



Integrating a differential evolution feature weighting scheme into prototype generation

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ABSTRACT

Prototype generation techniques have arisen as very competitive methods for enhancing the nearest neighbor classifier through data reduction. Within the prototype generation methodology, the methods of adjusting the prototypes' positioning have shown an outstanding performance. Evolutionary algorithms have been used to optimize the positioning of the prototypes with promising results. However, these results can be improved even more if other data reduction techniques, such as prototype selection and feature weighting, are considered.

In this paper, we propose a hybrid evolutionary scheme for data reduction, incorporating a new feature weighting scheme within two different prototype generation methodologies. Specifically, we will focus on a self-adaptive differential evolution algorithm in order to optimize feature weights and the placement of the prototypes. The results are contrasted with nonparametric statistical tests, showing that our proposal outperforms previously proposed methods, thus showing itself to be a suitable tool in the task of enhancing the performance of the nearest neighbor classifier.

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1. Introduction

The designing of classifiers can be considered to be one of the most important tasks in machine learning and data mining [1,2]. Most machine learning methods build a model during the learning process, known as eager learning methods [3], but there are some approaches where the algorithm does not need a model. These algorithms are known as lazy learning methods [4].

The Nearest Neighbor (NN) rule [5] is a simple and effective supervised classification technique which belongs to the lazy learning family of methods. NN is a nonparametric classifier, which requires that all training data instances are stored. Unseen cases are classified by finding the class labels of the closest instances to them. The extended version of NN to k neighbors (k NN) is considered one of the most influential data mining algorithms [6] and it has attracted much attention and research in recent years [7,8]. However, NN may have several disadvantages, such as high computational cost, high storage requirement and sensitivity to noise, which can affect its performance. Furthermore, NN makes predictions over existing data and it

assumes that input data perfectly delimits the decision boundaries among classes.

Many approaches have been proposed to improve the performance of the NN rule. One way to simultaneously tackle the computational complexity, storage requirements, and sensitivity to noise of NN is based on data reduction [9]. These techniques try to obtain a reduced version of the original training data, with the double objective of removing noisy and irrelevant data. Taking into consideration the feature space, we can highlight Feature Selection (FS) [10–13] and feature generation/extraction [14] as the main techniques. FS consists of choosing a representative subset of features from the original feature space, while feature generation creates new features to describe the data. From the perspective of the instances, data reduction can be divided into Prototype Selection (PS) [15–17] and Prototype Generation (PG) [18,19]. The former process consists of choosing an appropriate subset of the original training data, while the latter can also build new artificial prototypes to better adjust the decision boundaries between classes in NN classification. In this way, PG does not assume that input data perfectly defines the decision boundaries among classes.

Another way to improve the performance of NN is the employment of weighting schemes. Feature Weighting (FW) [20] is a well known technique which consists of assigning a weight to each feature of the domain of the problem to modify the way in which distances between examples are computed [21]. This technique

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can be viewed as a generalization of FS algorithms, allowing us to obtain a soft approximation of the feature relevance degree assigning a real value as a weight, so different features can receive different treatments.

Evolutionary algorithms [22] have been successfully used in different data mining problems [23,24]. Given that PS, PG and FW problems could be seen as combinatorial and optimization problems, evolutionary algorithms have been used to solve them with excellent results [25]. PS can be expressed as a binary space search problem. To the best of our knowledge, memetic algorithms [26] have provided the best evolutionary model proposed for PS, called SSMA [27]. PG is expressed as a continuous space search problem. Evolutionary algorithms for PG are based on the positioning adjustment of prototypes [28–30], which is a suitable methodology to optimize the location of prototypes. Concretely, Differential Evolution (DE) [31,32] and its advanced approaches [33] have been demonstrated as being the most effective positioning adjustment techniques [34]. Regarding FW methods, many successful evolutionary proposals, most of them based on genetic algorithms, have been proposed, applied to the NN algorithm [35].

Typically, positioning adjustment methods [28,36,30] focus on the placement process and they do not take into consideration the selection of the most appropriate number of prototypes per class. Recently, two different approaches have been proposed in order to tackle this problem. First, in [37,38], this problem is addressed by an iterative addition process that determines which classes need more prototypes to be represented. This algorithm is denoted as IPADECS. Secondly, in [34], the algorithm SSMA-DEPG is presented, in which a previous PS stage is applied to provide the appropriate choice of the number of prototypes per class.

In these techniques, the increase in the size of the data set is a crucial problem. It has been addressed in PS and PG by using stratification techniques [39,40]. They split the data set into various parts to make the application of a prototype reduction technique easier, using a mechanism to join the solutions of each part into a global solution.

The aim of this work is to propose a hybrid approach which combines these two PG methodologies with FW to enhance the NN rule addressing its main drawbacks. In both schemes, the most promising feature weights and location of the prototypes are generated by the SFLSDE algorithm [41] acting as an FW and PG method respectively. Evolutionary PG methods usually tend to overfit the training data in a small number of iterations. For this reason we apply, during the evolutionary optimization process, an FW stage to modify the fitness function of the PG method and determine the relevance of each feature.

The hybridization of the PG and FW problems is the main contribution of this paper, which can be divided into three objectives:

- To propose a new FW technique based on a self-adaptive DE. To the best of our knowledge, DE has not yet been applied to the FW problem.
- To carry out an empirical study to analyze the hybridization models in terms of classification accuracy. Specifically, we will analyze whether the integration of an FW stage with PG methods improves the quality of the resulting reduced sets.
- To check the behavior of these hybrid approaches when dealing with huge data sets, developing a stratified model with the proposed hybrid scheme.

To test the behavior of these approaches, the experimental study will include a statistical analysis based on nonparametric statistical tests [42]. We shall conduct experiments involving a total of 46 classification data sets with different properties.

In order to organize this paper, Section 2 describes the background of PS, PG, FW, DE and stratification. Section 3 explains the hybridization algorithms proposed. Section 4 discusses the experimental framework and Section 5 presents the analysis of results. Finally, in Section 6 we summarize our conclusions.

2. Background

This section covers the background information necessary to define and describe our proposals. Section 2.1 presents a formal definition of PS and PG problems. Section 2.2 describes the main characteristic of FW. Section 2.3 explains the DE technique. Finally, Section 2.4 details the characteristics of the stratification procedure.

2.1. PS and PG problems

This section presents the definition and notation for both PS and PG problems.

A formal specification of the PS problem is the following: let \mathbf{x}_p be an example where $\mathbf{x}_p = (\mathbf{x}_{p1}, \mathbf{x}_{p2}, \dots, \mathbf{x}_{pD}, \omega)$, with \mathbf{x}_p belonging to a class ω given by $\mathbf{x}_{p\omega}$ and a D -dimensional space in which \mathbf{x}_{pi} is the value of the i -th feature of the p -th sample. Then, let us assume that there is a training set TR which consists of \mathbf{n} instances \mathbf{x}_p and a test set TS composed of \mathbf{t} instances \mathbf{x}_q , with ω unknown. Let $SS \subseteq TR$ be the subset of selected samples resulting from the execution of a PS algorithm, then we classify a new pattern \mathbf{x}_q from TS by the NN rule acting over SS .

