MSc Data Mining Topic 05: Classification Part 04: K Nearest Neighbours Unsupervised Dr Bernard Butler and Dr Kieran Murphy Association Rules Regression Department of Computing and Mathematics, SETU Waterford. (bernard.butler@setu.ie; kmurphy@wit.ie) Recommender Systems **Anomaly Detection Basic Classification** Spring Semester, 2023 **Advanced Classification** Outline K Nearest Neighbours (KNN) algorithm

k-Nearest Neighbour Methods

General Idea

- Given m labeled observations (▲, ■, and ★), how should we classify a new unlabelled observation (?)?
- We could use the labels of the *k*-nearest neighbouring points.
 - "Nearest" means distance how should we calculate this?
 - How do we pick the value for *k*?
- What is our decision rule?
 - Assign new observation to most frequent occurring class in *k*-nearest neighbours.
 - What to do if there is a tie?

Distance Functions

We frequently want to measure how close/near/similar two points (think observations/instances/cases) are. For this we need a distance function.

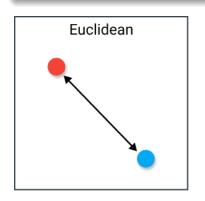
Distance Function

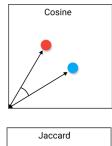
A distance function, D(a, b), is any function that satisfies the properties:

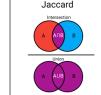
non-negativity: $D(a,b) \ge 0$, distance between any two points is non-negative and is only zero if a = b.

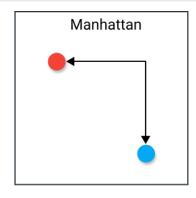
symmetric: D(a,b) = D(b,a)

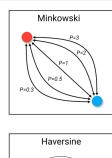
triangular inequality: $D(a,c) \leq D(a,b) + D(b,c)$

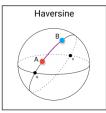


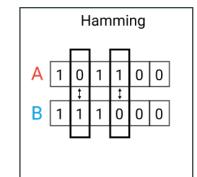


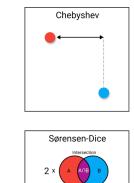




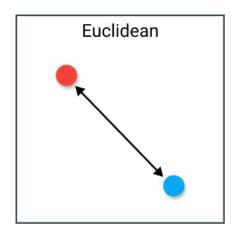


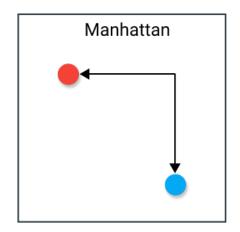


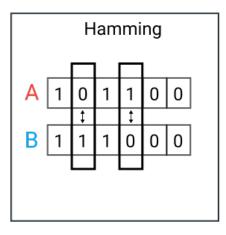




Distance Functions — Euclidean, Manhattan, and Hamming







• Pythagorean theorem

$$D(a,b) = \sqrt{\sum_{i=1}^{n} [a^{(i)} - b^{(i)}]^2}$$

- "As the crow flies"
- Features should be normalised before use
- ✓ Most commonly used metric.
- ✗ Becomes less useful for large dimensions

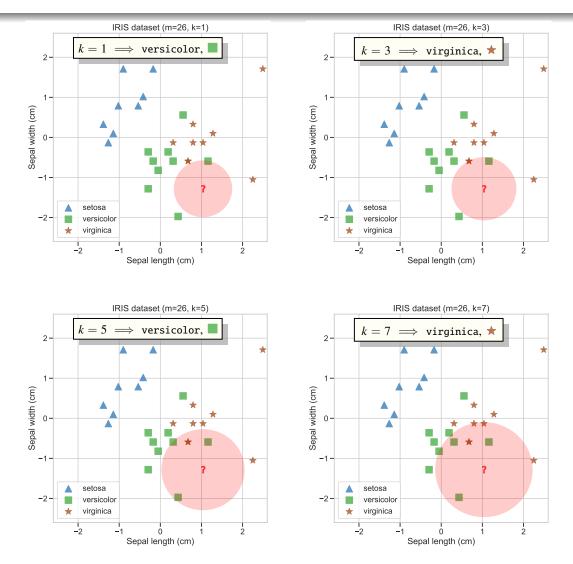
• Taxi-cab distance

$$D(a,b) = \sum_{i=1}^{n} |a^{(i)} - b^{(i)}|$$

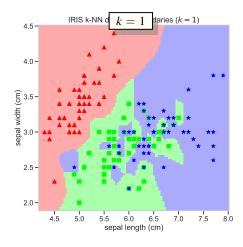
- Seems to work better than

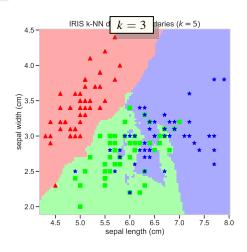
 Euclidean for high-dimensional data
- Suitable for datasets with discrete and/or binary features.
- Count of the number of differences (bits/letters/levels etc) between two points.
- Can be used between categorical variables.
- Difficult to use when two vectors are not of equal length.
- Should not be used when magnitude is important.

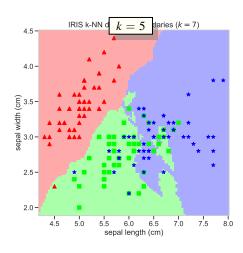
Effect of *k*

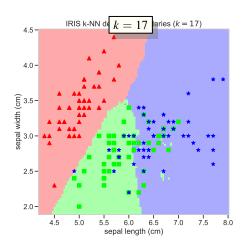


Effect of k on Decision Boundary









k-Nearest Neighbour Methods — Review

When to Consider

- Observations/instances map to points in \mathbb{R}^n
- Less than 20 features/attributes per instance
- Lots of training data

> Advantages

- Training is very fast
- Learn complex target functions
- Do not lose information

Disadvantages `

- Slow at query time
- Memory-based technique
- Easily fooled by irrelevant features/attributes

Hyper-Parameters

- Distance metric
- Number of neighbours, *k*

(quantitative/numerical features)

(low dimensionality)

(more points means closer neighbours)

(instantaneous, since lazy learner)

(lazy learner)

(uses training data not model to predict)

(must pass over (nearly) all points for each classification)

(Euclidean — "as the crow flies")

(Increasing *k* reduces variance, increases bias)

Resources

• 9 Distance Measures in Data Science

towardsdatascience.com/9-distance-measures-in-data-science-918109d069fa Non-technical comparison of common distances functions (source of images used here).