

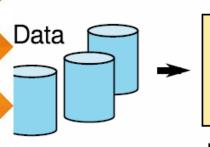
COMP809 Data Mining and Machine Learning

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K-Nearest Neighbors (KNN)





Pre-processing Normalization Feature selection

- Handling missing data
- Outliers
- PCA
- Signal-to-noise ratio

Optimization

- GA
- PSO
- D/E
- EDA
- ES

Modelling Learning

- Naive Bayes
- kNN, wkNN
- Decision Trees
- Linear Regression
- Neural Networks
- k-means clustering
- Association Rules

Evaluation and performance metrics

- Cross-validation
- Metrics in classification
- Metrics in regression
- Significance tests

K-Nearest Neighbours (KNN)

KNN is an algorithm that is an example of lazy learning.

- Non-parametric means that it makes no assumptions. The model is made up entirely from the data given to it rather than assuming its structure is normal.
- Lazy learning means that the algorithm makes no generalizations. This means that there is little training involved when using this method. Because of this, all of the training data is also used in testing when using KNN.



Instance-Based Classifiers

Set of Stored Cases

| | , | | | | | | | |
|---|---|-------|------|-------|--|--|--|--|
| | Atr1 | ••••• | AtrN | Class | | | | |
| 1 | | | | A | | | | |
| | V. | | | В | | | | |
| | 81 | | | В | | | | |
| | | | | С | | | | |
| | | | | A | | | | |
| | a) | | | C | | | | |
| | | | | В | | | | |

- Store the training records
- Use training records to predict the class label of unseen cases

Unseen Case

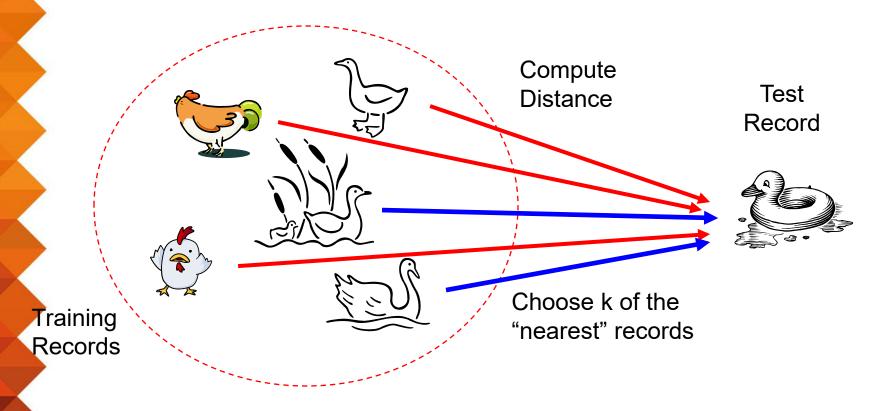
| Atr1 | AtrN |
|------|----------|
| | |



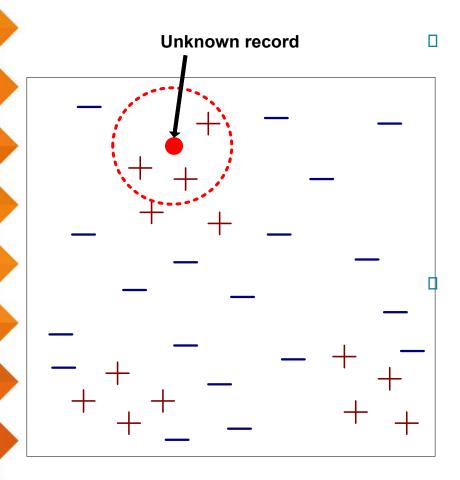
- Examples:
 - Rote-learner
 - Memorizes entire training data and performs classification only if attributes of record match one of the training examples exactly
 - Nearest neighbor
 - Uses k "closest" points (nearest neighbors) for performing classification

Nearest Neighbor Classifiers

- Basic idea:
 - If it walks like a duck, quacks like a duck, then it's probably a duck



