Multilabel Prototype Generation for Data Reduction in k-Nearest Neighbour classification

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Abstract

Prototype Generation (PG) methods are typically considered for improving the efficiency of the k-Nearest Neighbour (kNN) classifier when tackling high-size corpora. Such approaches aim at generating a reduced version of the corpus without decreasing the classification performance when compared to the initial set. Despite their large application in multiclass scenarios, very few works have addressed the proposal of PG methods for the multilabel space. In this regard, this work presents the novel adaptation of four multiclass PG strategies to the multilabel case. These proposals are evaluated with three multilabel kNN-based classifiers, 12 corpora comprising a varied range of domains and corpus sizes, and different noise scenarios artificially induced in the data. The results obtained show that the proposed adaptations are capable of significantly improving—both in terms of efficiency and classification performance—the only reference multilabel PG work in the literature as well as the case in which no PG method is applied, also presenting a statistically superior robustness in noisy scenarios. Moreover, these novel PG strategies allow prioritising either the efficiency or efficacy criteria through its configuration depending on the target scenario, hence covering a wide area in the solution space not previously filled by other works.

Keywords: Multilabel classification, Prototype Generation, Efficient kNN

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1. Introduction

The \( k \)-Nearest Neighbour (\( k \text{NN} \)) classifier represents one of the most well-known algorithms for non-parametric supervised classification, mostly due to its conceptual simplicity and good statistical error properties [1]. For a given query, this method hypothesises about its category by querying the \( k \) nearest neighbours of a reference corpus, following a specified similarity measure [2]. In this regard, this classification strategy has been largely considered in a wide range of disparate fields as, for instance, diabetes detection [3], musical key estimation [4], or handwritten signature verification [5], among others.

However, as a representative case of the lazy learning paradigm, \( k \text{NN} \) does not derive a model out of the reference corpus [6]. In contrast, for every query, this method requires an exhaustive search among the elements of the aforementioned corpus, thus entailing low-efficiency figures in both classification time and memory usage [7]. Note that, while this inefficiency issue may be obviated in scenarios with limited amounts of data, when considering large data collections, \( k \text{NN} \) becomes intractable [8].

Data Reduction (DR) stands as one of the main existing approaches in the related literature for tackling this drawback [9]. This group of methods aims to reduce the size of the reference set for improving the efficiency of the scheme while keeping—or even increasing—the classification performance obtained with the original data. Among them, the Prototype Generation (PG) family represents one of the most competitive alternatives due to its remarkable reduction capabilities compared to other DR strategies [10]. In a broad sense, PG derives an alternative reference set for the classifier by performing different selection and merging operations on the elements of the initial corpus following certain heuristics [11].

Due to the relevance of PG for efficient \( k \text{NN} \)-based classification, a considerable amount of research effort has been invested in proposing novel strategies as well as improving the existing ones [12]. However, such research works have typically addressed \textit{multiclass} scenarios—classification tasks in which every sin-
gle query is assigned to one category out of a set of mutually excluding labels—, hence neglecting the more general multilabel scenario—case in which an undetermined number of categories is assigned to each query [13].

The work by Ougiaroglou et al. [14] represents one of the scarce works of a PG strategy devised to address multilabel scenarios. More precisely, this work proposes the adaptation of the state-of-the-art Reduction through Homogeneous Clustering (RHC) method [15] to the multilabel space, obtaining the so-called Multilabel Reduction through Homogeneous Clustering (MRHC). The authors not only conclude that such adaptation remarkably improves the efficiency of the kNN classifier in multilabel scenarios but also state the need for contriving multilabel PG strategies due to the shortage of existing alternatives.

In this context, the present work further explores the proposal and use of PG methods for improving the efficiency of kNN classification in multilabel scenarios. More precisely, we introduce the novel adaptation of four PG strategies from their original multiclass formulation to the multilabel case. These proposals have been comprehensively evaluated considering several multilabel classification approaches based on kNN with a wide variety of corpora. Additionally, different percentages of label-level noise particularly devised for this multilabel framework—artificial alterations of the classes or labels of the data—have been induced in the corpora to assess the robustness of the proposals and their capability of dealing with such adverse scenarios. The results obtained report a statistical improvement in terms of both reduction capabilities and classification performance for all scenarios and noise levels contemplated compared to the exhaustive search carried out by the base kNN method and the reference MRHC reduction approach. In this regard, these novel proposals not only fill a gap in the scarce multilabel PG literature but also reportedly outperform the only existing strategy in the field, the commented MRHC algorithm.

The rest of the work is structured as follows: Section 2 provides the theoretical background of the work; Section 3 presents the proposed PG methods; Section 4 introduces the experimental set-up; Section 5 shows and discusses the results; and finally, Section 6 concludes the work and poses future research lines.
to pursue.

2. Background

To adequately describe multilabel classification, we initially introduce the multiclass framework, as it conceptually represents a simpler task. Formally, let \( \mathcal{X} \in \mathbb{R}^f \) denote an \( f \)-dimensional feature space and \( Y_{mc} \) a set of discrete labels. Additionally, let \( T_{mc} = \{ (x_i, y_i) : x_i \in \mathcal{X}, y_i \in Y_{mc} \} \) represent an annotated collection of data where each datum \( x_i \in \mathcal{X} \) is related to label \( y_i \in Y_{mc} \) by an underlying function \( h_{mc} : \mathcal{X} \rightarrow Y_{mc} \). The goal of multiclass classification is retrieving the most accurate approximation \( \hat{h}_{mc}(\cdot) \) to that underlying function.

Among the different alternatives for performing such an approximation task, the well-known \( k \)NN stands as one of the most common choices given its relevance in the Pattern Recognition field \[16\]. Formally, given a query \( q \in \mathcal{X} \), this method models \( \hat{h}_{mc} \) as:

\[
\hat{h}_{mc}(q) = \text{mode}\left( Y_{mc}^k\left( \arg \min_{x_i \in \mathcal{T}_{mc}}\{ d(q, x_i) \} \right) \right)
\]

where \( k \) stands for the number of neighbours considered, \( d : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_0^+ \) is a dissimilarity measure, \( \text{mode} : Y_{mc} \rightarrow Y_{mc} \) denotes the mode operator, and \( Y_{mc}^k \) is the set of labels retrieved from the closest \( k \) elements to the query \( q \).

