Estudio de Métodos de Selección de Instancias

Programa de Doctorado «Tecnologías Industriales e Ingeniería Civil»

Por

Álvar Arnaiz González

Universidad de Burgos

Memoria presentada para optar al título de doctor por la Universidad de Burgos.

January 9, 2018

La investigación realizada en esta tesis doctoral ha sido parcialmente subvencionada por el Ministerio de Economía, Industria y Competitividad, la Junta de Castilla y León y el Fondo Europeo para el Desarrollo Regional, proyectos TIN 2011-24046, TIN 2015-67534-P (MINECO/FEDER) y BU085P17 (JCyL/FEDER).

Resumen

En un sentido amplio del término, la inteligencia artificial es cualquier tipo de inteligencia de la que disponga una máquina. Más concretamente, es una rama del conocimiento que trata de construir agentes inteligentes, entendiendo estos como entidades que utilizan las percepciones del entorno para llevar a cabo acciones que maximicen alguna medida de rendimiento. Dentro del variado número de tareas que engloba la inteligencia artificial, esta tesis se centra en el aprendizaje automático. Este término ha evolucionado a partir del estudio del reconocimiento de patrones. La idea subyacente es la de diseñar algoritmos que sean capaces de aprender y hacer predicciones sobre los datos. El rendimiento en este caso viene dado por cómo de buenas son las predicciones hechas sobre los datos. Las percepciones los valores numéricos de los datos, y las acciones la modificación de valores de parámetros y la emisión de la predicción.

Tradicionalmente, el aprendizaje automático se ha dividido en tres grandes grupos: supervisado (donde se dispone de ejemplos etiquetados que sirven como modelos para aprender), no supervisado (donde los ejemplos no se encuentran etiquetados) y por refuerzo (inspirado en la psicología conductista, donde los agentes deciden sus acciones con el objetivo de aumentar la recompensa). El foco de la presente tesis se centra en el aprendizaje supervisado. En el aprendizaje supervisado, los algoritmos deben ser entrenados con un conjunto de ejemplos etiquetados (la etiqueta es el atributo objetivo a predecir), los cuales son utilizados por los algoritmos para realizar futuras predicciones. Dos tareas ampliamente estudiadas en el área son clasificación y regresión, dependiendo de si lo que se desea predecir es un valor categórico o numérico respectivamente.

A medida que las bases de datos, utilizadas para entrenar los sistemas previamente explicados, se hacen cada vez más grandes, aparecen nuevos retos para los algoritmos de aprendizaje. La minería de datos, un subcampo de las ciencias de la computación íntimamente ligado al aprendizaje automático y el reconocimiento de patrones, surge para dar solución a estos problemas. Una de las primeras fases en el proceso de descubrimiento de conocimiento (KDD) son las técnicas de preprocesado, que adecúan los conjuntos de datos para permitir su posterior tratamiento. Una de estas técnicas, llamada selección de instancias, trata de reducir el tamaño de las muestras mediante la eliminación de todas aquellas instancias que no aporten información relevante al conjunto.

Esta tesis se centra en el estudio de métodos de selección de instancias. Se han analizado las técnicas del estado del arte y desarrollado nuevos métodos para cubrir algunas áreas que no habían recibido la debida atención hasta el momento.

Abstract

In the broadest sense of the term, artificial intelligence is any type of intelligence that a machine can demonstrate. More specifically, it is a branch of knowledge that seeks to construct intelligent agents, where these are understood as entities that use perceptions from the environment to carry out actions that maximize some measure of performance. Within the broad spectrum of tasks that artificial intelligence encompasses, this thesis focuses on machine learning; a term that evolved from the study of pattern recognition. The underlying idea is to design algorithms that are capable of learning and making predictions from data sets.

Traditionally, Machine Learning has been organized into three large groups: supervised learning (with labelled data set examples that are used for learning), unsupervised learning (with data set examples that are not labelled), and reinforcement learning (inspired by behaviourist psychology, where the behaviour of each agent aims to maximize its reward). This thesis focuses on supervised learning. The algorithms of supervised learning must be trained with labelled data sets (the label is the attribute to be predicted), which are used by the algorithms to make future predictions. Two widely studied tasks in this area are classification and regression, depending on whether the predicted value is either nominal or numeric, respectively.

