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Efficient k-NN Classification based on Homogeneous Clusters

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Abstract The k-NN classifier is a widely used classification algorithm. However, exhaustively searching the whole dataset for the nearest neighbors is prohibitive for large datasets because of the high computational cost involved. The paper proposes an efficient model for fast and accurate nearest neighbor classification. The model consists of a non-parametric cluster-based preprocessing algorithm that constructs a two-level speed-up data structure and algorithms that access this structure to perform the classification. Furthermore, the paper demonstrates how the proposed model can improve the performance on reduced sets built by various data reduction techniques. The proposed classification model was evaluated using eight real-life datasets and compared to known speed-up methods. The experimental results show that it is a fast and accurate classifier, and, in addition, it involves low pre-processing computational cost.

Keywords nearest neighbors · classification · clustering

1 Introduction

A classifier is a data mining algorithm that assigns new data items to a set of predefined classes (Han et al, 2011). There are two major categories of classifiers: eager and lazy (James, 1985). Eager classifiers, e.g., decision trees (Rokach, 2007), build a model based on the available training data, and then, they classify all new data items using this model. On the other hand, lazy classifiers do not build any model. They consider the whole Training Set (TS) as a model. When a new item arrives and must be classified, they perform classification by scanning the available training data.

The main lazy classification method is the k-Nearest Neighbor (k-NN) classifier (Dasarathy, 1991). It makes classification predictions by searching in TS for the k nearest items (neighbors) to a new item. The latter is assigned to the most

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common class among the retrieved k nearest neighbors. Ties (two or more classes are most common) are resolved either randomly or by the one nearest neighbor. The latter is the approach adopted in this paper. The k-NN classifier, in its simplest form, must compute all distances between the new item and all items in TS. Therefore, the computational cost of searching depends on the size of TS and it may be prohibitive for large datasets and time-constrained applications.

The reduction of the cost of k-NN classifier remains an open research issue that has attracted the interest of many researchers. Many methods have been proposed to speed-up k-NN searching. A possible categorization of these methods is: (i) Multi-attribute Indexes, (ii) Data Reduction Techniques (DRTs)[1], and, (iii) Cluster-Based Methods (CBMs). DRTs, contrary to the other two categories, have the extra benefit of the reduction of storage requirements. The effectiveness of traditional multi-dimensional indexes (Samet, 2006) highly depends on the data dimensionality. In dimensions higher than ten, the curse of dimensionality may render their performance even worse than that of sequential search.

DRTs reduce the computational cost of k-NN classifier by building a small representative set of the initial training data. This set is called Condensing Set (CS). The idea behind DRTs is to apply the k-NN classifier over the CS attempting to achieve accuracy as high as when using the original TS. DRTs can be divided into two main categories: (i) selection (or filtering) (Garcia et al, 2012), and, (ii) abstraction (or generation) (Triguero et al, 2012) algorithms. Both have the same motivation but differ on the way that they build the CS. Selection algorithms select some "real" TS items as representatives (or prototypes). In contrast, abstraction algorithms generate representatives by summarizing similar items. In general, all DRTs produce their CS by keeping or generating for each class, a sufficient number of representatives.

CBMs pre-process the training items and group them into clusters. For each new item, they dynamically form an appropriate training subset of the initial TS, which then is used to classify the new item. This subset is usually called reference set. Contrary to DRTs, CBMs do not reduce the size of TS.

In our previous work (Ougiaroglou et al, 2012), we demonstrated that DRTs and CBMs can be combined in a hybrid classification method to achieve the desirable performance. In particular, we proposed a pre-processing algorithm to construct a data structure and a fast algorithm to classify new items by accessing this structure. The main disadvantage of our method was that both algorithms were parametric and required a trial-and-error procedure to properly adjust their parameters.

In Ougiaroglou and Evangelidis (2012b), our motivation was the development of a fast and non-parametric classification model for large and high dimensional data. Here, we extend this work by presenting a new model variation and new experiments. The complete contribution of our work is: (i) the development of an efficient and non-parametric classification model that combines two speed-up strategies, namely, DRTs and CBMs, and, (ii) the proposal of a variation of our model that is applied on data stored in a CS and is able to further improve the performance of DRTs. The main goal of the variation is extra fast classification.

[1] DRTs have two points of view: (i) item reduction, and, (ii) dimensionality reduction. We consider them from the first point of view.

The rest of this paper is organized as follows. Section 2 briefly presents related work. Sections 3 and 4 consider in detail the proposed classification model and its variation, respectively. Section 5 presents the experimental evaluation, and, finally, Section 6 concludes the paper.

2 Related work

The earliest and best known DRT is the Condensing Nearest Neighbor (CNN) rule (Hart, 1968) that belongs to the selection category. CNN-rule keeps for each class a sufficient number of representatives for the close-class-borders data areas and removes the items of the "internal" class data areas. The idea is that, since the "internal" items do not define decision boundaries between classes, they can be removed without affecting accuracy.

CNN uses two lists, S and T. Initially, it places an item in S and all the other items in T. Then, it classifies the content of T using the content of S by employing the 1-NN classifier. The misclassified items are moved from T to S. This procedure continues until all items of T are correctly classified by the content of S or, in other words, until there is no move from T to S during a complete pass of T. The content of S constitutes the Condensing Set (CS). At the end, the remaining items of T can be correctly classified by the contents of S. The idea is that if an item is misclassified, it probably lies in a close-class-border data area, and so, it should be placed in CS. An advantage of CNN-rule is that it automatically determines the size of CS based on the level of noise in the data and the number of classes (the higher the number of classes, the more the decision boundaries). On the other hand, a disadvantage of CNN-rule is that the resulting CS depends on the order of items in TS.

Many other selection algorithms either extend CNN-rule or are based on the same idea. Some of them are: the Reduced NN rule (Gates, 1972), the Selective NN rule (Ritter et al, 1975), the Modified CNN rule (Devi and Murty, 2002), the Generalized CNN rule (Chou et al, 2006), and, the IB algorithms (Aha et al, 1991; Aha, 1992). However, CNN-rule continues to be the reference algorithm and is used for comparison purposes in many research papers.

IB2 is an incremental one-pass version of CNN-rule. Therefore, it is a very fast algorithm. It belongs to the family of IB selection algorithms (Aha et al, 1991; Aha, 1992). IB2 works as follows: When a new TS item x arrives, it is classified by the 1-NN rule by examining the contents of the current CS. If x is misclassified, it is put in CS. Then, x is removed. IB2 is a non-parametric algorithm that highly depends on the order of items in TS. Contrary to CNN-rule, IB2 does not ensure that its CS can correctly classify all examined training data.

Chen and Jozwik's algorithm (CJA) (Chen and Jóźwik, 1996) is also a well-known DRT that belongs to the abstraction category. CJA initially retrieves the most distant items, X and Y in TS. The distance of X and Y defines the diameter of the dataset. Then, based on these two items, CJA divides the TS into two subsets: items that lie closer to X are placed in S_X while items that lie closer to Y are placed in S_Y. The algorithm continues by dividing the subset with the largest diameter. This procedure terminates when the number of subsets is equal to a user-predefined threshold. Finally, for each created subset, CJA places in CS a mean item (centroid) labeled by the most common class in the subset.

CJA is the ancestor of the family of Reduction by Space Partitioning (RSP) algorithms (Sánchez, 2004) that are a popular set of three abstraction algorithms known as RSP1, RSP2, and RSP3. RSP1 computes as many centroids as the number of different classes in each subset. Obviously, it builds larger CSs than CJA. However, it can achieve higher classification accuracy. RSP1 and RSP2 differ to each other on how they choose the next subset that will be split. RSP1 uses the criterion of the larger diameter while RSP2 uses the criterion of overlapping degree. Finally, RSP3 does not depend on the criterion used. It continues splitting the non-homogeneous subsets and terminates when all of them become homogeneous (i.e., contain items of a specific class). RSP3 is the only RSP algorithm (CJA included) that automatically determines the size of CS. Moreover, contrary to CNN-rule, CJA and RSP build CSs that do not depend on the data order in TS.

