Newly Proposed k-NN Method for More Efficient Classification

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Abstract: The purpose of this paper is to examine a new classification algorithm based on the well-known k nearest neighbors technique that achieves better efficiency in terms of accuracy, precision and time when classifying test observations in comparison to classic k nearest neighbors. The proposed methodology splits the input dataset into n folds containing all observations. Each record is allocated to one of the folds. One of the folds is saved for testing purposes and the rest of the folds are used for training. The process is executed n times. The pair of train/test subsets which produces the highest accuracy result is selected as final model for the respective input data. 18 different datasets are used for experiments. For each dataset, the classic k-NN is compared to the proposed method (MK-NN) using accuracy, F1 score and execution time as metrics. The proposed approach achieves better results than classic k-NN according to all used metrics. Based on experiments with validation subsets, evidence of overfitting was not found. This paper suggests a novel method for improvement in accuracy, precision, recall and time when classifying test observations from a dataset. The approach is based on the concept of k nearest neighbors. However, what separates it from classic k nearest neighbors is that it tries to find train and test subsets of the original dataset that best represent the input dataset using the k-fold method.

Keywords: Classification problems, k Nearest Neighbors, Machine Learning Algorithms

I. INTRODUCTION

In the realm of machine learning, specifically classification problems, one of the most popular [17] and long-standing techniques is k Nearest Neighbors (k-NN). The method has been around since 1967 [5] and since then has gained considerable popularity in both application and research fields. In a nutshell, the technique selects a class for a new observation by finding its k nearest neighbors whose class is known. The nearest neighbors are determined on the basis of their distance (Euclidean, Manhattan or another) to the new data point. Although it is used primarily for solving classification problems, it is not uncommon for k-NN to be applied in pattern recognition, text categorization, object recognition and etc. [15]. The idea of k-NN is applicable to a wide range of problems – business, medicine, media and others. Classic k-NN can be applied in customer relations processes by filtering potential buyers of a specific product or service more efficiently, as it can classify them as either buyers or non-buyers [1]. Spatial database is another area where k-NN techniques have an important application. From simply using k-NN to find nearest target points to a query point, to accommodating road networks, obstacles and etc. along with k-NN for more accurate distance evaluations [19]. Social media has become very powerful source of users’ data for marketing departments. Knowing as much as possible for your current customers and having effective process for targeting new ones is a key component for the success of many companies. Even though, specific user characteristics (gender, age, marital status and similar) are usually not available publicly, careful selection of appropriate features and inferencing with the help of classifiers, like k-NN, can produce promising predictions for both age and gender, as concluded by a case study on Korean Facebook users [4]. In the area of software quality, missing data can create serious obstacles when analyzing or modeling a dataset. Imputing the missing data with the help of k-NN has proven to be an adequate alternative solution [13]. In the field of medicine, an active learning method using fuzzy k-NN has been applied to classify cancer type from microarray gene expression datasets [11]. Human emotions are often unpredictable and pose a challenge for machine learning problems. In a study for emotion recognition, six men aged 26-50 were asked to simulate 6 common facial expressions. Muscle movements were recorded and thanks to the data, the scientists managed to build a model for classifying facial expressions using k-NN [20]. Many modifications of the classic k-NN algorithm have been proposed since its initial introduction and continue to be proposed to present day, proving its relevance and robustness. Researches are driven most often either by specific case studies or further developments of the algorithm. Weighted k Nearest Neighbor (WkNN) assigns different weights to the k neighbors based on their distance to the test point which makes use of training observations [6]. Similar to WkNN, the Modified k Nearest Neighbor also uses weights, but in addition it also looks for the validity of the data point when classifying nearest neighbor [18]. Reduced Nearest Neighbor ignores redundant patterns in the training phase of the classification [8]. Model based k nearest neighbor models the input data and uses the model to classify the data. This modification strives to achieve both improved accuracy and more efficient execution time, while also automatically chooses appropriate value for k [10]. Another modification based on the classic k-NN that tries to improve accuracy without sacrificing cost in time is Rank Nearest Neighbor (rRNN). It suggests assigning ranks to training data for each category [3]. A suggested approach for improving accuracy results of classifiers (including k-NN) is creating synthetic attributes which can be utilized in the modeling stage. Synthetic attributes can be created using other different features and data on subjects [2]. Image classification accuracy using k-NN based algorithm is proposed to be increased with Nearest Feature Line Neighbor (NFL) which takes advantage of multiple templates per class [16].
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approach, aimed specifically at text recognition, proposes the training sample sets to be clustered with the help of k-means and then use the cluster centers as the actual training samples [22].