New challenges have arisen for learning algorithms, as the data bases that are used for training systems have grown in size. Data Mining emerges as a field of computer science closely related to both machine learning and pattern recognition that can address those sorts of problems. Preprocessing techniques represented one of the very first phases of the process of "Knowledge Discovery in Databases" (KDD). Their purpose is to adjust data sets to make their subsequent treatment easier. One of those techniques, instance selection, is used to reduce the size of a data set by removing the instances that provide no valuable information to the whole data set.

This thesis focuses on the study of instance selection methods. State-of-the-art techniques are analysed and new methods are designed to cover some of the areas that have not, up until now, received the attention they deserve.

Agradecimientos

Mis mayores agradecimientos son para mis dos tutores, César y Juanjo, sin cuya sabiduría y paciencia infinita, esta tesis no habría podido acabar antes del final del próximo siglo. Sus correcciones, sugerencias e innovadoras ideas han hecho de la presente tesis algo de lo que estar orgulloso. Además, quiero aprovechar para agradecerles todo el camino que hemos recorrido juntos, desde que comencé mis estudios de ingeniero, pasando por los años en los que estuve trabajando y en los que nunca se olvidaron de mí, siendo dos de las mentes más brillantes que he conocido.

Pese a no haber participado en la dirección de la tesis, Jose también tiene responsabilidad en el éxito de este documento. En especial agradezco sus mil y una propuestas e ideas que siempre rondan su cabeza, y que hacen que cada reunión con él sea una auténtica inyección de originalidad.

No puedo seguir estas líneas sin agradecer enormemente a Lucy la estancia que pasé con ella en Bangor. Su dedicación a la investigación es de todos conocida, pero también quiero destacar su calidad humana, que fue un apoyo indispensable durante aquellos meses. Ella es la gran responsable de que mi estancia sea algo que recordaré durante toda mi vida.

Renglón aparte merecen todos los investigadores y compañeros del grupo de investigación ADMIRABLE. Por las reuniones y colaboraciones que hemos realizado (Andrés), por los cursos que hemos sacado adelante (Carlos y Raúl), y por las charlas en la cafetería que hacen las mañanas de inverno más cálidas (Carlos y Jesús).

No quiero dejar pasar la ocasión para agradecer a todos los demás profesores del área y de la universidad que siempre han contado conmigo para todo. Citaré a Chelo y Joaquín, por tener siempre un ojo encima mío y ayudarme en todo lo que han podido.

Tampoco quiero olvidarme de todos los alumnos a los que he tenido el gusto de impartir docencia en estos años, porque he aprendido mucho, y porque es el motivo por el que mi trabajo en la universidad cobre un sentido más amplio. Especialmente aquellos a los que he tenido el gusto de dirigir el trabajo de fin de grado y he podido crecer con ellos.

Pero no puedo pasar más tiempo de esta dedicatoria sin agradecerle a Alexia su apoyo durante todos estos años, por ayudarme, por mimarme, por hacerme reir, y por todo, puesto que es quien está en el sillín trasero de mi tándem, dando el impulso que a veces es necesario para subir las cuestas. Y, por supuesto, a mis padres y mi hermana por cuidarme, criarme y creer en mí cuando ni tan siquiera yo creía. Comprendisteis lo importante que es para mí este trabajo y habéis hecho lo posible para que llegase a conseguirlo, aunque en muchos casos haya significado estar menos tiempo juntos. Siempre habéis estado en mi cabeza, sobre todo cuando más lo he necesitado.

Por ir finalizando, agradecer a todos mis amigos que han tenido que soportarme en las juergas, en las acampadas, en el monte y en cualquier sitio de los muchos que hemos conocido juntos durante todos estos años que llevamos de trayectoria. No os nombraré uno a uno, para evitar un derroche en papel, cuestión de ecología, sé que lo entendéis.

Siempre es difícil enfrentarse al final de unos agradecimientos por el miedo a dejarse a alguien sin nombrar, no obstante si alguien falta, que sepa que se debe a mi mala memoria.

Por todo ello y a todos vosotros: Gracias.

Acknowledgements

My greatest thanks go to my directors, César and Juanjo, without whose assistance, this thesis could never have been finished before the end of the next century. Their corrections, suggestions and innovative ideas have made this thesis a source of pride. Moreover, I wish to take this opportunity to thank them for the long path we have travelled together since I began my studies as an Engineer, including the years I spent working and during which time I was never out of their minds; the two most brilliant minds that I have ever known.

