A Taxonomy and Experimental Study on Prototype Generation for Nearest Neighbor Classification

Isaac Triguero, Joaquín Derrac, Salvador García, Francisco Herrera

Abstract—The nearest neighbor rule is one of the most successfully used techniques for resolving classification and pattern recognition tasks. Despite its high classification accuracy, this rule suffers from several shortcomings in time response, noise sensitivity and high storage requirements. These weaknesses have been tackled from many different approaches, among them, a good and well-known solution that we can find in the literature consists of reducing the data used for the classification rule (training data). Prototype reduction techniques can be divided into two different approaches, known as prototype selection and prototype generation or abstraction. The former process consists of choosing a subset of the original training data, whereas prototype generation builds new artificial prototypes to increase the accuracy of the nearest neighbor classification.

In this paper we provide a survey of prototype generation methods specifically designed for the nearest neighbor rule. From a theoretical point of view, we propose a taxonomy based on the main characteristics presented in them. Furthermore, from an empirical point of view, we conduct a wide experimental study which involves small and large data sets for measuring their performance in terms of accuracy and reduction capabilities. The results are contrasted through non-parametrical statistical tests. Several remarks are made to understand which prototype generation models are appropriate for application to different data sets.

Index Terms—Prototype generation, nearest neighbor, taxonomy, classification, learning vector quantization.

I. INTRODUCTION

T HE Nearest Neighbors algorithm (NN) [1] and its derivatives have been shown to perform well, like a nonparametric classifier, in machine learning and data mining (DM) tasks [2]–[4]. It is included in a more specific field of DM known as lazy learning [5], which refers to the set of methods that predict the class label from raw training data and do not obtain learning models. Although NN is a simple technique, it has demonstrated itself to be one of the most interesting and effective algorithms in DM [6] and pattern recognition [7] and it has been considered one of the top ten methods in DM [8]. A wide range of new real problems have been stated as classifications problems [9], [10], where NN has been a great support for them, for instance [11], [12].

The most intuitive approach to pattern classification is based on the concept of similarity [13]–[15], obviously, patterns that are similar, in some sense, have to be assigned to the same class. The classification process involves partitioning samples into training and testing categories. Let \mathbf{x}_p be a training sample from n available samples in the training set. Let \mathbf{x}_t be a test sample, and let ω be the true class of a training sample and $\hat{\omega}$ be the predicted class for a test sample ($\omega, \hat{\omega} = 1, 2, ..., \Omega$). Here, Ω is the total number of classes. During the training process, we use only the true class ω of each training sample to train the classifier, while during testing we predict the class $\hat{\omega}$ of each test sample. With the 1NN rule, the predicted class of test sample \mathbf{x}_t is set equal to the true class ω of its nearest neighbor, where \mathbf{n}_t is a nearest neighbor to \mathbf{x}_t if the distance

$$d(\mathbf{nn}_t, \mathbf{x}_t) = \min_i \{ d(\mathbf{nn}_i, \mathbf{x}_t) \}.$$

For NN, the predicted class of test sample \mathbf{x}_t is set equal to the most frequent true class among k nearest training samples. This forms the decision rule $D : \mathbf{x}_t \to \hat{\omega}$.

Despite its high classification accuracy, it is well known that NN suffers from several drawbacks [4]. Four weaknesses could be mentioned as the main causes that prevent the successful application of this classifier. The first one is the necessity of high storage requirements in order to retain the set of examples which defines the decision rule. Furthermore, storing all of the data instances also leads to high-computational costs during the calculation of the decision rule, caused by multiple computations of similarities between the test and training samples. Regarding the third one, NN (especially 1NN) presents low tolerance to noise, due to the fact that it considers all data relevant even when the training set may contain incorrect data. Finally, NN makes predictions over existing data and it assumes that input data perfectly delimits the decision boundaries among classes.

Several approaches have been suggested and studied in order to tackle the drawbacks mentioned above [16]. The research on similarity measures to improve the effectiveness of NN (and other related techniques based on similarities) is very extensive in the literature [15], [17], [18]. Other techniques reduce overlapping between classes [19] based on local probability centers, increasing the tolerance to noise. Researchers also investigate about distance functions suitable for use under high dimensionality conditions [20].

A successful technique which simultaneously tackles the computational complexity, storage requirements and noise tolerance of NN is based on data reduction [21], [22]. These techniques aim to obtain a representative training set with a lower size compared to the original one and with a similar or even higher classification accuracy for new incoming data. In the literature, these are known as reduction techniques [21],

I. Triguero, J. Derrac and F. Herrera are with the Department of Computer Science and Artificial Intelligence, CITIC-UGR (Research Center on Information and Communications Technology), University of Granada, 18071, Granada, Spain (email: triguero@decsai.ugr.es, jderrac@decsai.ugr.es and herrera@decsai.ugr.es).

S. García is with the Department of Computer Science, University of Jaén, 23071, Jaén, Spain (e-mail: sglopez@ujaen.es).

instance selection [23]–[25], Prototype Selection (PS) [26], Prototype Generation (PG) [22], [27], [28], also known as Prototype Abstraction methods [29], [30].

Although the PS and PG problem are frequently confused and considered to be the same problem, they each relate to different problems. PS methods concern the identification of an optimal subset of representative objects from the original training data, discarding noisy and redundant examples. PG methods, by contrast, besides selecting data, can generate and replace the original data with new artificial data [27]. This process allows it to fill regions in the domain of the problem which have no representative examples in original data. Thus, PS methods assume that the best representative examples can be obtained from a subset of the original data whereas PG methods generate new representative examples if needed, tackling also the fourth weakness of NN mentioned above.

The PG methods that we study in this survey are those specifically designed for enhancing NN classification. Nevertheless, many other techniques could be used for the same goal as PG methods that are out of the scope of this survey. For instance, clustering techniques allow us to obtain a representative subset of prototypes or cluster centers, but they are obtained for more general purposes. A very good review of clustering can be found in [31].

Nowadays, there is no a general categorization for PG methods. In the literature a brief taxonomy for prototype reduction schemes was proposed in [22]. It includes both PS and PG methods and compares them in terms of classification accuracy and reduction rate. In this paper, the authors divide the prototype reduction schemes into creative (PG) and selecting methods (PS), but it is not exclusively focused on PG methods and especially on studying the similarities among them. Furthermore, a considerable number of PG algorithms have been proposed and some of them are rather unknown. The first approach we can find in the literature, called PNN [32] is based on merging prototypes. One of the most important families of methods are those based on Learning Vector Quantization (LVQ) [33]. Other methods are based on splitting the dimensional space [34] and even evolutionary algorithms and particle swarm optimization [35] have been also used for tackling this problem [36], [37].

Because of the absence of a focused taxonomy in the literature, we have observed that the new algorithms proposed are usually compared with only a subset of the complete family of PG methods and, in most of the studies, no rigorous analysis has been carried out.

These are the reasons that motivate the global purpose of this paper, which can be divided into three objectives:

- To propose a new and complete taxonomy based on the main properties observed in the PG methods. The taxonomy will allow us to know the advantages and drawbacks from a theoretical point of view.
- To make an empirical study for analyzing the PG algorithms in terms of accuracy, reduction capabilities and time complexity. Our goal is to identify the best methods in each family, depending on the size and type of the data sets and to stress the relevant properties of each one.