As previously introduced, the multilabel paradigm constitutes a generalisation of the multiclass framework in which each individual instance may be associated to more than a single label \[17\]. Formally, the set of multilabel data \( T_{ml} = \{ (x_i, y_i) : x_i \in \mathcal{X}, y_i \subseteq Y_{ml} \} \) relates datum \( x_i \in \mathcal{X} \) to a subset of classes \( y_i \subseteq Y_{ml} \), namely labelset, where \( Y_{ml} = \{ \lambda_1, \lambda_2, \ldots, \lambda_L \} \) is an \( L \)-size collection of mutually non-exclusive labels \[18\]. As in the multiclass case, the goal is retrieving the most accurate approximation \( \hat{h}_{ml}(\cdot) \) to the underlying function \( h_{ml} : \mathcal{X} \rightarrow Y_{ml} \).

To leverage the advantages of multiclass classifiers in multilabel scenarios, the literature considers two main approaches \[19\]: problem transformation and
algorithm adaptation. We now describe these paradigms and report some commonly considered methods within them for \( k \)NN schemes as it represents the focus of the work.

The problem transformation paradigm disentangles the multilabel task into several single-label problems for then applying a multiclass \( k \)NN-based strategy for performing the classification task. Some of the most common alternatives are: the Binary Relevance \( k \)NN (BR\( k \)NN), which decomposes the task into \( L \) independent binary classification problems [20]; the Label Powerset \( k \)NN (LP-\( k \)NN), which derives an alternative single-label corpus where each labelset is considered as a different class [21]; and Random \( k \)-Labelsets (RA\( k \)EL), which divides the initial set of labels into a number of small random subsets for then performing LP-\( k \)NN and creating an ensemble-based classifier [22].

In contrast, the algorithm adaptation approach focuses on modifying the base multiclass classifier to fit the multilabel scenario. In this regard, the Multilabel \( k \)NN (ML-\( k \)NN) proposed by Zhang and Zhou [23] expands the base \( k \)NN method resorting to a maximum-a-posteriori principle to determine the labelset of the query based on its neighbouring instances. Some extensions to this approach are the Dependent ML-\( k \)NN [24], which models the different dependencies among the set of labels, the IBLR-ML method [25], which expands the base ML-\( k \)NN one by combining it with logistic regression, or the combination of ensembles and ML-\( k \)NN as in the work by Zhu et al. [26].

Nevertheless, while these transformations and adaptations allow the use of \( k \)NN in multilabel classification tasks, the inherent efficiency issue of these classifiers has been neglected in the literature. Note that, while some multilabel schemes such as the ML-\( k \)NN depict similar inefficiency figures to that of the multiclass \( k \)NN formulation since they explore the entire reference \( T_{ml} \) set, the BR\( k \)NN case is of particular relevance as it requires iterating through the \( T_{ml} \) set \( L \) different times.

The Prototype Generation (PG) family of methods stands as one of the most successful approaches for efficient \( k \)NN classification in multiclass cases [9]. As a representative case of DR strategy, PG aims to obtain an alternative set \( R_{mc} \)
by performing certain combinations and transformations on the elements of \( \mathcal{J}_{mc} \) so that \( |\mathcal{R}_{mc}| < |\mathcal{J}_{mc}| \) while keeping—or even improving—the classification performance. However, as aforementioned, to the best of our knowledge, there is a remarkable lack of methods for performing PG in multilabel scenarios. The sole exception to this assertion is the work by Ougiaroglou et al. \[14\] where the state-of-the-art multiclass PG method RHC was adapted to the multilabel space. In that work, the authors experimentally proved the usefulness of their PG proposal to improve the efficiency of the multilabel classification and stated the need for devising other alternatives to fill this existing gap in the literature.

In this context, the present work proposes the novel adaptation to the multilabel space of four well-known multiclass PG algorithms. More precisely, we consider the classic Chen reduction algorithm \[27\] as well as the three different versions of the reference Reduction through Space Partitioning (RSP) strategy by Sánchez \[28\]. For this first-time adaptation to the multilabel space of such PG algorithms, this work proposes several mechanisms for both partitioning and integrating the labels of the multilabel prototypes of the initial corpus for eventually generating the instances of the reduced multilabel set. These novel methods are thoroughly compared, in terms of both performance and efficiency, to the state-of-the-art proposal by Ougiaroglou et al. \[14\] and to the case in which no reduction is performed considering different multilabel \( k \)NN-based classifiers, corpora, and noise scenarios. Such study shall provide insights on whether the proposed multilabel PG methods cope with the commented efficiency issue without decreasing the classification performance and on their robustness as well as data cleansing capabilities in cases depicting the presence of noise in the data.

3. Prototype Generation in the multilabel space

This section presents the proposed PG methods for the multilabel space. As commented, we focus on the first-time adaptation of four algorithms originally devised for multiclass cases: the Chen method \[27\] and the three versions of the
Reduction through Space Partitioning (RSP) strategy \cite{28}. In this regard, the first part of the section introduces the original multiclass formulations of these algorithms and the second one presents their respective multilabel adaptations proposed in this work.

3.1. Reference multiclass PG

The considered multiclass PG strategies—the Chen method as well as the different RSP versions—constitute representative examples of the so-called space splitting policy \cite{29}, which typically follows a two-step approach: a first stage, space partitioning, divides the feature space of the multiclass set $T_{mc}$ into different regions using certain heuristics; after that, the prototype merging stage computes new prototypes from each region attending to different criteria, producing the reduced set $R_{mc}$. The existing PG strategies under this framework, therefore, essentially differ in the particular splitting and prototype generation heuristics considered.

In the specific case of the Chen and RSP PG families, the aforementioned heuristics depict some similarities. In this regard, we first present the particular approach followed by the Chen method in Algorithm\[\text{1}\] \footnote{Algorithm\[\text{1}\]} \footnote{Algorithm\[\text{1}\]} \footnote{Algorithm\[\text{1}\]} \footnote{Algorithm\[\text{1}\]} aided by the graphical illustration in Figure\[\text{1}\] \footnote{Figure\[\text{1}\]} for then commenting the different points on which the three RSP strategies differ from it.

As it may be checked in the algorithm, the method iteratively divides the feature space of $T_{mc}$ into $n_d$—user parameter—disjoint subsets which are denoted as $C_{mc}(i)$ where $\bigcup_{i=1}^{n_d} C_{mc}(i) = T_{mc}$. For that, the largest subset in each iteration is divided in two attending to the distance between the two farthest prototypes in it. Eventually, for each of the $n_d$ regions, a new prototype is obtained as the median of the features of the elements in it and labelled after the most common class. Hence, the size of the resulting reduced set equals the number of partitions selected by the user, \textit{i.e.}, $|R_{mc}| = n_d$.