The purpose of PG is to obtain a prototype generated set GS , which consists of \mathbf{r} , $\mathbf{r} < \mathbf{n}$, prototypes, which are either selected or generated from the examples of TR . The prototypes of the generated set are determined to efficiently represent the distributions of the classes and to discriminate well when used to classify the training objects. Their cardinality should be sufficiently small to reduce both the storage and evaluation time spent by an NN classifier.

Both methodologies have been widely studied in the specialized literature. More than 50 PS methods have been proposed. In general, they can be categorized into three kinds of methods: condensation [43], edition [44] or hybrid models [27]. A complete review of this topic is proposed in [17]. Regarding PG techniques, they can be divided into several families depending on the main heuristic operation followed: positioning adjustment [30], class re-labeling [45], centroid-based [18] and space-splitting [46]. A recent PG review is proposed in [19].

More information about PS and PG approaches can be found at the SCI2S thematic public website on *Prototype Reduction in Nearest Neighbor Classification: Prototype Selection and Prototype Generation*.¹

2.2. Feature weighting

The aim of FW methods is to reduce the sensitivity to redundant, irrelevant or noisy features in the NN rule, by modifying its distance function with weights. These modifications allow us to perform more robust classification tasks, increasing in this manner the global accuracy of the classifier.

The most well known distance or dissimilarity measure for the NN rule is the Euclidean Distance (Eq. (1)), where x_p and x_q are two examples and D is their number of features. We will use it throughout this study as it is simple, easy to optimize, and has

¹ <http://sci2s.ugr.es/pr/>

been widely used in the field of instance based learning [47]

$$\text{EuclideanDistance}(X, Y) = \sqrt{\sum_{i=0}^D (x_{pi} - x_{qi})^2} \quad (1)$$

FW methods often extend this equation to apply different weights to each feature (W_i) which modify the way in which the distance measure is computed (Eq. (2))

$$\text{FWDist}(X, Y) = \sqrt{\sum_{i=0}^D W_i \cdot (x_{pi} - x_{qi})^2} \quad (2)$$

This technique has been widely used in the literature. As far as we know, the most complete study performed can be found in [20], in which a review of several FW methods for lazy learning algorithms is presented (with most of them applied to improve the performance of the NN rule). In this review, FW techniques were categorized by several dimensions, according to its weight learning bias, the weight space (binary or continuous), the representation of features, their generality and the degree of employment of domain specific knowledge.

A wide number of FW techniques are available in the literature, both classical (see [20]) and recent (for example, [21,35]). The most well known group of them is the family of *Relief-based* algorithms. The Relief algorithm [48] (which was originally an FS method) has been widely studied and modified, producing some interesting versions of the original approach [49]. Some of them are based on ReliefF [50] which is the first step of development of *Relief-based* methods as FW techniques [51].

Finally, it is important to note that it is possible to find some approaches dealing simultaneously with FW and FS tasks, for instance, inside a Tabu Search procedure [52] or by managing ensemble-based approaches [53].

2.3. Differential evolution

DE follows the general procedure of an evolutionary algorithm [33]. DE starts with a population of NP solutions, so-called individuals. The initial population should cover the entire search space as much as possible. In some problems, this is achieved by uniformly randomizing individuals, but in other problems, such as the PG problem, basic knowledge of the problem is available and the use of other initialization mechanisms is more effective. The subsequent generations are denoted by $G = 0, 1, \dots, G_{max}$. In DE, it is common to denote each individual as a D -dimensional vector $X_{i,G} = \{x_{i,G}^1, \dots, x_{i,G}^D\}$, called a “target vector”.

After initialization, DE applies the mutation operator to generate a mutant vector $V_{i,G}$, with respect to each individual $X_{i,G}$, in the current population. For each target $X_{i,G}$, at the generation G , its associated mutant vector $V_{i,G} = \{V_{i,G}^1, \dots, V_{i,G}^D\}$. The method of creating this mutant vector is that which differentiates one DE scheme from another. In this work, we will focus on the *RandToBest/1* which generates the mutant vector as follows:

$$V_{i,G} = X_{i,G} + F \cdot (X_{best,G} - X_{i,G}) + F \cdot (X_{r_1,G} - X_{r_2,G}) \quad (3)$$

The indices r_1, r_2 are mutually exclusive integers randomly generated within the range $[1, NP]$, which are also different from the base index i . The scaling factor F is a positive control parameter for scaling the different vectors.

After the mutation phase, the crossover operation is applied to each pair of the target vector $X_{i,G}$ and its corresponding mutant vector $V_{i,G}$ to generate a new trial vector that we denote $U_{i,G}$. We will focus on the binomial crossover scheme, which is performed on each component whenever a randomly picked number between 0 and 1 is less than or equal to the crossover rate (CR), which controls the fraction of parameter values copied from the

mutant vector. Then, we must decide which individual should survive in the next generation $G+1$. The selection operator is described as follows:

$$X_{i,G+1} = \begin{cases} U_{i,G} & \text{if } \mathcal{F}(U_{i,G}) \text{ is better than } \mathcal{F}(X_{i,G}) \\ X_{i,G} & \text{Otherwise} \end{cases}$$

where \mathcal{F} is the fitness function to be minimized. If the new trial vector yields a solution equal to or better than the target vector, it replaces the corresponding target vector in the next generation; otherwise the target is retained in the population. Therefore, the population always gets better or retains the same fitness values, but never deteriorates. This one-to-one selection procedure is generally kept fixed in most of the DE algorithms.

The success of DE in solving a specific problem crucially depends on choosing the appropriate mutation strategy and its associated control parameter values (F and CR) that determine the convergence speed. Hence, a fixed selection of these parameters can produce slow and/or premature convergence depending on the problem. Thus, researchers have investigated the parameter adaptation mechanisms to improve the performance of the basic DE algorithm [54–56].

One of the most successful adaptive DE algorithms is the Scale Factor Local Search in Differential Evolution (SFLSDE) proposed by [41]. This method was established as the best DE technique for PG in [34].

2.4. Stratification for prototype reduction schemes

When performing data reduction, the scaling up problem appears as the number of training examples increases beyond the capacity of the prototype reduction algorithms, harming their effectiveness and efficiency. This is a crucial problem which must be overcome in most practical applications of data reduction methods. In order to avoid it, in this work we will consider the use of the stratification strategy, initially proposed in [39] for PS, and [40] for PG.

This stratification strategy splits the training data into disjoint strata with equal class distribution. The initial data set D is divided into two sets, TR and TS , as usual (for example a 10th of the data for TS , and the rest for TR in a 10-fold cross validation). Then, TR is divided into t disjoint sets TR_j , strata of equal size, TR_1, TR_2, \dots, TR_t , maintaining class distribution within each subset. In this manner, the subsets TR and TS can be represented as follows:

$$TR = \bigcup_{j=1}^t TR_j, \quad TS = D \setminus TR \quad (4)$$

Then, a prototype reduction method should be applied to each TR_j , obtaining a reduced set RS_j for each partition.