Nearest Neighbour Algorithm



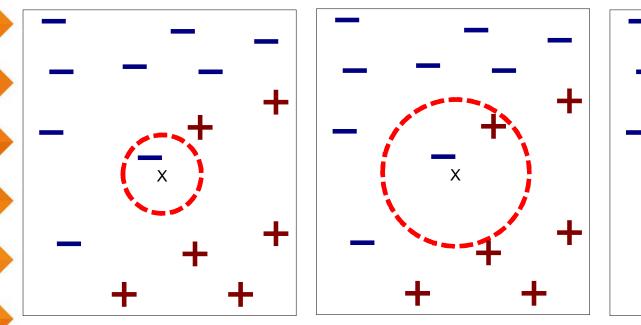
Requires three things

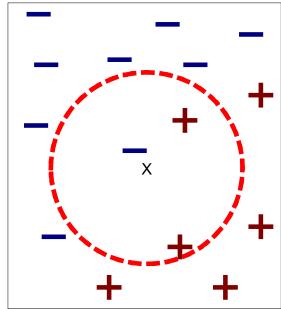
- The set of stored records
- Distance Metric to compute distance between records
- The value of k, the number of nearest neighbors to retrieve

To classify an unknown record:

- Compute distance to other training records
- Identify k nearest neighbors
- Use class labels of nearest neighbors to determine the class label of unknown record (e.g., by taking majority vote)

Definition of Nearest Neighbor

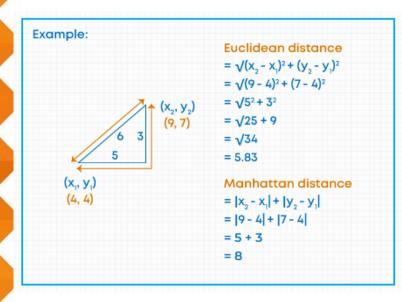


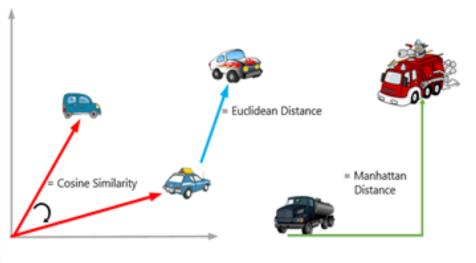


- (a) 1-nearest neighbor
- (b) 2-nearest neighbor
- (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

Similarity Distance Measures





Cosine similarity defined as the dot product of the vectors divided by their magnitude. For example, if we have two vectors, A and B, the similarity between them is calculated as:

$$similarity(A,B) = cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$$

$$\begin{array}{c} -\text{Angle } \theta \text{ close to } \theta \\ -\text{Cos}(\theta) \text{ close to } 1 \\ -\text{Similar vectors} \end{array}$$

Nearest Neighbor Classification

Compute distance between two points:

- Euclidean distance
- Manhattan distance
- q norm distance

$$d(p,q) = \sqrt{\sum_{i} (p_i - q_i)^2}$$

$$d(p,q) = \sum_{i} |p_i - q_i|$$

$$d(p,q) = (\sum_{i} |p_{i} - q_{i}|^{q})^{1/q}$$

Determine the class from nearest neighbor list

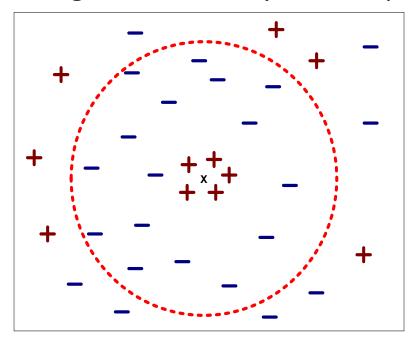
- take the majority vote of class labels among the k-nearest neighbors
- Weigh the vote according to distance
 - weight factor, $w = 1/d^2$

Nearest Neighbor Classification...

- Choosing the value of k:
 - If k is too small, sensitive to noise points

If k is too large, neighborhood may include points from

other classes



Nearest Neighbor Classification...

- Scaling issues
 - Attributes may have to be scaled to prevent distance measures from being dominated by one of the attributes
 - Example:
 - height of a person may vary from 1.5m to 1.8m
 - weight of a person may vary from 40kg to 150kg
 - income of a person may vary from \$10K to \$1M

Example

| Name | Age | Gender | Income |
|------|-----|--------|----------|
| Jim | 53 | М | \$68,000 |
| Mary | 20 | F | \$61,000 |
| John | 49 | М | \$36,000 |

$$d(Jim, Mary) \approx \sqrt{(68000 - 61000)^2}$$
$$\approx \sqrt{(7000)^2}$$
$$\approx 7000$$

$$d(Jim, John) \approx \sqrt{(68000 - 36000)^2}$$
$$\approx \sqrt{(32000)^2}$$
$$\approx 32000$$

Nearest neighbor Classification...