Although k-NN is very popular machine learning technique for classification problems, it doesn’t always produce satisfactory results in terms of efficiency, thus leaves room for improvement in this aspect. Especially, in fields like medicine, accuracy is of crucial importance as poor scores may have severe consequences. A key step in the modelling process is the split of the dataset to train and test. Herein, we propose a new algorithm for applying the concept of k-NN, which we call Mk-NN. By searching for the pair of train and test subset which best represents a given dataset, we try to achieve significant improvement in the accuracy results when classifying new observations. Furthermore, the concept of the proposed algorithm implies it would affect positively accuracy, specificity and sensitivity scores regardless of the nature of the input dataset which makes it applicable to wide range of business.

One of the most popular and widely used supervised classification techniques is k-nearest neighbors. Often used in a number of areas such as bankruptcy prediction, customer relationship management, fraud detection, intrusion detection, recommender systems and others[17].

When a new test observation is classified, the distance (usually Euclidean or Manhattan) is computed with each training data point. The class of the k nearest train points (neighbors) is considered at the next stage. The predominant class within the k nearest neighbors determines the class of the test observation at the end.

The simplicity of k-NN makes it a very attractive tool for solving classification problems at hand. The technique is easily understandable by users with different professional background which also makes it recognizable in a wide range of fields. Results can easily be visualized to an audience. The training process is expected to be very fast and stable even in the presence of noisy data. Furthermore, as with most classifiers, the larger the train dataset, the more effective the classifier would be[9], [15].

Naturally, k-NN is associated with drawbacks as well. Overall, the computation time is significant and since it is a lazy supervised technique, the testing as well needs considerable time. Using k-NN requires an appropriate amount of space for storage which can turn out to be quite huge. Observations used for training can have big impact on accuracy, so working with representative training dataset is a challenge. Furthermore, the selection of the variables for the model should be done with care, as irrelevant features humanitarian, social and other areas. Additionally, we create two modifications of the proposed Mk-NN algorithm. The first one splits the input dataset into train and test subsets. We call this modification – MK-NN(TA). We use this modification of Mk-NN to showcase the improved efficiency in comparison to the traditional k-NN. On the other hand, the second modification splits the source dataset into three subsets – validation, train and test, where the validation subset is used to compute the accuracy of the model. This variation is referred to as MK-NN(VA). Experiments with this modification disprove worries of overfitting. The rest of the paper is organized as follows: in Section II. we provide a brief review of the classic k-NN. We specify metrics for evaluating the performance of classifiers. We then propose a new modification of k-NN in Section III. Experiments and Results are presented in Section IV. We provide our conclusions and future work intentions in the final Section V.

II. LITERATURE REVIEW

Table 1: Confusion Matrix

| Predicted | Actual |
|-----------|--------|
| True Positives (TP) | False Positives (FP) |
| False Negatives (FN) | True Negatives (TN) |

Positives refer to correctly classified observations, whereas negatives refer to misclassified observations. More specifically, True Positives (TP) gives us the observations which are observed positive and are actually positive, True Negatives (TN) are the observations which are observed negative and are actually negative, False Positives (FP) are observed positive and are actually negative, False Negatives (FN) are observed negative and are actually positive.

Accuracy as a performance measure looks at the sum of all correctly classified observations divided by the total number of observations in the subset[21].

\[ \text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \]
Sensitivity provides information on the accuracy of only positive predictions [21].

\[
\text{Sensitivity} = \frac{TP}{TP + FN} \quad (2)
\]

Specificity represents the accuracy only of negative predictions [21].

\[
\text{Specificity} = \frac{TN}{TN + FP} \quad (3)
\]

F1 score is a statistical test that takes into consideration both sensitivity and specificity. In other words, it is the weighted average of the sensitivity and specificity [21].

\[
F1 = 2 \times \frac{\text{Sensitivity} \times \text{Specificity}}{\text{Sensitivity} + \text{Specificity}} \quad (4)
\]

Time should not be neglected as a performance factor in solving classification problems. It can make a huge difference to choose the most effective solution for decision making involving enormous databases and complex computations. When using k-NN classifier, it is expected the time needed for training and testing to depend on the number of nearest neighbors used as part of the decision rule. The bigger the value of k is, the more calculations are involved, hence the time needed for executing the method increases.

