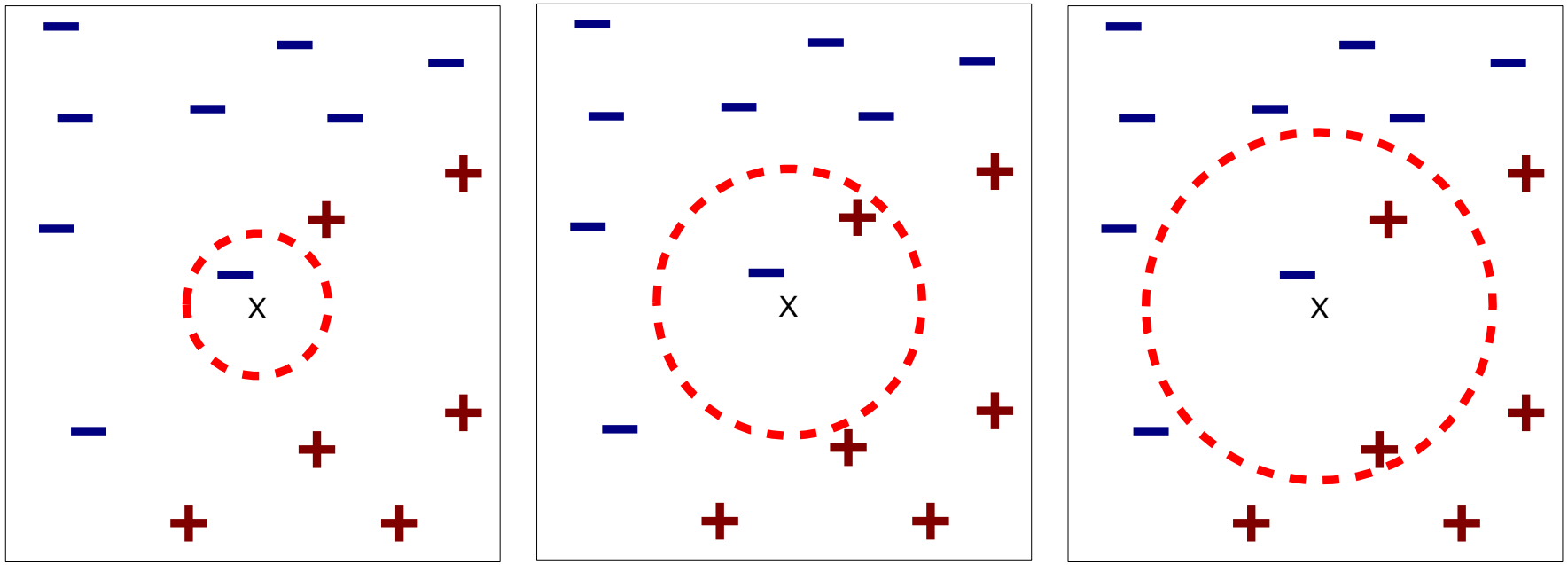
- **k-Nearest Neighbors** of a record x are data points that have the k shortest distance to x




(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

# Nearest Neighbours – KNN Algorithm

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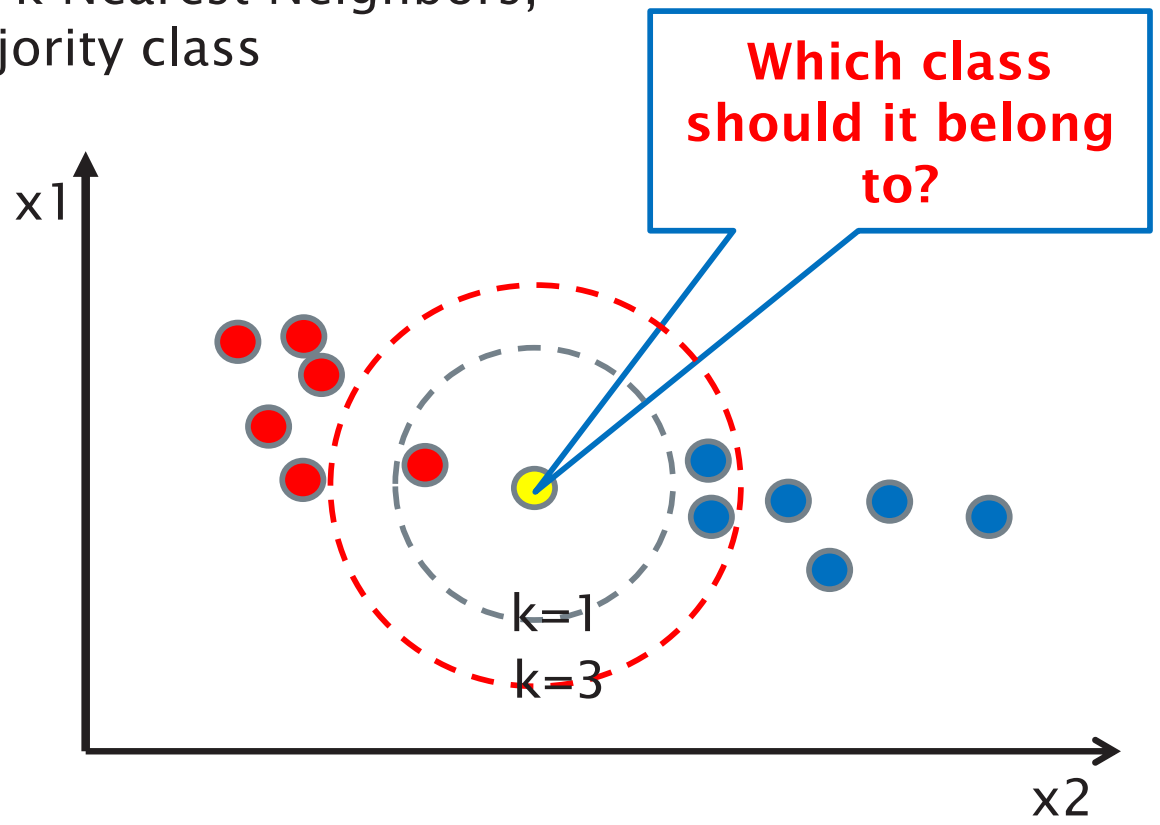
## How k-NN works?