RHC is a recently proposed abstraction DRT (Ougiaroglou and Evangelidis, 2012a). Like RSP3, it is based on the concept of homogeneity. RHC keeps on constructing clusters until all of them are homogeneous. In particular, it iteratively executes k-Means clustering (McQueen, 1967) on the data of each non-homogeneous cluster. Moreover, like CJA and RSP algorithms and contrary to CNN-rule, RHC is independent on the data order in TS. Finally, RHC is faster and achieves higher reduction rates than RSP3 and CNN, and also has acceptable accuracy.

The reduction rates of many DRTs depend on the level of noise in the data. Thus, achieving high reduction rates usually requires the application of a noise removal routine before the data reduction procedure (Lozano, 2007; Toussaint, 2002). These noise removal routines are known as editing algorithms. Editing algorithms remove noisy items and smooth the decision boundaries by removing some close-class-border items. Although editing algorithms cannot be characterized as typical DRTs (they do not aim at high reduction rates), they constitute a subcategory of selection DRTs. A well-known editing algorithm is ENN-rule (Wilson, 1972). It removes the irrelevant items by employing a simple rule: if the class label of a TS item does not agree with the majority of its k nearest neighbors, it is removed. Thus, ENN-rule computes all distances among the items in TS, i.e., $\frac{N\times(N-1)}{2}$ distances. Finally, some DRTs, such as IB3 (Aha et al, 1991), integrate the idea of editing in their main data reduction procedure (see Garcia et al (2012); Triguero et al (2012) for details).

Many other DRTs have been proposed during the past decades. Since our purpose is not to extensively review all DRTs, in this paper we present in detail only the DRTs that were used in our experiments. For the interested reader, selection and abstraction algorithms are reviewed and compared to each other in Garcia et al (2012) and Triguero et al (2012), respectively. Also, both of these papers present interesting taxonomies. Other relevant reviews can be found in Jankowski and Grochowski (2004); Grochowski and Jankowski (2004); Lozano (2007); Toussaint (2002); Wilson and Martinez (2000); Brighton and Mellish (2002); Olvera-López et al (2010).

Hwang and Cho proposed a CBM (Hwang and Cho, 2007) that uses the k-Means algorithm (McQueen, 1967) to find clusters in the data. Each cluster is divided into the core and the peripheral sets. Items lying in a certain distance from the cluster centroid are characterized as "core" items, whereas the rest are characterized as "peripheral" items. If an unclassified item x lies within the "core area" of the nearest cluster, it is classified by applying the k-NN classifier on the items of this cluster. Otherwise, the k-NN classifier is applied on the reference

set formed by the union of the items of the nearest cluster and the "peripheral" items of adjacent clusters. The performance of Hwang and Cho method depends on three input parameters as well as the selection of the initial means for k-means clustering.

We have used the Hwang and Cho method in our experiments. However, there are many other CBMs of interest. The Cluster-based Tree (Zhang and Srihari, 2004) is a CBM which is based on searching in a cluster hierarchy and can be used for either metric or non-metric spaces. Wang (2011) presented an algorithm for fast k-NN classification that prunes the search space by using the k-Means clustering and the triangle inequality. Finally, Karamitopoulos and Evangelidis (2009) proposed a CBM for fast time series classification.

3 SUDS Classification Model

The proposed classification model includes two major stages: (i) pre-processing, which is applied on the TS items in order to construct a Speed-up Data Structure (SUDS), and, (ii) classification, which uses SUDS and applies the proposed hybrid classifier. In this section, we present the pre-processing algorithm as well as the hybrid classifier.

3.1 Speed-Up Data Structure Construction Algorithm (SUDSCA)

The pre-processing algorithm builds SUDS by finding homogeneous clusters in TS. A cluster is homogeneous if it contains items of a specific class only. The SUDS Construction Algorithm (SUDSCA) repetitively executes the k-Means clustering algorithm until all of the identified clusters become homogeneous. SUDS is a two-level data structure. Its first level is a list of centroids (or representatives) of the identified homogeneous clusters. Each one represents a data area of a specific class and indexes the "real" cluster items which are in the second level of SUDS. Figure 1 shows how SUDS is constructed and Algorithm 1 summarizes the steps of the corresponding algorithm.

Initially, SUDSCA finds the mean items (class-centroids) of each class in TS by averaging its items (Figure 1(b)). Then, it executes the k-Means clustering algorithm using these class centroids as initial means. Thus, for a dataset with M classes, SUDSCA initially identifies M clusters (Figure 1(c)). SUDSCA continues by analyzing the M clusters. If a cluster is homogeneous, it is added to SUDS. The cluster centroid is added to the first level of SUDS as representative of the specific class and indexes the cluster items that are added to the second level. On the other hand, for each non-homogeneous cluster X, k-Means is executed on its items and identifies as many clusters as the number of distinct classes in X following the aforementioned procedure(Figure 1(d)). The repetitive execution of k-Means terminates when all constructed clusters are homogeneous. Following this algorithm, SUDSCA constructs few large clusters for internal class data areas, and many small clusters for close-class-border data areas.

SUDSCA can be easily implemented using a simple queue data structure that stores the unprocessed clusters. Initially, the whole TS constitutes an unprocessed cluster and it becomes the head of the queue (line 1 in Algorithm 1). In each

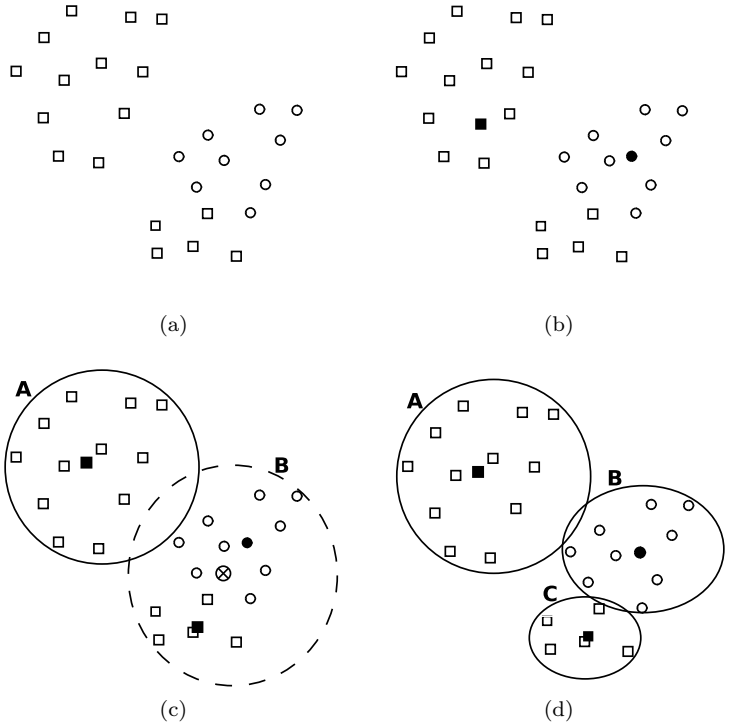


Fig. 1 SUDS construction by finding homogeneous clusters in the training dataset

iteration, SUDSCA checks if cluster C in the head of the queue is homogeneous or not (line 4). If it is, the cluster is added to SUDS (lines 5-7). Otherwise, the algorithm computes a mean item for each class ($ClassCentroids$) present in C (lines 9-13). SUDSCA continues by calling the k-Means clustering algorithm for the items of C (line 14). This procedure returns a list of clusters ($NewClusters$) that are added to the queue structure (line 15-17) as unprocessed clusters. This procedure is repeated until the queue becomes empty (line 19), which means that all constructed clusters are homogeneous.