III. NEW ALGORITHM

Here we propose a new method when building the k-NN classifier. The observations in the dataset are shuffled and then split into n folds containing all observations. Each observation is allocated to one of the folds. One of the folds is used as test data and the rest of the folds as train data. This process runs n times.

For example, let us say we have a dataset with 100 observations. We choose 10 folds. The observations are shuffled and allocated to 10 folds. Every fold has 10 observations.

For the experiments with Mk-NN and traditional k-NN, we use 18 different datasets. We use accuracy score, F1 score and time to evaluate the Mk-NN and traditional k-NN. Confusion matrix is used as well to present the result from using the classifiers. With the exception of Marital Satisfaction dataset, all datasets are taken from Knowledge Extraction Evolutionary Learning (KEEL) available at https://sci2s.ugr.es/keel/index.php.Marital Satisfaction observations. One of the folds is reserved as test data and the observations in the other 9 folds constitute the train data. At the next run the same folds are used, but another fold is selected as test data. The process will take place 10 times and each time a different fold is selected as test data.

Every time a fold is selected as test data we fit k-NN classifier and score the output in terms of accuracy. The accuracy is determined as percent of the correctly classified observations in the test data to the total number of observations in the test data. The observations in the train folds which produce the highest accuracy are saved and used to train the k-NN classifier. Following the fit of the test data, we compute the final accuracy, which should be the same as the highest accuracy during the train process.

We name the described method Mk-NN.

Algorithm: Mk-NN
1: Input dataset X;
2: Shuffle data points in X by keeping the initial indexes of each observation;
3: Split X into n folds (N1, N2, N3, N4 … Nn);
4: for i=1 to n do:
   4.1. Reserve Ni as Test data points and the rest of the folds use as Train data points;
   4.2. Define value for k in k-Nearest Neighbors;
   4.3. Train and fit k-NN algorithm;
   4.4. Compute accuracy score of the data points in Ni by dividing the number of correctly predicted class of test data points by the total number of test data points;
end for
5: Select the data points from (N1, N2, N3, N4 … Nn) producing the highest accuracy score as final test dataset and the rest of the data points in X as train dataset;
6: The train set in step 5 is used in the Mk-NN algorithm;

IV. EXPERIMENTAL RESULTS AND DISCUSSION

Table II gives an overview of the datasets used for the experiments. Each of the selected datasets has at least 1 000 observations and their expected accuracy score using classic k-NN is below 97%. We consider it impractical to compare the proposed modification Mk-NN with classic k-NN, when there is no real room for improvement in terms of accuracy, as classic k-NN already gives extremely satisfactory results.

| Dataset          | Number of observations | Number of features | Number of Classes |
|------------------|------------------------|--------------------|-------------------|
| Marital Satisfaction | 7178                 | 11                 | 2                 |
| Banana           | 5300                  | 2                  | 2                 |
| Titanic          | 2201                  | 3                  | 2                 |
| Phoneme          | 5404                  | 5                  | 2                 |
| Kr-vs-K          | 28056                 | 6                  | 18                |
| Yeast            | 1484                  | 8                  | 10                |
A. Classifiers

- k-NN
  For the experiments performed using k-NN, each dataset is split into two subsets (train and test) where the test subset includes 30% of the total number of observations in the respective dataset. The rest of the observations are kept for training. Twelve k-NN classifiers are used with values of k equal to 1, 3, 5, 7, 9, 11, 13, 15, 30, 45, 60 and √n for the classic k-NN. Manhattan distance is implemented when classifying the observations. Random allocation of observations to test and train subsets is used. The procedure is executed ten times for each value of k.