• To illustrate through graphical representations the trend of generation performed by the schemes studied in order to justify the results obtained in the experiments.

The experimental study will include a statistical analysis based on nonparametric tests and we will conduct experiments involving a total of 24 PG methods and 59 small and large size data sets. The graphical representations of selected data will be done by using a 2-dimensional data set called *banana* with moderate complexity features.

This paper is organized as follows. A description of the properties and an enumeration of the methods, as well as related and advanced work on PG, are given in Section II. Section III presents the taxonomy proposed. In section IV we describe the experimental framework, and Section V examines the results obtained in the empirical study and presents a discussion of them. Graphical representations of generated data by PG methods are illustrated in Section VI. Finally, Section VII concludes the paper.

II. PROTOTYPE GENERATION: BACKGROUND

PG builds new artificial examples from the training set, a formal specification of the problem is the following: Let \mathbf{x}_p be an instance where $\mathbf{x}_p = (\mathbf{x}_{p1}, \mathbf{x}_{p2}, ..., \mathbf{x}_{pm}, \mathbf{x}_{p\omega})$, with \mathbf{x}_p belonging to a class ω given by $\mathbf{x}_{p\omega}$ and a *m*-dimensional space in which 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 TRwhich consists of n instances \mathbf{x}_p and a test set TS composed of s instances \mathbf{x}_t , with $\mathbf{x}_{t\omega}$) unknown. The purpose of PG is to obtain a prototype generate set TG, which consists of r, r < n, prototypes, which are either selected or generated from the examples of TR. The prototypes of the generated set are determined to represent efficiently 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 a NN classifier. In this paper, we will focus on the use of the NN rule, with k=1, to classify the examples of TR and TS using the TG as reference.

This section presents an overview of the PG problem. Three main topics will be discussed:

- In Subsection II-A, the main characteristics which will define the categories of the taxonomy proposed in this paper, will be outlined. They refer to the type of reduction, resulting generation set, generation mechanisms and evaluation of the search. Furthermore, some criterias to compare PG methods are established.
- In Subsection II-B, we briefly enumerate all the PG proposed in the literature. The complete and abbreviated name will be given together with the proposal reference.
- Finally, Subsection II-C explores other areas related to PG and gives an interesting summary of advanced work in this research field.

A. Main characteristics in Prototype Generation Methods

This section establishes different properties of PG methods that will be necessary for the definition of the taxonomy in the next section. The issues discussed here include the type of reduction, resulting generation set, generation mechanisms and evaluation of the search. Finally, some criteria will be set in order to compare PG methods.

1) Type of Reduction: PG methods search for a reduced set TG of prototypes to represent the training set TR, there are also a variety of schemes in which the size of TG can be established:

- Incremental: An incremental reduction starts with an empty reduced set *TG* or with only some representative prototypes from each class. Next, a succession of additions of new prototypes or modifications of previous prototypes occurs. One important advantage of this kind of reduction is that these techniques can be faster and need less storage during the learning phase than non-incremental algorithms. Furthermore, this type of reduction allows the technique to adequately establish the number of prototypes required for each data set. Nevertheless, this could obtain adverse results due to the requirement of a high number of prototypes to adjust *TR* producing overfitting.
- **Decremental:** The decremental reduction begins with TG = TR, and then the algorithm starts reducing TG or modifying the prototypes in TG. It can be accomplished by following different procedures, such as merging, moving or removing prototypes and re-labeling classes. One advantage observed in decremental schemes, is that all training examples are available for examination to make a decision. On the other hand, a shortcoming of these kind of methods is that they usually present a high computational cost.
- Fixed: It is common to use a fixed reduction in PG. These methods establish the final number of prototypes for TG using a user previously defined parameter related to the percentage of retention of TR. This is the main drawback of this approach, apart from that is very dependent on each data set tackled. However, these techniques only focus on increasing the classification accuracy.
- **Mixed:** A mixed reduction begins with a pre-selected subset TG, obtained either by random selection with fixed reduction or by the run of a PS method, and next, additions, modifications and removals of prototypes are done in TG. This type of reduction combines the advantages of the previously seen, allowing several rectifications to solve the problem of fixed reduction. However, these techniques are prone to overfit the data and they usually have high computational cost.

2) *Resulting generation set:* This factor refers to the resulting set generated by the technique, that is, whether the final set will retain border, central or both types of points.

• **Condensation:** This set includes the techniques which return a reduced set of prototypes which are closer to the decision boundaries, also called border points. The reasoning behind retaining border points is that internal points do not affect the decision boundaries as much as border points, and thus can be removed with relatively little effect on classification. The idea behind these methods is to preserve the accuracy over the training set,

but the generalization accuracy over the test set can be negatively affected. Nevertheless, the reduction capability of condensation methods is normally high due to the fact that border points are less than internal points in most of the data.

- Edition: These schemes instead seek to remove or modify border points. They act over points that are noisy or do not agree with their nearest neighbors leaving smoother decision boundaries behind. However, such algorithms do not remove internal points that do not necessarily contribute to the decision boundaries. The effect obtained is related to the improvement of generalization accuracy in test data, although the reduction rate obtained is lower.
- Hybrid: Hybrid methods try to find the smallest set TG which maintains or even increases the generalization accuracy in test data. To achieve this, it allows modifications of internal and border points based on some specific criteria followed by the algorithm. The NN classifier is highly adaptable to these methods, obtaining great improvements even with a very small reduced set of prototypes.

3) Generation mechanisms: This factor describes the different mechanisms adopted in the literature to build the final TG set.

- Class re-labeling: This generation mechanism consists of changing the class labels of samples from *TR* which could be suspicious of being errors and belonging to other different classes. Its purpose is to cope with all types of imperfections in the training set (mislabeled, noisy and atypical cases). The effect obtained is closely related to the improvement in generalization accuracy of the test data, although the reduction rate is kept fixed.
- **Centroid based:** These techniques are based on generating artificial prototypes by merging a set of similar examples. The merging process is usually made from the computation of averaged attribute values over a selected set, yielding the so-called centroids. The identification and selection of the set of examples are the main concerns of the algorithms that belong to this category. These methods can obtain a high reduction rate but they are also related to accuracy rate losses.
- Space Splitting: This set includes the techniques based on different heuristics for partitioning the feature space, along with several mechanisms to define new prototypes. The idea consists of dividing TR into some regions which will be replaced with representative examples establishing the decision boundaries associated with the original TR. This mechanism works on a space level, due to the fact that the partitions are found in order to discriminate, as well as possible, a set of examples from others, whereas centroid based approaches work on the data level, mainly focusing on the optimal selection of only a set of examples to be treated. The reduction capabilities of these techniques usually depend on the number of regions that are needed to represent TR.
- **Positioning Adjustment:** The methods that belong to this family aim to correct the position of a subset of

prototypes from the initial set by using an optimization procedure. New positions of prototype can be obtained using the movement idea in the m-dimensional space, adding or subtracting some quantities to the attribute values of the prototypes. This mechanism is usually associated to a fixed or mixed type of reduction.

