K-Nearest Neighbour Classification

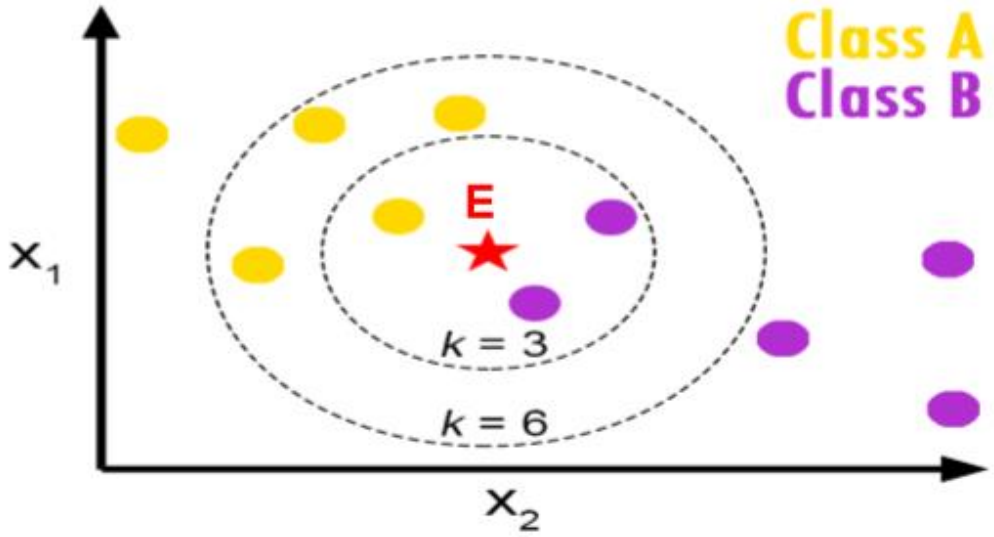
Introduction

- K-nearest neighbor classifier is one of the introductory supervised classifier, which every data science learner should be aware of
- Fix & Hodges proposed K-nearest neighbor classifier algorithm in 1951 for performing pattern classification task
- For simplicity, this classifier is called as KNN Classifier
- K-nearest neighbor classifier mostly represented as KNN, even in many research papers too
- KNN addresses the pattern recognition problems and also the best choices for addressing some of the classification related tasks
- The simple version of the K-nearest neighbor classifier algorithms is to predict the target label by finding the nearest neighbor class
- The closest class will be identified using the distance measures like Euclidean distance

K - Nearest Neighbour Algorithm

To determine the class of a new example E:

- Calculate the distance between E and all examples in the training set
- Select K-nearest examples to E in the training set
- Assign E to the most common class among its K-nearest neighbors



Distance Between Neighbours

$$D(X,Y) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

- “Closeness” is defined in terms of the Euclidean distance between two examples
- The Euclidean distance between X=(x1, x2, x3,…xn) and Y =(y1,y2, y3,…yn) is defined as:

K - Nearest Neighbors: Example

Customer	Age	Income	No. credit cards	Response
Jay	35	35K	3	No
Rina	22	50K	2	Yes
Hema	63	200K	1	No
Tommy	59	170K	1	No
Neil	25	40K	4	Yes
Dravid	37	50K	2	?

K - Nearest Neighbors: Example

Customer	Age	Income	No. credit cards	Response	Distance from Dravid
Jay	35	35K	3	No	$\sqrt{(35-37)^2+(35-50)^2+(3-2)^2} = 15.16$
Rina	22	50K	2	Yes	15
Hema	63	200K	1	No	152.23
Tommy	59	170K	1	No	122
Neil	25	40K	4	Yes	15.74
Dravid	37	50K	2	?	0

Normalizing features

Distance between neighbors could be dominated by some attributes with relatively large numbers (e.g., income in our example)

Important to normalize some features(e.g., map numbers to numbers between 0-1)

Example: Income

Highest income = 200K

Jay's income is normalized to 35/200, Rina income is normalized to 50/200, etc.)