Contrary to the pre-processing algorithm proposed in Ougiaroglou et al (2012), SUDSCA is non-parametric. It automatically determines the length of SUDS (i.e., the number of clusters) based on the dataset used. SUDSCA extends the idea of a previous work of ours that introduced a fast DRT called Reduction through Homogeneous Clusters (RHC) (Ougiaroglou and Evangelidis, 2012a). Here, our purpose is not the development of a DRT, but the development of a hybrid, non-parametric method that combines DRTs and CBMs. We note that the SUDS construction algorithm does not depend on the order of items in TS. Contrary to SUDSCA, other speed-up methods based on k-means clustering highly depend on the selection of the initial means (Hwang and Cho, 2007; Olvera-Lopez et al, 2010).

Algorithm 1 SUDS Construction Algorithm

Input: TS **Output:** $SUDS$

```
1: Enqueue(Queue, TS)
2: repeat
3:    C ← Dequeue(Queue)
4:    if C is Homogeneous then
5:       Compute the mean vector (class-centroid) M of C
6:       Put M into the first level of SUDS
7:       Put the items of C into the second level of SUDS and associate them to M
8:    else
9:       ClassCentroids ← ∅
10:      for each Class L in C do
11:         Centroid_L ← Compute the mean vector of items that belong to L
12:         ClassCentroids ← ClassCentroids ∪ Centroid_L
13:      end for
14:      NewClusters ← k-Means(C, ClassCentroids)
15:      for each cluster X in NewClusters do
16:         Enqueue(Queue, X)
17:      end for
18:   end if
19: until Queue is empty
20: return SUDS
```

3.2 Hybrid Classification Algorithm based on Homogeneous Clusters (HCAHC)

The second part of the proposed model is a classifier that uses SUDS. It is called Hybrid Classification Algorithm based on Homogeneous Clusters (HCAHC) and is described in Algorithm 2. When a new item x arrives and must be classified (line 1 in Algorithm 2), HCAHC initially scans the first level of SUDS and retrieves the Rk nearest representatives to x (lines 2-4). We call this scan a first level search. If all Rk retrieved representatives vote a specific class, x is classified to this class (lines 5-6). Otherwise, HCAHC goes to the second level of SUDS and x is classified by searching its k "real" nearest neighbors within the data subset dynamically formed by the union of the clusters of the Rk representatives (lines 8-10). We call this search a second level search.

second level search usually involves higher computational cost than a first level search. However, even in this case, HCAHC searches only a small subset of the initial TS data. For instance, suppose that SUDSCA has built a SUDS with 200 nodes and we have set Rk=8. HCAHC performs the first level search and retrieves the eight nearest representatives. Suppose that not all eight of them belong to the same class. As a result, HCAHC searches for the k nearest neighbors in the union of the eight clusters that correspond to the eight representatives and performs the classification. Even in this case, HCAHC significantly prunes the search space by ignoring the items of the rest 192 clusters.

A new item can be classified via either a first or a second level search. Practically, the first level search is an abstraction DRT, while the second level search is a CBM. That is why HCAHC is a hybrid method. Furthermore, when HCAHC performs a second level search, it accesses an almost noise-free subset of the initial TS. Since each cluster contains items of a specific class only, the subset (union of the Rk clusters) will not contain noisy items of other irrelevant classes, i.e., classes which are not represented by the Rk representatives. Thus, classification

Algorithm 2 HCAHC Algorithm

Input: $SUDS$, Rk, k

```
1: for each new item x do
2:    Scan 1st level of SUDS and retrieve the Rk Nearest Representatives (NR) to x
3:    Find the majority class MC1 of the Rk NR (ties are resolved by 1-NR)
4:    MCC ← COUNT(representatives of the majority class)
5:    if MCC = Rk then
6:       Classify x to MC1
7:    else
8:       Scan within the set formed by the union of clusters of the Rk representatives and
         retrieve the k Nearest Neighbors (NNs) to x {Second level search}
9:       Find the majority class MC2 of the k NNs (ties are resolved by 1-NN)
10:      Classify x to MC2
11:   end if
12: end for
```

performance may not be affected as much by noisy data of other classes. Of course, the length of SUDS and the size of the constructed clusters depends on the level of noise. The more the noise in TS, the smaller the size of the constructed clusters and the higher the final number of homogeneous clusters (or length of SUDS).

Since we aim to a non-parametric method, we must find a way to automatically determine Rk. In the experiments of the following section, we have tested the effect of the value of Rk on the performance of our method. In addition, we adopt the empirical rule: $Rk = \lfloor\sqrt{|SUDS|}\rfloor$, where $|SUDS|$ is the number of nodes (clusters) in SUDS. The adoption of this empirical rule was initially motivated by the rule of thumb $C = \lfloor\sqrt{\frac{n}{2}}\rfloor$ (Mardia et al, 1979) used for determining the number of clusters in the context of k-means clustering. Of course, we adopted the empirical rule by evaluating the performance of HCAHC on multiple datasets.

4 SUDS Classification Model over condensing sets

The motive behind the SUDS model presented in Section 3 is fast classification. In addition, we claim that our model could improve the performance of DRTs. More specifically, we suggest our SUDS classification model to be applied on the data stored in a Condensing Set (CS) that has been constructed by a DRT. Then, a classifier that uses SUDS will be executed faster than a classifier that searches for nearest neighbors in the full CS and without a negative impact on accuracy. Since SUDSCA will be applied on a CS (i.e., a small dataset), the preprocessing overhead it will introduce will be almost insignificant.

Suppose that a CS stores the close-class-border items of a dataset with four classes (Fig. 2(a)). Figures 2 (b)–(d) demonstrate the execution of SUDSCA. The result is the construction of a SUDS which contains five clusters. The SUDS construction procedure is similar to that presented in Figure 1.

Here, the classifier that uses SUDS to perform the classification is almost similar to HCAHC. However, there is a major difference: seldomly all Rk nearest representatives will belong to the same class. Almost in all cases, HCAHC proceeds to a second level search. Therefore, when the SUDS model is applied on a CS, the "if statement" (line 4 in Algorithm 2) regarding the first level classification is unnecessary (actually, it is meaningful only when Rk is very small). Thus,

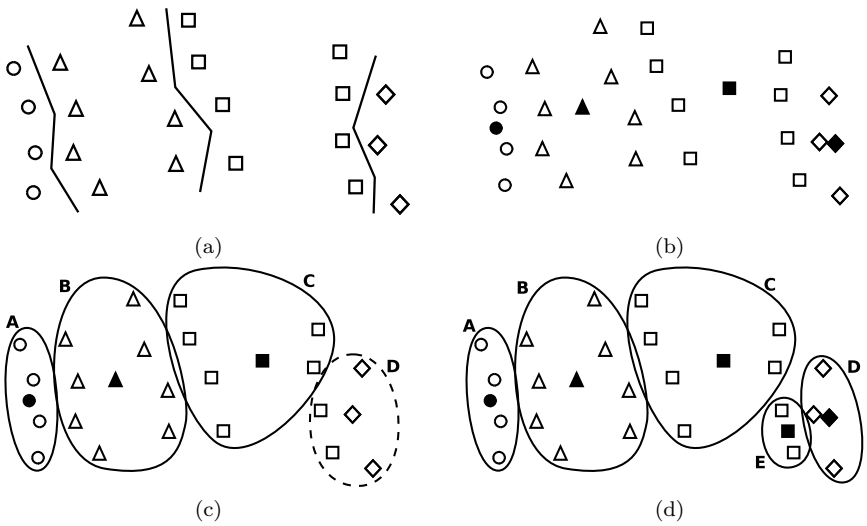


Fig. 2 SUDS construction by finding homogeneous clusters in the condensing set

Algorithm 3 HCA Algorithm

Input: $SUDS$, Rk, k

1: **for** each new item x **do**
2: Scan 1st level of $SUDS$ and retrieve the Rk Nearest Representatives (NR) to x
3: Scan within the set formed by the union of clusters of the Rk representatives and retrieve the k Nearest Neighbors (NNs) to x
4: Find the majority class MC of the k NNs (ties are resolved by 1-NN)
5: Classify x to MC
6: **end for**

a classifier that avoids classification though a first level search is a sufficient approach. We call this approach Homogeneous Clusters Algorithm (HCA) and we present it in Algorithm 3.