In PS and PG stratification procedures, the final reduced set is obtained joining every RS_j obtained, and it is denoted as Stratified Reduced Set (SRS)

$$\text{SRS} = \bigcup_{j=1}^t RS_j \quad (5)$$

When the SRS has been obtained, it is ready to be used by an NN classifier to classify the instances of TS .

The use of the stratification procedure does not have a great cost in time. Usually, the process of splitting the training data into strata, and joining them when the prototype reduction method has been applied, is not time-consuming, as it does not require any kind of additional processing. Thus, the time needed for the

stratified execution is almost the same as that taken in the execution of the prototype reduction method in each strata, which is significantly lower than the time spent if no stratification is applied, due to the time complexity of the PS and PG methods, which most of the time is $O(N^2)$ or higher.

The prototypes present in *TR* are independent of each other, so the distribution of the data into strata will not degrade their representation capabilities if the class distribution is maintained. The number of strata, which should be fixed empirically, will determine the size of them. By using a proper number it is possible to greatly reduce the training set size. This situation allows us to avoid the drawbacks that appeared due to the *scaling* up problem.

3. Hybrid evolutionary models integrating feature weighting and prototype generation

In this section we describe in depth the proposed hybrid approaches and their main components. First of all, we present the proposed FW scheme based on DE (Section 3.1). Next, as we established previously, we will design a hybrid model with the proposed FW for each of the two most effective PG methodologies, IPAECS [37] (Section 3.2) and SSMA-DEPG [34] (Section 3.3). Finally, we develop a stratified model for our hybrid proposals (Section 3.4).

3.1. Differential evolution for feature weighting

As we stated before, FW can be viewed as a continuous space search problem in which we want to determine the most appropriate weights for each feature in order to enhance the NN rule. Specifically, we propose the use of a DE procedure to obtain the best weights, which allows a given reduced set to increase the performance of the classification made in *TR*. We denote this algorithm as DEFW.

DEFW starts with a population of NP individuals $X_{i,G}$. In order to encode a weight vector in a DE individual, this algorithm uses a real-valued vector containing D elements corresponding to D attributes, which range in the interval $[0,1]$. It means that each individual $X_{i,G}$ in the population encodes a complete solution for the FW problem. Following the ideas established in [54,55,41], the initial population should better cover the entire search space as much as possible by uniformly randomizing individuals within the defined range.

After the initialization process, DEFW enters in a loop in which mutation and crossover operators, explained in Section 2.3, guide the optimization of feature weights by generating new trial vectors $U_{i,G}$. After applying these operators, we check if there have been values out of range of $[0,1]$. If a computed value is greater than 1, we truncate it to 1. Furthermore, based on [48], if this value is lower than a threshold θ , we consider this feature to be irrelevant, and therefore, it is established at 0. In our experiments, θ has been fixed empirically to 0.2.

Finally, the selection operator must decide which generated trial vectors should survive in the population of the next generation $G+1$. For our purpose, the NN rule guides this operator. The instances in *TR* are classified with the prototypes of the reduced set given, but in this case, the distance measure for the NN rule is modified according to Eq. (2), where the weights W_i are obtained from $X_{i,G}$ and $U_{i,G}$. Their corresponding fitness values are measured as the $accuracy(\cdot)$ obtained, which represents the number of successful hits (correct classifications) relative to the total number of classifications. We try to maximize this value, so the

selection operator can be viewed as follows:

$$X_{i,G+1} = \begin{cases} U_{i,G} & \text{if } accuracy(ReducedSet, U_{i,G}) \\ & > = accuracy(ReducedSet, X_{i,G}) \\ X_{i,G} & \text{Otherwise} \end{cases} \quad (6)$$

In case of a tie between the values of accuracy, we select the $U_{i,G}$ in order to give the mutated individual the opportunity to enter the population.

In order to overcome the limitation of the parameters' selection (F and CR), we use the ideas established in [41] to implement a self-adaptive DE scheme.

3.2. IPAECS-DEFW: hybridization with IPAECS

The IPAECS algorithm [37] follows an iterative prototype adjustment scheme with an incremental approach. At each step, an optimization procedure is used to adjust the position of the prototypes, adding new ones if needed. The aim of this algorithm is to determine the most appropriate number of prototypes per class and adjust their positioning during the evolutionary process. Specifically, IPAECS uses the SFLSDE technique as an optimizer with a complete solution per individual codification. At the end of the process, IPAECS returns the best GS found.

The hybrid model which composes IPAECS and DEFW can basically be described as the combination of an IPAECS stage and then a DEFW to determine the best weights. Fig. 1 shows the pseudo-code of this hybrid scheme. The algorithm proceeds as follows:

- Initially, we perform an IPAECS algorithm in which all the features have a relevance degree of 1.0 (Instructions 1–4).
- Then, the algorithm enters in a loop in which we try to find the most appropriate weights and placement of the prototypes:
 - Instruction 6 performs a DE optimization of the feature weights, so that, the best GS obtained from the IPAECS algorithm is used to determine the appropriate weights, as we described in Section 3.1. Furthermore, the current weights are inserted as one of the individuals of the FW population. In this way, we ensure that the FW scheme does not degrade the performance of the GS obtained with IPAECS, due to the selection operator used in DEFW.
 - Next, Instruction 7 generates a new GS , with IPAECS, but in this case, the optimization process takes into consideration the new weights to calculate the distances between prototypes (see Eq. (2)). The underlying idea of this instruction is that IPAECS should generate a different GS due to the fact that the distance measure has changed, and therefore, the continuous search space has been modified.

```

1: Weights [1..D] = 1.0
2: bestWeights [1..D] = Weights [1..D]
3: GS = IPAECS (Weights);
4: Accuracy = Evaluate With Weights (GS, TR, Weights)
5: for i = 1 to MAXITER do
6:   newWeights[1..D] = DEFW (GS, Weights)
7:   GSaux = IPAECS (newWeights)
8:   Accuracytrial = EvaluateWithWeights (GSaux, TR, newWeights)
9:   if Accuracytrial > Accuracy then
10:     Accuracy = Accuracytrial
11:     GS = GSaux
12:   end if
13:   Weights = newWeights
14: end for
15: return GS, Weights

```

Fig. 1. Hybridization of IPAECS and DEFW.

- After this process, we have to ensure that the new positioning of prototypes GS_{aux} with its respective weights has reported a successful improvement of the accuracy rate with respect to the previous GS . If the computed accuracy of the new GS_{aux} and its respective weights is greater than the best accuracy found, we save GS_{aux} as the current GS (Instructions 8–12).
- Instruction 13 stored the obtained weights and they will be used in the next iteration.
- After a previously fixed number of iterations, the hybrid model returns the best GS and its respective best feature weights.

3.3. SSMA-DEPGFW: hybridization with SSMA-DEPG

The SSMA-DEPG approach [34] uses a PS algorithm prior to the adjustment process to initialize a subset of prototypes, finding a promising selection of prototypes per class.

Specifically, the SSMA algorithm is applied [27]. This is a memetic algorithm which makes use of a local search or meme specifically developed for the PS problem. The interweaving of the global and local search phases allows the two to influence each other. The resulting SS is inserted as one of the individuals of the population in the SFLSDE algorithm, which, in this case, is acting as a PG method. Next, it performs mutation and crossover operations to generate new trial solutions. Again, the NN rule guides the selection operator, therefore the SSMA-DEPG returns the best location of the prototypes, which increases the classification rate.