4) Evaluation of Search: NN itself is an appropriate heuristic to guide the search of a PG method. The decisions made by the heuristic must have an evaluation measure that allows the comparison of different alternatives. The evaluation of search criterion depends on the use or not of NN in such an evaluation:

- **Filter:** We refer to filters techniques when they do not use the NN rule during the evaluation phase. Different heuristics are used to obtain the reduced set. They can be faster than NN but the performance in terms of accuracy obtained could be worse.
- Semi-Wrapper: NN is used for partial data to determine the criteria of making a certain decision. Thus, NN performance can be measured over localized data, which will contain most of prototypes that will be influenced in making a decision. It is an intermediate approach, where a trade-off between efficiency and accuracy is expected.
- Wrapper: In this case, the NN rule fully guides the search by using the complete training set with the leaveone-out validation scheme. The conjunction in the use of the two mentioned factors allows us to get a great estimator of generalization accuracy, thus obtaining better accuracy over test data. However, each decision involves a complete computation of the NN rule over the training set and the evaluation phase can be computationally expensive.

5) Criteria to Compare PG Methods: When comparing PG methods, there are a number of criteria that can be used to compare the relative strengths and weaknesses of each algorithm. These include storage reduction, noise tolerance, generalization accuracy and time requirements.

- *Storage reduction:* One of the main goals of the PG methods is to reduce storage requirements. Furthermore, another goal closely related to this is to speed up classification. A reduction in the number of stored instances will typically yield a corresponding reduction in the time it takes to search through these examples and classify a new input vector.
- *Noise tolerance:* Two main problems may occur in the presence of noise. The first is that very few instances will be removed because many instances are needed to maintain the noisy decision boundaries. Secondly, the generalization accuracy can suffer, especially if noisy instances are retained instead of good instances, or these are not re-labelled with the correct class.
- *Generalization accuracy:* A successful algorithm will often be able to significantly reduce the size of the training set without significantly reducing generalization accuracy.
- *Time requirements:* Usually, the learning process is carried out just once on a training set, so it seems not to

TABLE I: PG methods reviewed

Complete name	Abbr. name	Reference
Prototype Nearest Neighbor	PNN	[32]
Generalized Editing using Nearest Neighbor	GENN	[39]
Learning Vector Quantization 1	LVQ1	[33]
Learning Vector Quantization 2	LVQ2	
Learning Vector Quantization 2.1	LVQ2.1	
Learning Vector Quantization 3	LVQ3	
Decision Surface Mapping	DSM	[40]
Vector Quantization	VQ	[41]
Chen Algorithm	Chen	[34]
Bootstrap Technique for Nearest Neighbor	BTS3	[42]
Learning Vector Quantization with Training Counter	LVQTC	[43]
MSE	MSE	[44]
Modified Chang's Algorithm	MCA	[45]
Generalized Modified Chang's Algorithm	GMCA	[46]
Integrated Concept Prototype Learner	ICPL	[29]
Integrated Concept Prototype Learner 2	ICPL2	
Integrated Concept Prototype Learner 2	ICPL3	
Integrated Concept Prototype Learner 2	ICPL4	
Depuration Algorithm	Depur	[47]
Hybrid LVQ3 algorithm	HYB	[48]
Reduction by space partitioning 1	RSP1	[30]
Reduction by space partitioning 2	RSP2	
Reduction by space partitioning 3	RSP3	
Evolutionary Nearest Prototype Classifier	ENPC	[36]
Adaptive Vector Quantization	AVQ	[49]
Learning Vector Quantization with Pruning	LVQPRU	[50]
Pairwise Opposite Class Nearest Neighbor	POC-NN	[51]
Adaptive Condensing Algorithm Based on Mixtures of Gaussians	MixtGauss	[27]
Self-generating Prototypes	SGP	[28]
Adaptive Michigan PSO	AMPSO	[52]
Prototype Selection Clonal Selection Algorithm	PSCSA	[53]
Particle Swarm Optimization	PSO	[37]

be a very important evaluation method. However, if the learning phase takes too long it can become impractical for real applications.

B. Prototype Generation Methods

More than 25 PG methods have been proposed in the literature. This section is devoted to enumerating and designating them according to a standard followed in this paper. For more details on their implementations, the reader can visit the URL http://sci2s.ugr.es/pgtax. Implementations of the algorithms in java can be found in KEEL software [38].

Table I presents an enumeration of PG methods reviewed in this paper. The complete name, abbreviation and reference is provided for each one. In the case of there being more than one method in a row, they were proposed together and the best performing method (indicated by the respective authors) is depicted in bold. We will use the best representantive method of each proposed paper, so only the methods in bold when more than one method is proposed will be compared in the experimental study.

C. Related and Advanced Work

Nowadays, much research in enhancing NN through data preprocessing is common and highly demanded. PG could represent a feasible and promising technique to obtain expected results, which justifies its relationship to other methods and problems. This section provides a brief review on other topics closely related to PG and describes other interesting work and future trends which have been studied in the last few years.

- *Prototype Selection*: With the same objective as PG, storage reduction and classification accuracy improvement, these methods are limited only to select examples from the training set. More than 50 methods can be found in the literature. In general, three kinds of methods are usually differentiated, those also based on edition [54], condensation [55] or hybrid models [21], [56]. Advanced proposals can be found in [24], [57]–[59].
- *Instance and rule learning hybridizations*: It includes all the methods which simultaneously use instances and rules in order to compute the classification of a new object. If the values of the object are within the range of a rule, its consequent predicts the class; otherwise, if no rule matches with the object, the most similar rule or instance stored in the data base is used to estimate the class. Similarity is viewed as the closest rule or instance based on a distance measure. In short, these methods can generalize an instance into a hyperrectangle or rule [60], [61].
- *Hyperspherical prototypes*: This area [62] studies the use of hyperspheres to cover the training patterns of each class. The basic idea is to cluster the space into several objects, each of them corresponding to only one class, and the class of the nearest object is assigned to the test example.
- *Weighting*: This task consists of applying weights to the instances of the training set, modifying the distance measure between them and any other instance. This technique could be integrated with PS and PG methods [16], [63]–[66] for improving the accuracy in classification problems and to avoid overfitting. A complete review dealing with this topic can be found in [67].
- *Distance Functions*: Several distance metrics have been used with NN, especially when working with categorical attributes [68]. Many different distance measures try to optimize the performance of NN [15], [64], [69], [70], and they have successfully increased the classification accuracy. Advanced work is based on adaptive distance functions [71].
- Oversampling: This term is frequently used in learning with imbalanced classes [72], [73] and is closely related to undersampling [74]. Oversampling techniques replicate and generate artificial examples that belong to the minority classes in order to strengthen the presence of minority samples and to increase the performance over them. SMOTE [75] is the most well known oversampling technique and it has been shown to be very effective in many domains of application [76].

III. PROTOTYPE GENERATION: TAXONOMY

The main characteristics of the PG methods have been described in Section II-A, and they can be used to categorize the PG methods proposed in the literature. The type of reduction, resulting generation set, generation mechanisms and the evaluation of the search constitute a set of properties which define each PG method. This section presents the taxonomy of PG methods based on these properties.