The RSP family, as commented, builds upon the Chen proposal by modifying some of the space partitioning and/or prototype merging stages. The first RSP version—RSP1—considers the Chen algorithm prone to discard underrep-
Algorithm 1: Chen algorithm for multiclass PG

Input: \( T_{mc} \subset X \times Y_{mc} \) \( \rightarrow \) Multiclass corpus
\( n_d \) \( \rightarrow \) Number of resulting partitions
\( d(\cdot, \cdot) \) \( \rightarrow \) Dissimilarity measure

Output: \( R_{mc} \) \( \rightarrow \) Reduced set

1. Let \( n_c = i = 1, C_{mc} = \emptyset, B = T_{mc} \) \( \triangleright \) Space partitioning
2. Let \( p_1, p_2 \) be the farthest prototypes in \( B \)
3. while \( n_c < n_d \) do
4.   Divide \( B \) into subsets:
5.     \( B_1 = \{ p \in B : d(p, p_1) \leq d(p, p_2) \} \)
6.     \( B_2 = \{ p \in B : d(p, p_1) > d(p, p_2) \} \)
7.   Set \( n_c = n_c + 1, C_{mc}(i) = B_1, \) and \( C(n_c) = B_2 \)
8.   Divide \( C_{mc} \) into subsets:
9.     \( G_1 = \{ i : |\{ y \in C_{mc}(i) \}| > 1 \} \)
10.    \( G_2 = \{ j : j \leq n_c \} - G_1 \)
11.   Let \( G = G_1 \) if \( G_1 \neq \emptyset \) else \( G_2 \)
12.   Find farthest points \( q_1(i), q_2(i) \) in \( C_{mc}(i) \) \( \forall i \in G \)
13.   Let \( j = \arg \max_{j \in [1, i]} d(q_1(i), q_2(j)) \)
14.   Set \( B = C_{mc}(j), p_1 = q_1(j), \) and \( p_2 = q_2(j) \)
15. end while
16. Compute \( R_{mc} = \{(x_i, y_i)\}_{i=1}^{n_d} \) as: \( \triangleright \) Prototype merging
17.   \( x_i = \text{median} \{ \{ x \in C_{mc}(i) \} \} \)
18.   \( y_i = \text{mode} \{ \{ y \in C_{mc}(i) \} \} \)

represented classes due to its prototype merging policy (lines 16-18 in Algorithm 1). Thus, instead of computing a single prototype for each of the \( n_d \) regions and labelling them after the most represented class in each partition, RSP1 only merges prototypes sharing the same label. Hence, each region is now represented by more than a single prototype, more precisely, as many as the number of classes it contains. In this case, therefore, the size of the reduced set may not be known in advance but accomplishes \( |R_{mc}| \geq n_d \).

The second version of RSP—RSP2—expands RSP1 by modifying the space partitioning policy and, more precisely, the criterion for selecting the region to split (lines 12-13 in Algorithm 1). RSP2 considers the overlapping degree
Figure 1: Graphical illustration of the multiclass Chen PG method. The example depicts the results of the space partitioning process (cases 1a to 1c) and the prototype merging phase (case 1d) when considering \( n_d = 3 \) subsets. Symbols \( p_1 \) and \( p_2 \) denote the two furthest prototypes in the cluster to be divided.

criterion, which is defined as the ratio of the average distance between instances belonging to different classes and the average distance between instances that are from the same class. The region with the largest overlapping degree is the one to be divided.

The third RSP reduction heuristic—RSP3—is based on the idea that each resulting region should represent a cluster of instances belonging to only one class. Thus, this approach modifies the Chen method so that it iteratively performs the space partitioning stage (line 3 in Algorithm 1) until all resulting sets are homogeneous in terms of class representation, remaining the prototype merging phase of the algorithm unaltered. Hence, unlike the RSP1 and RSP2 strategies, the RSP3 approach does not require the \( n_d \) user parameter related...
to the number of resulting regions since the method exclusively relies on this
class homogeneity criterion to accomplish the space partitioning stage.

3.2. Multilabel PG proposals

Having introduced the four reference PG methods in their multiclass formulation, we now present their respective multilabel adaptations proposed in the work.

The multilabel space splitting PG framework may be formulated in an analogous manner to that of the multiclass case. Initially, the space partitioning phase divides the multilabel set $\mathcal{T}_{ml} \subset \mathcal{X} \times \mathcal{Y}_{ml}$ into $n_d$ non-overlapping multilabel regions $C_{ml}$ such that $\bigcup_{i=1}^{n_d} C_{ml}(i) = \mathcal{T}_{ml}$. After the convergence of this stage, the prototype merging step retrieves the multilabel set of data $\mathcal{R}_{ml}$ generated out of these $C_{ml}$ clusters by following a certain approach, where $|\mathcal{R}_{ml}| \leq |\mathcal{T}_{ml}|$. Within this framework, we introduce the different modifications proposed in the work for accommodating the presented multiclass PG methods to such scenario.

Our first proposal is the adaptation of the Chen algorithm, namely Multilabel Chen or MChen. Since the space partitioning stage (lines 1-15) computes the set of clusters $C_{mc}$ only relying on the set of features $\mathcal{X}$, no adaptation is required for its multilabel formulation to obtain set $C_{ml}$. Oppositely, given that the prototype merging stage (lines 16-18) usually requires combining elements from different classes, the question arises about the proper approach to do so in multilabel spaces since the simple selection of the most common label in the $C_{ml}$ cluster is not suitable for the considered scenario.

In this regard, we resort to the policy devised by Ougiaroglou et al. for the MRHC method in which the resulting prototype keeps the labels present in at least half of the instances of the cluster. Mathematically, the labelset assigned to the resulting element in cluster $C_{ml}(i)$ is given by:

$$ y_i = \left\{ \lambda : |C_{ml}(i)|_\lambda \geq \frac{|C_{ml}(i)|}{2} \quad \forall \ \lambda \in C_{ml}(i) \right\} $$

where $|C_{ml}(i)|_\lambda$ denotes the cardinality of label $\lambda$ in subset $C_{ml}(i)$. This expression replaces that in line 18 of Algorithm whereas the policy followed for
obtaining the set of features (line 17) is not modified. Figure 2c provides a graphical example of this merging procedure considering the space partitioning result shown in Figure 2b.

The second proposal is the Multilabel RSP1 or MRSP1. As aforementioned, the RSP1 states that, during the prototype merging stage and for each cluster $C_{mc}(i)$ of multiclass data, one prototype must be retrieved for each class present in it. The MRSP1 adapts such stage by resorting to a labelset approach (lines 16-18), i.e. each labelset is considered a different class and the instances with the same labelset are merged and assigned to it. Mathematically, set $R_{ml}$ is obtained as:

$$R_{ml} = \{(\text{median}(\{(x_j : (x_j, y_j) \in C_{ml}(i), y_j = y_k\})), y_k)\}_{i=1}^{n_d}$$

where $k = |\{y \in C_{ml}(i)\}|$ is the number of labelsets in the $i$-th cluster $C_{ml}(i)$ and $j \in [1,|C_{ml}(i)|]$. Figure 2d provides a graphical example of this procedure based on the space partitioning result depicted in Figure 2b.

