K-Nearest Neighbor Classification

Agenda

- KNN Classification Algorithm
- Solving Business Problems using KNN Algorithm
- Hands-on
- Compare Multiple Classification Algorithms

Sample Business Problem

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- Let’s assume a money lending company “XYZ” like UpStart, IndiaLends, etc.
- Money lending XYZ company is interested in making the money lending system comfortable & safe for lenders as well as for borrowers. The company holds a database of customer’s details.
- Using customer’s detailed information from the database, it will calculate a credit score(discrete value) for each customer.
- The calculated credit score helps the company and lenders to understand the credibility of a customer clearly.
- So they can simply take a decision whether they should lend money to a particular customer or not.

Sample Business Problem

- The customer's details could be:
  - Educational background details
    - Highest graduated degree
    - Cumulative grade points average (CGPA) or marks percentage
    - The reputation of the college
    - Consistency in his lower degrees
    - Whether to take the education loan or not
    - Cleared education loan dues
  - Employment details
    - Salary
    - Year of experience
    - Got any onsite opportunities
    - Average job change duration

Sample Business Problem

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- The company(XYZ) use's these kinds of details to calculate credit score of a customer
- The process of calculating the credit score from the customer's details is expensive
- To reduce the cost of predicting credit score, they realized that the customers with similar background details are getting a similar credit score
- So, they decided to use already available data of customers and predict the credit score using it by comparing it with similar data
- These kinds of problems are handled by the K-nearest neighbor classifier for finding the similar kind of customers

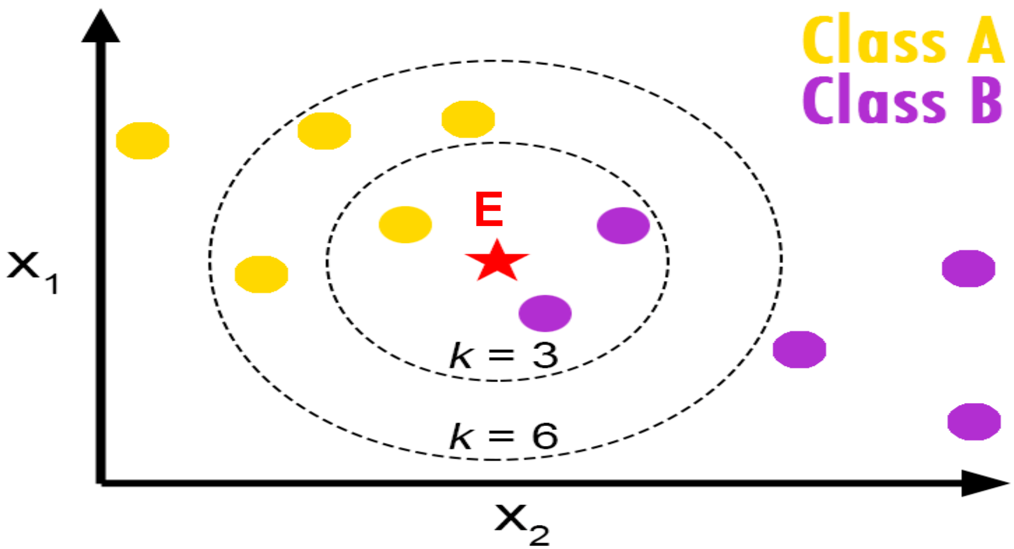
Introduction

- 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 Neighbors

Each example is represented with a set of numerical attributes

Jay:
Age=35
Income=95K
No. of credit cards=3

Rina:
Age=41
Income=215K
No. of credit cards=2

- “Closeness” is defined in terms of the Euclidean distance between two examples

- The Euclidean distance between X=(x_1, x_2, x_3,…x_n) and Y =(y_1,y_2, y_3,…y_n) is defined as:

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

$$\text{Distance (Jay,Rina)} = \sqrt{(35-41)^2+(95{,}000-215{,}000)^2+(3-2)^2}$$

K_Nearest Neighbours: 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 Neighbours: 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

K_Nearest Neighbours

Jay:
Age=35
Income=95K
No. of credit cards=3

Rina:
Age=41
Income=215K
No. of credit cards=2

Distance (Jay, Rina)=sqrt $[(35-45)^2 + \mathbf{(95{,}000-215{,}000)^2} + (3-2)^2]$

- 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 = 500K
  Davis's income is normalized to 95/500, Rina income is normalized to 215/500, etc.)

K_Nearest Neighbours

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

K-Nearest Neighbor

- Distance works naturally with numerical attributes
  d(Rina,Johm)= $\sqrt{(35-37)^2+(35-50)^2+(3-2)^2}$ =**15.16**
- What if we have nominal attributes?