In Figure 1, we show the PG map with the representative methods proposed in each paper ordered in time, following Table I. We refer to representantive methods those which are preferred by the authors or have reported the best results in the corresponding proposal paper. Some interesting remarks can be seen in Figure 1.

- Only two class re-labeling methods have been proposed for PG algorithms. The reason is that both methods obtain great results for this approach in accuracy, but the underlying concept of these methods does not achieve high reduction rates, which is one of the most important objectives of PG. Furthermore, it is important to point out that both algorithms are based on decremental reduction and that they have noise filtering purposes.
- The condensation techniques are a wide group. They usually use a semi-wrapper evaluation with any type of reduction. It is considered a classic idea due to the fact that, in recent years, hybrid models are preferred over condensation techniques, with few exceptions. ICPL2 was the first PG method with a hybrid approach, combining edition and condensation stages.
- Recent efforts in proposing positioning adjustment algorithms are noted for mixed reduction. Most of the methods following this scheme are based on LVQ and the recent approaches try to alleviate the main drawback of the fixed reduction.
- There are many efforts in centroid-based techniques because they have reported a great synergy with the NN rule since the first algorithm PNN. Furthermore, many of them are based on simple and intuitive heuristics which allow them to obtain a reduced set with high quality accuracy. By contrast, those with decremental and mixed reduction are slow techniques.
- Wrapper evaluation appeared a few years ago, and is only presented in hybrid approaches. This evaluation search is intended to optimize a selection, without taking into account computational costs.

Figure 2 illustrates the categorization following a hierarchy based on this order: generation mechanisms, resulting generation set, type of reduction, and finally, evaluation of the search.

The properties studied here can help to understand how the PG algorithms work. In the next sections, we will establish which methods perform best for each family considering several metrics of performance with a wide experimental framework.

IV. EXPERIMENTAL FRAMEWORK

In this section we show the factors and issues related to the experimental study. We provide the measures employed to evaluate the performance of the algorithms (subsection IV-A, details of the problems chosen for the experimentation (subsection IV-B), parameters of the algorithms (subsection IV-C), and finally, the statistical tests employed to contrast the results obtained are described (subsection IV-D).

A. Performance measures for standard classification

In this work, we deal with multi-class data sets. In these domains, two measures are widely used because of their sim-



Fig. 2: Prototype Generation Hierarchy

TABLE III: Confusion Matrix for an Ω -class problem

Correct Class	Predicted Class									
	ω_1	ω_2		ω_{Ω}	Total					
ω_1	h_{11}	h_{12}		$h_{1\Omega}$	T_{r1}					
ω_2	h_{12}	h_{22}		$h_{2\Omega}$	T_{r2}					
:			۰.		:					
ω _Ω	$h_{1\Omega}$	$h_{2\Omega}$		$h_{\Omega\Omega}$	$T_{r\Omega}$					
Total	T_{c1}	T_{c2}		$T_{c\Omega}$	Т					

plicity and successful application. We refer to the classification rate and Cohen's kappa rate measures, which we will now explain:

- *Classification rate*: is the number of successful hits (correct classifications) relative to the total number of classifications. It has been by far the most commonly used metric for assessing the performance of classifiers for years [2], [77].
- *Cohen's kappa (Kappa rate)*: is an alternative measure to the *classification rate*, since it compensates for random hits [78]. In contrast to the classification rate, kappa evaluates the portion of hits that can be attributed to the classifier itself (i.e., not to mere chance), relative to all the classifications that cannot be attributed to chance alone. An easy way of computing Cohen's kappa is by making use of the resulting confusion matrix (Table III) in a classification task. With the expression (1), we can obtain Cohen's kappa:

$$kappa = \frac{n \sum_{i=1}^{\Omega} h_{ii} - \sum_{i=1}^{\Omega} T_{ri} T_{ci}}{n^2 - \sum_{i=1}^{\Omega} T_{ri} T_{ci}},$$
 (1)

where h_{ii} is the cell count in the main diagonal (the number of true positives for each class), n is the number of examples, Ω is the number of class labels, and T_{ri} , T_{ci} are the rows' and columns' total counts, respectively $(T_{ri} = \sum_{j=1}^{\Omega} h_{ij}, T_{ci} = \sum_{j=1}^{\Omega} h_{ji})$. Cohen's kappa ranges from -1 (total disagreement)

Cohen's kappa ranges from -1 (total disagreement) through 0 (random classification) to 1 (perfect agreement). For multi-class problems, kappa is a very useful, yet simple, meter for measuring a classifier's classification rate while compensating for random successes.

The main difference between the classification rate and Cohen's kappa is the scoring of the correct classifications. Classification rate scores all the successes over all classes, whereas Cohen's kappa scores the successes independently for each class and aggregates them. The second way of scoring is less sensitive to randomness caused by a different number of examples in each class.

B. Data sets

In the experimental study, we selected 59 data sets from the UCI repository [79] and KEEL-dataset¹ [38]. Table II summarizes the properties of the selected data sets. It shows, for each data set, the number of examples (#Ex.), the number of attributes (#Atts.), the number of numerical (#Num.) and nominal (#Nom.) attributes, and the number of classes (#Cl.). The data sets are grouped into two categories depending on the size they have. Small data sets have less than 2,000 instances and large data sets have more than 2,000 instances. The data sets considered are partitioned using the ten fold cross-validation (10-fcv) procedure.

C. Parameters

Many different method configurations have been established by the authors in each paper for the PG techniques. In our experimental study, we have used the parameters defined in the reference where they were originally described, 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 IV. Note that some PG methods have no parameters to be fixed, so they are not included in this table.

In most of the techniques, euclidean distance is used as the similarity function, to decide which neighbors are closest. Furthermore, to avoid problems with a large number of attributes and distances, all data sets have been normalized between 0 and 1. This normalization process allows to apply all the PG methods over each data set, independently of the types of attributes.

TABLE IV: Parameter specification for all the methods employed in the experimentation

Algorithm	Parameters
LVQ3	Iterations = 100 , $alpha = 0.1$, WindowWidth= 0.2
	epsilon = 0.1
DSM	Iterations = 100 , $alpha = 0.1$
VQ	Iterations = 100 , $alpha = 0.1$
BTS3	NN selected = 1, Random Trials = 3
LVQTC	Iterations = 100, $alpha_R = 0.1$,
	$alpha_W = 0.1$, Retention Threshold = 3,
	Number of Epoches= 4
MSE	Gradient Step = 0.5 , Initial Temperature = 100
ICLP2	Filtering method = RT2
Depur	k' = 2, $k = 3$
HYB	Search Iterations = 200 , Optimal search Iterations = 1000
	alpha = 0.1, Initial $epsilon = 0$, Final $epsilon = 0.5$
	Initial WindowWidth = 0, Final WindowWidth = 0.5
	delta = 0.1, delta WindowWidth = 0.1
	Initial Selection = SVM
RSP3	Subset Choice = Diameter
ENPC	Iterations $= 250$
AVQ	Iterations = 100 , T set percentage= 80% ,
	epsilon = 0.1
LVQPRU	Iterations = 100 , $alpha = 0.1$, WindowWidth = 0.5
POCNN	alpha ratio = 0.2
SGP	Rmin = 0.01, Rmis = 0.2
AMPSO	Iterations = 300 , C1 = 1.0 , C2 = 1.0 , C3 = 0.25 ,
	Vmax = 1, W = 0.1, X = 0.5, Pr = 0.1, Pd = 0.1
PSCSA	HyperMutation Rate = 2 , Clonal Rate = 10 ,
	Mutation Rate = 0.01 , Stimulation Threshold = 0.89 ,
	Alpha = 0.4
PSO	SwarmSize = 20 , Iterations = 250 , C1 = 1,
	C2 = 3, $Vmax = 0.25$, $Wstart = 1.5$, $Wend = 0.5$
Note: The par	amotor Poduction Pate on fixed reduction algorithms has been