Normalizing features

Normalization of Variables				
Customer	**Age**	**Income**	**No. credit cards**	**Response**
Jay	55/63= 0.175	35/200= 0.175	3/4= 0.75	No
Rina	22/63= 0.34	50/200= 0.25	2/4= 0.5	Yes
Hema	63/63= 1	200/200= 1	1/4= 0.25	No
Tommy	59/63= 0.93	170/200= 0.175	1/4= 0.25	No
Neil	25/63= 0.39	40/200= 0.2	4/4= 1	Yes
Dravid	37/63= 0. 58	50/200= 0.25	2/4= 0.5	Yes

KNN & Nominal attributes

- Distance works naturally with numerical attributes
- d(Jay,Dravid)= $(35-37)2+(35-50)2+(3-2)2$ =**15.16**
- What if we have nominal attributes?

Customer	Married	Income	No. credit cards	Response
Jay	Yes	35K	3	No
Rina	No	50K	2	Yes
Hema	No	200K	1	No
Tommy	Yes	170K	1	No
Neil	No	40K	4	Yes
Dravid	Yes	50K	2	Yes

Non-Numeric Data

- Feature values are not always numbers
- Example
  - Boolean values: Yes or no, presence or absence of an attribute
  - Categories: Colors, educational attainment, gender
- How do these values factor into the computation of distance?

Dealing with Non-Numeric Data

- Boolean values => convert to 0 or 1
  - Applies to yes-no/presence-absence attributes
- Non-binary characterizations
  - Use natural progression when applicable; e.g., educational attainment: GS, HS, College, MS, PHD => 1,2,3,4,5
  - Assign arbitrary numbers but be careful about distances; e.g., color: red, yellow, blue => 1,2,3

Pre-processing Your Dataset

- Dataset may need to be preprocessed to ensure more reliable data mining results
- Conversion of non-numeric data to numeric data
- Calibration of numeric data to reduce effects of disparate ranges
- Particularly when using the Euclidean distance metric

Distance measures

- How to determine similarity between data points
  - –using various distance metrics
- Let x = (x1,…,xn) and y = (y1,…yn) be n-dimensional vectors of data points of objects g1 and g2
  - –g1, g2 can be two different genes in microarray data
  - –n can be the number of samples

Distance measures

- Euclidean distance

$$d(g_1, g_2) = \sum_{i=1}^{n} \left| (x_i - y_i) \right|$$

- Manhattan distance

$$d(g_1, g_2) = \sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}$$

- Minkowski distance

$$d(g_1, g_2) = \sqrt[m]{\sum_{i=1}^{n} (x_i - y_i)^m}$$

Correlation distance

$$r_{xy} = \frac{Cov(X,Y)}{\sqrt{(Var(X) \cdot Var(Y)}}$$

- Correlation distance
  - –Cov(X,Y) stands for covariance of X and Y
    - degree to which two different variables are related
  - –Var(X) stands for variance of X
    - measurement of a sample differ from their mean

Correlation distance

- Variance

$$Var(X) = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \overline{X})^2}{n-1}}$$

- Covariance

$$CoVar(X,Y) = \frac{\sum_{i=1}^{n}(x_i - \overline{X})(y_i - \overline{Y})}{n-1}$$

– Positive covariance
  - two variables vary in the same way

– Negative covariance
  - one variable might increase when the other decreases

– Covariance is only suitable for heterogeneous pairs

Summary of similarity measures

- Using different measures for clustering can yield different clusters
- Euclidean distance and correlation distance are the most common choices of similarity measures for microarray data
- Euclidean vs Correlation Example
  - g1 = (1,2,3,4,5)
  - g2 = (100,200,300,400,500)
  - g3 = (5,4,3,2,1)

–Which genes are similar according to the two different measures?

KNN variations

- Value of k
  - –Larger k increases confidence in prediction
  - –Note that if k is too large, decision may be skewed
- Weighted evaluation of nearest neighbors
  - –Plain majority may unfairly skew decision
  - –Revise algorithm so that closer neighbors have greater “vote weight”