- Mk-NN
  For the experiments performed using the proposed Mk-NN classifier, each dataset is split into 10 folds where each observation is used and one observation can be allocated to only one fold. Each fold is used once as test subset with the rest of the folds saved for training, hence the classifier runs ten times with unique pair of test/train subsets each time. The observations are shuffled before being distributed to the folds. As with the k-NN experiments, the same twelve values for k are used here, namely 1, 3, 5, 7, 9, 11, 13, 15, 30, 45, 60 and √n. The Manhattan distance is used when classifying the observations. The train/test subset pair with highest accuracy score per k is selected for the final models, where k equals 1, 3, 5, 7, 9, 11, 13, 15, 30, 45, 60 and √n respectively.

  We create two modifications of the described Mk-NN classifier.
  a. Mk-NN with Testing Accuracy (Mk-NN(TA)) – we use the full input dataset to create 10 folds. We apply this variation to all datasets. We use this modification of Mk-NN to compare its accuracy results, F1 score results and time for execution with the results achieved using k-NN. Since the performed experiments with Mk-NN(TA) give rise to suspicion related to overfitting, we use the described in b. modification to check these concerns.
  b. Mk-NN with Validation Accuracy (Mk-NN(VA)) – we create an additional subset with randomly selected observations from the input dataset, which we call validation subset. This validation subset constitutes 10 percent of the input dataset and its observations are not used in the 10 folds for training and testing. This modification is applied to 10 of the datasets (Banana, Abalone, Ring, Thyroid, Chess, Marital Satisfaction, Phoneme, Satimage, Wine Quality – White and Spambase). We record the accuracy achieved on the basis of both test subset and validation subset in order to investigate the possibility of overfitting in the model.

B. Metrics

- Testing Accuracy
  For classic k-NN, the testing accuracy of each classifier (each value of k) is evaluated by computing the average accuracy from all ten runs, whereas the testing accuracy for Mk-NN(TA) is computed using only the train/test pair selected for the final model per each k. The testing accuracy corresponds to the portion of correctly classified observations from the total observations in the test subset.

- Validation Accuracy
  The validation accuracy is computed by dividing the correctly classified observations by the total number of observations in the validation subset. It is applicable to Mk-NN(VA), which is used on 10 of the datasets (Banana, Abalone, Ring, Thyroid, Chess, Marital Satisfaction, Phoneme, Satimage, Wine Quality – White and Spambase).

- F1 score
  Apart from accuracy, we also use F1 score to evaluate the results of both classic k-NN and Mk-NN(TA) when applied to all datasets. Thus, we are looking how Mk-NN(TA) performs in terms of precision and recall compared to k-NN. The score is computed for all 18 datasets and for each value of k (1, 3, 5, 7, 9, 11, 13, 15, 30, 45, 60 and √n).

Since we are using F1 score as available from scikit-learn package in python, average is an important parameter for the computation. When there are two classes in the dataset, the parameter is used as it is by default. Otherwise, when we have multiclass targets (more than two classes), we set the parameter to micro, which calculates metrics globally by counting the total true positives, false negatives and false positives.

- Confusion Matrix
  Confusion matrix is presented for three of the datasets, namely these are Nursery, Satimage and Ring. The matrices are compiled using both the classic k-NN and the proposed Mk-NN(TA) classifier, where the value for k is 1 in both instances. The confusion matrices are built on all observations since the number of test observations would differ applying each classifier.

### Dataset Statistics

| Dataset          | Observations | Train | Test |
|------------------|--------------|-------|------|
| Abalone          | 4174         | 8     | 28   |
| Nursery          | 12960        | 8     | 5    |
| Contraceptive    | 1473         | 9     | 3    |
| Flare            | 1066         | 11    | 6    |
| Wine quality – red | 1599       | 11    | 6    |
| Wine quality – white | 4898     | 11    | 7    |
| Ring             | 7400         | 20    | 2    |
| Thyroid          | 7200         | 21    | 3    |
| Chess            | 3196         | 36    | 2    |
| Satimage         | 6435         | 36    | 7    |
| Spambase         | 4597         | 57    | 2    |
| Splice           | 3190         | 60    | 3    |
MK-NN(TA) uses ten folds to split the dataset, whereas k-NN splits the dataset using 30% percent of it for test cases. Another important note is that since MK-NN(TA) determines one best train/test split used as model for prediction, and k-NN select different subsets on each run, randomly one result from the ten runs of 1-NN is chosen and confusion matrix is created using it.