**Key idea:** 1) find k-Nearest Neighbors,
2) assign the majority class



# Nearest Neighbours – K-NN Algorithm

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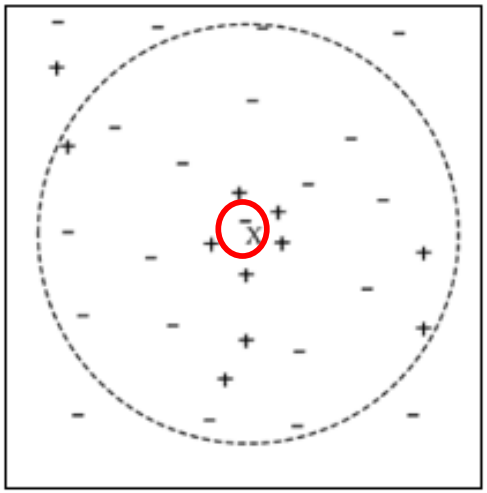
- On choosing K:
  - *K* must not be multiples of the total class number when each vote is equally weighted
    - Odd numbers (1, 3, 5, 7, 9,…) for majority voting on 2-class classification
    - 1, ~~**3 (not good),**~~ 5, 7, ~~**9 (not good)…**~~ for 3-class classification
  - If K is too small, sensitive to noise points
  - If K is too large, neighborhood may include points from other classes



# Nearest Neighbours – Example

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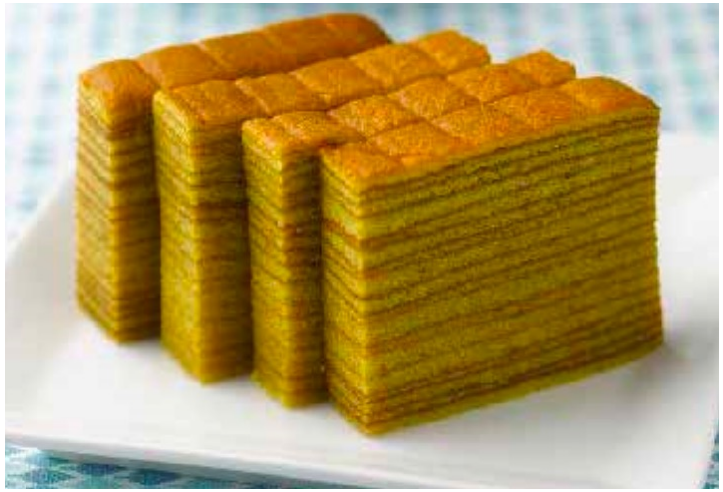
- We want to train a model to decide an unknown goodie is a *Chocolate Cake* or *Pineapple Tart*

*Chocolate Cake*

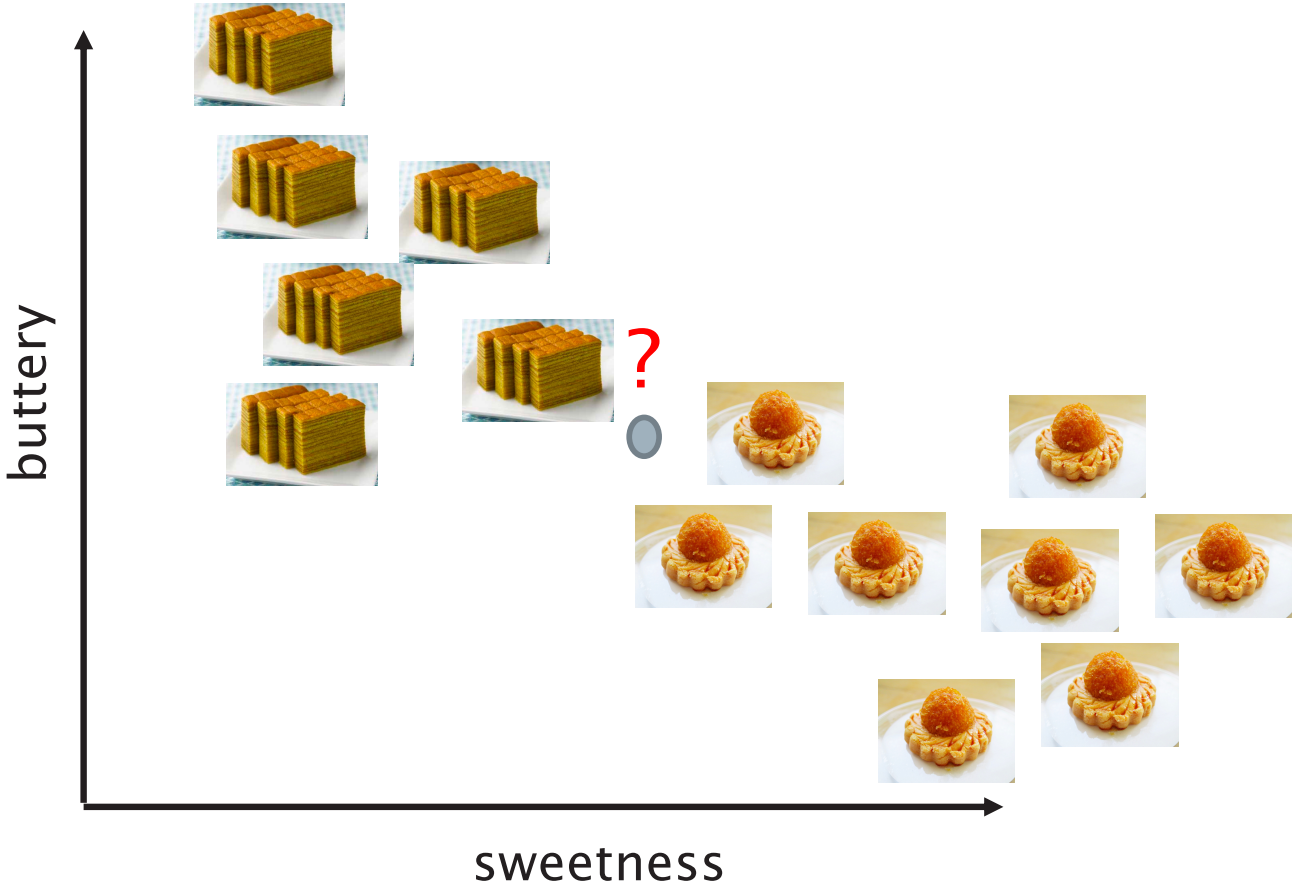


Pineapple Tart

Evaluate on 2 attributes: “sweetness” and “buttery” level

# Nearest Neighbours – Example

- Suppose we have k set to 3 (k = 3 nearest neighbors)
  - 2 neighbors are *Pineapple Tarts* and 1 neighbor is *Chocolate Cake*