Contrary to HCAHC, HCA is not a hybrid classifier. Basically, it is a typical CBM. For each new item, it dynamically forms a training subset (reference set) of the initial CS on which the search for the nearest neighbors is executed. The training subset is the union of the Rk clusters that have been constructed by SUDSCA. As in the case of HCAHC, HCA adopts the empirical rule $Rk = \lfloor\sqrt{|SUDS|}\rfloor$ for the determination of Rk.

5 Performance Evaluation

The experimentation contains two main stages[2]. First, we evaluate the performance of SUDS classification model over original data, and then, over CSs that have been built by three DRTs. In all cases, our experiments were conducted us-

[2] Detailed experimental results are available at `http://users.uom.gr/~stoug/AIRJ_experiments.zip`

Table 1 Description of used datasets

Dataset	Size	Attributes	Classes
Letter Recognition (LR)	20000	16	26
Magic Gamma Telescope (MGT)	19020	10	2
Pen-Digits (PD)	10992	16	10
Landsat Satellite (LS)	6435	36	6
Shuttle (SH)	58000	9	7
Texture (TXR)	5500	40	11
Phoneme (PH)	5404	5	2
KddCup (KDD)	141481	23	36

ing eight real life datasets distributed by KEEL dataset Repository[3](Alcalá-Fdez et al, 2009) (see Table 1). We used the Euclidean distance as the distance metric. Ties during nearest neighbors voting (two or more classes are major classes) were resolved by the 1-NN rule.

SUDS classification model was compared to five speed-up methods by measuring three comparison criteria: classification accuracy, computational (classification) cost, and, preprocessing cost. We evaluated: (i) CNN-rule (Hart, 1968), the first and one of the most popular selection DRTs, (ii) the fast IB2 algorithm (Aha et al, 1991; Aha, 1992), (iii) RSP3 (Sánchez, 2004), the well-known abstraction DRT, (iv) the CBM proposed by Hwang and Cho (2007) (Hwang's method), and, (v) our abstraction DRT called RHC (Ougiaroglou and Evangelidis, 2012a).

All methods were implemented in C and evaluated using 5-fold cross validation. For each one of the seven datasets (except KDD), we used the five already constructed pairs of Training/Testing sets hosted by KEEL repository. These sets are appropriate for 5-fold cross validation. With the exception of KDD, we run all experiments without any previous knowledge about the datasets. Therefore, we did not perform normalization or any other data transformation.

KDD contains 41 attributes and 494,020 items. However, some attributes are unnecessary and huge amounts of data are duplicates. We removed the 5 unnecessary attributes (three nominal and two fixed-value attributes) and all duplicate items. Therefore, the transformed dataset includes 36 attributes and 141,481 unique items. We note that duplicate items are useless especially in the context of 1-NN classification. They do not influence the accuracy and negatively affect the computational cost. On the other hand, in the context of k-NN classification (with $k > 1$), duplicates influence the accuracy. However, when the goal is to speed-up k-NN classification, they can be removed (Xi et al, 2006). Moreover, we observed extreme variation on the value ranges of the attributes of KDD. Thus, we normalized all attributes to the value range [0-1]. Finally, we randomized the dataset and prepared it for 5-fold cross-validation.

[3] `http://sci2s.ugr.es/keel/datasets.php`

5.1 Performance of SUDS classification model over original data

5.1.1 Experimental Setup

CNN-rule, IB2, RSP3 and RHC are non-parametric methods, that is, they do not use user-defined parameters in order to reduce the training data. On the other hand, Hwang's method is parametric. In addition to parameter k (number of nearest neighbors to search), which is used by all methods during the classification step, it uses three extra parameters: (i) C: the number of clusters constructed by the k-Means clustering algorithm, (ii) D: the distance threshold used to divide each cluster into core and peripheral sets, and, (iii) L: the number of adjacent clusters that will be used. C and D are used during the preprocessing step, while L during the classification step (see Section 2 or Hwang and Cho (2007) for details). These parameters should be tuned. For each dataset, we built eight Hwang's classifiers using eight different C values. More specifically, each classifier i=1,...,8, used $C = \lfloor\sqrt{\frac{n}{2^i}}\rfloor$, where n is the number of TS items. The first classifier, i.e. i=1, is based on the rule of thumb $C = \lfloor\sqrt{\frac{n}{2}}\rfloor$ (Mardia et al, 1979). We decided to build additional classifiers that use smaller C values than $C = \lfloor\sqrt{\frac{n}{2}}\rfloor$ based on the observation that Hwang and Cho defined C=10 for a dataset with 60919 items (they did not find the optimal C value). For the other two parameters, we adopted the values suggested by Hwang and Cho in their experiments.

Although SUDSCA is non-parametric, HCAHC is a parametric classifier. In addition to k, it uses the Rk parameter. We built 29 HCAHC classifiers, for Rk=2,3,...,30, and we also considered the automatic determination of Rk (see Section 3). We refer to that classifier as HCAHC-sqrt. For both HCAHC and Hwang's method, we report only the most accurate classifiers for each cost level, i.e., the performance of a classifier was omitted if it achieved lower accuracy and involved higher computational cost than another classifier that achieved equal or higher accuracy and involved lower computational cost.

During the classification step, all methods involve parameter k. The DRTs perform k-NN classification using their CS, while Hwang's method does this over a small reference set that is dynamically formed for each new item. Finally, HCAHC searches for k nearest neighbors when it performs a second level search. We used the best k values for each method and dataset, i.e., the value that achieved the highest classification accuracy. In effect, we ran the cross validation many times for different k values and kept the best one. Of course, we did not use different k values for each fold.

For the first seven datasets, we run all experiments twice: on non-edited and on edited data (noise-free datasets). For editing purposes, we used ENN-rule (Wilson, 1972) by setting k=3 (according to Wilson and Martinez (2000), k=3 is a good value). The goal was to study how noise affects the performance of each method. The complete procedure that we followed during our experimentation is shown in Figure 3. For KDD, ENN-rule eliminates all items of some rare classes. More specifically, the ENN-rule edited KDD dataset contains fewer than 23 classes (from 4 to 7 fewer classes - depending on the fold). Therefore, we decided to skip the edited version of KDD. We note that the execution of ENN-rule on KDD was an extremely costly procedure. It involved the computation of $\frac{113{,}185\times 113{,}184}{2} \times 5$ folds $\simeq$ 32 billion distances. SH is also imbalanced as it contains two rare classes.

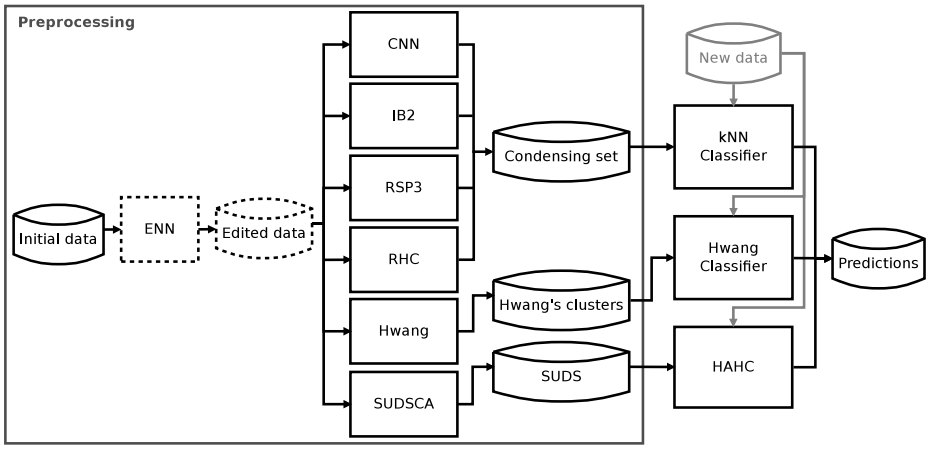


Fig. 3 Classification procedure of the experimental study

However, ENN-rule did not eliminate these rare classes. Thus, we decided to run experiments on the edited SH.