**Execution Time**

For each value of k, the execution time has been recorded using the time library and method available in python 3.6. The experiments were performed on 64-bit Windows 10 with Intel Core i7-7500 and 8.00GB RAM using Spyder 3.2.8 as integrated development environment. It should be noted that the duration for classifying will always vary slightly from one execution to the other, but these differences would not affect the overall conclusions.

**C. Results**

The testing accuracy results of the experiments are summarized in Table III. It shows the maximum accuracy achieved with classic k-NN and MK-NN(TA) respectively, the number of neighbors with which the maximum accuracy was achieved, and the execution time needed to classify with the k neighbors reaching maximum accuracy. In case, multiple values of k achieve maximum accuracy, we take the execution time from the smallest k value achieving the maximum accuracy. In the two rightmost columns are computed the differences in both accuracy and time between classic k-NN and MK-NN(TA), again referring to maximum accuracy. The following key points can be noted from the summary table:

- In all instances, the MK-NN(TA) classifiers outperform the classic k-NN classifiers.
- There is no specific value for k that predominately gives the best accuracy results.
- Big improvements in accuracy when comparing classic k-NN and MK-NN(TA) can be observed for Yeast, Wine quality - white, Flare and Wine quality – red, with improvements of 0.08, 0.08, 0.09 and 0.10 respectively.
- The execution time needed for reaching maximum accuracy is always less using MK-NN(TA) in comparison to classic k-NN.
- Overall, it can be concluded MK-NN(TA) is more efficient than classical k-NN in both accuracy and execution time.

### Table III: MAX Testing Accuracy Results

| Dataset                | MAX Testing Accuracy | k-NN Neighbors | Execution Time in seconds | MAX Testing Accuracy | k-NN Neighbors | Execution Time in seconds | Accuracy Difference | Difference in Time Needed |
|------------------------|----------------------|----------------|---------------------------|----------------------|----------------|---------------------------|---------------------|--------------------------|
| Marital Satisfaction   | 0.80                 | 7, 9, 15       | 3.00                      | 0.83                 | 9, 11, 13      | 0.65                      | 0.03                | -2.35                    |
| Banana                 | 0.90                 | 9, 11, 13, 15, 30, 45, √n | 0.22                      | 0.92                 | 11, 30, 45, 60 | 0.06                      | 0.02                | -0.16                    |
| Titanic                | 0.79                 | 11, 60         | 0.28                      | 0.85                 | 9, 11, 13, 15 | 0.08                      | 0.06                | -0.20                    |
| Phoneme                | 0.90                 | 1              | 0.22                      | 0.92                 | 1              | 0.02                      | 0.02                | -0.20                    |
| Kr-vs-K                | 0.75                 | 7              | 8.34                      | 0.81                 | 7, 9           | 1.28                      | 0.06                | -7.06                    |
| Yeast                  | 0.59                 | 45             | 0.47                      | 0.67                 | 30, 45, 60     | 0.09                      | 0.08                | -0.38                    |
| Abalone                | 0.27                 | 60             | 1.36                      | 0.33                 | 30             | 0.19                      | 0.06                | -1.17                    |
| Nursery                | 0.96                 | 7              | 5.98                      | 0.98                 | 7, 9, 11       | 0.91                      | 0.02                | -5.07                    |
| Contraceptive          | 0.55                 | 30             | 0.23                      | 0.62                 | 15             | 0.04                      | 0.07                | -0.19                    |
| Flare                  | 0.74                 | 9, 13, 30, √n  | 0.12                      | 0.83                 | 13             | 0.04                      | 0.09                | -0.08                    |
| Wine quality - red     | 0.57                 | 1              | 0.08                      | 0.67                 | 1              | 0.01                      | 0.10                | -0.07                    |
| Wine quality - white   | 0.57                 | 1              | 0.23                      | 0.65                 | 1              | 0.06                      | 0.08                | -0.17                    |
| Ring                   | 0.71                 | 1              | 7.53                      | 0.75                 | 1              | 1.92                      | 0.04                | -5.61                    |
| Thyroid                | 0.94                 | 3, 5, 7, 9, 11, 13 | 6.11                      | 0.95                 | 3, 5, 7, 9, 11, 13 | 1.59                  | 0.01                | -4.52                    |
| Chess                  | 0.95                 | 3              | 2.95                      | 0.98                 | 5, 7           | 0.61                      | 0.03                | -2.34                    |
| Satimage               | 0.91                 | 3, 5, 7        | 6.91                      | 0.93                 | 3, 5           | 1.42                      | 0.02                | -5.49                    |
| Spambase               | 0.84                 | 1              | 0.94                      | 0.87                 | 1, 3, 5        | 0.26                      | 0.03                | -0.68                    |
| Splice                 | 0.89                 | 60, √n         | 8.42                      | 0.93                 | 60             | 1.69                      | 0.04                | -6.73                    |
In table IV, we present the testing and validation accuracy results for the 10 datasets subject of experiments with the Mk-NN(VA) variation of Mk-NN. For each dataset, we provide the maximum Mk-NN(VA) validation accuracy and its corresponding testing accuracy. We also add a column in the table computing the difference between the testing and validation accuracy.

