Advanced kNN: A Mature Machine Learning Series

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Abstract

k-nearest neighbour (kNN) is one of the most prominent, simple and basic algorithm used in machine learning and data mining. However, kNN has limited prediction ability, i.e., kNN cannot predict any instance correctly if it does not belong to any of the predefined classes in the training data set. The purpose of this paper is to suggest an Advanced kNN (A-kNN) algorithm that will be able to classify an instance as unknown, after verifying that it does not belong to any of the predefined classes. Performance of kNN and A-kNN is compared on three different data sets namely iris plant data set, BUPA liver disorder data set, and Alpha Beta detection data set. Results of A-kNN are significantly accurate for detecting unknown instances.

Keywords: kNN, Machine Learning.

1. Introduction

k-nearest neighbour is among the top 10 classification algorithms as described by [1], [2], and [3] used in KDD\textsuperscript{1} and data mining. kNN algorithm is a simple but effective non-parametric classification method [4]. The principle behind Nearest Neighbour Classification is quite elementary. The instances are categorized based on the class of their nearest neighbours. It is often useful to take more than one neighbours into account so the technique is more commonly referred as k-Nearest Neighbour classification where k nearest neighbours are utilized in determining the class [5]. It is called a lazy learner, as it performs classification tasks without building its model [6].

\textsuperscript{1}KDD: Knowledge Discovery in Databases (KDD) is the process of discovering useful knowledge from a collection of data.
Model-based classifiers are those which builds a model and learns from given and existing training data set. Then using that model its accuracy is tested with test data set. The same model is used to predict the label of new instances. Unlike these model-based classifiers, kNN keeps all previous examples in memory. So for new prediction, kNN finds k nearest instances and decides class of new instance to be the class same as of neighbors. Imbalanced data set also has some impacts on classifier performance. kNN is a type of supervised machine learning (ML) algorithm which can be used for both classification as well as regression predictive problems. However, it is mainly used for classification. The main purpose of kNN is to estimate the classification of an unseen instance using the class label of the instance or instances that are nearest to it.

Besides various improvements over the years in kNN, it still has limited capacity of prediction. kNN cannot predict any instance correctly if it does not belong to any of the predefined classes in the training data set. As an example, if kNN is trained with a data set of patients who are either healthy or suffering from cancer, and in test set there is a patient of diabetes. The traditional kNN algorithm will classify that diabetes patient as a healthy or a cancer patient as it has only two options, while both the options are wrong.

To overcome this issue, Advanced kNN (A-kNN) will identify it as an unknown instance and will inform the domain expert about it. Domain expert will guide the algorithm on this instance, whether to add it as separate class to training set or classify it as one of the predefined classes. In this way, by employing concepts of Training Class Area, Area of class and Gap Constant, A-kNN will be quite mature to identify unknown instances without requiring any predefined data in the training set. All these concepts are explored in coming sections.

Section 2 will cover related work with respect to improvement in kNN algorithm. We introduce our Advanced kNN algorithm in section 3. Section 4 will cover the experiments and results and in the last section we will discuss the conclusion and directions for future research.

\footnote{In this paper, label and class is used interchangeably.}

\footnote{Data set having different number of instances in positive and negative class.}
2. Related work

kNN methodology is still a hot topic for research in machine learning and data mining despite the fact that the algorithm was first proposed in 1967. The kNN rule as described by Devijver and Kittler, has been widely used since it is effective, when probability distributions of the feature variables are not known [8]. Various researchers have proposed various methods to improve this algorithm. Hart proposed a computationally simple local search method as Condensed Nearest Neighbour (CNN) by minimizing the number of stored patterns and storing only a subset of the training set for classification [9]. The basic idea is that patterns in the training set may be very similar and many of the instances do not add extra information and thus may be discarded. Gates proposed the Reduced Nearest Neighbour (RNN) rule that aims to further reduce the stored subset after having applied CNN [10]. It simply removes those elements from the subset which will not cause an error.