<u>Example</u>: Married

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-Neumeric 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
- How about unavailable data?
  (0 value not always the answer)

Preprocessing 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 measure

- Euclidean distance

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

- Manhattan distance

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

- Minkowski distance

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

Correlation distance

- Correlation distance

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

  – 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

Correlation distance

- Correlation

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

  - maximum value of 1 if X and Y are perfectly correlated
  - minimum value of 0 if X and Y are exactly opposite
  - $d(X,Y) = (1 + r_{xy})/2$

Cosine distance

- Cosine distance
  - Used in document comparison

$$-\cos(\theta) = \frac{X^T Y}{\|X\| \|Y\|}$$

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?

k-NN 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 distance measures

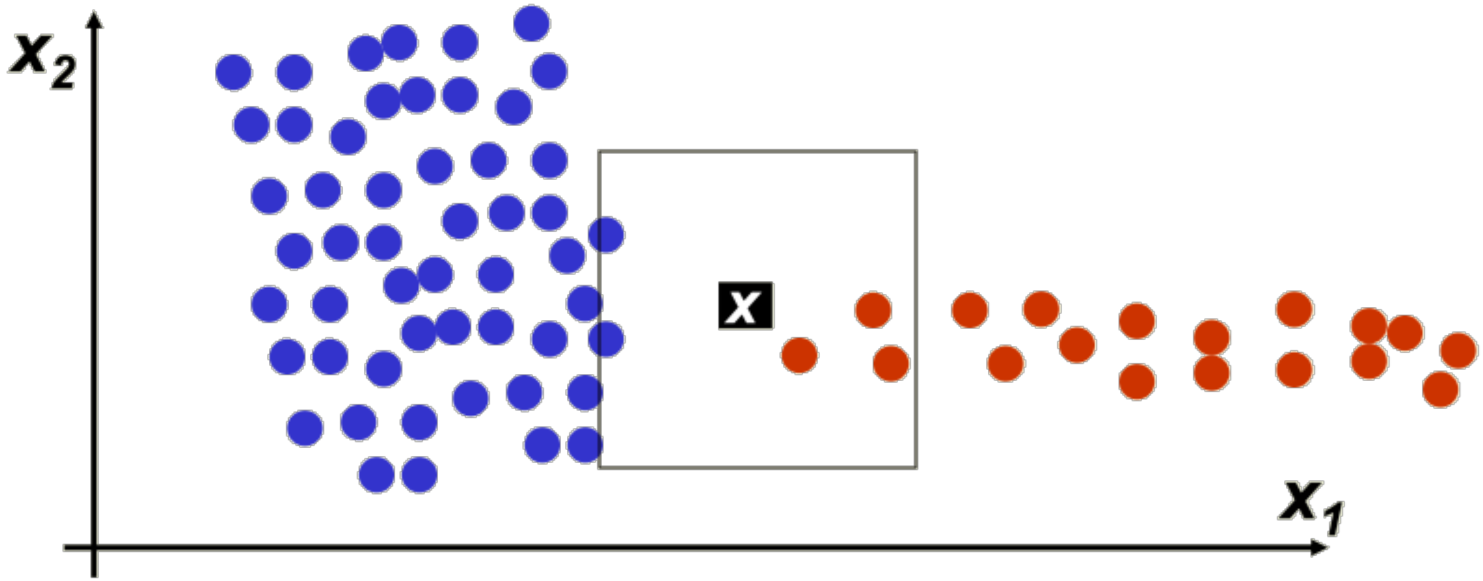
Other Distance Measures

- 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)
- Others

Distance-Weighted Nearest Neighbor 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 (X_i, C_i) where $i = 1,2,\cdots,n$ be data points. X_i denotes feature values & C_i denotes labels for X_i for each i
- Assuming the number of classes as c, $C_i \in \{1,2,3,\cdots,c\}$ 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 $d(x, x_i)$, $i = 1,2, \cdots, n$; where d denotes the Euclidean distance between the points.
- Let's consider a setup with n training samples, where x_i 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 k_i denotes no. of points belonging to the i^{th} class among k points.
- If $k_i > k_j$ for all $i \neq j$ then put x in class i