Although José has not directly participated in the direction of this thesis, he also has some responsibility for its success. I especially thank him for his one-thousand-and-one proposals and ideas that are always buzzing through his mind, turning each and every meeting with him into a very real injection of originality.

I cannot continue without thanking Lucy very warmly for my stay with her in Bangor. Her dedication to research is well-known to all, but I also wish to mention her human virtues and the supportive attitude she has shown over those months that we shared. She is highly responsible for making my stay there something that I will always remember.

All the researchers and colleagues of the ADMIRABLE research group deserve a special line: for the meetings and collaborative works that we have completed (Andrés), for the study modules that we carried out (Carlos and Raúl), and for those discussions in the cafeteria that enlivened many a winter morning (Carlos and Jesús). I also wish to acknowledge all of my other colleagues from the Area and the University who have always relied on me for so much, especially Chelo and Joaquín for keeping an eye on me at all times and helping me in as much as they were able.

Neither do I wish to forget my students, whom I have had the privilege of teaching over these years, because I have learnt a lot from them, and because they are the reason why my work at the university has assumed a broader meaning. Especially those students whose final degree projects I have had the pleasure of directing; I have been able to grow together with them.

But I can go no further with these acknowledgements without thanking Alexia for her support throughout these years, for helping me, for pampering me, for making me laugh, and for everything, because she is the one on the rear saddle of my tandem, giving the extra boost that is sometimes necessary to climb steep slopes. And, of course, I would also like to extend my thanks to my parents and my sister for caring for me, raising me, and believing in me even when I did not believe in myself. You understand how important this work is to me and you have done as much as possible for me to achieve it, although in many cases it may have meant less time together. You have always held me in mind, especially when I needed it most of all.

I should like to close by giving thanks to my friends who have had to get along with me in their games, on camping trips, trekking and any one of the many places we have known together during these years we have behind us. I will not name you one by one to avoid wasting paper, a question of ecology; I know will you understand.

It is always difficult to confront the end of the acknowledgements out of a fear of having forgotten to mention someone, nevertheless, if somebody is missing, rest assured it is due to my poor memory.

In consequence, my thanks to you all.

Author's declaration

La tesis «Estudio de Métodos de Selección de Instancias», que presenta D. Álvar Arnaiz González para optar al título de doctor, ha sido realizada dentro del programa «Tecnologías Industriales e Ingeniería Civil», en el área de Lenguajes y Sistemas Informáticos, perteneciente al departamento de Ingeniería Civil de la Universidad de Burgos, bajo la dirección de los doctores D. Juan José Rodríguez Diez y D. César Ignacio García Osorio. Los directores autorizan la presentación del presente documento como memoria para optar al grado de Doctor por la Universidad de Burgos.

V. B. del Director:	V. B. del Director:	El doctorando:
Dr. D. César Ignacio García Osorio	Dr. D. Juan José Rodríguez Diez	D. Álvar Arnaiz González

Burgos, January 9, 2018

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In God we trust. All others must bring data.

W. Edwards Deming

Chapter 1

Introduction

This chapter introduces the reader to the basics of Machine Learning, paying particular attention to preprocessing techniques. The experimental methodology commonly used in the literature is also presented in this chapter.

Preprocessing methods are essential for achieving accurate models. It should never be forgotten that a trained model can only be as accurate as the data used in the training phase. The focus of this thesis is supervised learning, the common name for prediction methods in Data Mining. The availability of massive data sets has been incessant, ever since the beginning of the Information Age. One of the major challenges of the data mining community is to achieve fast, scalable and accurate approaches (Chawla et al., 2004) to data management. Among the possible solutions to cope with overwhelming volumes of data is the reduction of the data sets. One successful reduction technique is instance[1] selection. Instance selection is in particular the topic of this thesis. It will be analysed in depth throughout the present chapter.

1.1 Supervised learning

The aim of supervised learning is to discover hidden relationships between input attributes (i.e. variables or features) and a target attribute. The target attribute can be numerical or categorical: if the target is numerical, the prediction task is named regression, as opposed to classification where the target attribute is discrete or categorical.