- k-NN classifiers are lazy learners
 - It does not build models explicitly
 - Unlike eager learners such as decision tree induction and rule-based systems
 - Classifying unknown records are relatively expensive

Nearest Neighbour Algorithm: Nominal Data

 For nominal data, Euclidean distance cannot be used and a distance measure based on whether an exact match exists or not can be used

Applying Nearest Neighbour to Credit Scoring

 For the credit scoring example we will use k=3 and distance between two instances is based on a 0/1 scheme

| Name | Debt | Income | Married? | Risk Actual | Probability: Good Risk | Probability: Poor Risk | Risk Predicted |
|------|------|--------|----------|----------------|---------------------------|---------------------------|-------------------|
| Joe | High | High | Yes | Good | 0.82 | 0.18 | Good |
| Sue | Low | High | Yes | Good | 0.69 | 0.31 | Good |
| John | Low | High | No | Poor | 0 | 1.0 | Poor |
| Mary | High | Low | Yes | Poor | 0 | 1.0 | Poor |
| Fred | Low | Low | Yes | Poor | 0 | 1.0 | Poor |

| | Joe | Sue | John | Mary | Fred |
|------|-----|-----|------|------|------|
| Joe | 0 | 1 | 2 | 1 | 2 |
| Sue | 1 | 0 | 1 | 2 | 1 |
| John | 2 | 1 | 0 | 3 | 2 |
| Mary | 1 | 2 | 3 | 0 | 1 |
| Fred | 2 | 1 | 2 | 1 | 0 |



- To classify Sam (Debt=High, Income=High, Married = Yes), we find the 3 nearest neighbours to Sam, who are Joe, Sue, and Mary
- The risk values of the neighbours are Good, Good and Poor, which means that Sam is classified as a Good risk

| Name | Debt | Income | Married? | Risk Actual | Probability: Good Risk | Probability: Poor Risk | Risk Predicted |
|------|------|--------|----------|----------------|---------------------------|---------------------------|-------------------|
| Joe | High | High | Yes | Good | 0.82 | 0.18 | Good |
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| John | Low | High | No | Poor | 0 | 1.0 | Poor |
| Mary | High | Low | Yes | Poor | 0 | 1.0 | Poor |
| Fred | Low | Low | Yes | Poor | 0 | 1.0 | Poor |
| | | | | | | | |

| | Joe | Sue | John | Mary | Fred |
|------|-----|-----|------|------|------|
| Joe | 0 | 1 | 2 | 1 | 2 |
| Sue | 1 | 0 | 1 | 2 | 1 |
| John | 2 | 1 | 0 | 3 | 2 |
| Mary | 1 | 2 | 3 | 0 | 1 |
| Fred | 2 | 1 | 2 | 1 | 0 |
| | | | | | |

Issues with k-NN

- Accuracy of prediction depends on the value of k and the choice of distance metric
- Most DM products choose a value of 10 as default for k
- Distance metric needs to be defined by the miner this requires some care
- In datasets that contain numeric data, need to be careful with attributes that are defined on different scale ranges eg *Income* and *Age*
- for nominal data (E.g. in age groupings) need to recognise that distance between pairs of age groupings are not always the same: d((21, 30), (51,60)) > d((21, 30), (41,50))

K-NN - Summary

Pros:

- Easy to use.
- Quick calculation time.
- Does not make assumptions about the data.

Cons:

- Accuracy depends on the quality of the data.
- Must find an optimal k value (number of nearest neighbours).
- Poor at classifying data points in a boundary where they can be classified one way or another.

References

- Chapter 4, Data Mining: Practical Machine Learning Tools and Techniques (3nd edition) / Ian Witten, Eibe Frank; Elsevier, 2011.
- Chapter 4, Introduction to Data Mining / Pang-Ning Tan,
 Michael Steinbach and Vipin Kumar, Pearson Education, Inc,
 2006.
- KNN Algorithm Using Python | How KNN Algorithm Works