Other measures

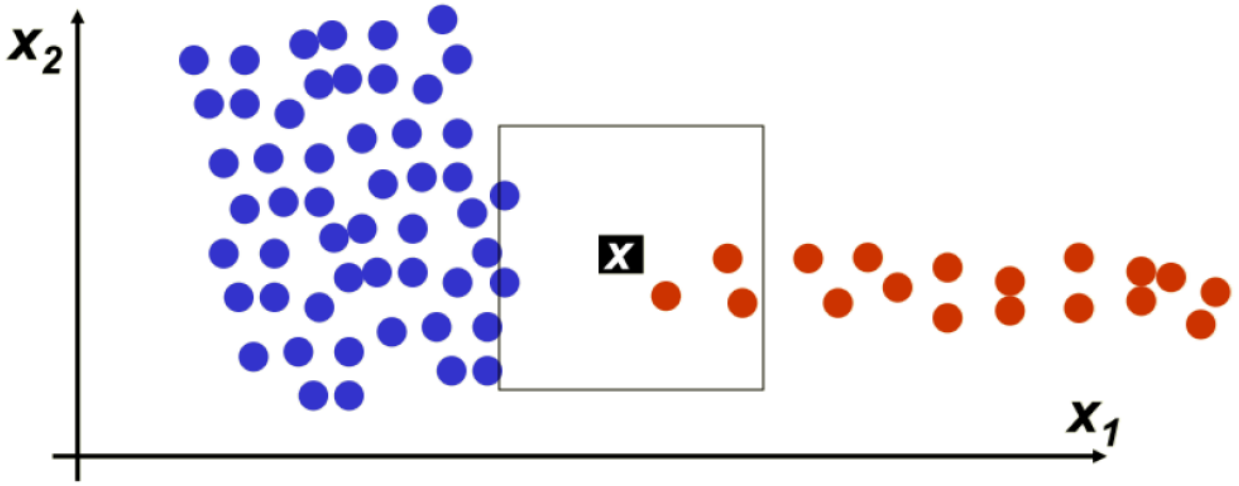
- City-block distance (Manhattan dist)
  - –Add absolute value of differences
- Cosine similarity
  - –Measure angle formed by the two samples (with the origin)
- Jaccard distance
  - –Determine percentage of exact matches between the samples (not including unavailable data)

Distance-Weighted Nearest Neighbour Algorithm

- Assign weights to the neighbors based on their ‘distance’ from the query point
- Weight ‘may’ be inverse square of the distances
- All training points may influence a particular instance

How to Choose ”K”?

- For k = 1, …,5 point x gets classified correctly
  - red class
- For larger k classification of x is wrong
  - blue class



How to Choose ”K”?

- Selecting the value of K in K-nearest neighbor is the most critical problem.
- A small value of K means that noise will have a higher influence on the result i.e., the probability of overfitting is very high.
- A large value of K makes it computationally expensive and defeats the basic idea behind KNN (that points that are near might have similar classes).
- A simple approach to select K is $K=\sqrt{n}$
- It depends on individual cases, at times best process is to run through each possible value of K and test our result

KNN algorithm Pseudo Code

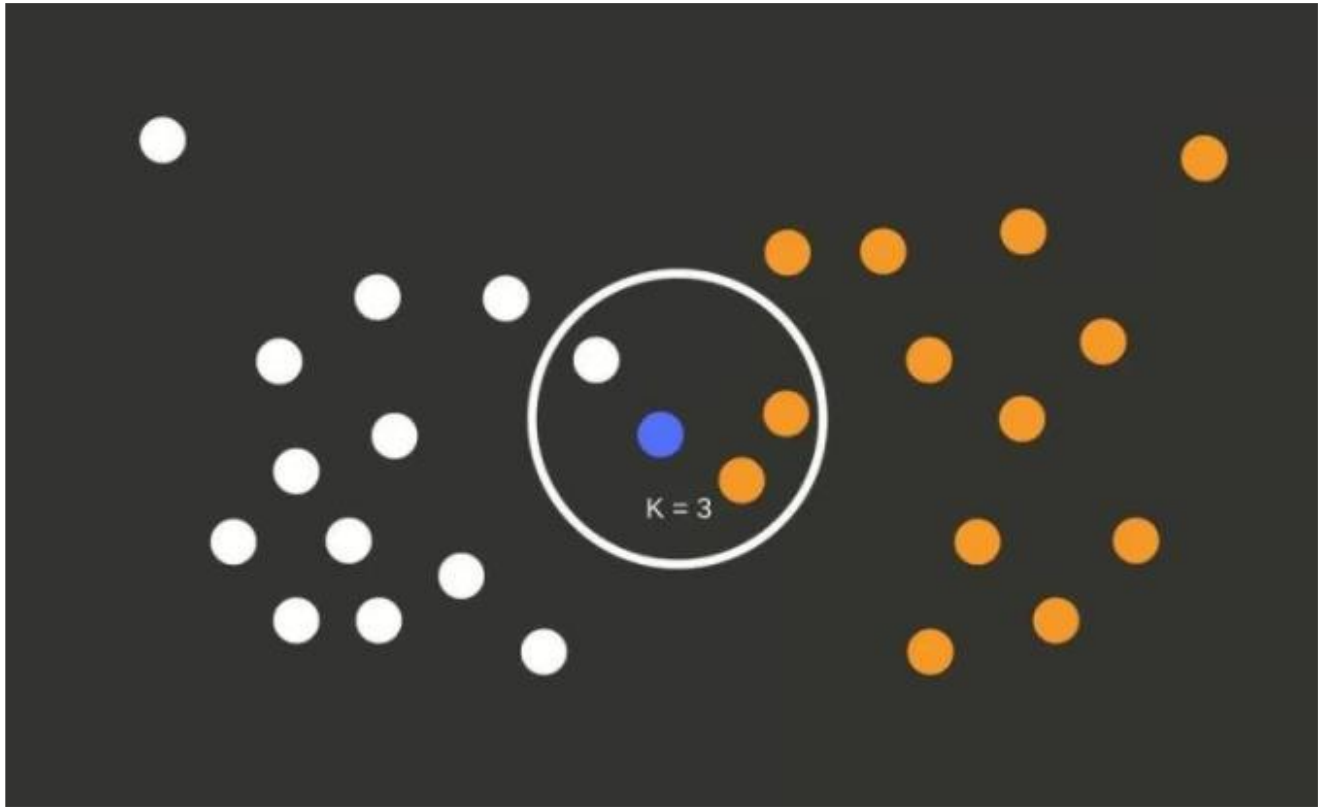
- Let $(Xi,Ci)$where $i=1,2,\cdots,n$be data points. Xidenotes feature values & Cidenotes labels for $Xi$for each i
- Assuming the number of classes as c, $Ci\in\{1,2,3,\cdots,c\}$for all values of i
- Let $x$be a point for which label is not known
- We would like to find the label class using k-nearest neighbor algorithms.