The Multilabel RSP2 or MRSP2 proposal generalises the space partitioning approach based on the overlapping degree from the RSP2 method to the multilabel space (lines 12-13). For that, as in the MRSP1 proposal, we resort to a labelset approach: each labelset is considered a different class and the overlapping degree $\Phi_i$ of the $i$-th $C_{ml}(i)$ region is computed as the ratio of the average distance between instances belonging to different labelsets—$D^\neq$—and the average distance between instances of the same labelset—$D^=$.

In formal terms, for the $i$-th region, these pairwise distance values $D^\neq$ and $D^=$ are respectively computed as:

$$D^\neq = \{d(x_j, x_k) : (x_j, y_j) \land (x_k, y_k) \in C_{ml}(i), j \neq k, y_j \neq y_k\}$$

$$D^= = \{d(x_j, x_k) : (x_j, y_j) \land (x_k, y_k) \in C_{ml}(i), j \neq k, y_j = y_k\}$$

with $1 \leq j, k \leq n_d$. Based on this, the overlapping degree $\Phi_i$ for the same $i$-th region is eventually obtained as:

$$\Phi_i = \frac{\sum_{j=1}^{D^\neq} D^\neq(j)}{\sum_{k=1}^{D=} D^=(k)} \cdot \frac{|D^=|}{|D^\neq|}$$
Figure 2: Graphical illustration of the multilabel PG proposals introduced in the work. Figure 2a represents a multilabel set of train data $T_{ml}$ to be reduced. Figure 2b shows the space partitioning results on which the different reduction proposals are based, except for the MRSP3 one, whose case is illustrated in Figure 2e. Prototype merging graphs 2c and 2f depict the number of prototypes—denoted as $\#prot$—and the cardinality of labels—$\#\Box$, $\#\diamond$, and $\#\circ$—for each of the original clusters.
Note that, after the convergence of the space partitioning stage, the prototype merging policy in Equation 2 introduced for MRSP1 is applied.

The last proposal is the Multilabel RSP3 or MRSP3. In this case, we must generalise the cluster homogeneity concept of the RSP3 method to automatically estimate the $n_d$ number of clusters. For that, we resort to the criterion posed by Ougiaroglou et al. [14] which states that a set of multilabel data is considered to be homogeneous if there is, at least, one common label among all the prototypes in the set, i.e. $\exists \lambda \in C_{ml}(i)$ s.t. $|C_{ml}(i)|_\lambda = |C_{ml}(i)|$. This substitutes the condition in line 3 in Algorithm 1 so that the process finishes when this homogeneity criterion is accomplished by all regions. After this space partitioning stage, the set of clusters $C_{ml}$ is further processed following the prototype merging approach of the MChen proposal in Equation 2.

Finally, Figures 2e and 2f respectively show the result of the space partitioning and prototype merging phases of the introduced MRSP3 proposal.

4. Experimental set-up

This section presents the experimental scheme designed for comparatively assessing the proposed multilabel PG methods. For an easier description, this procedure is graphically illustrated in Figure 3.

During the training phase of the procedure, the set of train data $T_{ml} \subset \mathcal{X} \times Y_{ml}$ is altered to induce certain noise level in the instances controlled by the user parameter $\theta \in [0, 1]$, retrieving set $T'_{ml}$. Then, this latter data collection
$T'_{ml}$ is processed by a multilabel PG method to obtain a reduced version of the set—namely $R_{ml}$—that is used as the reference set for the multilabel $k$NN-based classifier. It must be noted that the noise induction process represents an optional stage in the posed pipeline. Hence, as it will be shown, the first experimental part does not induce any noise by setting $\theta = 0$ while the second one will analyse the robustness and data cleansing capabilities of the reduction methods to the data corruption process by considering $\theta > 0$.

During the inference stage, a test set of multilabel data $S_{ml} \subset X \times Y_{ml}$ drawn from the same distribution as the train data $T_{ml}$ but disjoint from it is considered for evaluating the method. Using a $\hat{h}_{ml} (\cdot)$ prediction function from the particular multilabel $k$NN-based classification strategy at hand, each sample $x_i \in S_{ml}$ is given a labelset that is eventually compared to that in the ground-truth based on certain evaluation criteria.

The remainder of the section presents the corpora used for assessing the multilabel PG proposals, the noise induction procedure used, the considered $k$NN-based classification strategies, and the contemplated evaluation protocol.

4.1. Corpora

We have considered 12 multilabel corpora from the Mulan repository [30] comprising a varied range of domains, corpus sizes, initial space dimensionalities, and target label spaces. The precise details in terms of size, features and label dimensionality of these sets are provided in Table 1. In addition, the cardinality—average number of labels associated with each instance—and density—ratio of cardinality and label dimensionality of the corpus—measures are provided for each corpus as they represent common descriptors in the multilabel classification field.

Note that, for the sake of reproducible research, we have used the partitions defined by Szymański and Kajdanowicz in these particular corpora [31].

4.2. Noise induction procedure

To examine the actual robustness of both the existing and the proposed multilabel PG methods, we artificially introduce noise in the data. For that, as
Table 1: Summary of the corpora considered for the experimentation. Each corpus is described in terms of its data domain, partition sizes, dimensionality of input data (features) and output space (labels), cardinality, and density.

| Name    | Domain | Corpus size | Dimensionality | Cardinality | Density |
|---------|--------|-------------|----------------|-------------|---------|
|         |        | Train | Test | Features | Labels |        |          |
| Bibtex  | Text   | 4,880 | 2,515 | 1,836    | 159     | 2.40   | 0.015    |
| Birds   | Audio  | 322   | 323   | 260      | 19      | 1.01   | 0.053    |
| Corel5k | Image  | 4,500 | 500   | 499      | 374     | 3.52   | 0.009    |
| Emotions| Music  | 391   | 202   | 72       | 6       | 1.87   | 0.311    |
| Genbase | Biology| 463   | 199   | 1,186    | 27      | 1.25   | 0.046    |
| Medical | Text   | 333   | 645   | 1,449    | 45      | 1.25   | 0.028    |
| rcvsubset1 | Text | 3,000 | 3,000 | 47,236   | 101     | 2.88   | 0.029    |
| rcvsubset2 | Text | 3,000 | 3,000 | 47,236   | 101     | 2.63   | 0.026    |
| rcvsubset3 | Text | 3,000 | 3,000 | 47,236   | 101     | 2.61   | 0.026    |
| rcvsubset4 | Text | 3,000 | 3,000 | 47,229   | 101     | 2.49   | 0.025    |
| Scene   | Image  | 1,211 | 1,196 | 294      | 6       | 1.07   | 0.179    |
| Yeast   | Biology| 1,500 | 917   | 103      | 14      | 4.24   | 0.303    |

commonly considered in the literature \cite{Zhou2019}, we induce this noise by swapping the labels of pairs of prototypes randomly chosen from the train partition $T_{ml}$. This procedure is detailed in Algorithm 2 in which the user parameter $\theta \in [0, 1]$ represents the induced noise rate, i.e., the percentage of prototypes that change their label.