Although for all five datasets the testing accuracy is greater than or equal to the validation accuracy, the difference can be considered as too small for overfitting to be considered. With the exception of Wine Quality – White, for all other datasets the difference between validation and testing accuracy is 0.02 at most in favor of the testing accuracy.

| Dataset                | Mk-NN(VA) Testing Accuracy | Mk-NN(VA) MAX Validation Accuracy | Mk-NN(VA) MAX Validation Accuracy - Testing Accuracy |
|------------------------|----------------------------|----------------------------------|-----------------------------------------------|
| Banana                 | 0.93                       | 0.92                             | -0.01                                         |
| Abalone                | 0.34                       | 0.32                             | -0.02                                         |
| Ring                   | 0.74                       | 0.73                             | -0.01                                         |
| Thyroid                | 0.95                       | 0.95                             | 0.00                                          |
| Chess                  | 0.97                       | 0.97                             | 0.00                                          |
| Marital Satisfaction   | 0.84                       | 0.82                             | -0.02                                         |
| Phoneme                | 0.93                       | 0.91                             | -0.02                                         |
| Satimage               | 0.93                       | 0.91                             | -0.02                                         |
| Wine Quality - White   | 0.62                       | 0.57                             | -0.05                                         |
| Spambase               | 0.86                       | 0.83                             | -0.02                                         |

Next, we provide the results from F1 score in table V for both classic k-NN and Mk-NN(TA). The table displays the maximum F1 score achieved with classic k-NN and Mk-NN(TA) respectively, the number of neighbors with which the maximum F1 score was achieved, and the execution time needed to classify with the k neighbors reaching maximum F1 score. In case, multiple values of k achieve maximum F1 score, we take the execution time from the smallest k value achieving the maximum F1 score. In the two rightmost columns are computed the differences in both F1 score and execution time between classic k-NN and Mk-NN(TA), again referring to maximum F1 score. Looking at the results we can conclude that:

- For all datasets, Mk-NN(TA) always gives the highest F1 score.
- The best F1 score is always achieved with k=1.
- The following datasets (6 datasets) have at least 0.10 increase in F1 score when using Mk-NN method compared to F1 score results of classic k-NN: Yeast, Abalone, Contraceptive, Wine quality – red and Wine quality – white. The biggest improvement can be observed in Abalone dataset – 0.17.
- In terms of execution time, again Mk-NN(TA) provides better results managing to reach higher F1 score in less time in comparison to classic k-NN.

| Dataset            | MAX F1 | k Neighbors | Execution Time in seconds | MAX F1 | k Neighbors | Execution Time in seconds | F1 Score Difference | Difference in Time Needed |
|--------------------|--------|-------------|----------------------------|--------|-------------|----------------------------|---------------------|--------------------------|
| Marital Satisfaction| 0.94   | 1           | 1.14                       | 0.98   | 1           | 0.25                       | 0.04                | -0.89                    |
| Banana             | 0.96   | 1           | 0.11                       | 0.99   | 1           | 0.02                       | 0.03                | -0.09                    |
| Titanic            | 0.58   | 3           | 0.28                       | 0.59   | 1, 7        | 0.08                       | 0.01                | -0.20                    |
| Phoneme            | 0.95   | 1           | 0.22                       | 0.99   | 1           | 0.02                       | 0.04                | -0.20                    |
Finally, in table VI, table VII and table VIII, we present confusion matrixes built from classic k-NN and Mk-NN(TA) for three datasets (Nursery, Satimage and Ring) where k has value of 1. The left part of each table displays the confusion matrix as a result of classic k-NN and the right part as a result of Mk-NN(TA). The values on the diagonal starting from the upper left are correctly classified and consequently all other values in a table are incorrectly classified.