5.1.2 Pre-processing performance

Tables 2 and 3 present the pre-processing computational costs in terms of millions (M) of distance computations (how many distances were computed during pre-processing) performed by each method on non-edited and edited data. As we expected, SUDSCA and RHC were executed very fast in comparison to the other approaches, and were comparable in performance to IB2, which is a one-pass algorithm. This happened because: (i) the construction of SUDS and of the RHC condensing set are based on the repetitive execution of the fast k-Means clustering algorithm, and, (ii) in both cases, k-Means uses the mean items of the classes as initial centroids, and thus, clusters are consolidated very quickly. It is worth mentioning that SUDSCA and RHC pre-processing could become even faster had we used a different k-Means stopping criterion than the full clusters consolidation (no item move from one cluster to another during a complete algorithm pass).

Table 2 Preprocessing Cost on non-edited data (in millions of distance computations)

Dataset	CNN	IB2	RSP3	Hwang's method				RHC/ SUDSCA
				i=1	i=3	i=5	i=7	
LR	163.03	23.37	326.52	88.88	63.66	26.35	10.89	41.85
MGT	277.18	34.61	511.67	120.22	72.64	21.74	10.64	4.09
PD	11.75	1.78	86.66	28.80	11.27	5.97	1.70	2.88
LS	18.59	2.22	37.70	16.74	12.44	4.54	0.81	1.69
SH	45.30	8.26	17410.12	744.82	399.23	105.13	34.78	16.83
TXR	5.57	0.84	27.63	14.86	7.43	3.89	0.83	3.63
PH	13.45	1.96	20.31	9.87	3.70	1.33	0.74	0.65
KDD	384.90	55.58	20278.87	5440.21	2155.75	955.06	309.97	81.59
Avg.	114.97	16.08	4837.43	808.05	340.77	140.50	46.29	19.15

Table 3 Preprocessing Cost on edited data (in millions of distance computations)

Dataset	CNN	IB2	RSP3	Hwang's method				RHC/ SUDSCA
				i=1	i=3	i=5	i=7	
LR	112.20	18.35	300.51	74.60	55.31	31.45	9.93	31.05
MGT	70.27	8.51	318.82	85.28	33.80	16.33	7.06	2.83
PD	9.25	1.51	85.15	26.76	12.06	5.18	1.83	2.83
LS	7.09	1.02	30.63	13.76	9.60	3.43	0.87	1.74
SH	26.02	6.35	15652.75	867.40	367.52	146.12	37.18	22.41
TXR	4.39	0.71	27.04	14.76	7.16	4.27	0.82	3.00
PH	5.57	0.86	15.67	5.58	2.65	1.03	0.48	0.47
Avg.	33.54	5.33	2347.22	155.45	69.73	29.69	8.31	9.19

Table 4 Cost of ENN-rule (in millions of distance computations)

	LR	MGT	PD	LS	SH	TXR	PH
Edited TS size:	15306.8	12160.2	8734	4681	46314.2	4345.6	3837.4
Accuracy (%):	94.98	80.96	99.30	90.41	99.79	98.64	880.14
Reduction Rate (%):	4.33	20.08	0.67	9.07	0.18	1.24	11.25
ENN Cost:	127.99	115.76	38.65	13.25	1076.46	9.68	9.35

Concerning the other methods, RSP3 was the most time consuming approach. This is because RSP3 repetitively executes a costly procedure for finding the most distant items in data groups. Hwang's method for $i \geq 5$ is executed very fast. However, in real applications, the user must perform a trial-end-error procedure for determining the parameters. This may render pre-processing a hard and extremely time consuming procedure. Although CNN-rule is quite faster than RSP3, its pre-processing cost remains at high levels.

Finally, as we expected, DRTs and SUDSCA are faster when executed on edited data. This happens because: (i) edited TSs include fewer items than non-edited TSs, and, (ii) noisy items have a negative effect on these methods. One one hand, in RHC, RSP3 and SUDCA that use the concept of homogeneity, noisy items lead to many and small groups of items and, thus, these methods involve a high cost to build them. On the other hand, in CNN, noisy items lead to the execution of many algorithm data passes and of course to a large CS. The preprocessing cost of Hwang's method is not affected by noisy items. However, for noisy datasets, even this method involved lower preprocessing cost because of the smaller edited TS.

Nevertheless, to obtain an edited (i.e., noise-free) dataset, the execution of an extra preprocessing procedure is necessary (see Figure 3). This procedure involves additional computational cost. Thus, the total preprocessing cost includes the cost of ENN that is $\frac{N*(N-1)}{2}$, where N is the number of TS items. Table 4 shows the cost required by ENN-rule as well as the size of the edited TS and the corresponding reduction rate. We observe that MGT, PH, and LS have a significant level of noise, while in the rest datasets, the level of noise is almost insignificant.

5.1.3 Classification performance

We performed the classification step by using eight classification methods on the eight datasets. The methods used were: (i) Conventional k-NN (conv-k-NN), (ii) IB2, (iii) HCAHC, (iv) HCAHC-sqrt, (v) RHC, (vi) CNN, (vii) RSP3, and, (viii) Hwang's method. The performance measurements of conv-k-NN are shown

in Table 5 while the measurements of the speed-up methods are depicted in Figures 4-20. In particular, each figure includes two diagrams for each dataset, one corresponding to the non-edited TS and one to the edited TS.

The figures show the cost measurements (in terms of millions or thousands distance computations) on the x-axis and the corresponding accuracy on the y-axis. The cost measurements indicate how many distances were computed in order to classify all testing items. Since, we used a cross-validation schema, cost measurements are average values.

Almost in all cases, HCAHC and HCAHC-sqrt had very good performance. HCAHC can even reach the accuracy level of conv-k-NN (see Table 5). All diagrams show that rule $Rk = \lfloor\sqrt{|SUDS|}\rfloor$ is a good choice for the determination of Rk. With the exception of the SH and KDD datasets, HCAHC achieved better classification performance than all DRTs. On the other hand, although HCAHC and HCAHC-sqrt achieved higher accuracy than Hwang's method in all datasets, for the MGT, SH, PH AND KDD datasets, Hwang's method may be preferable because it achieved accuracies close to those of HCAHC and HCAHC-sqrt at a lower computational cost.

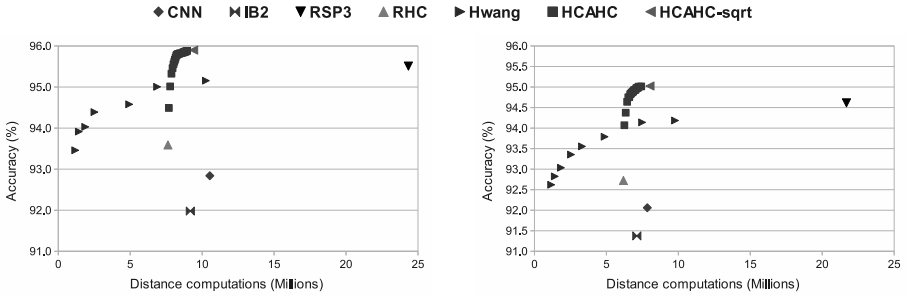
Table 5 compares the performance on non-edited data of conv-k-NN with that of HCAHC with an Rk value that achieves the highest possible accuracy (note that we have not conducted experiments for $Rk > 30$ and for $Rk \neq \lfloor\sqrt{|SUDS|}\rfloor$). Observe that the accuracy measurements are almost similar with significant gains in computational cost. In LS and PH, HCAHC achieved slightly better accuracy than conv-k-NN. This is because the reference sets formed by HCAHC during the second level searches do not contain items of irrelevant classes.

Concerning the SH and KDD dataset, all DRTs built very small CSs. Thus, the k-NN classifiers that were applied on these CSs, were not only accurate but very fast as well. HCAHC and HCAHC-sqrt were able to achieve even higher accuracy levels than all DRTs but, it involves higher computational cost.