Model is the term that denotes the structure generated by some learning algorithms after the learning phase. This phase consists in training the algorithm with a labelled data set, so that the algorithm can discover the underlying relationship between the input attributes and the target

[1]The terms object, instance, and example will be used interchangeably throughout this thesis.

Hair	Feathers	Eggs	Milk	Airborne	Aquatic	Predator	Legs	Type
true	false	false	true	true	false	false	4	mammal
false	true	true	false	true	false	false	2	bird
false	false	true	false	false	true	true	8	invertebrate
false	false	true	false	true	true	true	4	amphibian

TABLE 1.1. Example of a classification data set, the goal is to predict the type of the animal.

Cylinders	Displacement	HP	Weight	Acceleration	Model Year	MPG
4	110	87	2 672	17.5	70	25.0
4	81	60	1 760	16.1	81	35.0
4	89	62	1 845	15.3	80	29.8
5	183	77	3 530	20.1	79	25.4
6	232	112	2 835	14.7	82	22.0
8	360	150	3 940	13.0	79	18.5

TABLE 1.2. Example of a regression data set, the goal is to predict the car city-cycle fuel consumption in miles per gallon.

one. The goal of the training phase is to achieve an explicit model that can be used to predict instances that have never been seen before. However, not all algorithms create a prediction model, accordingly, algorithms can be grouped into two clusters: eager learning and lazy learning (both concepts are detailed further on).

Data sets used for training are usually described as a set of instances. Each instance is a vector of attribute values, one of them is the variable of interest or "target". Usually, the attribute values are nominal or numerical, but there are many others such as date, Boolean...

As previously stated, the type of target attribute defines two different problems: classification, when the target is either categorical or nominal, and regression, when the target is continuous. Tables 1.1 and 1.2 show a tabular representation of two data sets: classification and regression, respectively.

Supervised learning has a myriad of application domains, such as bio-informatics, finance, medicine, engineering, telecommunications, among others.

1.1.1 Lazy learning

Lazy algorithms construct no models throughout the training phase; instead they simply store the whole data set and postpone its evaluation until a query is submitted; exactly the opposite procedure to the one that eager algorithms follow.

The advantages and disadvantages of these methods are due to their way of working, as previously explained. They need large spaces to fit the whole training set and are slow when they have to evaluate a query. The advantages include a fast training phase (they only store the whole data set) and good local approximators. Moreover, they can add new examples with no need for retraining, because they only need to add the new examples to their data base. This last advantage makes them especially suitable for changing environments, such as concept drift on streaming learning (Tsymbal, 2004).

Examples of lazy learning algorithms are k nearest neighbours and case-based reasoning, among others.

1.1.2 Eager learning

Eager algorithms construct a predictive model during the learning phase. The model that is generated differs according to the algorithm: decision trees, neural networks, etc. The model that is constructed is used by the algorithm to make predictions when new queries are submitted.

Training instances are used to build the model and, when the training phase ends, the algorithm only needs the model to decide the target of the new instance. Accordingly, eager algorithms have no need to store the whole data set, but only the model, which usually requires much less space. It is commonly named *batch* or *off-line* learning, because the training phase is only done once.

Examples of eager algorithms are those that build decision/regression trees, artificial neural networks, and support vector machines, among others.

1.2 Introduction to data preprocessing

As previously stated, input data are the cornerstone of Machine Learning. Algorithms need accurate and well-formed data sets for training purposes. Unfortunately, external factors usually degrade data consistency in the real world, e.g. presence of noise, superfluous data, huge amount of instances or features (García et al., 2014). Hence, data preprocessing tasks take up a significant length of time in Machine Learning work-flows. Two main groups are commonly used to bring different preprocessing techniques together: data preparation and data reduction.

1.2.1 Data preparation

Data preparation gathers several different techniques used to suit data for Data Mining processes and it is usually a mandatory step. Why is it so important? Imagine a problem of interest: the data sets have first of all to be gathered from the source or sources and then prepared for use[2]. The steps for data preparation are grouped and briefly explained below:

- Data cleaning: includes tasks like noise identification and treatment of missing values. In a nutshell, the aim of data cleaning is to obtain a well-formed data set suitable to feed algorithms.
- Data transformation: usually done under human supervision, it comprises such tasks as discretization, summarization, and aggregation...
- Data integration: comprises the processes of merging data from multiple data sources. Special care must be taken to avoid duplicated instances, and different data domains, among others.
- Data normalization: different attributes can have different ranges and some methods, such as distance-based methods, are very sensitive to the scale of the features. Normalization processes provide the same range and scale for all attributes.