Note: The parameter Reduction Rate on fixed reduction algorithms has been established to 95% for small size data set, 98% for large

D. Statistical tests for performance comparison

In this paper, we use the hypothesis testing techniques to provide statistical support for the analysis of the results [80],

Data Set	#Ex.	#Atts.	#Num.	#Nom.	#Cl.	Data Set	#Ex.	#Atts.	#Num.	#Nom.	#Cl.
abalone	4,174	8	7	1	28	marketing	8,993	13	13	0	9
appendicitis	106	7	7	0	2	monks	432	6	6	0	2
australian	690	14	8	6	2	movement_libras	360	90	90	0	15
automobile	205	25	15	10	6	newthyroid	215	5	5	0	3
balance	625	4	4	0	3	nursery	12,960	8	0	8	5
banana	5,300	2	2	0	2	pageblocks	5,472	10	10	0	5
bands	539	19	19	0	2	penbased	10,992	16	16	0	10
breast	286	9	0	9	2	phoneme	5,404	5	5	0	2
bupa	345	6	6	0	2	pima	768	8	8	0	2
car	1,728	6	0	6	4	ring	7,400	20	20	0	2
chess	3,196	36	0	36	2	saheart	462	9	8	1	2
cleveland	297	13	13	0	5	satimage	6,435	36	36	0	7
coil2000	9,822	85	85	0	2	segment	2,310	19	19	0	7
contraceptive	1,473	9	9	0	3	sonar	208	60	60	0	2
crx	690	15	6	9	2	spambase	4,597	57	57	0	2
dermatology	366	33	1	32	6	spectheart	267	44	44	0	2
ecoli	336	7	7	0	8	splice	3,190	60	0	60	3
flare-solar	1,066	11	0	11	2	tae	151	5	5	0	3
german	1,000	20	7	13	2	texture	5,500	40	40	0	11
glass	214	9	9	0	7	thyroid	7,200	21	21	0	3
haberman	306	3	3	0	2	tic-tac-toe	958	9	0	9	2
hayes-roth	160	4	4	0	3	titanic	2,201	3	3	0	2
heart	270	13	13	0	2	twonorm	7,400	20	20	0	2
hepatitis	155	19	19	0	2	vehicle	846	18	18	0	4
housevotes	435	16	0	16	2	vowel	990	13	13	0	11
iris	150	4	4	0	3	wine	178	13	13	0	3
led7digit	500	7	7	0	10	wisconsin	699	9	9	0	2
lymphography	148	18	3	15	4	yeast	1484	8	8	0	10
magic	19,020	10	10	0	2	Z00	101	16	0	16	7
mammographic	961	5	0	5	2						

TABLE II: Summary description for classification data sets

[81]. Specifically, we use non-parametric tests, due to the fact that the initial conditions that guarantee the reliability of the parametric tests may not be satisfied, causing the statistical analysis to lose credibility with these parametric tests. These tests are suggested in the studies presented in [80], [82]–[84], where its use in the field of Machine Learning is highly recommended.

The Wilcoxon test [82], [83] is adopted considering a level of significance of $\alpha = 0.1$. More information about statistical tests and the results obtained can be found in the web site associated with this paper (http://sci2s.ugr.es/pgtax).

E. Other considerations

We want to outline that the implementations are based only on the descriptions and specifications given by the respective authors in their papers. No advanced data structures and enhancements for improving the efficiency of PG methods have been carried out. All methods are available in KEEL software [38].

V. ANALYSIS OF RESULTS

This section presents the average results collected in the experimental study and some discussions of them, the complete results can be found on the web page associated with this paper. The study will be divided into two parts: analysis of the results obtained over small size data sets (Subsection V-A) and over large data sets (Subsection V-B). Finally, a global analysis is added in (Subsection V-C).

A. Analysis and Empirical Results of Small Size Data Sets

Table V presents the average results obtained by the PG methods over the 40 small size data sets. *Red.* denotes reduction rate achieved, *train Acc* and *train Kap* present the accuracy and kappa obtained in the training data, respectively; on the other hand *tst Acc* and *tst Kap* present the accuracy and kappa obtained over the test data. Finally, *Time* denotes the average time elapsed in seconds to finish a run of PG method. The algorithms are ordered from the best to the worst for each type of result. Algorithms highlighted in bold are those which obtain the best result in their corresponding family, according to the first level of the hierarchy in Figure 2.

Red.		train Acc.		train Kap.		tst Acc.		tst Kap.		Time (s)	
PSCSA	0.9858	MCA	0.8772	MCA	0.7717	GENN	0.7564	GENN	0.5400	1NN	-
AVQ	0.9759	GMCA	0.8405	GMCA	0.7067	ICPL2	0.7560	ICPL2	0.5366	LVQTC	0.1644
LVQTC	0.9551	HYB	0.8309	HYB	0.6988	PSO	0.7501	PSO	0.5332	DSM	0.1780
MixtGauss	0.9552	ICPL2	0.8254	ENPC	0.6800	GMCA	0.7351	GMCA	0.5062	BTS3	0.2079
MSE	0.9520	ENPC	0.8247	PSO	0.6791	1NN	0.7326	RSP3	0.5004	LVQ3	0.2316
Chen	0.9519	PSO	0.8238	ICPL2	0.6690	RSP3	0.7325	MSE	0.4925	VQ	0.2469
BTS3	0.9519	GENN	0.8002	GENN	0.6243	Depur	0.7296	1NN	0.4918	Chen	0.2675
SGP	0.9512	RSP3	0.7924	RSP3	0.6112	MSE	0.7237	MCA	0.4867	Depur	0.2777
LVQPRU	0.9503	Depur	0.7801	Depur	0.5815	MCA	0.7219	Depur	0.4826	LVQPRU	0.5592
PSO	0.9491	MSE	0.7566	MSE	0.5388	ENPC	0.7167	ENPC	0.4818	AVQ	0.6561
VQ	0.9491	1NN	0.7369	LVQTC	0.5224	HYB	0.7153	HYB	0.4790	MixtGauss	0.8125
DSM	0.9491	LVQTC	0.7327	Chen	0.5116	LVQPRU	0.6997	LVQPRU	0.4592	SGP	1.3597
LVQ3	0.9488	LVQPRU	0.7304	LVQPRU	0.5110	LVQTC	0.6981	MixtGauss	0.4546	GENN	1.4285
PNN	0.9447	SGP	0.7256	AMPSO	0.5039	SGP	0.6949	LVQTC	0.4541	RSP3	1.8505
AMPSO	0.9430	AMPSO	0.7227	1NN	0.4985	MixtGauss	0.6932	AMPSO	0.4440	PSCSA	1.9562
MCA	0.8568	MixtGauss	0.7138	MixtGauss	0.4888	AMPSO	0.6903	PNN	0.4369	MSE	2.4794
ICPL2	0.8371	DSM	0.7036	SGP	0.4852	DSM	0.6810	SGP	0.4360	HYB	5.5888
RSP3	0.7329	PNN	0.7015	PNN	0.4718	PNN	0.6786	AVQ	0.4326	AMPSO	8.2870
ENPC	0.7220	Chen	0.6964	AVQ	0.4660	Chen	0.6770	DSM	0.4239	GMCA	8.4947
GMCA	0.6984	LVQ3	0.6931	DSM	0.4627	LVQ3	0.6763	PSCSA	0.4231	PNN	14.0066
POC	0.6071	AVQ	0.6869	PSCSA	0.4461	PSCSA	0.6682	LVQ3	0.4114	PSO	42.3168
HYB	0.4278	PSCSA	0.6787	LVQ3	0.4421	AVQ	0.6672	Chen	0.4026	ENPC	47.1377
Depur	0.3531	BTS3	0.6713	BTS3	0.3923	BTS3	0.6626	BTS3	0.3784	POC	151.9278
GENN	0.1862	VQ	0.6614	VQ	0.3866	VQ	0.6549	VQ	0.3770	ICPL2	163.9147
1NN	0.0000	POC	0.6487	POC	0.3601	POC	0.6493	POC	0.3700	MCA	190.4930