All figures show that when the speed-up methods are performed over edited data, they are faster than when they performed over non-edited data. However, in some cases, either the cost gains are not very high or the classification accuracy is significantly reduced. On the other hand, in the cases of MGT, which is a very noisy dataset, editing is a necessary preprocessing procedure for all speed-up methods. In Figure 5, we observe that the cost gains are high, while the classification accuracy is not reduced significantly.

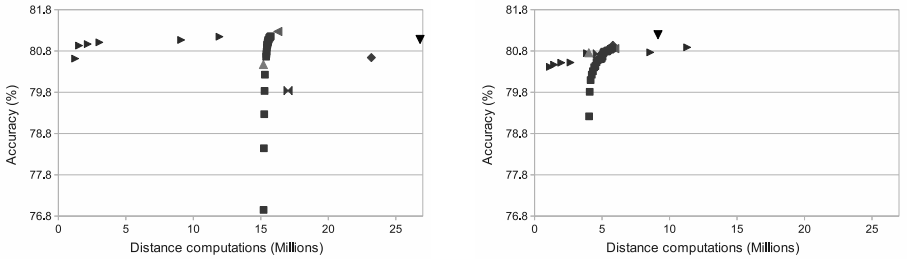
Table 5 Conv-k-NN vs HCAHC over non-edited data

Dataset	**Conv-k-NN**		**HCAHC**		
	Acc(%)	**Cost(M)**	**Acc(%)**	**Cost(M)**	***Rk***
LR	96.01	64.00	95.90	9.41	43
MGT	81.32	57.88	81.27	16.26	63
PD	99.37	19.34	99.33	2.45	20
LS	91.22	6.63	91.25	1.10	15
SH	99.82	538.24	99.82	227.26	29
TXR	99.02	4.84	99.02	0.71	18
PH	90.10	4.67	90.23	1.08	11
KDD	99.71	3202.68	99.71	429.31	10
Avg.	94.5715	487.29	94.5663	85.97	



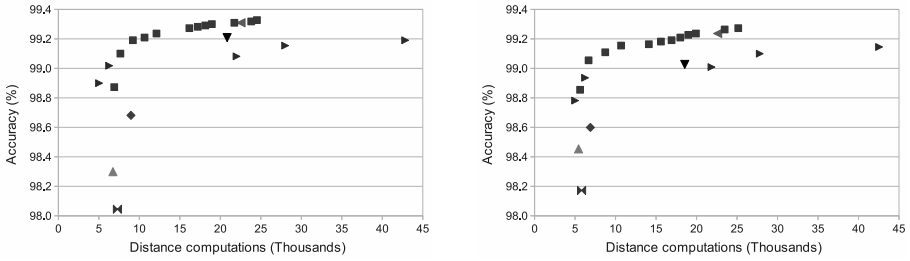
(a) Non-edited data (b) Edited data

Fig. 4 LIR dataset (Accuracy vs Computational cost)



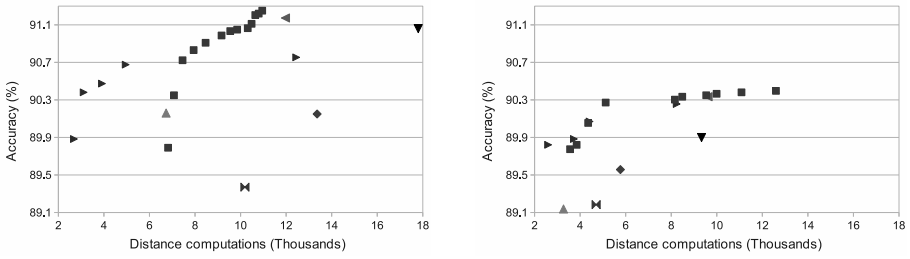
(a) Non-edited data (b) Edited data

Fig. 5 MGT dataset (Accuracy vs Computational cost)



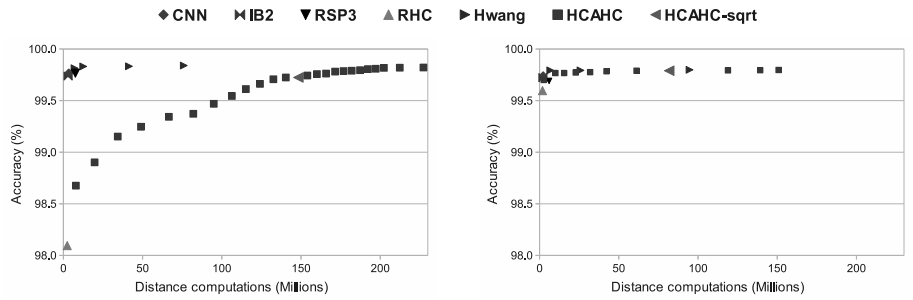
(a) Non-edited data (b) Edited data

Fig. 6 PD dataset (Accuracy vs Computational cost)



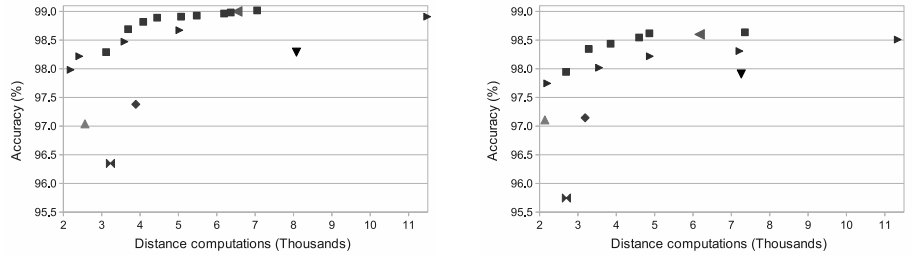
(a) Non-edited data (b) Edited data

Fig. 7 LS dataset (Accuracy vs Computational cost)



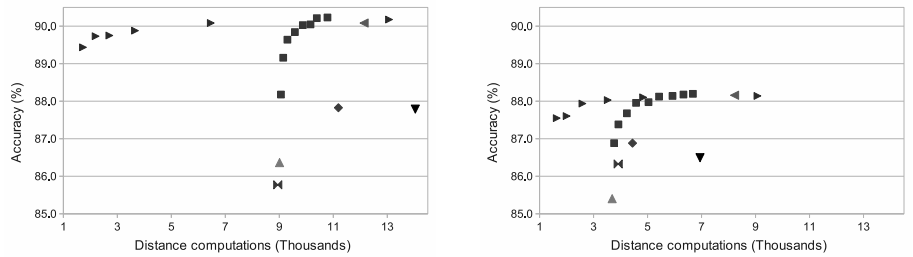
(a) Non-edited data (b) Edited data

Fig. 8 SH dataset (Accuracy vs Computational cost)



(a) Non-edited data (b) Edited data

Fig. 9 TXR dataset (Accuracy vs Computational cost)



(a) Non-edited data (b) Edited data

Fig. 10 PH dataset (Accuracy vs Computational cost)

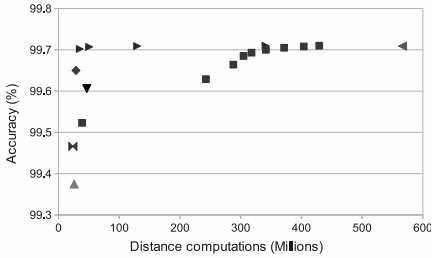


Fig. 11 Non-edited KDD dataset (Accuracy vs Computational cost)

5.1.4 Non parametric statistical test of significance

The experimentation is complemented by the application of a non-parametric statistical test of significance (Sheskin, 2011; García et al, 2009). More specifically, the experimental measurements were validated by the Wilcoxon signed ranks test (Demšar, 2006), which compares each pair of methods taking into consideration their performance in each dataset used. We ran Wilcoxon test considering all comparison criteria as having the same significance. As a consequence, we ran the test on 45 measurements, 24 for non-edited data and 21 for edited data.

Of course, we could not include tests for all variations of HCAHC and Hwang's method (for the different tested values of Rk and i parameters respectively). For each dataset we chose a good representative variation for each one of these parametric algorithms. Our criterion was high performance, i.e., relatively high accuracy and low classification cost (we do take into account the cost of the corresponding preprocessing algorithms). The parameter values for the selected classifiers are shown in Table 6.