KNN algorithm: Example

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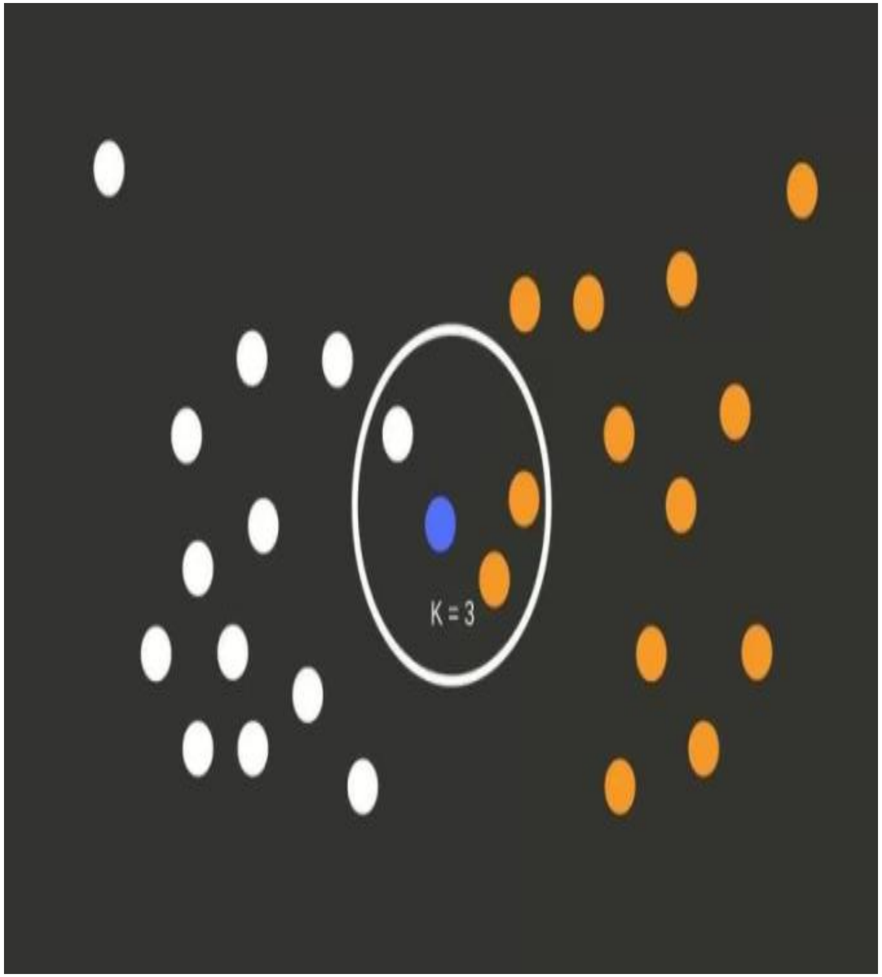
- Let’s consider the image shown here where we have two different target classes white and orange circles.
- We have total 26 training samples.
- Now we would like to predict the target class for the blue circle
- Considering k value as three, we need to calculate the similarity distance using similarity 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.

Nearest Neighbor Algorithm

- Nearest neighbor is a special case of k-nearest neighbor class.
- In this case k value is 1 ($k = 1$).
- In this case, new data point target class will be assigned to the 1^{st} closest neighbor

Radius Neighbor Algorithm

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- KNN classifier is also considered to be an instance based learning / non-generalizing algorithm.
- It stores records of training data in a multidimensional space.
- For each new sample & particular value of K, it recalculates Euclidean distances and predicts the target class
- So, it does not create a generalized internal model
- Similar to KNN classifier, we can use Radius Neighbor Classifier for classification tasks.
- As in KNN classifier, we specify the value of K, similarly, in Radius neighbour classifier the value of R should be defined.
- The RNC classifier determines the target class based on the number of neighbors within a fixed radius, r, for each training data point.

Radius Neighbor Algorithm

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- Measuring similarity with distance between the points using Euclidian method
- Other distance measurement methods include Manhattan distance, Minkowski distance, Mahalanobis distance, Bhattacharya distance etc.
- Scikit-learn implements two different nearest neighbors classifiers:
  - K Nearest Neighbor Classifier
  - Radius Neighbor Classifier
- Radius Neighbor Classifier implements learning based on number of neighbors within a fixed radius ‘r’ of each training point, where ‘r’ is a floating point value specified by the user
- Determining the optimal K is the challenge in K Nearest Neighbor classifiers. In general, larger value of K supresses impact of noise but prone to majority class dominating
- Radius Neighbor Classifier may be a better choice when the sampling is not uniform. However, when there are many attributes and data is sparse, this method becomes ineffective due to curse of dimensionality

Advantages and Disadvantages

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- 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))


Demo Using Python

Sample Code in Python

```
X = [[0], [1], [2], [3]]
y = [0, 0, 1, 1]
from sklearn.neighbors import KNeighborsClassifier
neigh = KNeighborsClassifier(n_neighbors=3)
neigh.fit(X, y) KNeighborsClassifier(...)
(neigh.predict([[1.1]])) [0]

(neigh.predict_proba([[0.9]])) [[ 0.66666667 0.33333333]]
```

Summary

- KNN classification algorithm
  - Different distance measures
  - KNN algorithm
  - Advantages and disadvantages
- Case study 1 (using KNN)
- Hands-on 1
- Case study 2 (comparing KNN with other classification methods)
- Hands-on 2

Thanks!