Fig. 2 outlines the hybrid model. To hybridize FW with SSMA-DEPG, this method is carried out as follows:

- Firstly, it is necessary to apply an SSMA stage to determine the number of prototypes per class (Instruction 1).
- Next, the rest of the individuals are randomly generated, extracting prototypes from the TR and keeping the same structure as the SS selected by the PS method, thus they must have the same number of prototypes per class, and the classes must have the same arrangement in the matrix $X_{i,G}$.
- At this stage, we have established the relevance degree of all features to 1.0. Then, Instruction 4 determines the best classification accuracy obtained in the NP population.
- After this, our hybrid model enters into a cooperative loop between FW and SFLSDE.
 - The proposed FW method is applied with the best GS found up to that moment. Once again, the current weights are inserted as one of the individuals of the FW population (Instruction 6).
 - Then, a new optimization stage is applied to all the individuals of the population, with the obtained weights modifying the distance measure between prototypes.
- Finally, the method returns the best GS with its appropriate feature weights, and it is ready to be used as a reference set by the NN classifier.

```

1:  $GS[1] = SSMA()$ ;
2: Generate  $GS[2..NP]$  randomly
   with the prototypes distribution of  $GS[1]$ 
3:  $Weights[1..D] = 1.0$ 
4: Determine the best  $GS$ 
5: for  $i = 1$  to  $MAXITER$  do
6:    $Weights[1..D] = DEFW(GS[best], Weights)$ 
7:    $GS[1..NP] = SFLSDE(GS[1..NP], Weights)$ 
8:   Determine the best  $GS$ 
9: end for
10: return  $GS[best], Weights$ 

```

Fig. 2. Hybridization of SSMA-DEPG and DEFW.

3.4. A stratified scheme for hybrid FW and PG methods

Since the immediate application of these hybrid methods over huge sets should be avoided due to their computational cost, we propose the use of a stratification procedure to mitigate this drawback, and thus develop a suitable approach to huge problems.

PS and PG stratified models join every resulting set RS_j , obtained as the application of these techniques to each strata TR_j . Nevertheless, in the proposed hybrid scheme, we obtain for each strata a generated reduced set and its respective feature weights. To develop a stratified method, we study two different strategies:

- **Join procedure:** In this variant, the SRS is also generated as the sum of each RS_j . However, the weight of each feature is recalculated, applying the DEFW algorithm. In this case, it uses the SRS set as a given reduced set. The stratified method returns SRS and its obtained weights to classify the instances of TS .
- **Voting rule:** This approach consists of applying a majority voting rule. Each strata RS_j and its respective weights are used to calculate the possible class of each instance of TS . The final assigned class is produced via majority voting of the computed class per strata. In our implementation, ties are randomly decided.

4. Experimental framework

In this section, we present the main characteristics related to the experimental study. Section 4.1 introduces the data sets used in this study. Section 4.2 summarizes the algorithms used for comparison with their respective parameters. Finally, Section 4.3 describes the statistical tests applied to contrast the results obtained.

4.1. Data sets

In this study, we have selected 40 classification data sets for the main experimental study. These are well-known problems in the area, taken from the KEEL data set repository² [57]. Table 1 summarizes the properties of the selected data sets. It shows, for each data set, the number of examples (#Ex.), the number of attributes (#Atts.), and the number of classes (#Cl.). The data sets considered in this study contain between 100 and 20 000 instances, and the number of attributes ranges from 2 to 85. In addition, they are partitioned using the 10 fold cross-validation (10-fcv) procedure and their values are normalized in the interval [0,1] to equalize the influence of attributes with different range domains. In addition, instances with missing values have been discarded before the execution of the methods over the data sets.

Furthermore, we will perform an additional experiment applying our hybrid models to six huge data sets, which contain more than 20 000 instances. Table 2 shows their characteristics, including the exact number of strata (#Strata.) and instances per strata (#Instances/Strata.).

4.2. Comparison algorithms and parameters

In order to perform an exhaustive study of the capabilities of our proposals, we have selected some of the main proposed models in the literature of PS, PG and FW. In addition, the NN rule with $k=1$ (1NN) has been included as a baseline limit of performance. Apart from SSMA, IPADECS and SSMA-DEPG, which

² <http://sci2s.ugr.es/keel/datasets>

Table 1
Summary description for classification data sets.

| Data set | #Ex. | #Atts. | #Cl. | Data set | #Ex. | #Atts. | #Cl. |
|---------------|------|--------|------|--------------|--------|--------|------|
| Sbalone | 4174 | 8 | 28 | Lym | 148 | 18 | 4 |
| Banana | 5300 | 2 | 2 | Magic | 19 020 | 10 | 2 |
| Bands | 539 | 19 | 2 | Mammographic | 961 | 5 | 2 |
| Breast | 286 | 9 | 2 | Marketing | 8993 | 13 | 9 |
| Bupa | 345 | 6 | 2 | Monks | 432 | 6 | 2 |
| Chess | 3196 | 36 | 2 | Newthyroid | 215 | 5 | 3 |
| Cleveland | 297 | 13 | 5 | Nursery | 12 690 | 8 | 5 |
| Coil2000 | 9822 | 85 | 2 | Pima | 768 | 8 | 2 |
| Contraceptive | 1473 | 9 | 3 | Ring | 7400 | 20 | 2 |
| Crx | 125 | 15 | 2 | Saheart | 462 | 9 | 2 |
| Dermatology | 366 | 33 | 6 | Spambase | 4597 | 57 | 2 |
| Flare-solar | 1066 | 9 | 2 | Sphearheart | 267 | 44 | 2 |
| German | 1000 | 20 | 2 | splice | 3190 | 60 | 3 |
| Glass | 214 | 9 | 7 | Tae | 151 | 5 | 3 |
| Haberman | 306 | 3 | 2 | Thyroid | 7200 | 21 | 3 |
| Hayes-roth | 133 | 4 | 3 | Titanic | 2201 | 3 | 2 |
| Heart | 270 | 13 | 2 | Twonorm | 7400 | 20 | 2 |
| Housevotes | 435 | 16 | 2 | Wisconsin | 683 | 9 | 2 |
| Iris | 150 | 4 | 3 | Yeast | 1484 | 8 | 10 |
| led7digit | 500 | 7 | 10 | Zoo | 101 | 16 | 7 |

Table 2
Summary description for huge classification data sets.

| Data set | #Ex. | #Atts. | #Cl. | #Strata. | #Instances/strata. |
|-----------|---------|--------|------|----------|--------------------|
| Adult | 48 842 | 14 | 2 | 10 | 4884 |
| Census | 299 285 | 41 | 2 | 60 | 4990 |
| Connect-4 | 67 557 | 42 | 3 | 14 | 4826 |
| Fars | 100 968 | 29 | 8 | 20 | 5048 |
| Letter | 20 000 | 16 | 26 | 4 | 5000 |
| Shuttle | 58 000 | 9 | 7 | 12 | 4833 |

have been explained above, the rest of the methods are described as follows:

- **TSKNN**: A Tabu search based method for simultaneous FS and FW, which encodes in its solutions the current set of features selected (binary codification), the current set of weights assigned to features, and the best value of k found for the kNN classifier. Furthermore, this method uses fuzzy kNN [58] to avoid ties in the classification process [52].
- **ReliefF**: The first *Relief-based* method adapted to perform the FW process [50]. Weights computed in the original Relief algorithm are not binarized to 0, 1. Instead, they are employed as final weights for the kNN classifier. This method was marked as the best *performance-based* FW method in [20].
- **GOCBR**: A genetic algorithm designed for simultaneous PS and FW process in the same chromosome. Weights are represented by binary chains, thus preserving binary codification in the chromosomes. It has been applied successfully to several real-world applications [59].