Li et al. suggested an improved kNN algorithm for text categorization. Their main focus is on the selection of the parameter k. In traditional kNN algorithms, the value of k is already fixed. If k is very large, then the big classes will overcome the small ones. Practically, the value of k is usually optimized by running various trials on the training and validation sets. However, this method is not suitable in those cases where there is no option to perform cross-validation, like in online classification. To tackle this problem, they proposed a revised k-Nearest Neighbor algorithm, which employs various values of k for various classes, rather than a fixed k value [11]. Zhang et al. proposed a computation method for k-parameter for the purpose of kNN approximate prediction based on Sparse learning [12], known as S-kNN [2]. Their proposed S-KNN algorithm works out an optimized value of k for each and every test sample. This implies that the value of k can be different for various test samples. Similarly Zhang et al. put forward a new kNN method to learn different values of k for different instances of test data by following the distribution of training data. They named it as Correlation Matrix kNN (CM-kNN) [13]. This method involves usage of previous knowledge inherent in training data, including the correlation among data points, the removal of noisy data, and preserving the local structures of the data.

Liu et al. also proposed a new method unlike traditional kNN methods and named it Mutual Nearest Neighbours (MNN) [14]. It makes use of the concept of mutual nearest neighbor of the unknown instance to determine its label. To approximate the label of that instance, MNN first identifies
its mutual nearest neighbors and then goes on to make a decision. Their claim is that the predicted label is more creditable as it is derived from the intimate neighbors. Moreover, some outliers will also be left out. Toyama et. al, by utilizing the marginal distribution of kth nearest neighbors in low dimensions, put forward a probably correct approach of kNN, which is a probabilistic modification of the partial distance searching [15]. Guo et. al formalized a method which he called MkNN to automatically determine a proper value of k for different datasets. It is quite similar to the cross-validation technique. MkNN firstly develops a kNN model for the data, and then chooses an optimal value of k on the basis of its classification accuracy [16].

3. Advanced kNN

Before going through A-kNN, we will first sift through the original kNN algorithm.

3.1. kNN Algorithm

The following steps depict the working of kNN algorithm[17]:

1. Collect training data set.
2. Set integer value of k.
3. To predict label of new instance/point,
   3.1 Calculate the distance between new instance and all instances of training data set.
   3.2 Sort list of distances in ascending order.
   3.3 Select only top k (lowest) distances and their class labels.
   3.4 Class of the new instance will be the most frequent class of top k selected instances.
4. End.

3.2. Improvement in traditional kNN

Till now, the bulk of research on kNN has been revolving around two areas. One is to select the best value of k, and the other is to select distance calculating method. Commonly used values of k are 1, 3, 5, 7, and so on. While the most used methods for distance calculation are following:
1. Euclidean Distance:

\[ d(\text{Euclidean}) = \sqrt{\sum_{i=1}^{k} (x_i - y_i)^2} \]  \hspace{1cm} (1)

2. Manhattan Distance:

\[ d(\text{Manhattan}) = \sum_{i=1}^{k} |x_i - y_i| \]  \hspace{1cm} (2)

3. Minkowski Distance:

\[ d(\text{Minkowski}) = \left( \sum_{i=1}^{k} (|x_i - y_i|)^q \right)^{\frac{1}{q}} \]  \hspace{1cm} (3)

3.3. Advanced kNN

As mentioned previously, our Advanced kNN will make use of a Training Class Area (TCA), Area of Class and Gap Constant to classify whether an instance belongs to some unknown class or not. Following steps show the working of Advanced kNN algorithm:

1. Collect training data set.
2. Set integer value of k.
3. Define TCA i.e., the training class area of each class (will be explained next).
4. To predict label of new instance/point,
   4.1 Calculate the distance between new instance and all instances of training data set.
   4.2 Sort list of distances in ascending order.
   4.3 Select only top k distances and their class labels. Smallest distances is called \textit{min\_dist}.
   4.4 Find most frequently occurring class in the list of top k instances called \textit{expected class}.
      \hspace{1cm} \textbf{if.} (\textit{min\_dist} > area of expected class)
      \hspace{1cm} then. Class of new instance is \textit{unknown}.
      \hspace{1cm} else. Class of new instance is label of expected class.
5. End.
3.3.1. Defining Area of a class

Defining an area for a class has no specific rules or an equation as it is a new area of research in A-kNN. Basically defining area of class majorly depends on the nature of the data. In this research we defined the area as given below:

1. Select one of the above distance calculation formula.
2. Using that formula calculate distance of all instances in the training set with each other.
3. Sort it in descending order and select maximum distance.
4. This distance will be called Training Class Area (TCA).
5. Using this TCA, domain expert will decide boundary of a class based on the nature of whole data. If classes are closer to each other, boundary will be narrow about 1.5 times of TCA or 2 times of TCA. As the distance among classes increases, gap can be widened and area of class can be decided to be about gc times of TCA, where gc is called Gap constant. Area of class can be more widened or tied nearer, depending upon the nature of data.

Table 1: Data set for analysis

| Employ | Salary($) | Scale | Original Title | Assigned Label |
|--------|-----------|-------|----------------|---------------|
| E1     | 581       | 17    | Gazetted       | G             |
| E2     | 710       | 18    | Gazetted       | G             |
| E3     | 370       | 15    | Non-Gazetted   | N             |
| E4     | 413       | 16    | Non-Gazetted   | N             |
| E5     | 329       | 16    | Non-Gazetted   | ?             |
| E6     | 626       | 18    | Gazetted       | ?             |
| E7     | 129       | 4     | Class-4        | ?             |
| E8     | 968       | 21    | Bureaucrat     | ?             |

Before moving on to broader experimentation, we have a dataset of simple eight points given in table [1] and visualized in figure [1]. Salary (in $) and employee scale are the two features which will be used to predict the title or label [4] of employee. Scale 15, and 16 represent non gazetted officers while

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[4] Here the words ‘title’ and ‘label’ are used in the same sense, title of last two employees

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scale 17 and 18 are called gazetted officers. Data of first four 
employs \( E1 - E4 \) is used for training. While label of next 
four \( E5 - E8 \) is to be predicted. So using simple 
kNN and setting \( k=1 \) prediction of \( E5 \) and \( E6 \) is very 
easy and obvious. \( E5 \) will be predicted as Non-gazetted (N), while 
label of \( E6 \) will be predicted as gazetted (G). \( E7 \) and \( E8 \) are the points 
of our interest. As the actual title of \( E7 \) is \textit{Class-4} while that of \( E8 \) is 
\textit{Bureaucrat}. However, there is no data of both of these titles in 
our training set. So according to kNN, 
\( E7 \) is near to Non-gazetted officer while \( E8 \) is near to gazetted officer. So 
kNN will classify \( E7 \) as N, while \( E8 \) as G, which are actually wrong. What 
will A-kNN do in this case? If there is point somewhere outside from the 
regions of already available classes in training data set, it will be classified as 
an unknown category. So a domain expert will be notified to guide A-kNN 
for this point.

In figure 1, the main area of interest in previous literature is the bold lined 
rectangle. To decide whether the instances in the area of bold rectangle will 
belong to G class or N. Here in this research we are interested in the instance 
beyond this area, which lies very far from all previous class like \( E7 \) and \( E8 \). 
Distance between \( E1 \) and \( E2 \) is marked as TCA for Gazetted class, while 
distance between \( E3 \) and \( E4 \) is marked as TCA for Non-gazetted class. Area 
of both classes is encircled.