Additionally to the parametric HCAHC (HCAHC-Rk), we ran the test for HCAHC-sqrt. Consequently, HCAHC-sqrt and HCAHC-Rk are compared to each one of the four other speed-up methods. Note that the execution of HCAHC implies the execution of SUDSCA during the preprocessing phase. Table 7 illustrates the results of Wilcoxon signed ranks tests. The last table column lists the Wilcoxon significant level. If that value is not higher than 0.05, one can claim that the difference between the pair of methods is significant.

As we expected, there is no statistically significant difference between HCAHC and RHC. Both have the same preprocessing cost, RHC classifiers are faster than HCAHC classifiers, but HCAHC classifiers are more accurate than RHC classifiers. One the other hand, the statistical test confirms that the proposed method performs better than all other methods, with the exception of IB2. In almost all cases (14/15), both HCAHC approaches achieve highest accuracies than IB2. However, they lose slightly in terms of the other two comparison criteria. The test shows that there is not significant difference between HCAHC-sqrt and Hwang-i. However, considering that both preprocessing and classification algorithms of Hwang's method are parametric and SUDSCA and HCAHC-sqrt are not parametric, one concludes that the SUDS model is preferable.

Table 6 Parameter values selected for the Wilcoxon signed ranks test

	LR	**MGT**	**PD**	**LS**	**SH**	**TXR**	**PH**	**KDD**
Non-edited data								
Rk	10	23	6	15	9	5	11	2
i	7	3	7	4	3	5	4	1
Edited data								
Rk	8	17	5	5	2	3	7	-
i	7	5	7	4	1	5	3	-

Table 7 Wilcoxon signed ranks test

Methods	wins/losses/ties	Wilcoxon
HCAHC-sqrt vs CNN	31/14/0	**0.039**
HCAHC-sqrt vs IB2	20/25/0	0.756
HCAHC-sqrt vs RSP3	36/9/0	**0.000**
HCAHC-sqrt vs Hwang-i	26/19/0	0.271
HCAHC-sqrt vs RHC	15/15/15	0.245
HCAHC-Rk vs CNN	33/12/0	**0.003**
HCAHC-Rk vs IB2	21/24/0	0.340
HCAHC-Rk vs RSP3	40/5/0	**0.000**
HCAHC-Rk vs Hwang-i	30/15/0	**0.027**
HCAHC-Rk vs RHC	15/15/15	0,111

5.2 Performance of SUDS classification model over Condensing Sets

5.2.1 Experimental Setup

The second part of our experimentation concerns the performance of SUDS model when applied on CSs. To build the CSs, we executed the four DRTs that we had used in Subsection 5.1, i.e. (i) CNN, (ii) IB2, (iii) RSP3, and (iv) RHC, on the training sets presented in Table 1. Then, we applied SUDS model on the four constructed CSs. Of course SUDS can be combined with any DRT. Once again, we executed all experiments twice on non-edited data and on edited data using ENN-rule. Figure 12 depicts the procedure that we followed during this stage of our experimentation.

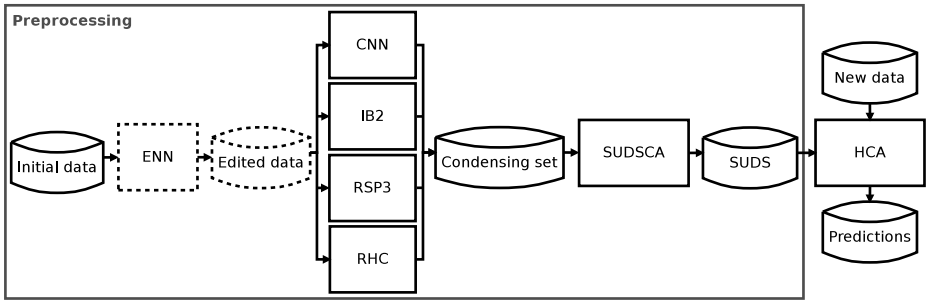


Fig. 12 Classification using SUDS model on the condensing set

During the classification step, we executed HCA (Algorithm 3). Like HCAHC, HCA uses the Rk parameter. We executed several experiments with different Rk parameter values. In addition, we built an HCA classifier that uses the empirical rule: $Rk = \lfloor\sqrt{|SUDS|}\rfloor$. In all cases, this rule was proven to be a good choice for the determination of Rk. For that reason, in the figures presented in Subsection 5.2.3 below, we have included only the performance of the HCA classifier that uses the empirical rule.

Additionally to the performance of HCA, the diagrams presented in subsection 5.2.3 include the performance measurements obtained by the three DRTs (i.e.,

application of k-NN classifier on their CSs). In this way, we can easily conclude whether the SUDS model can significantly improve the performance of the DRTs. Finally, as in Section 5.1, for each method and dataset, we used the k parameter that achieved the highest classification accuracy.

5.2.2 Preprocessing performance

SUDS construction constitutes an extra preprocessing step that is applied after the construction of CS (see Figure 12). Thus, additionally to the cost shown in Tables 4-3, the total preprocessing cost involves the cost overhead of SUDSCA execution. Table 8 shows the preprocessing overheads for each DRT on non-edited and edited training sets.

The computational cost overheads depend on the size of each CS. RSP3 achieved the lowest reduction rates, and so, it involves the highest overhead. In contrast, RHC achieves the highest reduction rates and thus it involves a small overhead. In all cases, overheads added by SUDSCA are almost insignificant. Considering that the preprocessing is executed only once, the small preprocessing overhead does not constitute a problem in real-life data mining applications. Actually, efficient data preprocessing implies fast predictions during the classification step.

Table 8 SUDSCA preprocessing overhead (in millions of distance computations)

Dataset	**Non-edited data**				**Edited data**			
	CNN	**IB2**	**RSP3**	**RHC**	**CNN**	**IB2**	**RSP3**	**RHC**
LR	2.777	2.158	8.489	1.512	1.688	1.478	7.425	1.072
MGT	1.375	0.914	1.577	0.802	0.220	0.159	0.358	0.131
PD	0.072	0.045	0.218	0.035	0.043	0.034	0.161	0.025
LS	0.208	0.122	0.333	0.076	0.054	0.042	0.104	0.025
SH	0.061	0.052	0.188	0.035	0.034	0.028	0.134	0.024
TXR	0.071	0.054	0.243	0.043	0.038	0.035	0.264	0.032
PH	0.102	0.080	0.144	0.083	0.032	0.025	0.055	0.024
KDD	0.323	0.247	0.624	0.285	-	-	-	-
Avg.	0.624	0.459	1.477	0.359	0.301	0.257	1.215	0.190

5.2.3 Classification performance

Figures 13-20 show the performance measurements for the classification stage of our experimentation. Each figure includes two diagrams, one for non-edited and one for edited data. The diagrams show the performance of the three DRTs when using or not using the SUDS model. Each diagram shows the performance of eight classifiers, two for each DRT: (i) k-NN classifier over its CS, (ii) HCA that uses the empirical rule over SUDS.

HCA classifier performed better than k-NN classifier over CSs. An HCA classifier avoids a large number of distance computations and, at the same time, keeps the classification accuracy as high as k-NN classifier. This happens because HCA avoids the distance computations between a new item and items that have been assigned to distant clusters. The performance improvements are significant in both

edited and non-edited datasets. However, they are higher in the case of non-edited data.

For RSP3, the cost gains are higher than those of the other two methods. For instance, in the cases of LIR, PD, SH, TXR datasets, the class labels of the testing items were predicted four or three times faster. The performance improvements for CNN and RHC are not as high but they deserve to be mentioned.

A final comment: SUDS classification model is able to significantly speed-up the predictions of class labels when it is applied on data stored in CSs constructed by DRTs by adding a small cost overhead during the preprocessing phase. This approach is appropriate when extremely fast classification is required.