1.2.2 Data reduction

Nowadays, available data sets are progressively increasing in size. As a consequence, many systems have difficulties when processing (big or huge) data sets to obtain exploitable knowledge (García-Pedrajas and de Haro-García, 2014).

The aim of data reduction is to decrease complexity and to improve the quality of the resulting data sets by reducing their size. The size of data sets can be reduced in terms of both features and instances. Some relevant techniques are grouped below:

- Discretization: the process of transforming numerical into discrete attributes. The challenge is how to find the best ranges or intervals into which the numerical values should be split. The discretization process can also be considered as part of the data preparation stage. The decision to include it as a data reduction task is explained in (García et al., 2014): the discretization stage actually maps data from a large range of numeric values onto a reduced subset of categorical ones.
- Feature extraction: includes several modifications to the features such as removing one or more attributes, merging a subset of them, or creating new artificial ones.

[2]In some cases, the data without preparation could be good enough to feed an algorithm, but its results would probably not make sense.

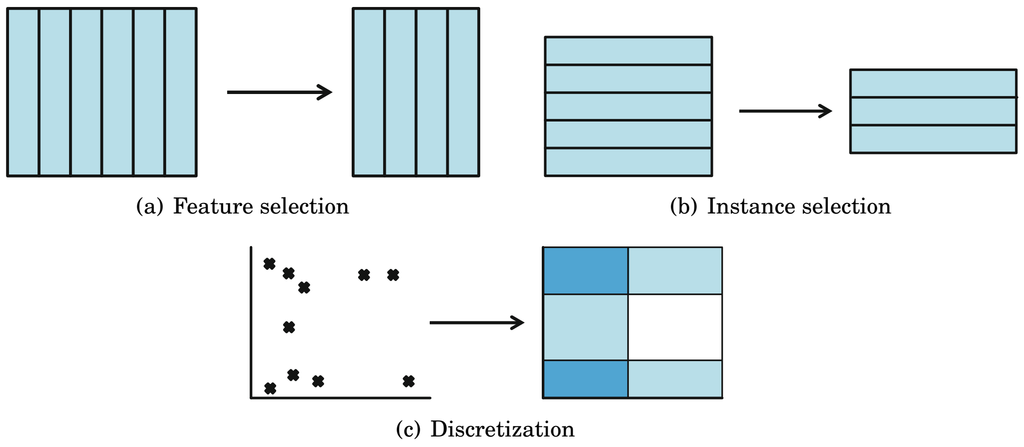


FIGURE 1.1. Main kinds of data reduction. Figures reproduced from (García et al., 2014).

- Instance generation: in this task, new artificial instances are created as a summary of the original ones. The new instances are created with the aim of improving the representativeness of the whole data set while reducing its size.

- Feature selection: the elimination of some attributes can make the learning process easier. The presence of irrelevant or duplicate features in the data set are challenges for the algorithms.

- Instance selection: attempts to find the most representative subset, of the initial data set, without lessening the predictive capabilities of original one. In other words, if we train one algorithm with the original data set, and another with the selected subset, both algorithms must perform in a similar manner (Nanni and Lumini, 2011). Instance selection can be seen as a special case of instance generation, where the instances to be generated are limited to the original ones. These methods play a central role in data reduction processes. Whereas feature selection or discretization processes reduce complexity, instance selection reduces the data set size (García et al., 2016).

1.3 Instance selection

As previously explained, instance selection algorithms are intended to reduce the complexity of learning algorithms by reducing the number of examples of data sets (Leyva et al., 2015). The purpose of these algorithms is to extract the most significant subset of instances by discarding those that do not provide valuable information. Figure 1.2 illustrates the instance selection process. The reduction of the data set has two main advantages: it reduces both the space requirements of the system and the processing time of learning tasks.