TABLE V: Average results obtained by the PG methods over small data sets

Figure 3 depicts a representation of an opposition between the two objectives: reduction and test accuracy. Each algorithm located inside the graphic gets its position from the average values of each measure evaluated (exact position corresponding to the beginning of the name of the algorithm). Across the graphic, there is a line that represents the threshold of test accuracy achieved by the 1-NN algorithm without preprocessing. Note that in Figure 3a the names of some PG methods overlap, and hence Figure 3b shows this overlapping zone.

To complete the set of results, the web site associated to this paper contains the results of applying the Wilcoxon test to all possible comparisons among all PG considered in small data sets.

Observing Tables V, Figure 3 and the Wilcoxon Test, we can point out some interesting facts:

- Some classical algorithms are at the top in accuracy and kappa rate. For instance, GENN, GMCA and MSE obtain better results than other recent methods over test data. However, these techniques usually have a poor associated reduction rate. We can observe this statement in the Wilcoxon test, where classical methods significantly overcome other recent approaches in terms of accuracy and kappa rates. However, In terms of Acc. * Red. and Kap. * Red. measures, typically, these methods do not outperform recent techniques.
- PSO and ENPC could be stressed from the *Positioning Adjustment* family as the best performing methods. Each one of them belongs to different sub-families, fixed and mixed reduction, respectively. PSO focuses on improving the classification accuracy and it obtains a good generalization capability. On the other hand, ENPC has

the overfitting as the main drawback, clearly discernible from Table V. In general, LVQ based approaches obtain worse accuracy rates than 1NN, but the reduction rate achieved by them is very high. MSE and HYB are the most outstanding techniques belonging to the subgroup of *Condensation* and *Positioning Adjustment*.

- With respect to *class re-labeling* methods, GENN obtains better accuracy/kappa rates but worse reduction rates than Depur. However, the statistical test informs that GENN does not outperform to the Depur algorithm in terms of accuracy and kappa rate. Furthermore, when the reduction rate is taken into consideration, that is, when the statistical test is based on the *Acc.***Red.* and *Kap.***Red.* measures, the Depur algorithm clearly outperforms to GENN.
- The decremental approaches belonging to the *centroids* family require high computation times but usually offer good reduction rates. MCA and PNN tend to overfit the data, but GMCA obtains excellent results.
- In the whole *centroids* family, two methods deserve particular mention: ICPL2 and GMCA. Both generate a reduced prototype set with good accuracy rates in test data. The other approaches based on Fixed and Incremental reduction are less appropriate to improve the effectiveness of 1NN, but they are very fast and offer much reduced generated sets.
- Regarding *space splitting* approaches, several differences can be observed. RSP3 is an algorithm based on Chen's algorithm but tries to avoid drastic changes in the form of the decision boundaries, and it produces a good tradeoff between reduction and accuracy. Although the POC algorithm is a relatively modern technique, this does not obtain great results. We can justify these results



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Fig. 3: Accuracy in test vs reduction in small data sets

because the α parameter is very sensitive for each data set. Furthermore, it is quite slow when tackling data sets with more than two classes.

- The best methods in accuracy/kappa rates for each one of the families are PSO, GENN, ICPL2 and RSP3, respectively and five methods outperform 1NN in accuracy.
- In general, hybrid methods obtain the best result in terms of accuracy and reduction rate.
- Usually, there is no difference between the rankings obtained with accuracy and kappa rates, except for some concrete algorithms. For example, we can observe that 1NN obtains a lower ranking with the kappa measure, it probably indicates that 1NN benefits of random hits.

Furthermore, in the web site associated to this paper, we can find an analysis of the results depending on the type of attributes of the data sets. We show the results in accuracy/kappa rate for all PG methods differentiating between numerical, nominal and mixed data sets. In numerical and nominal data sets all attributes must be numerical and nominal respectively, whereas in mixed data sets, we include those data sets with numerical and nominal attributes mixed. Observing these tables, we want to outline different properties of the PG methods.

- In general, there is no difference in performance between numerical, nominal and mixed data sets, except for some concrete algorithms. For example, in mixed data sets, we can see that a class-relabeling method, GENN, is on the top, due to the fact that it does not produce modifications to the attributes. However, in numerical data sets, PSO is the best performing method, indicating to us that the positioning adjustment strategy is usually well-adapted to numerical data sets.
- In fact, comparing these tables, we observe that some representative techniques of the positioning adjustment family, such as PSO, MSE, and ENPC have a close accuracy/kappa rate to 1NN. However, over nominal and mixed data sets, they decrease their accuracy rates.
- ICPL2 and GMCA techniques obtain good accu-

racy/kappa rates independently of the type of input data.

Finally, we perform an study depending on the number of classes of the data sets. In the web site associated to this paper, we show the average results in accuracy/kappa rate differentiating between binary and multi-class data sets. We can analyze several details from the results collected:

- Eight techniques outperform 1NN in accuracy when they tackle binary data sets. However, over multi-class data sets, there are only three techniques that are able to overcome 1NN.
- Centroid-based techniques usually perform well when dealing with multi-class data sets. For instance, we can highlight the MCA, SGP, PNN, ICPL2 and GMCA techniques, which increase their respective rankings with multi-class data sets.
- GENN and ICPL2 techniques obtain good accuracy/kappa rates independently of the number of classes.
- PSCSA has a good behavior with binary data sets. However, over multi-class data sets, PSCSA decrease its performance.
- Some methods present significant differences between accuracy and kappa measures when dealing with binary data sets. We can stress MSE, Depur, Chen and BTS3 like techniques penalized by the kappa measure.