Credit: Zhaoxia Wang

# Nearest Neighbours – Example

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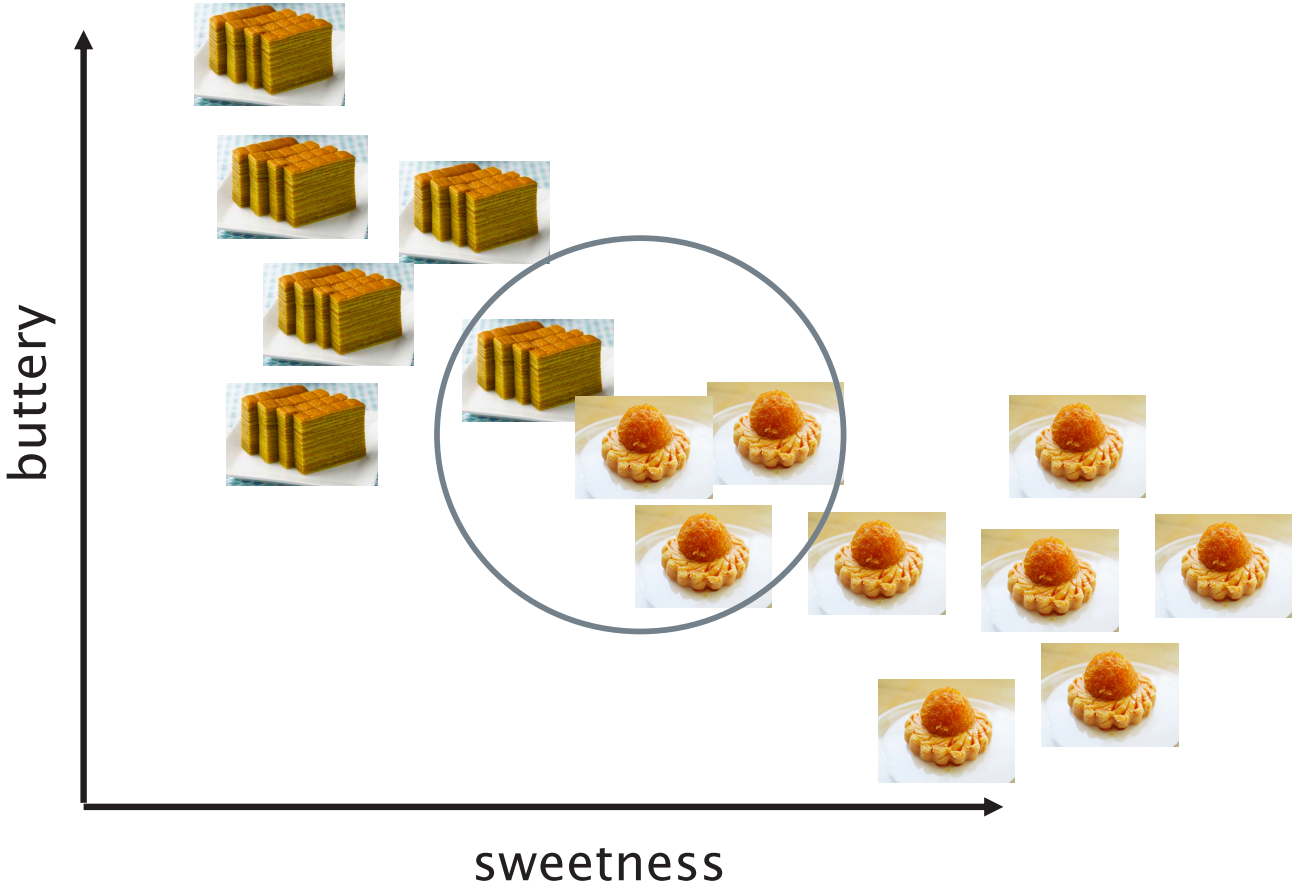
- Using majority voting, we will predict that the unknown goodie is likely to be a *Pineapple Tart*




Credit: Zhaoxia Wang

# Nearest Neighbours – Example

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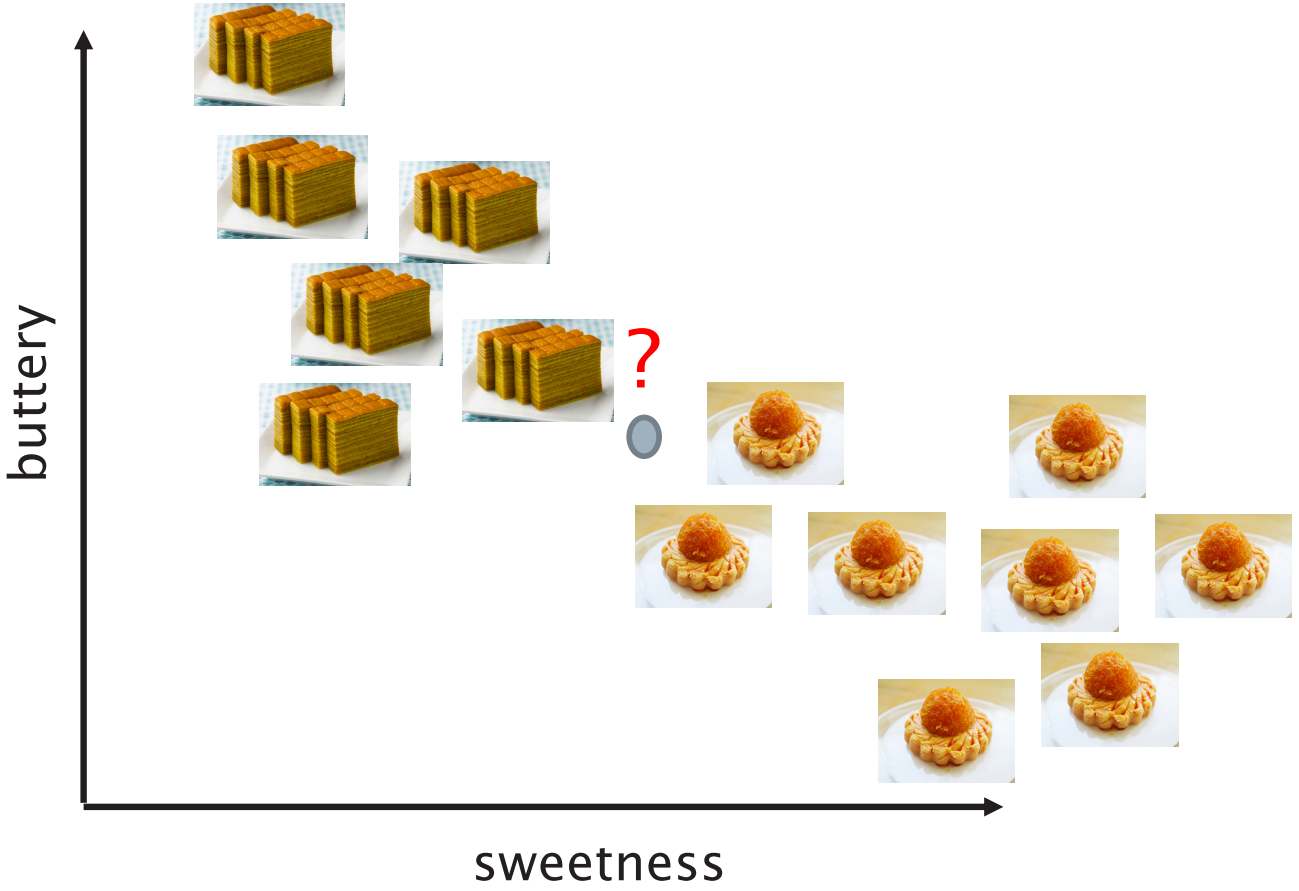
- However, for the situation shown below: suppose we have k set to 7 (k = 7 nearest neighbors)
  - 3 neighbors are *Pineapple Tarts* and 4 neighbors are *Chocolate Cakes*