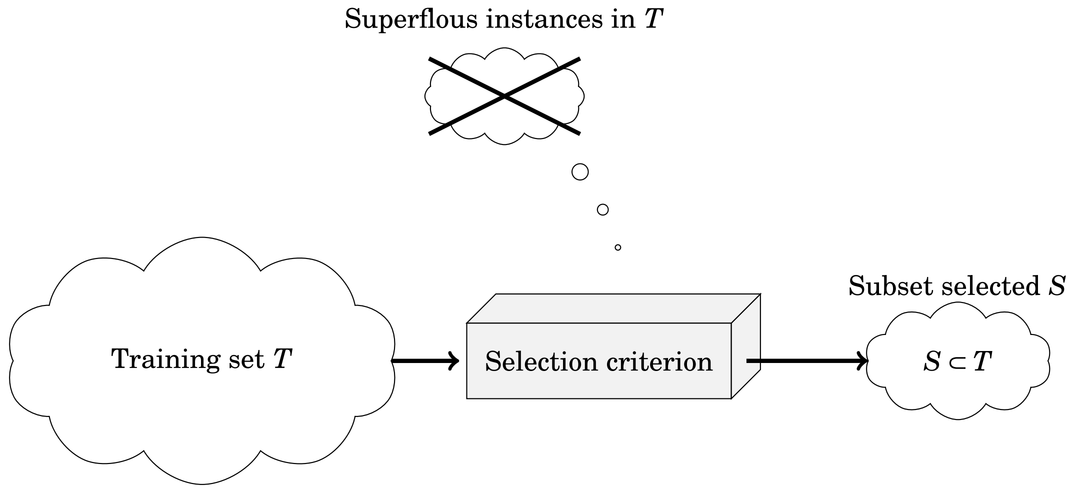


FIGURE 1.2. Instance selection process. Figure based on (Olvera-López et al., 2010).

The selected set of instances can be used for training any kind of algorithm but, traditionally, many instance selection algorithms have been developed for the k nearest neighbours classifier (Cover and Hart, 1967), or kNN for short. For this reason, the term used for the selection process is also prototype selection (García et al., 2014). In this thesis, the term instance selection is used to refer to the task that involves the selection of a subset of instances from the original data set, without considering the subsequent algorithm that has to be trained.

When real-world data sets are examined, the imperative need for instance selection algorithms becomes increasingly clear. On the one hand, the average data set size is becoming larger and larger. On the other hand, real data sets usually contain noisy instances, outliers, and anomalies. Attempts to train a classifier, for example, on the basis of millions of instances can be a difficult, or even an intractable task. The selection of a proper subset of instances is therefore a good option for shrinking the size of the sample, enabling its subsequent treatment.

1.3.1 Taxonomy

Instance selection methods are usually categorized under the following headings: the direction of the search, the type of selection, and the evaluation of the search (Garcia et al., 2012). Figure 1.3 shows the instance selection methods from their origins up until to 2012. Table 1.3 gathers some important characteristics of well-known instance selection algorithms. The different properties of the taxonomy are explained below.