B. Analysis and Empirical Results of Large Size Data Sets

This section presents the study and analysis of large size data sets. The goal of this study is to analyze the effect of scaling up the data in PG methods. For time complexity reasons, several algorithms cannot be run over large data sets. PNN, MCA, GMCA, ICPL2 and POC are extremely slow techniques and their time complexity quickly increases when the data scales up or manages more than five classes.

Table VI shows the average results obtained and Figure 4 illustrates the comparison between the accuracy and reduction rates of the PG methods over large size data sets. Finally, the web site associated to this paper contains the results

Red.		train Acc.		train Kap.		tst Acc.		tst Kap.		Time (s)	
PSCSA	0.9988	ENPC	0.8809	ENPC	0.7613	GENN	0.8133	GENN	0.6269	1NN	
AVQ	0.9980	GENN	0.8428	GENN	0.6806	1NN	0.8060	1NN	0.6181	DSM	1.6849
LVQTC	0.9975	Depur	0.8250	Depur	0.6322	ENPC	0.8029	ENPC	0.6170	LVQ3	1.7037
MSE	0.9936	PSO	0.8158	RSP3	0.6299	Depur	0.8004	Depur	0.5863	VQ	1.7193
SGP	0.9823	1NN	0.8057	1NN	0.6178	PSO	0.8000	PSO	0.5861	MSE	17.4228
BTS3	0.9801	RSP3	0.7922	PSO	0.6173	MSE	0.7674	RSP3	0.5597	HYB	18.6338
Mixtgauss	0.9801	HYB	0.7888	HYB	0.5992	Chen	0.7621	HYB	0.5567	LVQPRU	24.4067
LVQPRU	0.9801	MSE	0.7759	MSE	0.5349	HYB	0.7618	MSE	0.5221	Depur	26.8656
Chen	0.9801	Chen	0.7682	Chen	0.5236	RSP3	0.7556	Chen	0.5116	AVQ	38.3665
LVQ3	0.9799	AMPSO	0.7436	BTS3	0.4859	AMPSO	0.7410	LVQPRU	0.4799	Chen	50.0435
DSM	0.9799	BTS3	0.7393	AMPSO	0.4836	BTS3	0.7399	DSM	0.4796	SGP	52.3400
VQ	0.9799	LVQPRU	0.7373	LVQPRU	0.4818	LVQPRU	0.7356	BTS3	0.4788	LVQTC	83.6030
PSO	0.9799	DSM	0.7353	DSM	0.4795	DSM	0.7341	AMPSO	0.4784	PSCSA	160.3864
AMPSO	0.9797	MixtGauss	0.7345	Mixtgauss	0.4711	Mixtgauss	0.7318	MixtGauss	0.4661	GENN	167.4849
ENPC	0.8205	LVQ3	0.7340	VQ	0.4689	LVQ3	0.7318	VQ	0.4651	BTS3	219.2394
RSP3	0.8100	VQ	0.7322	LVQ3	0.4683	VQ	0.7316	LVQ3	0.4627	AMPSO	587.7181
HYB	0.5727	LVQTC	0.7065	AVQ	0.4321	LVQTC	0.7056	AVQ	0.4280	RSP3	258.6881
Depur	0.2708	PSCSA	0.6730	LVQTC	0.4185	PSCSA	0.6707	LVQTC	0.4165	MixtGauss	639.3139
GENN	0.1576	AVQ	0.6546	PSCSA	0.3900	AVQ	0.6518	PSCSA	0.3842	PSO	909.9820
1NN	0.0000	SGP	0.6162	SGP	0.3568	SGP	0.6086	SGP	0.3466	ENPC	10931.1977

TABLE VI: Average results obtained by the PG methods over large data sets



Fig. 4: Accuracy in test vs reduction in large data sets

of applying the Wilcoxon test over all possible comparisons among all PG considered in large data sets.

These tables allow us to highlight some observations of the results obtained:

- Only the GENN approach outperforms the performance of 1NN in accuracy/kappa rate.
- Some methods present clear differences when dealing with large data sets. For instance, we can highlight the PSO and RSP3 techniques. The former may suffer from a lack of convergence due to the fact that the performance obtained in training data is slightly higher than that obtained by 1NN; hence, it may be a sign that more iterations are needed to tackle large data sets. On the other hand, the techniques based on space partitioning present some drawbacks when the data scales up and is made up of more attributes. This is the case with RSP3.
- In general, LVQ based methods do not work well when

the data scales up.

- BTS3 stands out as the best centroids-based method over large size data sets because the best-performing ones over small data sets were also the most complex in time and they cannot be run here.
- Although ENPC overfits the data, it is the best performing method considering the trade-off between accuracy/kappa and reduction rates. PSO can also be stressed as a good candidate in this type of data set.
- There is no significant differences between the accuracy and kappa rankings when dealing with large data sets.

Again, we differentiate between numerical, nominal and mixed data sets. Complete results can be found in the web site associated to this paper. Observing these results, we want to outline different properties of PG methods over large data sets. Note that there is only one data set with mixed attributes, for this reason we focus this analysis in the differences between numerical and nominal data sets.

- When only numerical data sets are taken into consideration, three algorithms outperform the 1NN rule: GENN, PSO and ENPC.
- Over nominal large data sets, no PG method outperforms 1NN.
- MixtGauss and AMPSO are highly conditioned on the type of input data, preferring numerical data sets. By contrast, RSP3 is better adapted to nominal data sets.

Finally, we perform again an analysis of the behavior of the PG techniques depending on the number of classes, but in this case, over large data sets. the web site associated to this paper presents the results. Observing these results, we can point out several comments:

- Over binary large data sets, there are four algorithms that outperform 1NN. However, when the PG techniques tackle multi-class data sets, no PG method overcome 1NN.
- When dealing with large data sets, there is no important differences between the accuracy and kappa ranking with binary data sets.
- Class-relabeling methods perform well independently of the number of classes.

C. Global Analysis

This subsection shows a global view of the obtained results. As a summary we want to outline several remarks on the use of PG, because the choice of a certain method depends on various factors.

- Several PG methods can be emphasized according to their test accuracy/kappa obtained: PSO, ICPL2, ENPC and GENN. In principle, in terms of reduction capabilities, PSCSA and AVQ obtain the best results but they offer poor accuracy rates. Taking into consideration the computational cost, we can consider DSM, LVQ3 and VQ to be the fastest algorithms.
- Edition schemes usually outperform the 1NN classifier, but the number of prototypes in the result set is too high. This fact could be prohibitive over large data sets, because there is no significant reduction. Furthermore, other PG methods have shown that it is possible to preserve high accuracy with a better reduction rate.
- A high reduction rate serves no purpose if there is not a minimum guarantee of performance accuracy. This is the case of PSCSA or AVQ. Nevertheless, MSE offers excellent reduction rates without losing performance accuracy.
- For the trade-off reduction-accuracy rate, PSO has been reported to have the best results over small size data sets. In the case of dealing with large data sets, the ENPC approach seems to be the most appropriate one.
- A good reduction-accuracy balance is difficult to achieve with a fast algorithm. Considering this restriction, we could say that RSP3 allows us to yield generated sets with a good tradeoff between reduction, accuracy and time complexity.