Comparing the values which do not belong to the diagonal with correctly classified observation, it is clearly visible that Mk-NN(TA) tends to outperform k-NN in terms of accuracy.

| k-NN | Actual | Predicted |
|------|--------|-----------|
| 0.86| 1  3.38 0.95 | 1  0.76 0.09 |
| Yeast | 0.86 | 1  0.12 0.96 | 1  0.04 0.10 |
| Abalone | 0.76 | 1  0.27 0.92 | 1  0.13 0.16 |
| Nursery | 0.97 | 5, 7, 9 4.86 0.98 | 1, 5, 7, 9, 11, 13 0.61 0.01 |
| Contraceptive | 0.81 | 1  0.06 0.91 | 1  0.04 0.10 |
| Flare | 0.78 | 1  0.08 0.82 | 1  0.04 0.04 |
| Wine quality - red | 0.87 | 1  0.08 0.97 | 1  0.01 0.10 |
| Wine quality - white | 0.87 | 1  0.23 0.97 | 1  0.06 0.10 |
| Ring | 0.92 | 1  7.53 0.98 | 1  1.92 0.06 |
| Thyroid | 0.98 | 1  0.12 0.99 | 1  1.42 0.01 |
| Chess | 0.97 | 1, 3, 5 2.45 0.99 | 1  0.46 0.02 |
| Satimage | 0.97 | 1  3.35 0.99 | 1  0.86 0.02 |
| Spambase | 0.94 | 1  0.94 0.98 | 1  0.26 0.04 |
| Splice | 0.92 | 1  3.95 0.98 | 1  0.95 0.06 |

Table VI: Nursery Confusion Matrix

| Mk-NN(TA) | Actual |
|-----------|--------|
| 4141 | 24 | 3 | 98 |
| 35 | 4256 | 1 | 30 |
| 16 | 2 | 310 | 0 |
| 52 | 14 | 0 | 3978 |

Table VII: Satimage Confusion Matrix

| Mk-NN(TA) | Actual |
|-----------|--------|
| 1529 | 0 | 3 | 0 | 1 | 0 |
| 0 | 700 | 0 | 0 | 3 | 0 |
| 0 | 0 | 1351 | 6 | 0 | 1 |
| 1 | 1 | 4 | 611 | 0 | 9 |
| 1 | 1 | 0 | 0 | 703 | 2 |
| 0 | 0 | 3 | 11 | 3 | 1491 |

Table VIII: Ring Confusion Matrix

| Predicated k-NN | Actual |
|-----------------|--------|
| 3051 | 613 |
| 7 | 3729 |

| Predicated Mk-NN(TA) | Actual |
|----------------------|--------|
| 3482 | 182 |
| 4 | 3732 |

V. CONCLUSION AND FUTURE WORK

This paper proposes a new method for applying k-NN, which strives to achieve better efficiency in classifying test observations. The method tries to select the most representative train dataset from the respective input dataset by splitting the input dataset in predefined number of folds and checking each fold as test dataset. The pair of train/test datasets that provides the highest score in terms of
correctly predicted test observations against all test observations is selected for the final modelling of the dataset in question.

Performing experiments with real datasets shows improved results in terms of accuracy, specificity, sensitivity and execution time compared to classic k-NN. On average, Mk-NN(TA) maximization testing accuracy outperforms classic k-NN by 5% and maximum F1 score has on average 6% improvement when comparing Mk-NN and classic k-NN. Experiments with Mk-NN(VA) did not indicate overfitting. Whereas the best F1 scores are predominately achieved with 1 nearest neighbor, the best accuracy results don’t seem to be related with a specific value of k.

As future work, finding a way to determine the most appropriate number of folds for a given dataset can be explored. Also, experiments with shuffling the input dataset many times and executing the proposed method each time could yield even better accuracy results, albeit increasing execution time.

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