**Algorithm 2**: Noise induction procedure

```
Input : $T_{ml} \subseteq X \times Y_{ml} \leftarrow$ Multilabel train corpus
\hspace{1cm}$\theta \leftarrow$ Noise level parameter

Output: $T_{ml}' \subseteq X \times Y_{ml} \leftarrow$ Noisy multilabel train corpus

1 Let $\Theta = \{(x_i, y_i)\}_{i=1}^{\theta \cdot |T_{ml}|} \in_R T_{ml}$ \hspace{1cm}$\triangleright$ Random sampling of set $T_{ml}$
2 Let $T_{ml}' = T_{ml} - \Theta$
3 for $i \in [0, \ldots, \lfloor \Theta/2 \rfloor]$ do
4 \hspace{1cm}Save labelset of the $i$-th element in set $\Theta$: $y' = y \in \Theta_i$
5 \hspace{1cm}Put labelset in $|\Theta| - i$ in the $i$-th sample: $y \in \Theta_i = y \in \Theta_{|\Theta| - i}$
6 \hspace{1cm}Set $y'$ as the labelset of the $|\Theta| - i$-th element: $y \in \Theta_{|\Theta| - i} = y'$
7 end for
8 Let $T_{ml}' = T_{ml}' \cup \Theta$
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As aforementioned, the particular case of $\theta = 0$ represents that in which no noise is induced in the corpus, hence being $T_{\text{ml}}' = T_{\text{ml}}$.

4.3. Classification strategies

We have selected three reference multilabel techniques based on $k$NN as classification methods: BR$k$NN and LP-$k$NN from the transformation paradigm as well as ML-$k$NN based on the algorithm adaptation premise. In all cases, the Euclidean distance has been used as the dissimilarity measure.

Regarding the $k$ parameter representing the number of neighbours, we have considered the values $k \in \{1, 3, 5, 7\}$. Note that this parameter is not optimised by any means during the experimentation since the aim is to examine its influence on the overall classification performance in relation to the PG mechanisms.

4.4. Evaluation metrics

To assess the goodness of the proposals, we consider two criteria: classification performance and efficiency figures.

With respect to the former criterion, we resort to the Hamming Loss (HL) as it constitutes a commonly considered approach for measuring the goodness of multilabel classifiers [33]. This metric, which is defined as the fraction of the wrong predicted labels with respect to the total number of labels, can be mathematically posed as:

$$HL = \frac{1}{|S_{\text{ml}}|} \sum_{i=1}^{|S_{\text{ml}}|} \frac{1}{L} \cdot |y_i \Delta \hat{h}_{\text{ml}}(x_i)| (7)$$

where $S_{\text{ml}} \subset \mathcal{X} \times \mathcal{Y}_{\text{ml}}$ denotes the multilabel set of test data, $\Delta$ is the symmetric difference of ground-truth $y_i$ and predicted $\hat{h}_{\text{ml}}(x_i)$ sets, and $L$ is the number of labels.

As commonly done in the DR field, efficiency is assessed by comparing the size of the reduced set $R_{\text{ml}}$ normalised by that of the training set $T_{\text{ml}}$ [34]. Computation time was discarded as an evaluation metric due to its variability depending on the load of the computing system.
It must be noted that PG methods for \( k \)NN seek to simultaneously optimise two contradictory goals, set size reduction and classification performance, being not possible to achieve a global optimum. Hence, as in reference works from the literature \cite{35,36}, we address it as a Multi-objective Optimisation Problem in which the two aforementioned objectives are meant to be optimised. The different solutions under this framework—there may exist more than one—are retrieved by resorting to the concept of non-dominance: one solution is said to dominate another if it is better or equal in each goal function and, at least, strictly better in one of them. Those elements, typically known as non-dominated, constitute the Pareto frontier in which all elements are deemed as optimal solutions without any order among them.

5. Results

This section introduces and discusses the results obtained by the proposed multilabel PG methods with the evaluation methodology considered. For comparison purposes, the reference MRHC method and the case in which no reduction process is applied—denoted as ALL—are included. Also, let subscript \( m \) represent the input parameter of the PG methods when required, i.e. \( \text{MChen}_m \), \( \text{MRSP1}_m \), and \( \text{MRSP2}_m \), which relates to the number of partitions as \( n_d = m \cdot |T_{ml}|/100 \). For assessing its influence in the scheme, we considered different values of this input parameter as \( m \in \{10, 30, 50, 70, 90\} \).

The remainder of the section presents two particular experiments: (i) a first part in which the PG methods are comparatively evaluated obviating the noise induction process; and (ii) a second one whose focus is the noise robustness and data cleansing capabilities of these PG schemes.

The implementation of the proposed PG methods and the experimental procedure considered is publicly available in: [https://github.com/jose-jvmas/multilabel_PG](https://github.com/jose-jvmas/multilabel_PG)
5.1. Comparative assessment of multilabel PG strategies

In this first experiment, we thoroughly compare the different reduction strategies using the aforementioned multilabel kNN-based classifiers as individual scenarios. In this regard, Table 2 and Figure 4 show the results obtained in which the performance and reduction figures constitute the average of the individual values obtained for the corpora considered.

Table 2: Results in terms of HL and resulting size for both the reference methods (exhaustive search, denoted as ALL, and MRHC) and our proposals (MChen, MRSP1, MRSP2, and MRSP3) when considering the different kNN-based classifiers. Non-dominated solutions per classifier are highlighted in bold type. Underlined values denote the best performance rates per PG scheme and classifier.

|             | Size | Reference  | BR\textsuperscript{kNN} | LP-kNN | ML-kNN |
|-------------|------|------------|-----------------------|-------|--------|
|             |      | ALL        | 100                   | 9.09  | 7.94   |
|             |      | MRHC       | 59.62                 | 8.76  | 7.40   |
| Proposals   |      | MChen\textsubscript{10} | 9.98                | 7.92  | 7.74   |
|             |      | MChen\textsubscript{30} | 29.94               | 8.00  | 7.58   |
|             |      | MChen\textsubscript{50} | 49.96               | 8.29  | 7.71   |
|             |      | MChen\textsubscript{70} | 69.97               | 8.51  | 7.72   |
|             |      | MChen\textsubscript{90} | 89.02               | 8.73  | 7.92   |
|             |      | MRSP1\textsubscript{10} | 61.88               | 8.95  | 7.96   |
|             |      | MRSP1\textsubscript{30} | 74.51               | 8.77  | 7.76   |
|             |      | MRSP1\textsubscript{50} | 80.11               | 8.80  | 7.78   |
|             |      | MRSP1\textsubscript{70} | 83.59               | 8.86  | 7.77   |
|             |      | MRSP1\textsubscript{90} | 87.21               | 8.80  | 7.67   |
|             |      | MRSP2\textsubscript{10} | 61.09               | 8.85  | 7.90   |
|             |      | MRSP2\textsubscript{30} | 78.07               | 8.79  | 7.87   |
|             |      | MRSP2\textsubscript{50} | 83.59               | 8.74  | 7.76   |