6 Conclusions

Speeding-up distance based classifiers is a very important issue in data mining. In this paper, we presented and evaluated a new classification model. The motivation of our work was the development of a non-parametric method that has low pre-processing cost and is able to classify new items fast and with high accuracy.

We presented an efficient classification model which includes a non-parametric fast pre-processing algorithm that builds a two-level data structure, and a classifier that makes predictions by accessing this structure. In addition, based on the same motivation, we applied the proposed classification model on data stored in condensing sets constructed by DRTs. The goal of this adoption is to improve the performance of the DRTs. The proposed HCAHC and HCA classifiers are parametric since they use parameter Rk (number of cluster representatives to use in a first level search). However, we demonstrated that Rk can be automatically determined and render the proposed classification model non-parametric. Experimental results based on eight real-life datasets showed that the proposed model achieved the aforementioned goals.

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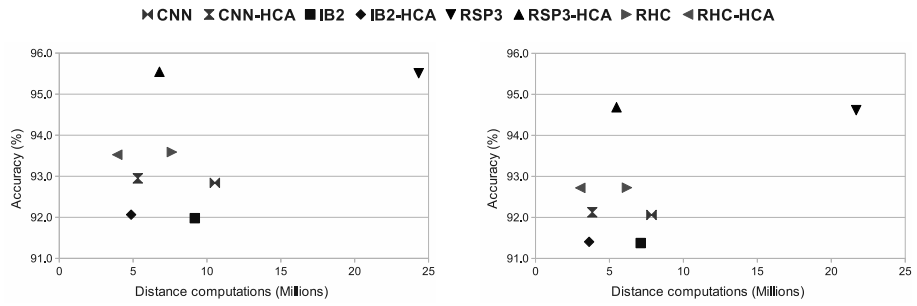
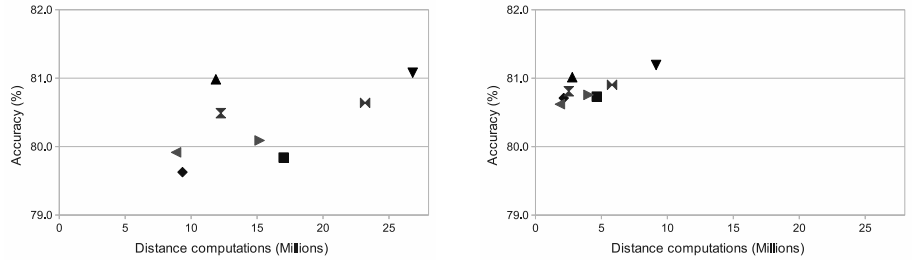


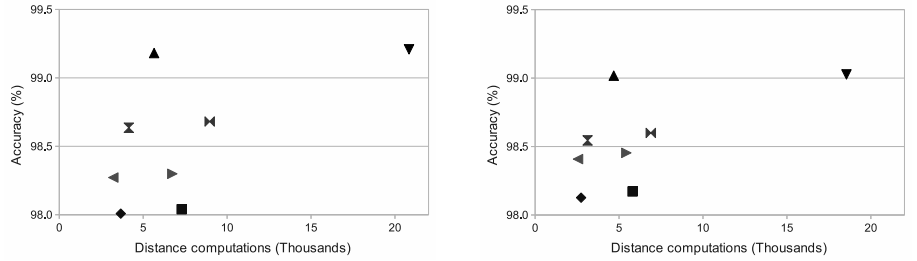
(a) Non-edited data (b) Edited data

Fig. 13 LIR dataset (Accuracy vs Computational cost)



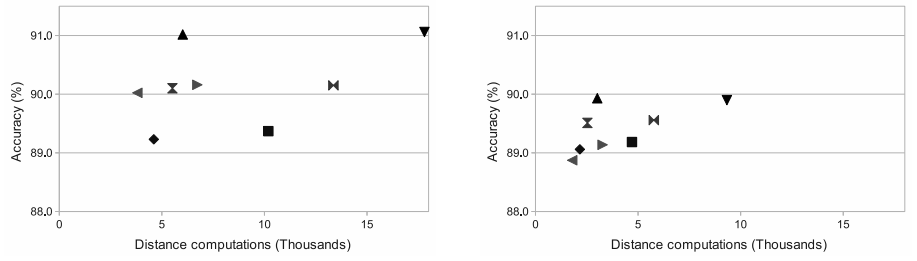
(a) Non-edited data (b) Edited data

Fig. 14 MGT dataset (Accuracy vs Computational cost)



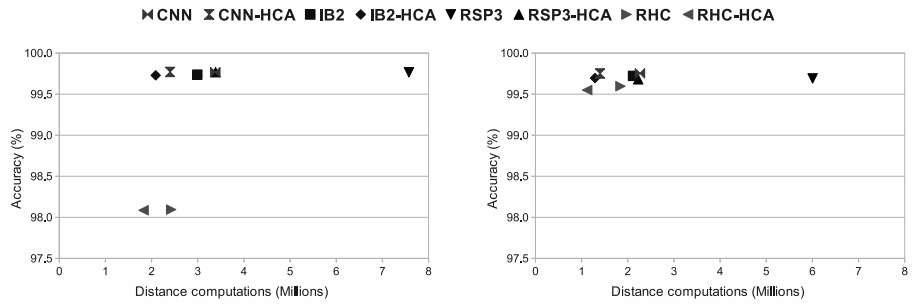
(a) Non-edited data (b) Edited data

Fig. 15 PD dataset (Accuracy vs Computational cost)



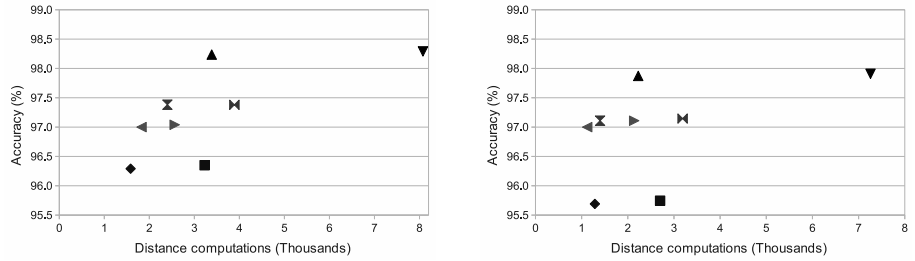
(a) Non-edited data (b) Edited data

Fig. 16 LS dataset (Accuracy vs Computational cost)



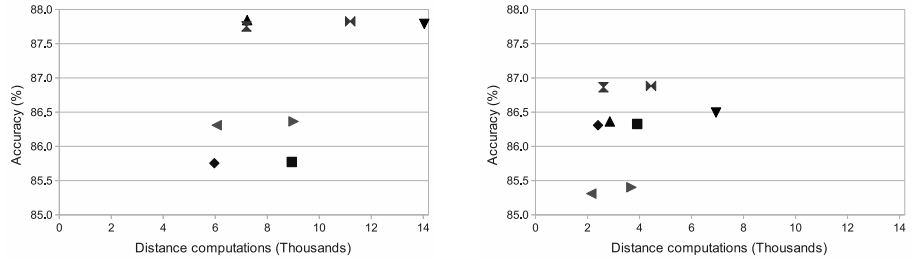
(a) Non-edited data (b) Edited data

Fig. 17 SH dataset (Accuracy vs Computational cost)



(a) Non-edited data (b) Edited data

Fig. 18 TXR dataset (Accuracy vs Computational cost)



(a) Non-edited data (b) Edited data

Fig. 19 PH dataset (Accuracy vs Computational cost)

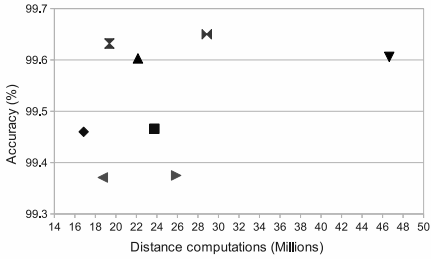


Fig. 20 Non-edited KDD dataset (Accuracy vs Computational cost)

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