Using euclidean distance on the data set in table 1, TCA of G class is 
129, while TCA of N class is 43. Value of gap constant is set to be 1.5. 
So area of G class is 193.5 while area of N class is calculated to be 64.37. 
Setting \( k = 1 \), \( E5 \) is very closed to \( E3 \). Euclidean distance between these two 
instances is 41 which is minimum, and lower than the area of N class (64.37), 
so obviously it will be classified as N. Similarly euclidean between \( E6 \) and \( E1 \) 
is 45.01 which is minimum and lower than area of G class (193.5), so its label 
will be predicted as G. On the other hand \( E7 \) is nearest to \( E3 \), but euclidean 
distance between \( E7 \) and \( E3 \) is 241.25 which very very greater than area of 
N class (64.37). It means that \( E7 \) is very very far from all the classes and 
will be classified as unknown class. So domain expert should be notified to 
guide the machine on this instance. Now it is in the hands of domain expert 
whether he classifies and add this instance to nearest class (Non-gazetted) 
or labels it as a new class (class-4), and retrain the machine. Similarly \( E8 \) is 
nearest to \( E2 \), their euclidean distance is 258 >> 193.5 (area of G class). So

\[ \text{is just for ease of the reader.} \]
domain expert will be requested for guidance on this instance too.

Figure 1: Data points

3.3.2. Impact of Gap Constant

Figure 2 depicts the impact of gap constant on area of class. Initially the training class only contains blue points (A, B, C, D, E, F and G). Maximum distance of this class is between point D and point F, so circle of diameter equal to maximum distance (i.e. inner circle) is TCA. When gc=1, all the points except blue are out of this class. For gc=2, area of class expands and black points (i.e. H and I) also become members of this class. J may get membership of this class by expanding area of class more to circle e with gc=3. Points N and O are even not members of this class with gc=5. So as we increase the gc, area of the class increases, and far more points will be classified as a members of this class.
4. Experiments and Results

We have carried out experiments to evaluate the performance of A-kNN in comparison with the traditional kNN algorithm. Experiments have been performed on data sets downloaded from UCI repository. The details of data sets are given in Table 2. Both A-kNN and traditional kNN have been implemented in Python.

4.1. Experimental procedure

Data sets are split into training and testing set in ratio of 70:30. Both A-kNN and traditional kNN are trained on the training set. Performances of both algorithms are evaluated in two ways. First both are evaluated using original test set, which means all the data in the test set belongs to one of the class and no unknown (very far from seen class) data is fed. In this case the performances of both A-kNN and traditional kNN is comparable. Now, instances of unknown data are added to the test set. These instances are very far from all previous classes, which means all these instances must not belong to any of the previous class and the algorithm should indicate them.
Table 2: Data sets details

| Data set Title            | Number of Instances | Number of Attributes | Number of Classes | Class Names                |
|---------------------------|---------------------|----------------------|-------------------|---------------------------|
| Iris Plants Database      | 150                 | 4                    | 3                 | Setosa, Versicolour, Virginica |
| BUPA liver disorders      | 345                 | 6                    | 2                 | 1, 2                      |
| Alpha Beta Detection      | 199                 | 2                    | 2                 | 0, 1                      |

as unknown instances. So that the domain expert may take necessary steps about this data. Here the importance of A-kNN will be highlighted. Because traditional kNN will not be able to indicate unknown data, but it will classify these instances as one of the previous classes, based on nearest neighbors.

4.2. Experiments on Iris Plants Data Set

Details of iris plants database is given in table 2. Total instances in iris data set are 150. By keeping 70:30 ratio, number of instances in training set is 105 while number of instances in original test set becomes 45. Number of unknown instances is 20. For k=1, 7 and using the test set without unknown instances, the results of KNN and A-KNN comes out to be similar. However, with unknown instances, it can be seen that results are highly different. KNN misclassified all of the unknown instances as one of the predefined class in training set. Whereas A-KNN discriminates unknown and known instances, and clearly identifies very far instances as unknown instances. Further A-KNN is strongly dependent on the value of gap constant. As the value of gap constant increases, area of class becomes widen. When any of the instances gets into the area of any class, it is classified as that class. With a gap constant of 1000, A-KNN miss-classifies 18 unknown instances too.