Many different configurations are established by the authors of each paper for the different techniques. We focus this experimentation on the recommended parameters proposed by their respective authors, assuming that the choice of the values of the parameters was optimally chosen. The configuration parameters, which are common to all problems, are shown in Table 3. In all of the techniques, Euclidean distance is used as a similarity function and those which are stochastic methods have been run three times per partition. Note that the values of the parameters F_i , F_u , $iterSFGSS$ and $iterSFHC$ remain constant in all the DE optimizations, and are the recommended values established in [41]. Implementations of the algorithms can be found in the KEEL software tool [57].

Table 3
Parameter specification for all the methods used in the experimentation.

| Algorithm | Parameters |
|--------------|--|
| SSMA | Population=30, Evaluations=10 000, Crossover Probability=0.5, Mutation Probability=0.001 |
| SSMA-DEPG | PopulationSFLSDE=40, IterationsSFLSDE=500, iterSFGSS=8, iterSFHC=20, $F_l=0.1$, $F_u=0.9$ |
| IPADECS | Population=10, iterations of Basic DE=500, iterSFGSS=8, iterSFHC=20, $F_l=0.1$, $F_u=0.9$ |
| TSKNN | Evaluations=10 000, $M=10$, $N=2$, $P=\text{ceil}(\sqrt{\#Features})$ |
| ReliefF | K value for contributions=Best in [1,20] |
| GOCBR | Evaluations=10 000, Population=100, Crossover Probability=0.7, Mutation Probability=0.1 |
| SSMA-DEPGFW | $MAXITER=20$, PopulationSFLSDE=40, IterationsSFLSDE=50, PopulationDEFW=25, IterationsDEFW=200, iterSFGSS=8, iterSFHC=20, $F_l=0.1$, $F_u=0.9$ |
| IPADECS-DEFW | $MAXITER=20$, PopulationIPADECS=10, iterations of Basic DE=50, PopulationDEFW=25, IterationsDEFW=200, iterSFGSS=8, iterSFHC=20, $F_l=0.1$, $F_u=0.9$ |

4.3. Statistical tools for analysis

Hypothesis testing techniques provide us with a way to statistically support the results obtained in the experimental study, identifying the most relevant differences found between the methods [60]. To this end, the use of nonparametric tests will be preferred over parametric ones, since the initial conditions that guarantee the reliability of the latter may not be satisfied, causing the statistical analysis to lose credibility.

We will focus on the use of the Friedman Aligned-ranks (FA) test [42], as a tool for contrasting the behavior of each of our proposals. Its application will allow us to highlight the existence of significant differences between methods. Later, post hoc procedures like Holm's or Finner's will find out which algorithms are distinctive among the $1:n$ comparisons performed. Furthermore, we will use the Wilcoxon Signed-Ranks test in those cases in which we analyze differences between pairs of methods not marked as significant by the previous tests.

More information about these tests and other statistical procedures specifically designed for use in the field of Machine Learning can be found at the SCI2S thematic public website on *Statistical Inference in Computational Intelligence and Data Mining*.³

5. Analysis of results

In this section, we analyze the results obtained from different experimental studies. Specifically, our aims are:

- To compare the proposed hybrid schemes to each other over the 40 data sets (Section 5.1).
- To test the performance of these models in comparison with previously proposed methods (Section 5.2).
- To check if the performance of hybrid models is maintained with huge data sets using the proposed stratified model (Section 5.3).

5.1. Comparison of the proposed hybrid schemes

We focus this experiment on comparing both hybrid schemes in terms of accuracy and reduction capabilities. Fig. 3 shows a star plot in which the obtained accuracy test of IPADECS-DEFW and SSMA-DEPGFW is presented for each data set, allowing us to see in an easier way how both algorithms behave in the same domains.

³ <http://sci2s.ugr.es/sicidm/>

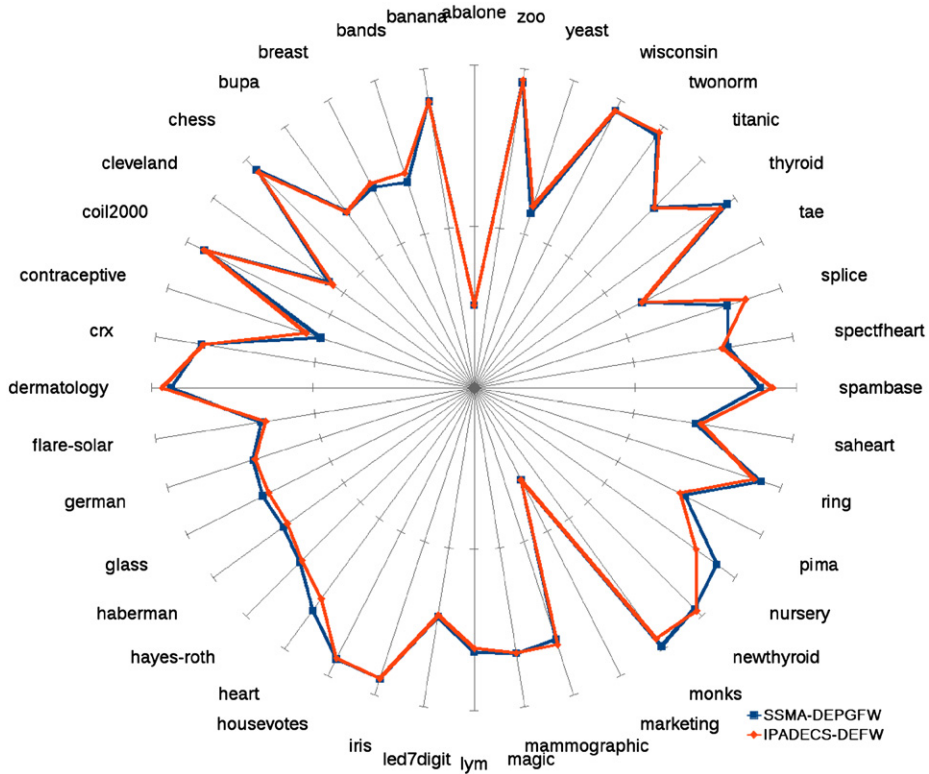


Fig. 3. Accuracy rate comparison.