|             |      | MRSP2\textsubscript{70} | 87.21               | 8.80  | 7.67   |
|             |      | MRSP2\textsubscript{90} | 89.28               | 8.76  | 7.68   |
|             |      | MRSP3\textsubscript{10} | 66.88               | 8.53  | 7.62   |

A first remark that may be observed is that the proposed methods fill a region in the space of possible solutions not previously occupied by existing multilabel PG methods. This is because some of the proposals (MChen, MRSP1, and MRSP2) allow selecting the size of the reduced set through a parameter.
Figure 4: Results in terms of HL and resulting size obtained with the $k$NN-based classifiers when considering the PG methods and the exhaustive search case (ALL) for the different $k$ values tested. Circed methods and dashed lines represent the non-dominated elements and the Pareto frontiers in each scenario, respectively. For easier comparison, shaded areas depict the regions in the solution space occupied by the baseline cases (MRHC and ALL).

Note that, while this may be considered a drawback, such a feature allows prioritising either the reduction rate or classification performance depending on
the particular application considered.

It can be also checked that, for all cases, MChen achieves the highest reduction rates, even when other parameter-based multilabel PG proposals consider the same $m$ value. This is somehow expected since, during the prototype merging stage, MChen only retrieves a single prototype for each region while MRSP1 and MRSP2 obtain a prototype per labelset in those subsets, hence inherently increasing the size of the $R_{ml}$ resulting set.

In terms of non-dominance, it may be noted that the obtained Pareto frontiers in the different classification scenarios considered only comprise examples of the novel multilabel PG strategies proposed in the work: BR$k$NN contains MChen$_{10}$, MChen$_{30}$, MRSP1$_{30}$, and MRSP2$_{70}$; LP-$k$NN depicts the MChen$_{10}$ and MChen$_{30}$ cases; and ML-$k$NN points out four of them, which are MChen$_{10}$, MChen$_{70}$, MRSP1$_{30}$, and MRSP2$_{90}$. Hence, the ALL and MRHC cases may not be considered optimal solutions to the task as they are consistently dominated by the novel proposals presented in this work.

Since the reduction process is applied before the classification stage, the resulting set sizes are the same for all scenarios, being the differences in performance only due to the particular capabilities of the classification scheme. In this regard, it can be observed that LP-$k$NN may be deemed as the least competitive alternative since, for the same reduction scheme, HL figures tend to be higher than the other alternatives. Oppositely, BR$k$NN and ML-$k$NN show similar performance results since the HL figures do not remarkably differ among them.

Finally, it may be also checked that the classification rates do generally improve as the number of neighbours considered—$k$ parameter of the classifiers—increases. This fact suggests the presence of some noise in the corpora that is somehow palliated by adequately tuning this parameter. Note that, among the different multilabel classifiers studied, LP-$k$NN is the one that shows the least improvement when increasing this $k$ value.
5.1.1. Statistical significance analysis

A significance analysis has been performed to statistically evaluate the results obtained. For that, we have considered the Wilcoxon signed-rank test [37] to assess whether the classification performance and reduction rate of the proposed PG methods significantly improve those of the baseline strategies. More precisely, for each classification scenario, we compare the results obtained by the elements of the particular Pareto frontier against the best figures obtained by the baseline MRHC and ALL methods. For that, we consider the individual results obtained—either performance or reduction—for each contemplated corpus in the experimentation. Table 3 shows the results of such analysis when considering a significance threshold of \( p < 0.05 \).

Table 3: Wilcoxon signed-rank test results with \( p < 0.05 \) for the classifiers considered. Symbols \( \checkmark, \times, \) and \( = \) respectively denote that, for each classification scenario, the non-dominated solution in the row significantly improves, worsens or does not differ from the reference one in the column for the performance (HL) or reduction (Size) criterion.

|                | ALL ■ |               | MRHC ▼ |               |
|----------------|-------|---------------|--------|---------------|
|                | HL    | Size          | HL     | Size          |
| **BR\(k\)NN** |       |               |        |               |
| MChen_{10}     | ✓     | ✓             | ✓      | ✓             |
| MChen_{30}     | ✓     | ✓             | ✓      | ✓             |
| MRSP_{130}     | ✓     | ✓             | ✓      | ✓             |
| MRSP_{270}     | ✓     | ✓             | ✓      | ×             |
| **LP\(-k\)NN**|       |               |        |               |
| MChen_{10}     | ✓     | ✓             | ✓      | ✓             |
| MChen_{30}     | ✓     | ✓             | ✓      | ✓             |
| **ML\(-k\)NN**|       |               |        |               |
| MChen_{10}     | ✓     | ✓             | ✓      | ✓             |
| MChen_{70}     | ✓     | ✓             | ✓      | ✓             |
| MRSP_{130}     | ✓     | ✓             | ✓      | ✓             |
| MRSP_{50}      | ✓     | ✓             | ✓      | ×             |

Focusing on the classification performance criterion (HL), it may be observed that the non-dominated elements in the Pareto frontier—exclusively defined by the proposals introduced in the work—statistically equal or improve the results
of the baselines considered. However, since the particular conclusions are quite
related to the actual classification scheme at hand, we shall now analyse them
in a separate manner.

When considering the BR$k$NN classifier, the proposals depicting the highest
reduction rates—$\text{MChen}^{10}$ and $\text{MChen}^{30}$—show a similar performance to both
ALL and MRHC baseline cases; on the contrary, those schemes with larger re-
sulting set sizes—MRSP1$^{30}$ and MRSP2$^{70}$—do improve the reference strategies.

In the case of the LP-$k$NN classifier, a similar trend to that of the BR$k$NN is
found: when performing a sharp reduction—$\text{MChen}^{10}$ strategy—, the reported
classification rate does not statistically differ to those of the baselines; however,
when allowing a larger set size—the $\text{MChen}^{30}$ method—, this performance in-
dicator does improve those of the reference cases.

The results obtained with the ML-$k$NN classifier, however, do not show a
similar tendency to the ones presented. As it may be observed, none of the non-
dominated cases is able to statistically outperform the ALL case, while they do
obtain similar performance scores with remarkably fewer prototypes. Regarding
the MRHC base case, two of the proposals—$\text{MChen}^{70}$ and MRSP2$^{50}$—do sig-
nificantly improve this base case while the other two non-dominated elements—