4.3. Experiments on BUPA Liver Disorders Data Set

In this particular data set, the total number of instances we have is 345. The total number of attributes are 6 while the target classes are two namely 1 in case of a liver disorder and 2 in case of absence. When it is divided in
Table 3: Results of Iris data set with kNN and A-kNN

| K   | gc | Accuracy                  | Misclassified unknown instances (out of 20) |
|-----|----|---------------------------|---------------------------------------------|
|     |    | Without unknown instances | With unknown instances                      | Total | classified as label setosa | classified as label versicolor | classified as label virginica |
| 1   | KNN- | 0.98                      | 0.68                                        | 20    | 4                           | 0                             | 16                     |
| 1   | AKNN | 1.00                       | 1.00                                        | 0     | 0                           | 0                             | 0                      |
| 1   | AKNN | 1.50                       | 1.00                                        | 0     | 0                           | 0                             | 0                      |
| 1   | AKNN | 2.00                       | 0.98                                        | 1     | 1                           | 0                             | 0                      |
| 1   | AKNN | 5.00                       | 0.94                                        | 4     | 4                           | 0                             | 0                      |
| 1   | AKNN | 10.00                      | 0.92                                        | 5     | 4                           | 0                             | 1                      |
| 1   | AKNN | 100.00                     | 0.75                                        | 16    | 6                           | 0                             | 10                     |
| 1   | AKNN | 1000.00                    | 0.72                                        | 18    | 6                           | 0                             | 12                     |
| 7   | KNN- | 0.98                       | 0.68                                        | 20    | 4                           | 0                             | 16                     |
| 7   | AKNN | 1.00                       | 0.97                                        | 0     | 0                           | 0                             | 1                      |
| 7   | AKNN | 1.50                       | 0.97                                        | 0     | 0                           | 0                             | 1                      |
| 7   | AKNN | 2.00                       | 0.95                                        | 1     | 1                           | 0                             | 1                      |
| 7   | AKNN | 5.00                       | 0.91                                        | 5     | 4                           | 0                             | 1                      |
| 7   | AKNN | 10.00                      | 0.89                                        | 6     | 4                           | 0                             | 2                      |
| 7   | AKNN | 100.00                     | 0.74                                        | 16    | 6                           | 0                             | 10                     |
| 7   | AKNN | 1000.00                    | 0.71                                        | 18    | 6                           | 0                             | 12                     |

the ratio of 70:30, the training set comes out to be of 241 and testing set to be 104. The results are shown in table 4. Unknown instances here are again 20 in number. For k=1 and 7, KNN shows almost dismal results both with and without unknown instances. On the contrary, A-KNN with k=1 outperforms KNN with k=1 & 7, and A-KNN with k=7. It can be seen that for A-KNN with both k=1 and 7, the number of misclassified instances rise when the value of gap constant is increased beyond 2.

4.4. Experiments on Alpha Beta Detection Data Set

This data set contains a total of 199 instances. Keeping training and testing ratio 70:30, the number of instances in training set are 139 while 60 are in test set. Similar to the previous experiments, 20 unknown instances have been kept here again. The results exhibit that 100% accuracy is achieved by both KNN and A-KNN employing k=1 and 7 when there are no unknown instances. With the introduction of unknown instances, the accuracy of KNN dips down by 25%, while that of A-KNN by a mere 7.5% when the gap constant is kept till 2. As also shown in our previous experimentations, the number of misclassified instances start increasing when we move the gap constant above 2.
### Table 4: Results of BUPA Liver Disorders Data Set with kNN and A-kNN