Credit: Zhaoxia Wang

# Nearest Neighbours – Example

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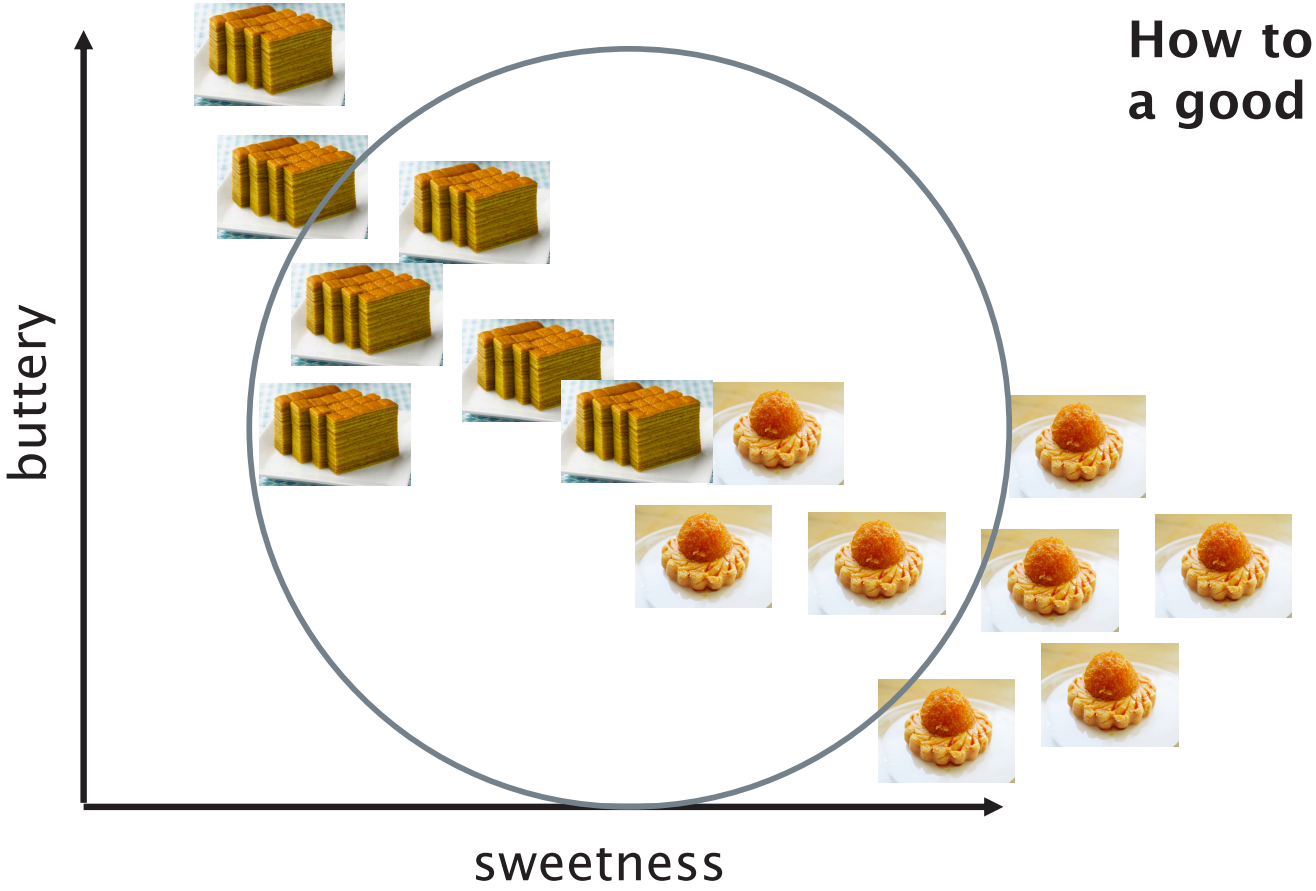
- In such situation, using majority voting, we will predict that the unknown goodie is likely to be a *Chocolate Cake? Yes?*




Credit: Zhaoxia Wang

# Nearest Neighbours – Weighted KNN

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Up to now, each value in the $k$ nearest neighbours has been treated equally.

Better: if closer neighbours are more important

We can use a range of weighting schemes to do this:

- Inverse Weighting
- Subtraction weighting
- Gaussian Weighting

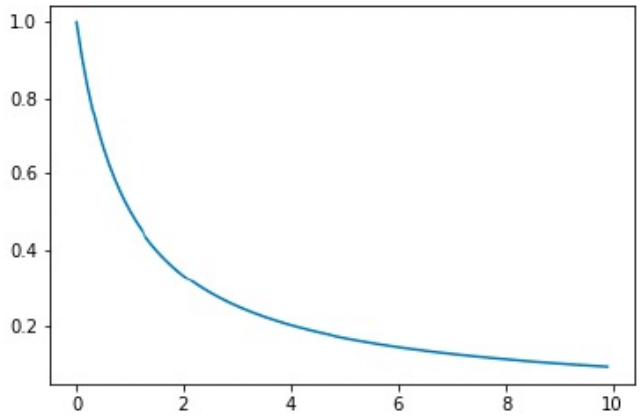
Credit: Jo Grundy

# Nearest Neighbours – Weighted KNN

Inverse Weighting:

$$w = \frac{1}{dist + c}$$

Where $c$ is a constant, avoiding division by zero error if $dist = 0$




Credit: Jo Grundy

# Nearest Neighbours – Weighted KNN

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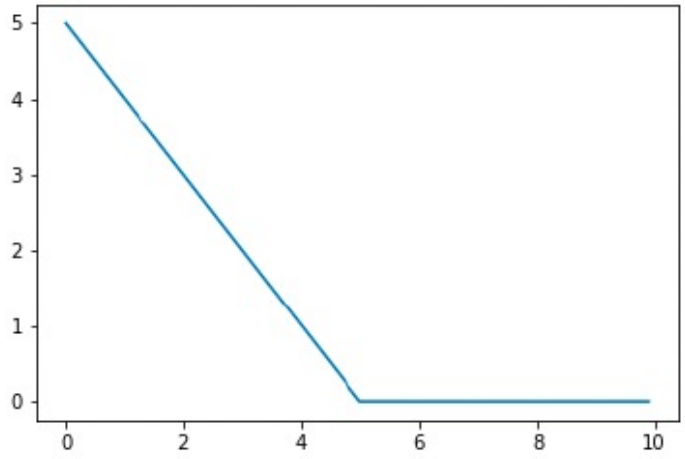
Subtraction Weighting:

$$w = \max(0, c - dist)$$

Where $c$ is a constant




Credit: Jo Grundy

# Nearest Neighbours – Weighted KNN

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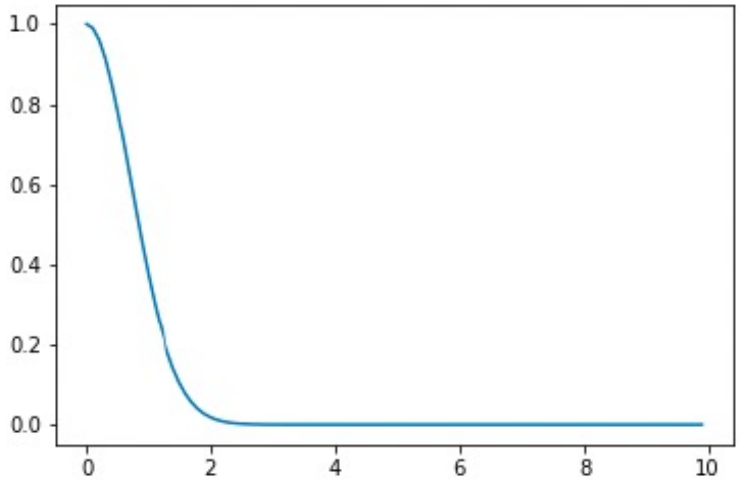
Gaussian Weighting:

$$w = \exp \frac{-dist^2}{c^2}$$

Where $c$ is a constant




Credit: Jo Grundy

# Nearest Neighbours – KNN

Advantages?

- No assumptions made
- No training phase
- Simple and easy to implement

Problems?

- Doesn't scale well with lots of data
- Doesn't scale well with many dimensions

Credit: Jo Grundy

# Nearest Neighbours – KNN

Again, to chose the best weighting scheme, measure performance using cross validation.

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

Problems?

- Heterogenous Data - features with larger ranges have greater effects
- Outliers affect data a good deal, especially for low $k$
- For larger $k$, less common classes can get ignored
- Distance metric determines similarity - usually Euclidean, works badly in high D
- Can use Hamming distance for categorical attributes
- Irrelevant data can force otherwise similar data samples to be far apart
- Computationally expensive if there are lots of data, or highly dimensional data

Credit: Jo Grundy

# Nearest Neighbours – KNN

Curse of dimensionality; For low dimensions, the size of a neighbourhood is small.

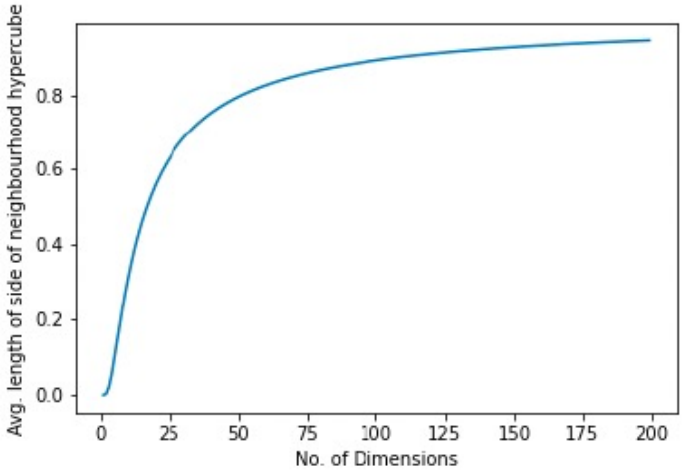
e.g. for $k = 10$, number of points $N = 1,000,000$

In a unit line, the average neighbourhood is $\frac{10}{10^6} = 0.00001$ long

In a unit square, the average side length is $\sqrt{\frac{10}{10^6}} = 0.003$ long

In a unit cube, the average side length is $\sqrt[3]{\frac{10}{10^6}} = 0.02$ long

As the dimensionality increases, the average neighborhood size for k=10 grows rapidly




In very high dimensions (like 200), to find the 10 nearest neighbors for a point, you essentially need to consider above 90% of the entire dataset of 1 million points.

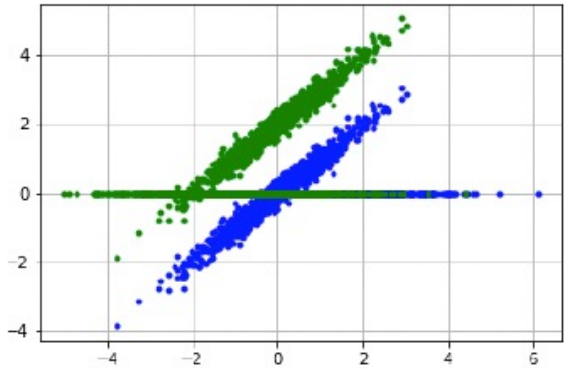
This can make it very difficult to work out which are closer, as the distances are nearly all the same

Credit: Jo Grundy

# Nearest Neighbours – KNN

Solutions for high D?

- Dimensionality reduction.. Care! Some aren't suitable (e.g. MDS, SOM) for extremely high dim
- Also.. PCA:




- A random direction could be better!
  Johnson Lindenstrauss lemma:
  if points in a vector space are of high enough dimensionality, they may be projected into a lower dimensional space in a way which approximately preserves the distances between the points, this basis can be generated randomly

Credit: Jo Grundy

# Nearest Neighbours – KNN

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## Solutions: For heterogenous data?

- For heterogenous data, can *normalise* using methods e.g., Z-score
- Better to scale factors for each feature to optimise performance

  Example:
  - height of a person may vary from 1.5m to 1.8m
  - weight of a person may vary from 30kg to 100kg
  - income of a person may vary from \$10K to \$1M

- Could use this to do feature selection
  eg. if works best when scale factor $= 0$, then feature is useless!