$\text{MChen}^{10}$ and MRSP1$^{30}$—report statistically similar classification rates.

In relation to the analysis of the reduction capabilities, as expected, the
results show that all non-dominated cases statistically improve the ALL case.
Oppositely, when compared to the MRHC, there is a larger variability in the
results: $\text{MChen}$ generally outperforms the reference method except for the case
of $\text{MChen}^{70}$ in the ML-$k$NN scenario, which shows no statistical difference; the
MRSP1$^{30}$—found in BR$k$NN and ML-$k$NN—also shows alike reduction capa-
bilities to MRHC as the analysis points out no difference; finally, MRSP2$^{70}$ and
MRSP2$^{50}$, respectively found in the BR$k$NN and ML-$k$NN scenarios, stand for
the cases in which the reduction results are statistically worse than MRHC,
given that these methods do not remarkably reduce the set size of the reference
corpus.
5.2. Noise robustness and data cleansing study

In this second experiment, we assess the performance of both the proposed multilabel PG strategies as well as the reference ones in scenarios with noisy data. For that, we consider the labelset swapping procedure introduced in Section 4.2 with $\theta \in \{20\%, 40\%\}$ as they stand as representative noise rates commonly considered in the related literature [32]. For comparative purposes, the case of $\theta = 0$ is also included to assess the base case in which no noise is induced in the data.

The results obtained in the different noise scenarios posed are depicted in Table 4 and Figure 5. Note that, for simplicity, these figures constitute the average performance—both in terms of recognition rate and reduction capabilities—of the individual results per PG method and $k$ classification parameter for the three $k$NN-based algorithms considered.

The induction of noise in the corpora clearly affects the overall performance since, in general, all studied cases depict lower classification rates as the noise level increases. It must be noted that, while the use of high $k$ classification values (e.g., $k = 5$ or $k = 7$) somehow palliates this effect, the best performance achieved in these noisy scenarios is indeed lower than that of the non-induced noise case.

Besides, all PG methods show, in general, worse reduction rates as the noise increases, being the MRHC and MRSP3 strategies particularly affected. The sole exception to this assertion is the MChen method whose reduction capabilities remain stable independently of the noise induced in the data.

Overall, it can be noted that MChen can be considered the best noise cleansing strategy since the classification schemes trained after that stage achieve the best overall HL performance figures. MRSP proposals, though, prove not to be that robust against this type of noise since the performance of the classification schemes trained with the set obtained with those methods degrades as the presence of noise increases. Regarding the reference MRHC method, it may be observed a similar performance trend to that of the MRSP family.

In terms of non-dominance, it may be observed that the different Pareto
Table 4: Results in terms of HL and resulting size for both the reference methods (exhaustive search, denoted as ALL, and MRHC) and our proposals (MChen, MRSP1, MRSP2, and MRSP3) when considering the different noise scenarios posed. Each value constitutes the average performance obtained for the three classification methods considered. Non-dominated solutions per noise scenario are highlighted in bold type. Underlined values denote the best performance rates per PG scheme and noise scenario.

| Noise 0% | Noise 20% | Noise 40% |
|----------|----------|----------|
|          | Size     | k        | Size     | k        | Size     | k        |
| Reference| ALL      | 100 9.09 | 8.19     | 7.98     | 7.89     | 100 9.80 | 8.50     | 8.22     | 8.03     | 100 10.65 | 9.17     | 8.73     | 8.53     |
| MRHC     | ▼        | 59.62    | 8.76     | 8.01     | 7.99     | 7.92     | 8.52     | 8.02     | 72.95     | 8.19     | 7.95     | 7.94     | 8.02     | 7.80     |
| Proposals| ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen10  | ■        | 59.62    | 8.76     | 8.01     | 7.99     | 7.92     | 8.52     | 8.02     | 72.95     | 8.19     | 7.95     | 7.94     | 8.02     | 7.80     |
| MChen20  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen30  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen40  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen50  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen60  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen70  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen80  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MChen90  | ▲        | 9.98     | 7.92     | 7.84     | 7.81     | 7.89     | 9.98     | 7.92     | 8.02     | 7.84     | 7.89     | 8.02     | 7.84     | 7.89     |
| MRSP110  | ▲        | 61.08    | 8.85     | 8.35     | 8.19     | 8.02     | 65.12    | 8.85     | 8.35     | 8.02     | 68.50    | 8.54     | 8.14     | 8.02     |
| MRSP130  | ▲        | 74.51    | 8.77     | 8.05     | 7.71     | 7.74     | 78.89    | 9.52     | 8.39     | 8.04     | 7.74     | 81.73    | 9.38     | 8.07     | 8.15     |
| MRSP150  | ▲        | 80.11    | 8.80     | 8.01     | 7.76     | 7.77     | 84.39    | 9.50     | 8.34     | 8.00     | 7.84     | 87.23    | 10.40    | 8.09     | 8.33     |
| MRSP170  | ▲        | 84.37    | 8.86     | 8.00     | 7.77     | 7.76     | 88.28    | 9.49     | 8.25     | 7.92     | 7.82     | 91.38    | 10.33    | 8.98     | 8.37     |
| MRSP190  | ▲        | 90.78    | 8.84     | 7.95     | 7.70     | 7.74     | 92.35    | 9.56     | 8.26     | 7.90     | 7.81     | 93.82    | 10.31    | 9.10     | 8.64     |
| MRSP210  | ▲        | 99.66    | 8.53     | 7.95     | 7.80     | 7.73     | 93.13    | 9.56     | 8.26     | 7.90     | 7.81     | 93.82    | 10.31    | 9.10     | 8.64     |
| MRSP230  | ▲        | 78.07    | 8.79     | 8.09     | 7.82     | 7.73     | 81.23    | 9.53     | 8.38     | 8.06     | 7.78     | 83.41    | 10.21    | 8.78     | 8.40     |
| MRSP250  | ▲        | 83.59    | 8.74     | 8.04     | 7.80     | 7.68     | 87.92    | 9.38     | 8.32     | 8.07     | 7.76     | 89.37    | 10.34    | 8.93     | 8.41     |
| MRSP270  | ▲        | 87.21    | 8.80     | 7.93     | 7.80     | 7.65     | 90.53    | 9.35     | 8.28     | 7.99     | 7.74     | 92.67    | 10.35    | 8.85     | 8.32     |
| MRSP290  | ▲        | 89.28    | 8.76     | 7.96     | 7.81     | 7.73     | 92.16    | 9.46     | 8.16     | 7.87     | 7.71     | 93.69    | 10.35    | 9.04     | 8.58     |
| MRSP310  | ▲        | 66.88    | 8.53     | 7.95     | 7.80     | 7.76     | 75.54    | 9.15     | 8.28     | 7.92     | 7.68     | 81.33    | 8.84     | 8.31     | 8.17     |