VI. VISUALIZATION OF DATA RESULTING SETS: A CASE STUDY BASED ON BANANA DATA SET

This section is devoted to illustrating the subsets selected resulting from some PG algorithms considered in our study. To do this, we focus on the *banana* data set, which contains 5,300 examples in the complete set. It is an artificial data set of 2 classes composed of three well-defined clusters of instances of the class -1 and two clusters of the class 1. Although the borders are clear among the clusters there is a high overlap between both classes. The complete data set is illustrated in Figure 5a.

The pictures of the generated sets by some PG methods could help to visualize and understand their way of working and the results obtained in the experimental study. The reduction rate, and the accuracy and kappa values in test data registered in the experimental study are specified for each one. In the original data set, the two values indicated correspond to accuracy and kappa with 1NN:

- Figure 5b depicts generated data by the algorithm GENN. It belongs to the edition approaches and the generated subset differs slightly from the original data set. Those samples found within the class boundaries can either be removed or be re-labeled. It is noticeable that the clusters of different classes are a little more separated.
- Figure 5c shows the resulting subset of the classical LVQ3 condensation algorithm. It can be appreciated that most of the points are moved to define the class boundaries, but a few interior points are also used. The accuracy and kappa decrease with respect to the original, as is usually the case with condensation algorithms.
- Figures 5d and 5e represent the sets generated by Chen and RSP3 methods respectively. These methods are based on a space splitting strategy, but the first one requires the specification of the final size of the generated sets while the latter does not. We can see that the Chen method generates prototypes keeping a homogeneous distribution of points in the space. RSP3 was proposed to fix some problems observed in the Chen method, but in this concrete data set, this method is worse in accuracy/kappa rates than its ancestor. However, the reduction type of Chen's method is fixed and it is very dependent on the data set tackled.
- Figures 5f and 5g represent sets of data generated by BTS3 and SGP methods. Both techniques are clusterbased and present very high reduction rates over this data set. SGP does not work well in this data set because it promotes the removal of prototypes and uses an incremental order, which does not allow us to choose the most appropriate decision. BTS3 uses a fixed reduction type, thus it focuses on improving accuracy rates, but its generation mechanisms are not well suited to in this type of data set.
- Figures 5h and 5i illustrate the sets of data generated by PSO and ENPC methods. They are wrapper and hybrid methods of the position adjusting family and iterate many times to obtain an optimal reallocation of prototypes. PSO requires as a parameter the final size of the subset selected



Fig. 5: Data Generated Sets in Banana Data Set

and this parameter is very conditioned to the complexity of the data set addressed. In the *banana* case, keeping a 2% of prototypes seems to work well. On the other hand, ENPC can adjust the number of prototypes required to fit a specific data set. In the case study presented, we can see that it obtains similar sets to those obtained by the Chen approach, because it also fills the regions with a homogeneous distribution of generated prototypes. In decision boundaries, the density of prototypes is increased and may produce quite noisy samples for further classification of the test data. It explains its poor behavior in this problem with respect to PSO, the lower reduction rate achieved and the decrement of accuracy/kappa rates with regard to the original data set classified with 1NN.

We have seen the resulting data sets of condensation, edition and hybrid methods and different generation mechanisms with some representative PG methods. Although the methods can be categorized as a specific family, they do not follow a specific behavior pattern, since some of the condensation techniques may generate interior points (like in LVQ3), others clusters of data (RSP3) or even points with a homogeneous distribution in space (Chen or ENPC). Nevertheless, visual characteristics of generated sets are also the subject of interest and can also help to decide the choice of a PG method.

VII. CONCLUSIONS

In this paper, we have provided an overview of Prototype Generation methods proposed in the literature. We have identified the basic and advanced characteristics. Furthermore, existing work and related fields have been reviewed. Based on the main characteristics studied, we have proposed a taxonomy of Prototype Generation methods.

The most important methods have been empirically analyzed over small and large sizes of classification data sets. To illustrate and strengthen the study, some graphical representations of data subsets selected have been drawn and statistical analysis based on nonparametric tests has been employed. Several remarks and guidelines can be suggested:

• A researcher, who needs to apply a PG method, should know the main characteristics of these kinds of methods in order to choose the most suitable. The taxonomy proposed and the empirical study can help a researcher to make this decision.

- To propose a new PG method, rigorous analysis should be considered to compare the most well known approaches and those which fit with the basic properties of the new proposal. To do this, the taxonomy and analysis of influence in the literature can help guide a future proposal to the correct method.
- This paper helps non-experts in PG methods to differentiate between them, to make an appropriate decision about their application and to understand their behavior.
- It is important to know the main advantages of each PG method. In this paper, many PG methods have been empirically analyzed but a specific conclusion cannot be drawn regarding the best performing method. This choice depends on the problem tackled but the results offered in this paper could help to reduce the set of candidates.

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Isaac Triguero received the M.Sc. degree in Computer Science from the University of Granada, Granada, Spain, in 2009.

He is currently a Ph.D. student in the Department of Computer Science and Artificial Intelligence, University of Granada, Granada, Spain. His research interests include data mining, data reduction and evolutionary algorithms.



Joaquín Derrac received the M.Sc. degree in Computer Science from the University of Granada, Granada, Spain, in 2008.

He is currently a Ph.D. student in the Department of Computer Science and Artificial Intelligence, University of Granada, Granada, Spain. His research interests include data mining, data reduction, lazy learning and evolutionary algorithms.



Salvador García received the M.Sc. and Ph.D. degrees in Computer Science from the University of Granada, Granada, Spain, in 2004 and 2008, respectively.

He is currently an Assistant Professor in the Department of Computer Science, University of Jaén, Jaén, Spain. His research interests include data mining, data reduction, data complexity, imbalanced learning, statistical inference and evolutionary algorithms.



Francisco Herrera received the M.Sc. degree in Mathematics in 1988 and the Ph.D. degree in Mathematics in 1991, both from the University of Granada, Spain.

He is currently a Professor in the Department of Computer Science and Artificial Intelligence at the University of Granada. He has published more than 150 papers in international journals. He is coauthor of the book *Genetic Fuzzy Systems: Evolutionary Tuning and Learning of Fuzzy Knowledge Bases* (World Scientific, 2001).

As edited activities, he has co-edited five international books and co-edited twenty special issues in international journals on different Soft Computing topics. He acts as associated editor of the journals: IEEE Transactions on Fuzzy Systems, Information Sciences, Mathware and Soft Computing, Advances in Fuzzy Systems, Advances in Computational Sciences and Technology, and International Journal of Applied Metaheuristics Computing. He currently serves as area editor of the Journal Soft Computing (area of genetic algorithms and genetic fuzzy systems), and he serves as member of several journal editorial boards, among others: Fuzzy Sets and Systems, Applied Intelligence, Knowledge and Information Systems, Information Fusion, Evolutionary Intelligence, International Journal of Hybrid Intelligent Systems, Memetic Computation.

His current research interests include computing with words and decision making, data mining, data preparation, instance selection, fuzzy rule based systems, genetic fuzzy systems, knowledge extraction based on evolutionary algorithms, memetic algorithms and genetic algorithms.