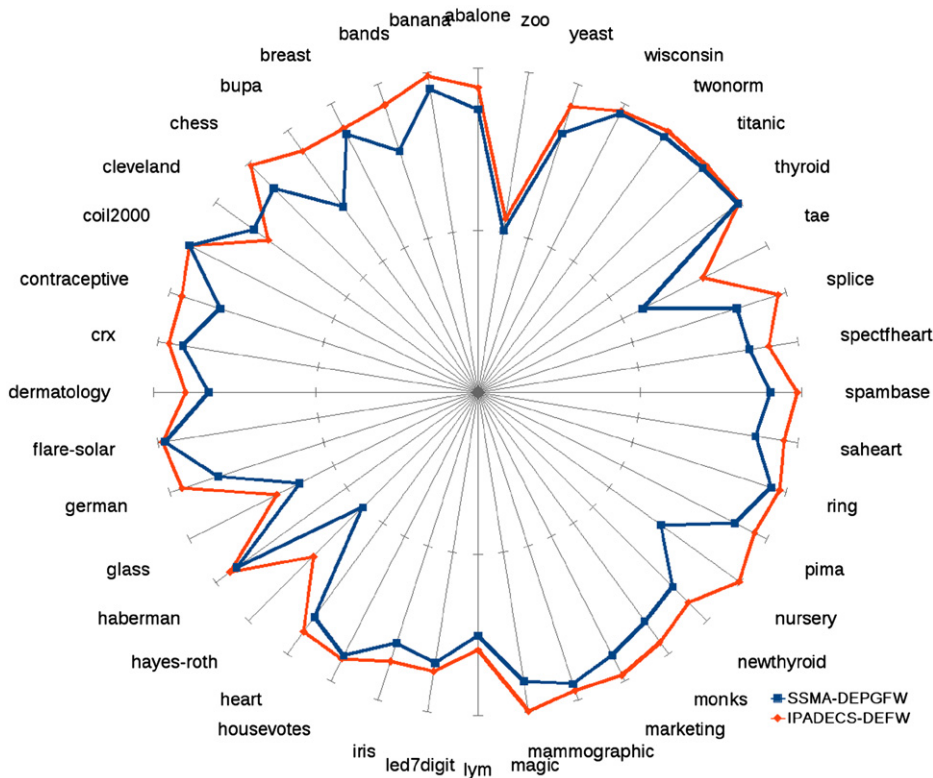


Fig. 4. Reduction rate comparison.

The reduction rate is defined as

$$Reduction\ Rate = 1 - \frac{size(GS)}{size(TR)} \quad (7)$$

It has a strong influence on the efficiency of the solutions obtained, due to the cost of the final classification process performed

by the 1NN classifier. Fig. 4 illustrates a star plot representing the reduction rate obtained in each data set for both hybrid models. These star plots represent the performance as the distance from the center; hence a higher area determines the best average performance. The plots allow us to visualize the

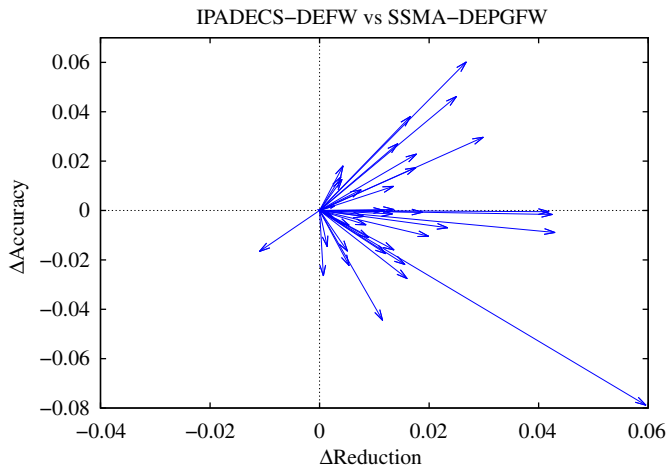


Fig. 5. Accuracy/reduction rates comparison.

Table 4
Results of the Wilcoxon signed-ranks test comparing hybrid schemes.

| Comparison | R+ | R– | p-Value |
|-----------------------------|-----|-----|---|
| <i>Accuracy rate</i> | | | |
| SSMA-DEPGFW vs IPADECS-DEFW | 442 | 338 | 0.4639 |
| <i>Reduction rate</i> | | | |
| IPADECS-DEFW Vs SSMA-DEPGFW | 802 | 18 | 4.602×10^{-10} |

performance of the algorithms comparatively for each problem and in general.

Fig. 5 shows a graphical comparison between these methods considering both objectives simultaneously (accuracy and reduction rate), by using a relative movement diagram [61]. The idea of this diagram is to represent with an arrow the results of two methods on each data set. The arrow starts at the coordinate origin and the coordinates of the tip of the arrow are given by the difference between the reduction (x -axis) and accuracy (y -axis) of IPADECS-DEFW and SSMA-DEPGFW, in this order. Furthermore, numerical results will be presented later in Tables 5 and 6.

Apart from these figures, we use the Wilcoxon test to statistically compare our proposals in both measures. Table 4 collects the results of its application to the accuracy and reduction rates. This table shows the rankings $R+$ and $R-$ values achieved and its associate p -value.

Observing Figs. 3–5 and Table 4 we want to make some comments:

- Fig. 3 shows that both proposals present similar behavior in many domains. Nevertheless, SSMA-DEPGFW obtains the best average result in 24 of the 40 data sets. The Wilcoxon test confirms this statement, showing that there are no significant differences between both approaches and the $R+$ is greater for SSMA-DEPGFW.
- In terms of reduction capabilities, IPADECS-DEFW is shown to be the best performing hybrid model. As the Wilcoxon test reports, it obtains significant differences with respect to SSMA-DEPGFW.
- In Fig. 5, we observe that most of the arrows point out to the right side of the plot. This means that IPADECS-DEFW obtains a lower reduction rate in the problems addressed. Moreover, there are a similar number of arrows pointing up-right and down-left, depicting that the accuracy of both methods is similar. Hence, we can state that IPADECS-DEFW finds the best trade-off between accuracy and reduction rate.

5.2. Comparison with previously proposed methods

In this subsection we perform a comparison between the two proposed hybrid models and the comparison methods established above. We analyze the results obtained in terms of the accuracy in test data and reduction rate.

Table 5 shows the accuracy test results for each method considered in the study. For each data set, the mean accuracy (Acc) and the standard deviation (SD) are computed. The best result for each column is highlighted in bold. The last row presents the average considering all the data sets.

Table 6 presents the reduction rate achieved. Reduction rates are only shown for those methods which perform a relevant reduction of the instances of the TR . In this table we can observe that those methods which are based on SSMA obtain the same average reduction rate. This is due to the fact that SSMA is used to obtain the appropriate number of prototypes per class, determining the reduction capabilities at the beginning of the hybrid models: SSMA-DEPG and SSMA-DEPGFW. IPADECS and IPADECS-DEFW obtains slightly different reduction rates because they use the same PG approach changing the fitness function with weights.

To verify the performance of each of our proposals, we have divided the nonparametric statistical study into two different parts. Firstly, we will compare IPADECS-DEFW and SSMA-DEPGFW with the rest of the comparison methods separately (excluding the other proposal) in terms of test accuracy.