Frontiers are entirely defined by the novel PG proposals introduced in this work: MChen10, MChen30, MChen50, and MRSP270 in the non-induced noise scenario; MChen10, MChen30, and MRSP130 when $\theta = 20\%$; and MChen10 and MChen30 when considering the noisiest scenario of the ones studied in the work. In this regard, it may be concluded that the MChen algorithm proves itself as a considerably robust method—both in terms of efficiency and classification performance—against noisy situations, especially when set to high reduction rates (e.g., $m = 10\%$ or $m = 30\%$).
Figure 5: Results in terms of HL and resulting size for the different noise scenarios when considering the PG methods and the exhaustive search case (ALL) for the $k$ values tested. Note that each sample constitutes the average performance obtained for the three classification methods studied. Circled methods and dashed lines represent the non-dominated elements and the Pareto frontiers in each scenario, respectively. For easier comparison, shaded areas depict the regions in the solution space occupied by the baseline cases (MRHC and ALL).
5.2.1. Statistical significance analysis

As in the first experiment, we have considered the Wilcoxon signed-rank test to statistically compare the results obtained by the elements of the Pareto frontier against the best results obtained by the baseline MRHC and ALL methods for each noise scenario. Table 5 shows the outcome of such analysis when considering a significance threshold of $p < 0.05$.

Table 5: Wilcoxon signed-rank test results with $p < 0.05$ for the noise scenarios posed. Symbols $\checkmark$, $\times$, and $=$ respectively denote that, for each classification scenario, the non-dominated solution in the row significantly improves, worsens or does not differ from the reference one in the column for the performance (HL) or reduction (Size) criterion.

| Noise 0%         | ALL  | MRHC |
|------------------|------|------|
|                  | HL   | Size | HL   | Size |
| MChen$_{10}$     | =    | =    | =    | =    |
| MChen$_{30}$     | =    | =    | =    | =    |
| MChen$_{50}$     | =    | =    | =    | =    |
| MRSP$_{270}$     | =    | =    | =    | =    |

| Noise 20%        | ALL  | MRHC |
|------------------|------|------|
|                  | HL   | Size | HL   | Size |
| MChen$_{10}$     | =    | =    | =    | =    |
| MChen$_{30}$     | =    | =    | =    | =    |
| MRSP$_{130}$     | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |

| Noise 40%        | ALL  | MRHC |
|------------------|------|------|
|                  | HL   | Size | HL   | Size |
| MChen$_{10}$     | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| MChen$_{30}$     | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |

As it may be observed, the multilabel PG strategies proposed in the work significantly improve the reduction rate of the baselines considered for all noise scenarios posed. Such a point suggests a remarkable robustness of our methods to the presence of noise in the data: while the reduction capabilities of the reference MRHC strategy severely degrade as the noise in the data increases, the MChen is not affected by such an alteration whereas the MRSP1 and MRSP2 strategies do not degrade as much as the MRHC.

In relation to the classification rate, it may be noted that all non-dominated
proposals either equal or improve the exhaustive search case with a significantly lower amount of prototypes. More precisely, our proposals improve the ALL case when inducing an elevated level of noise in the data while, when addressing scenarios with low levels of induced noise, the proposed multilabel methods in the Pareto frontier do not significantly differ from the results of the exhaustive search.

Regarding the classification performance of the MRHC baseline method, it may be observed that this strategy is remarkably affected by the noise, being significantly outperformed by all the multilabel PG proposals in the non-dominated frontier. The sole exception to this assertion is the MChen10 in the Noise 0% scenario that does not significantly differ from the MRHC case.

Overall, this analysis proves the superior robustness and noise cleansing capabilities of the proposed multilabel PG alternatives since, in the worst-case scenario, the classification rate achieved is similar to that of the exhaustive search but with a significantly lower amount of samples. Besides, it is also proved that the only existing multilabel PG method in the literature—the MRHC algorithm—is severely affected by these noisy scenarios—both in terms of efficiency and classification rate—, being hence outperformed by the novel multilabel PG proposals introduced in this work.

6. Conclusions and Future Work

Prototype Generation (PG) represents one of the most competitive approaches for improving the efficiency of the $k$-Nearest Neighbour ($k$NN) classifier, which is typically related to low efficiency figures when tackling scenarios with large amounts of data. Nevertheless, while PG methods are commonly considered in multiclass scenarios, very scarce works have addressed such a task in multilabel frameworks.

This work presents the first-time adaptation of four multiclass PG methods to the multilabel case: the reference Chen method [27] and the three versions of the well-known Reduction through Space Partitioning [28]. For that, we gener-
alise to the multilabel space the different criteria considered by each method for gathering sets of prototypes (space partitioning stage) which are then combined according to certain policies (prototype merging). These novel PG proposals have been evaluated with 3 multilabel kNN-based classifiers, 12 multilabel corpora comprising a varied range of domains and corpus sizes, and different noise scenarios obtained by exchanging the labels of the instances in the train partition.

The results obtained show that the proposed adaptations are capable of significantly improving, both in terms of efficiency and efficacy, the only reference work in the literature—Multilabel Reduction through Homogeneous Clustering method by Ougiaroglou et al. [14]—as well as the case in which no PG method is applied—the exhaustive search. It is also proved that some of these adaptations show high robustness and data cleansing capabilities in the presence of noise. More precisely, when set to high reduction rates, the proposed Multilabel Chen strategy allows training classification schemes that statistically outperform those trained with the existing baseline approaches. Moreover, the user parameter of these methods allows prioritising either the efficiency or performance features of the scheme, depending on the particular application.

Future work considers the adaptation of other PG schemes to multilabel scenarios. The second point of interest is the further exploration of alternative criteria for the gathering and merging prototype stages, which may result in more efficient and/or robust classifiers. Finally, in light of the noise robustness capabilities of the proposals, we consider their use as preprocessing techniques for other classification schemes such as Support Vector Machine or neural models in task-oriented cases as, for instance, music tagging or image classification, among others.

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