Credit: Jo Grundy

# Nearest Neighbours – KNN

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## More solutions for high D?

- Use different metric:
  - Hamming distance for categorical attributes
  - BM25 or TF-IDF for text data
  - Minkowski distance (p-norm) - generalisation of Euclidean distance
  - Kullback - Liebler Divergence for histograms

The symbols may be letters, bits, or decimal digits, among other possibilities. For example, the Hamming distance between:

- "**karolin**" and "**kathrin**" is 3.
- "**karolin**" and "**kerstin**" is 3.
- "**kathrin**" and "**kerstin**" is 4.
- **0000** and **1111** is 4.
- **2173896** and **2233796** is 3.

https://en.wikipedia.org

Credit: Jo Grundy

# Nearest Neighbours – KNN

Solutions for lots of data?

- Need to quickly find the nearest neighbour to a particular point in a highly dimensional space
  - Could index points in a tree structure?
  - Could hash the points?
  - Could break up the space

Credit: Jo Grundy

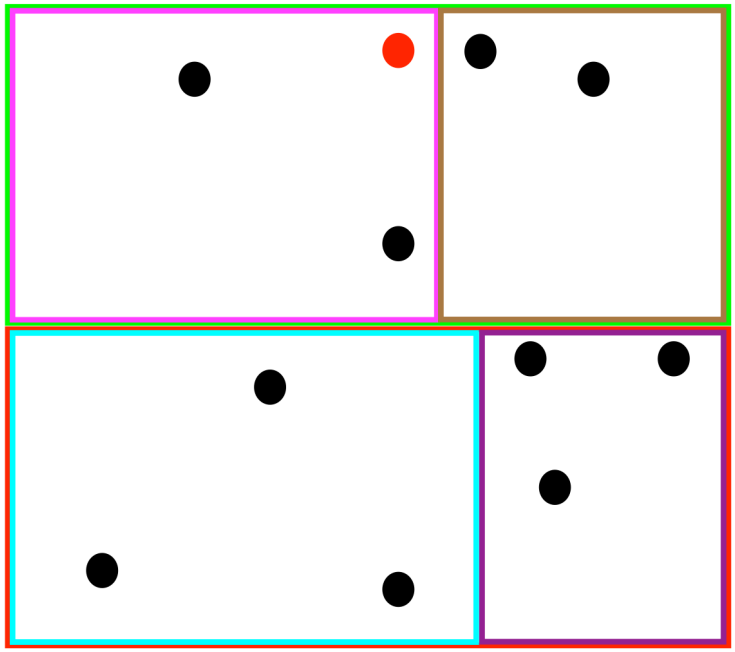
# Nearest Neighbours – K-D trees

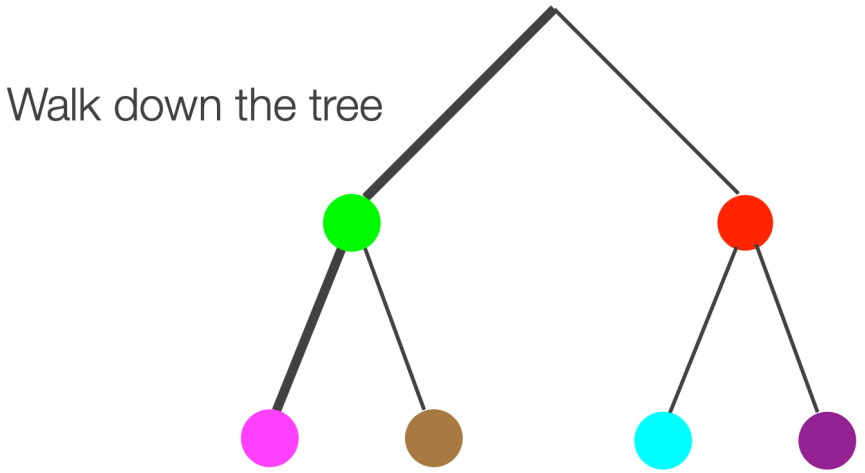
K-D trees are binary tree structures that partition the space along an axis-aligned hyperplane

- Chose random dimension
- Divide along median value
- Repeat until depth limit reached or certain number of items in each leaf