Tables 7 and 8 present the results of the FA test for IPADECS-DEFW and SSMA-DEPGFW respectively. In these tables, the computed FA rankings, which represent the associated effectiveness, are presented in the second column. Both tables are ordered from the best (lowest) to the worst (highest) ranking. The third column shows the adjusted p -value (APV) with Holm's test. Finally, the fourth column presents the APV with Finner's test. Note that IPADECS-DEFW and SSMA-DEPGFW are established as control algorithms because they have obtained the best FA ranking in their respective studies. Those APVs highlighted in bold are methods outperformed by the control, at an $\alpha = 0.1$ level of significance.

In this study, we have observed that hybrid schemes perform well with large data sets (those data sets that have more than 2000 instances). We select large data sets, from Table 1, and we compare weighted and unweighted proposals. Fig. 6 shows this comparison. The x -axis position of the point is the accuracy of the original proposal on a single data set, and the y -axis position is the accuracy of the weighted algorithm. Therefore, points above the $y=x$ line correspond to data sets for which new proposals perform better than the original algorithm.

Given Fig. 6 and the results shown before, we can make the following analysis:

- SSMA-DEPGFW and IPADECS-DEFW achieve the best average results. It is important to note that the two hybrid models clearly outperform the methods upon which they are based. The good synergy between PG and FW methods is demonstrated with the obtained results. Specifically, if we focus our attention on those data sets with a large number of features (see splice, chess, etc.), we can state that, in general, the hybridization between PG and a DEFW scheme can be useful to increase the classification accuracy obtained.
- Furthermore, Fig. 6 shows that the proposed weighted algorithms are able to overcome, in most cases, the original proposal when dealing with large data sets.
- Both SSMA-DEPGFW and IPADECS-DEFW achieve the lowest (best) ranking in the comparison. The p -value of the FA test is

Table 6
Reduction rates obtained.

| Data sets | SSMA | SSMA-DEPG | SSMA-DEPGFW | IPADECs | IPADECs DEFw |
|---------------|--------|-----------|-------------|---------------|--------------|
| Abalone | 0.9749 | 0.9749 | 0.9749 | 0.9886 | 0.9882 |
| Banana | 0.9900 | 0.9900 | 0.9900 | 0.9981 | 0.9981 |
| Bands | 0.9567 | 0.9567 | 0.9567 | 0.9872 | 0.9866 |
| Breast | 0.9790 | 0.9790 | 0.9790 | 0.9820 | 0.9829 |
| Bupa | 0.9417 | 0.9417 | 0.9417 | 0.9848 | 0.9842 |
| Chess | 0.9782 | 0.9782 | 0.9782 | 0.9981 | 0.9981 |
| Cleveland | 0.9710 | 0.9710 | 0.9710 | 0.9600 | 0.9600 |
| Coil2000 | 0.9999 | 0.9999 | 0.9999 | 0.9997 | 0.9997 |
| Contraceptive | 0.9672 | 0.9672 | 0.9672 | 0.9926 | 0.9922 |
| Crx | 0.9844 | 0.9844 | 0.9844 | 0.9929 | 0.9929 |
| Dermatology | 0.9663 | 0.9663 | 0.9663 | 0.9806 | 0.9806 |
| Flare-solar | 0.9955 | 0.9955 | 0.9955 | 0.9969 | 0.9969 |
| German | 0.9686 | 0.9686 | 0.9686 | 0.9940 | 0.9920 |
| Glass | 0.9237 | 0.9237 | 0.9237 | 0.9393 | 0.9393 |
| Haberman | 0.9840 | 0.9840 | 0.9840 | 0.9904 | 0.9891 |
| Hayes-roth | 0.9006 | 0.9006 | 0.9006 | 0.9436 | 0.9436 |
| Heart | 0.9716 | 0.9716 | 0.9716 | 0.9853 | 0.9831 |
| Housevotes | 0.9826 | 0.9826 | 0.9826 | 0.9849 | 0.9849 |
| Iris | 0.9630 | 0.9630 | 0.9630 | 0.9748 | 0.9748 |
| Led7digit | 0.9693 | 0.9693 | 0.9693 | 0.9747 | 0.9747 |
| Lym | 0.9504 | 0.9504 | 0.9504 | 0.9594 | 0.9594 |
| Magic | 0.9808 | 0.9808 | 0.9808 | 0.9996 | 0.9996 |
| Mammographic | 0.9895 | 0.9895 | 0.9895 | 0.9938 | 0.9938 |
| Marketing | 0.9825 | 0.9825 | 0.9825 | 0.9961 | 0.9961 |
| Monks | 0.9750 | 0.9750 | 0.9750 | 0.9910 | 0.9910 |
| Newthyroid | 0.9700 | 0.9700 | 0.9700 | 0.9835 | 0.9835 |
| Nursery | 0.9396 | 0.9396 | 0.9396 | 0.9992 | 0.9992 |
| Pima | 0.9780 | 0.9780 | 0.9780 | 0.9916 | 0.9916 |
| Ring | 0.9902 | 0.9902 | 0.9902 | 0.9956 | 0.9956 |
| Saheart | 0.9735 | 0.9735 | 0.9735 | 0.9931 | 0.9911 |
| Spambase | 0.9805 | 0.9805 | 0.9805 | 0.9971 | 0.9971 |
| Spectfheart | 0.9696 | 0.9696 | 0.9696 | 0.9817 | 0.9817 |
| Splice | 0.9679 | 0.9679 | 0.9679 | 0.9947 | 0.9947 |
| Tae | 0.9139 | 0.9139 | 0.9139 | 0.9558 | 0.9558 |
| Thyroid | 0.9982 | 0.9982 | 0.9982 | 0.9992 | 0.9989 |
| Titanic | 0.9960 | 0.9960 | 0.9960 | 0.9990 | 0.9987 |
| Twonorm | 0.9952 | 0.9952 | 0.9952 | 0.9993 | 0.9993 |
| Wisconsin | 0.9932 | 0.9932 | 0.9932 | 0.9951 | 0.9951 |
| Yeast | 0.9681 | 0.9681 | 0.9681 | 0.9858 | 0.9858 |
| Zoo | 0.9010 | 0.9010 | 0.9010 | 0.9086 | 0.9086 |
| Average | 0.9695 | 0.9695 | 0.9695 | 0.9842 | 0.9840 |

Table 7
Average FA rankings of IPADECs-DEFw and the rest of the comparison methods.

| Algorithm | FA ranking | Holm APV | Finner APV |
|--------------|------------|---------------|---------------|
| IPADECs-DEFw | 97.6750 | – | – |
| SSMA-DEPG | 106.8875 | 0.6561 | 0.6561 |
| IPADECs | 133.9000 | 0.1599 | 0.0926 |
| SSMA | 149.0250 | 0.0392 | 0.0182 |
| TSKNN | 153.1375 | 0.0294 | 0.0128 |
| GOCBR | 190.4875 | 0 | 0 |
| Relieff | 209.0500 | 0 | 0 |
| 1NN | 243.8375 | 0 | 0 |

p -Value by the FA test = 9.915×10^{-6} .

reduction rate achieved for each method. In this table, both IPADECs-DEFw variants obtain the same average reduction rate.