KNN algorithm Pseudo Code

- Calculate $d(x,xi)$, i=1,2,⋯,n;where d denotes the Euclidean distance between the points.
- Let's consider a setup with n training samples, where xi is the training data point.
- The training data points are categorized into c classes.
- Using KNN, we want to predict class for the new data point.
- So, the first step is to calculate the distance(Euclidean) between the new data point and all the training data points.
- Next step is to arrange all the distances in non-decreasing order.
- Assuming a positive value of $k$and filtering $k$least values from the sorted list.
- Now, we have $k$top distances.
- Let kidenotes no. of points belonging to the ith class among $k$points.
- If $ki>kj$for all $i\neq j$then put $x$in class i

KNN algorithm: Example

- Let’s consider the image shown here where we have two different target classes white and orange circles.
- We have total 26 training samples.
- Now we would like to predict the target class for the blue circle
- Considering *k*value as three, we need to calculate the similarity distance using similarity measures like Euclidean distance.
- If the similarity score is less which means the classes are close.
- In the image, we have calculated distance and placed the less distance circles to blue circle inside the Big circle.



Condensed Nearest Neighbor Data Reduction Rule

- Working on a big dataset can be an expensive task.
- Using the condensed nearest neighbor rule, we can clean our data and can sort the important observations out of it.
- This process can reduce the execution time of the machine learning algorithm. But there is a chance of accuracy reduction.
- The steps to condense are to divide data points into the following:
  - Outliers: Observations that lie at an abnormal distance from all the data points. Most of these are extreme values. Removing these observations will increase the accuracy of the model.
  - Prototypes: Minimum points in training set required to recognize non-outlier points.
  - Absorbed points : These are points that are correctly identified to be non-outlier points.

Advantages and Disadvantages

Advantages

- Makes no assumptions about distributions of classes in feature space
- Don’t need any prior knowledge about the structure of data in the training set
- No retraining is required if the new training pattern is added to the existing training set
- Can work for multi-classes simultaneously
- Easy to implement and understand
- Not impacted by outliers
- KNN executes quickly for small training data sets
- Performance asymptotically approaches the performance of the Bayes Classifier

Disadvantages

- Fixing the optimal value of K is a challenge
- Will not be effective when the class distributions overlap
- Does not output any models. Calculates distances for every new point (lazy learner)
- For every test data, the distance should be computed between test data and all the training data. Thus a lot of time may be needed for the testing
- Computationally intensive (O(N^2))

Example in Python

- Iris dataset