Credit: Jo Grundy

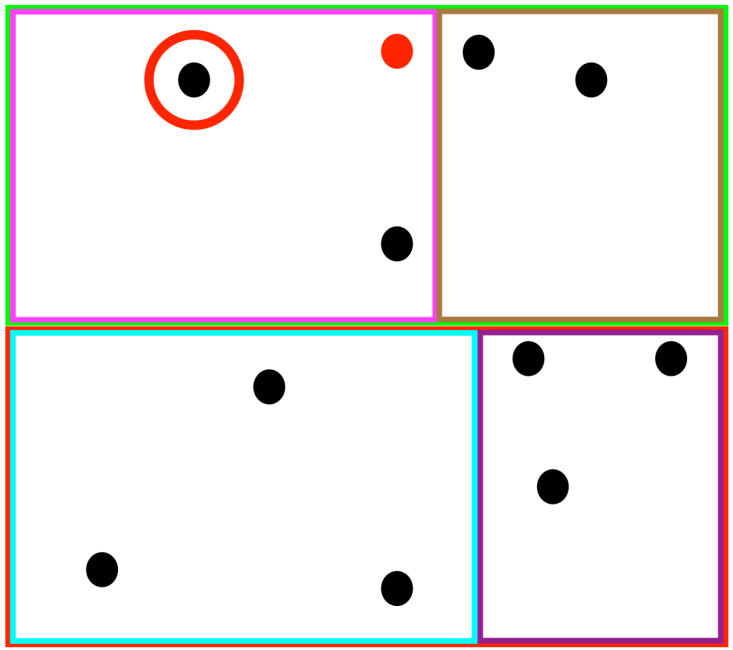
# Nearest Neighbours – K-D trees



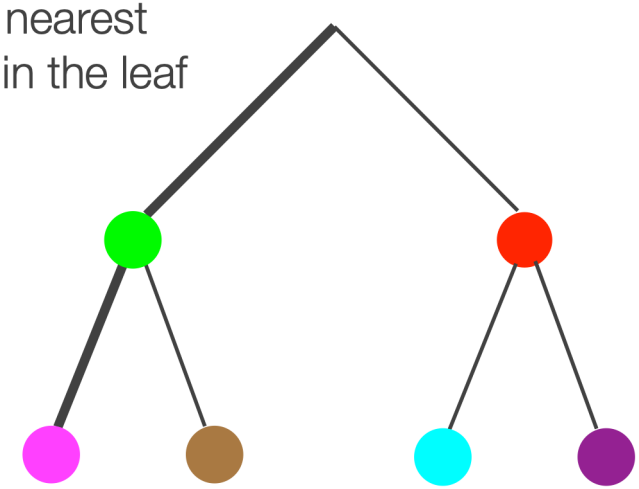



Credit: Jon Hare

# Nearest Neighbours – K-D trees

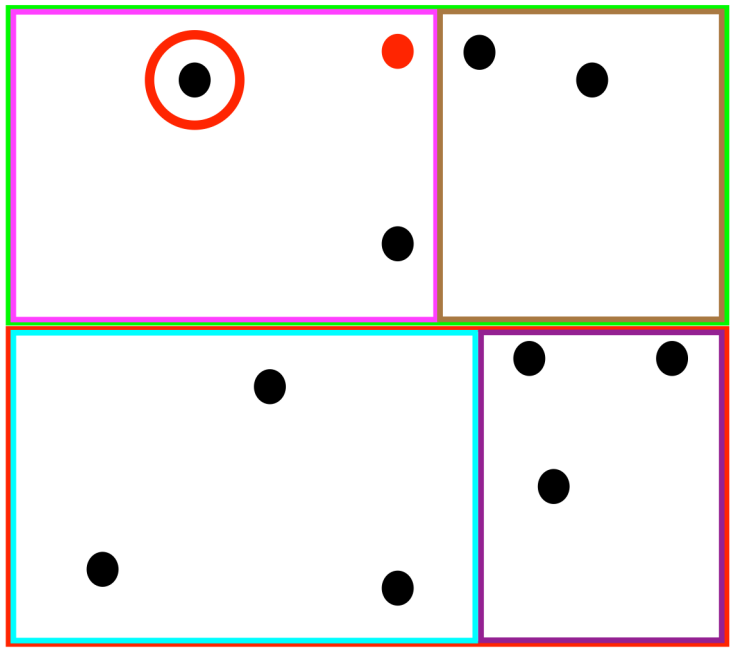


Find the nearest neighbour in the leaf

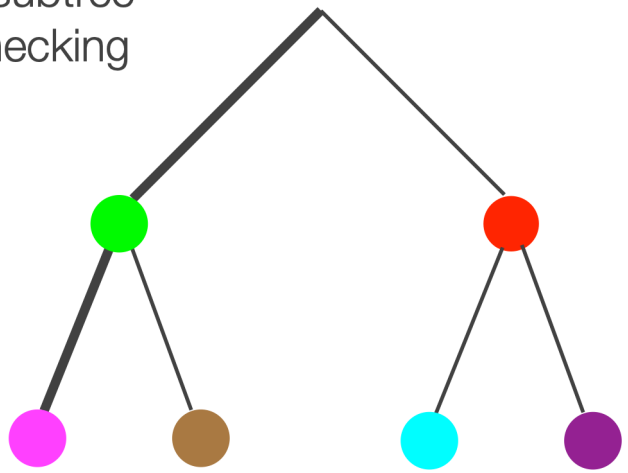


Credit: Jon Hare

# Nearest Neighbours – K-D trees

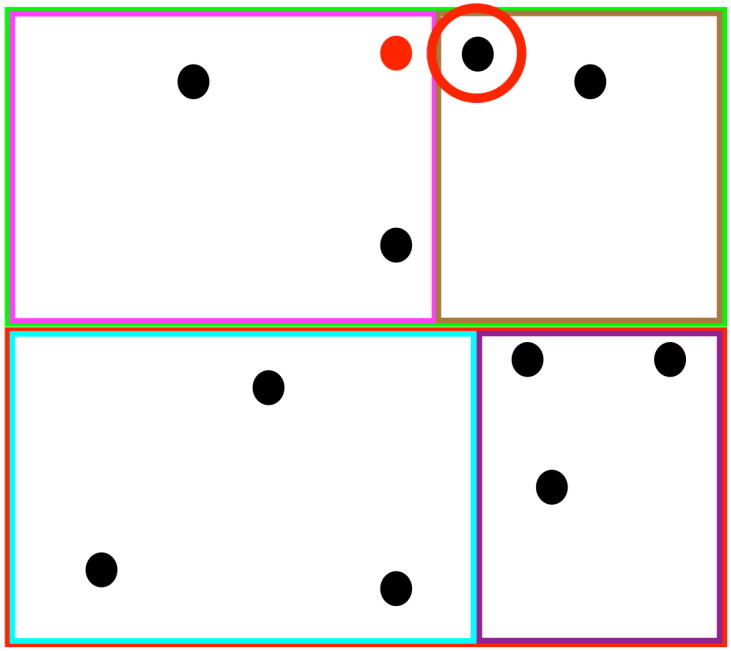


Backtrack, and see if the next subtree needs checking



Credit: Jon Hare

# Nearest Neighbours – K-D trees



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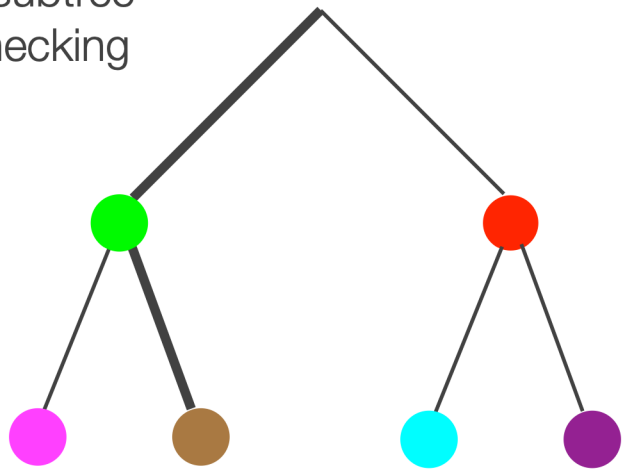
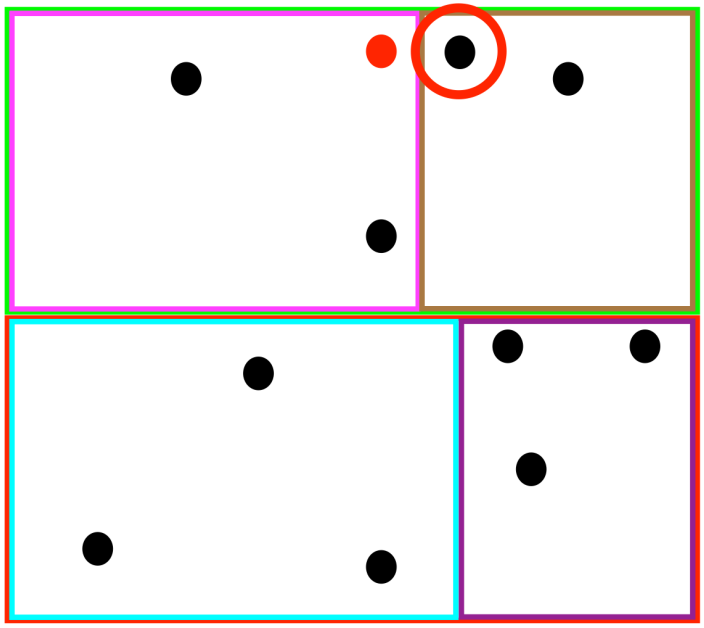