In Table 10, we observe that the IPADECs-DEFw model with the join procedure has obtained the best average accuracy result. The Wilcoxon test has been conducted comparing this method with the rest. Table 12 shows the results of its application.

As in the former study, IPADECs-DEFw obtains a slightly lower reduction power than IPADECs as we can see in Table 11.

Observing these tables, we can summarize that with an appropriate stratification procedure, the idea of combining PG and FW is also applicable to huge data sets, obtaining good

Table 8
Average FA rankings of SSMA-DEPGFW and the rest of the comparison methods.

| Algorithm | FA ranking | Holm APV | Finner APV |
|-------------|------------|---------------|---------------|
| SSMA-DEPGFW | 93.8875 | – | – |
| SSMA-DEPG | 108.0750 | 0.4929 | 0.4929 |
| IPADECs | 133.5250 | 0.1107 | 0.0643 |
| SSMA | 149.5250 | 0.0215 | 0.0100 |
| TSKNN | 155.2250 | 0.0121 | 0.0053 |
| GOCBR | 190.8000 | 0 | 0 |
| Relieff | 208.7250 | 0 | 0 |
| 1NN | 244.2375 | 0 | 0 |

p -Value by the FA test = 9.644×10^{-6} .

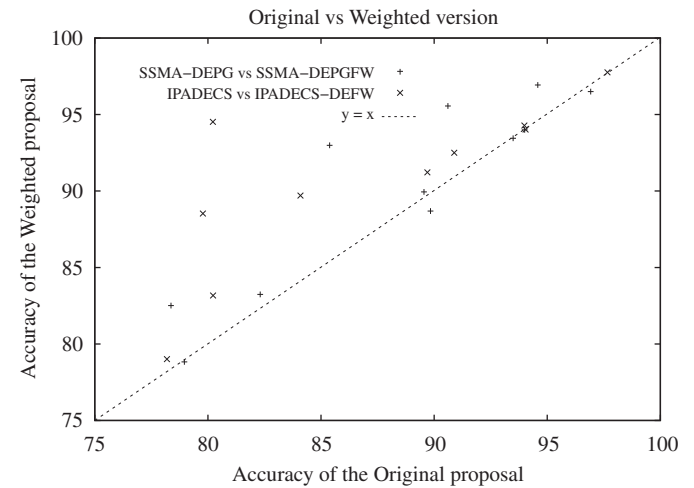


Fig. 6. Accuracy results over large data sets.

Table 9
Results of the Wilcoxon signed-ranks test.

| Comparison | R+ | R– | p -Value |
|---------------------------|-------|-------|---------------|
| SSMA-DEPGFW vs SSMA-DEPG | 586.5 | 233.5 | 0.0469 |
| IPADECs-DEFw vs SSMA-DEPG | 521 | 259 | 0.0682 |

results. The Wilcoxon test supports this statement, showing that IPADECs-DEFw, with the join procedure, is able to significantly outperform IPADECs, SSMA-DEPG and 1NN to a level of $\alpha = 0.1$.

6. Conclusions

In this paper, we have introduced a novel data reduction technique which exploits the cooperation between FW and PG to improve the classification performance of the NN, storage requirements and its running time. A self-adaptive DE algorithm has been used to optimize feature weights and the positioning of the prototypes for the nearest neighbor algorithm, acting as an FW scheme and a PG method, respectively.

The proposed DEFw scheme has been incorporated within two of the most promising PG methods. These hybrid models are able to overcome isolated PG methods due to the fact that FW changes the way in which distances between prototypes are measured, and therefore the adjustment of prototypes can be more refined. Furthermore, we have proposed a stratified procedure specifically designed to deal with huge data sets.

The wide experimental study performed has allowed us to contrast the behavior of these hybrid models when dealing with a wide variety of data sets with different numbers of instances and

Table 10
Accuracy test results in huge data sets.

| Data sets | 1NN | | IPADECs | | SSMA-DEPG | | IPADECs-DEFW | | IPADECs-DEFW | |
|----------------|---------------|--------|---------|--------|-----------|--------|---------------|--------|---------------|--------|
| | Acc | SD | Acc | SD | Acc | SD | Join | | Voting rule | |
| | | | | | | | Acc | SD | Acc | SD |
| Adult | 0.7960 | 0.0035 | 0.8263 | 0.0032 | 0.8273 | 0.0098 | 0.8335 | 0.0077 | 0.8313 | 0.0031 |
| Census | 0.9253 | 0.0010 | 0.9439 | 0.0005 | 0.9460 | 0.0009 | 0.9477 | 0.0007 | 0.9428 | 0.0300 |
| Connect-4 | 0.6720 | 0.0036 | 0.6569 | 0.0009 | 0.6794 | 0.0061 | 0.6847 | 0.0058 | 0.6624 | 0.0045 |
| Fars | 0.7466 | 0.0034 | 0.7439 | 0.0218 | 0.7625 | 0.0036 | 0.7676 | 0.0039 | 0.7536 | 0.0033 |
| Letter | 0.9592 | 0.0002 | 0.9420 | 0.0082 | 0.9053 | 0.0082 | 0.9632 | 0.0121 | 0.9699 | 0.0075 |
| Shuttle | 0.9993 | 0.0004 | 0.9941 | 0.0021 | 0.9967 | 0.0021 | 0.9967 | 0.0008 | 0.9967 | 0.0015 |
| Average | 0.8497 | 0.0020 | 0.8512 | 0.0061 | 0.8529 | 0.0051 | 0.8656 | 0.0052 | 0.8595 | 0.0083 |

Table 11
Reduction rate results in huge data sets.

| Data sets | IPADECs | SSMA-DEPG | IPADECs-DEFW | IPADECs-DEFW |
|-----------|---------------|-----------|---------------|---------------|
| | | | Join | Voting rule |
| Adult | 0.9986 | 0.9882 | 0.9986 | 0.9986 |
| Census | 0.9994 | 0.9973 | 0.9987 | 0.9987 |
| Connect-4 | 0.9990 | 0.9822 | 0.9981 | 0.9981 |
| Fars | 0.9968 | 0.9808 | 0.9957 | 0.9957 |
| Letter | 0.9924 | 0.9805 | 0.9901 | 0.9901 |
| Shuttle | 0.9986 | 0.9981 | 0.9971 | 0.9971 |
| Average | 0.9975 | 0.9878 | 0.9964 | 0.9964 |

Table 12
Results obtained by the Wilcoxon test for algorithm IPADECs-DEFW join.

| IPADECs-DEFW join VS | R+ | R– | p-Value |
|--------------------------|------|-----|---------------|
| 1NN | 20.0 | 1.0 | 0.0625 |
| IPADECs | 21.0 | 0.0 | 0.0312 |
| SSMA-DEPG | 15.0 | 0.0 | 0.0625 |
| IPADECs-DEFW voting rule | 12.0 | 3.0 | 0.1775 |

features. The proposed stratified procedure has shown that this technique is useful to tackle the scaling up problem. The results have been compared with several nonparametric statistical procedures, which have supported the conclusions drawn.

As future work, we consider that this methodology could be extended by using different learning algorithms such as support vector machines, decision trees, and so on, following the guidelines given in similar studies for training set selection [62–64].

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