| K | gc | Accuracy | Misclassified unknown instances (out of 20) |
|---|----|----------|---------------------------------------------|
|   |    | Without unknown instances | With unknown instances | Total | classified as label 1 | classified as label 2 |
| 1 | KNN | - | 0.57 | 0.48 | 20 | 1 | 19 |
| 1 | AKNN | 1 | 1 | 1 | 0 | 0 | 0 |
| 1 | AKNN | 1.5 | 1 | 0.99 | 1 | 0 | 1 |
| 1 | AKNN | 2 | 1 | 0.99 | 1 | 0 | 1 |
| 1 | AKNN | 5 | 1 | 0.90 | 12 | 1 | 11 |
| 1 | AKNN | 10 | 1 | 0.86 | 17 | 2 | 15 |
| 1 | AKNN | 100 | 1 | 0.83 | 20 | 4 | 16 |
| 1 | AKNN | 1000 | 1 | 0.83 | 20 | 4 | 16 |
| 7 | KNN | - | 0.61 | 0.51 | 20 | 2 | 18 |
| 7 | AKNN | 1 | 0.73 | 0.77 | 0 | 0 | 0 |
| 7 | AKNN | 1.5 | 0.73 | 0.76 | 1 | 0 | 1 |
| 7 | AKNN | 2 | 0.73 | 0.76 | 1 | 0 | 1 |
| 7 | AKNN | 5 | 0.73 | 0.67 | 12 | 1 | 11 |
| 7 | AKNN | 10 | 0.73 | 0.66 | 17 | 2 | 15 |
| 7 | AKNN | 100 | 0.73 | 0.61 | 20 | 2 | 18 |
| 7 | AKNN | 1000 | 0.73 | 0.61 | 20 | 2 | 18 |

### Table 5: Results of Alpha Beta Detection data set with kNN and A-kNN

| K | gc | Accuracy | Misclassified unknown instances (out of 20) |
|---|----|----------|---------------------------------------------|
|   |    | Without unknown instances | With unknown instances | Total | classified as label 0 | classified as label 1 |
| 1 | KNN | - | 1 | 0.75 | 20 | 14 | 6 |
| 1 | AKNN | 1 | 1 | 0.925 | 6 | 3 | 3 |
| 1 | AKNN | 1.5 | 1 | 0.925 | 6 | 3 | 3 |
| 1 | AKNN | 2 | 1 | 0.925 | 6 | 3 | 3 |
| 1 | AKNN | 5 | 1 | 0.89 | 9 | 5 | 4 |
| 1 | AKNN | 10 | 1 | 0.85 | 13 | 5 | 8 |
| 1 | AKNN | 100 | 1 | 0.75 | 20 | 12 | 8 |
| 1 | AKNN | 1000 | 1 | 0.75 | 20 | 12 | 8 |
| 7 | KNN | - | 1 | 0.75 | 20 | 14 | 6 |
| 7 | AKNN | 1 | 1 | 0.925 | 6 | 3 | 3 |
| 7 | AKNN | 1.5 | 1 | 0.925 | 6 | 3 | 3 |
| 7 | AKNN | 2 | 1 | 0.925 | 6 | 3 | 3 |
| 7 | AKNN | 5 | 1 | 0.887 | 9 | 5 | 4 |
| 7 | AKNN | 10 | 1 | 0.887 | 13 | 5 | 8 |
| 7 | AKNN | 100 | 1 | 0.75 | 20 | 12 | 8 |
| 7 | AKNN | 1000 | 1 | 0.75 | 20 | 12 | 8 |
5. Conclusions and Future Work

The presented results of our experiments clearly demonstrate the utility of our Advanced-KNN algorithm over the traditional KNN when dealing with instances that cannot be categorised under any of the prescribed classes. By varying the gap constant which is linked with the area of class and making use of two values of $k$, we have observed various scenarios where the unknown instances being categorised under an unknown class. It is also depicted that when the gap constant is increased above 2, the amount of misclassified unknown instances start increasing. We in our study have striven to offer a new avenue of research. For the days to come, calculating an optimal value of the gap constant (area of the class) for more accurate classifications, is one area which can be researched.
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