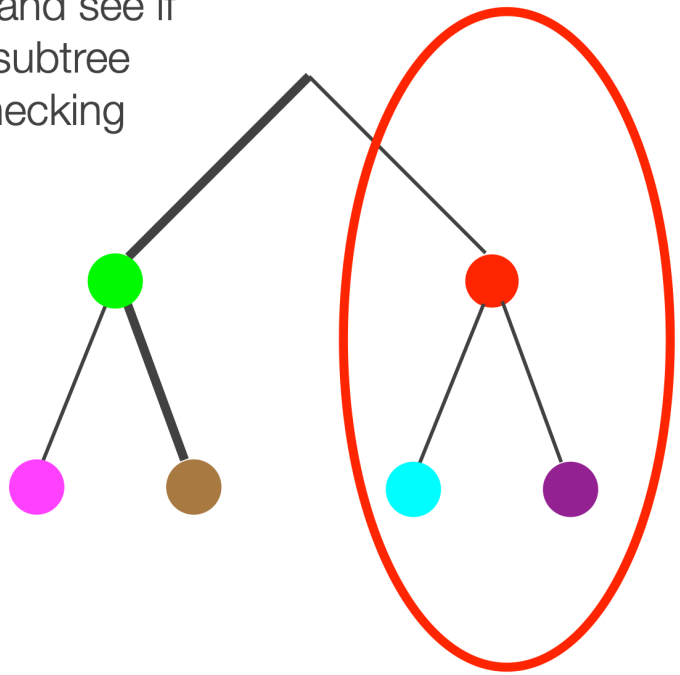
Credit: Jon Hare

# Nearest Neighbours – K-D trees



Backtrack, and see if the next subtree needs checking

No need to check this subtree



Credit: Jon Hare

# Nearest Neighbours – K-D trees

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Problems?

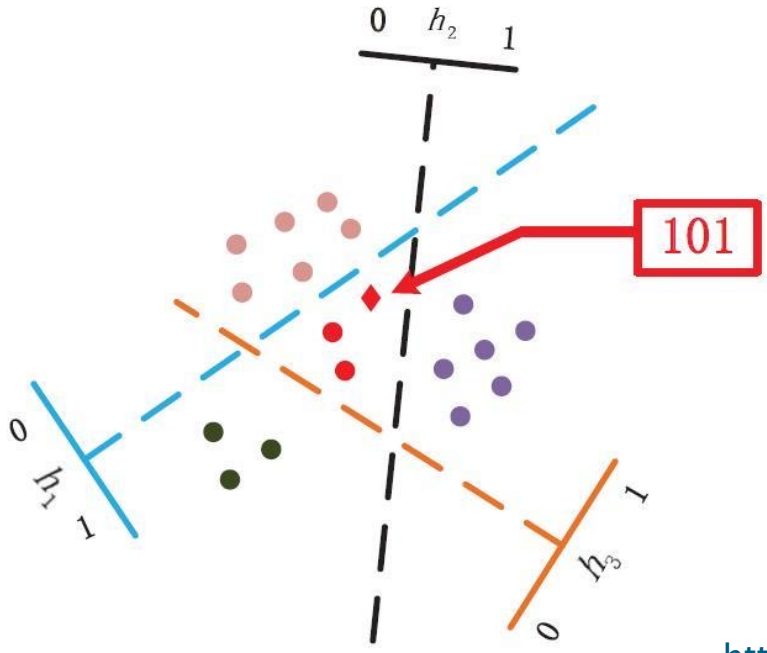
- Doesn't scale well to high dimensions
- Often need to search much of the tree
- Need *many* more examples than there are dimensions, at least $2^n$
- There are approximate versions, not guaranteed exact answer but do scale
  - Based on ensembles of trees with a randomised split dimension

Credit: Jo Grundy

# Nearest Neighbours – LSH

Locality Sensitive Hashing
Makes hash codes that are similar for similar vectors

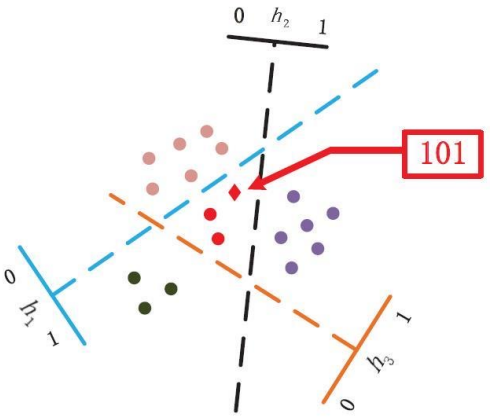
- Similar items map to the same buckets with high probability
- number of buckets much smaller than number of data samples
- Aims to maximise the probability of a collision for similar items




https://www.researchgate.net

Credit: Jo Grundy

# Nearest Neighbours – LSH




Accomplished by:

- Chose random hyperplanes $(h_1, h_2, \ldots, h_k)$
- Each hyperplane with split the space in to 2 regions
- $\therefore$ the space will be sliced in to $2^k$ regions (buckets)
- Giving a simple code for each of the data points, depending on which side of each hyperplane the data points are
- The same code for each of the data points within the same region
- Compare new point only to training points in the same region
- Repeat with different random hyperplanes $(h_1, h_2, \ldots, h_k)$

on board

Gives low complexity , $\approx O(d \log n)$, as compare new data to only $\frac{n}{2^k}$

Credit: Jo Grundy

# Nearest Neighbours – Summary

KNN can be used for regression as well as classification

- Using weighting can improve performance
- Poor performance with large data sets
- Can use K-D trees to help overcome these issues
  - Still can have issues with highly dimensional data
  - Often not much improvement in performance
- Curse of dimensionality
  - Affects neighbourhood size
- Can use dimensionality reduction to help (but be careful!)
- Fast approximate Nearest Neighbourhood methods - LSH

Also: *Final presentation does not need to be for full coursework, it is to show what you have done so far*

Credit: Jo Grundy