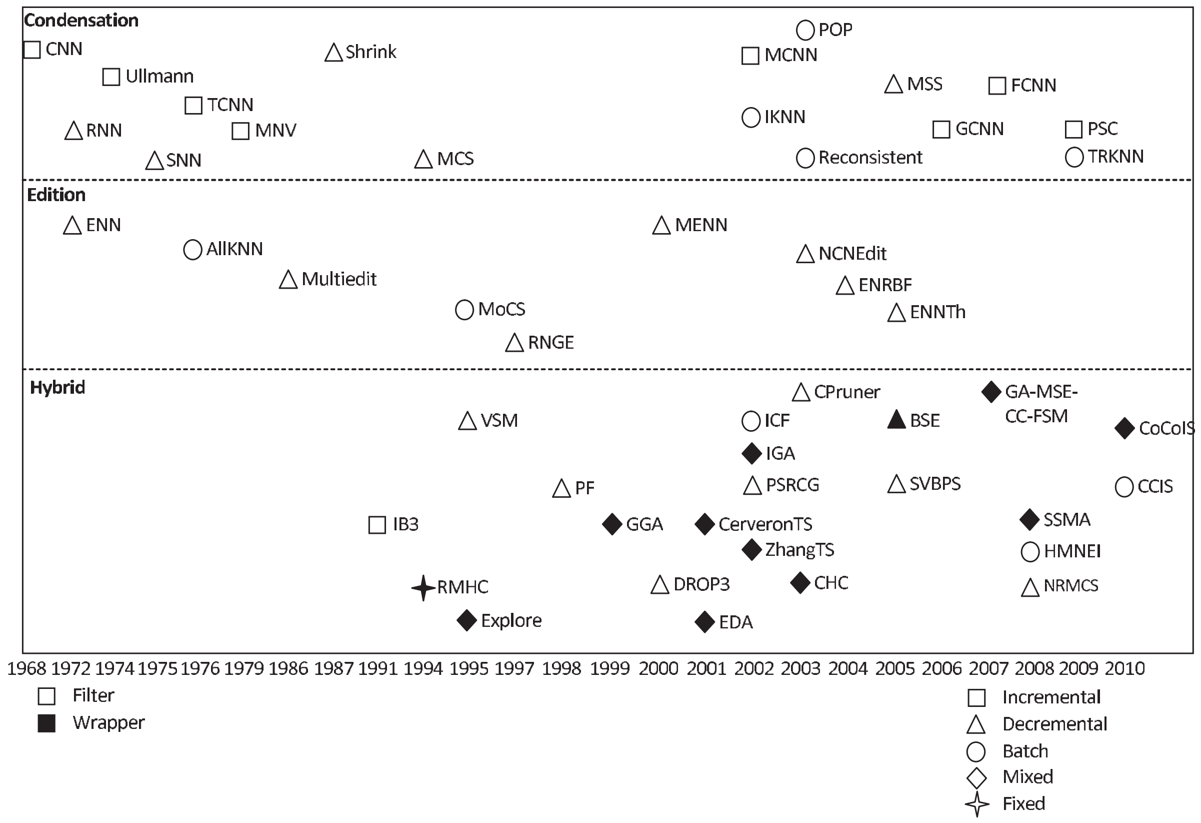


FIGURE 1.3. Instance selection methods according to the established taxonomy. Figure reproduced from (Garcia et al., 2012).

TABLE 1.3. A brief sample of state-of-the-art instance selection methods as per the aforementioned taxonomy. Computational complexity extracted from (Jankowski and Grochowski, 2004) and authors' papers.

Strategy	Direction	Algorithm	Complexity	Year	Authors
Edition	Incremental	LSSm	$\mathcal{O}(n^2)$	2015	Leyva et al. (2015)
	Decremental	ENN	$\mathcal{O}(n^2)$	1972	Wilson (1972)
	Batch	All-kNN	$\mathcal{O}(n^2)$	1976	Tomek (1976)
Condensation	Incremental	CNN	$\mathcal{O}(n^3)$	1968	Hart (1968)
	Incremental	PSC	$\mathcal{O}(n \log n)$	2010	Olvera-López et al. (2009a)
	Decremental	RNN	$\mathcal{O}(n^3)$	1972	Gates (1972)
	Decremental	MSS	$\mathcal{O}(n^2)$	2002	Barandela et al. (2005)
Hybrid	Decremental	DROP1-5	$\mathcal{O}(n^3)$	2000	Wilson and Martinez (2000)
	Batch	ICF	$\mathcal{O}(n^2)$	2002	Brighton and Mellish (2002)
	Batch	HMN-EI	$\mathcal{O}(n^2)$	2008	Marchiori (2008)
	Batch	LSBo	$\mathcal{O}(n^2)$	2015	Leyva et al. (2015)

1.3.1.1 Direction of search

Instance selection can be considered as a search problem; given a particular measure, its goal is to find the most representative subset of instances for that measure (Cano et al., 2005b). Five groups may be defined on the basis of the search direction:

- Incremental: they start with an empty data set and add those instances that fulfil a predefined criterion. Their problem is that they are highly sensitive to the order in which instances appear. Their main advantages are that data can be processed on stream, they are usually faster, and they need low storage requirements.
- Decremental: they work in the opposite direction, starting with the whole data set, and they then remove instances following a predefined criteria. The order is again important, but not so much as in the previous group. Their main drawback is that the whole data set has to fit in the memory.
- Batch: instances are analysed in batch mode, i.e. they are processed successively and are marked for deletion, but the removal process only occurs once at the end of the algorithm. Their essential advantage is that they retain the overall view of the whole data set at all times.
- Mixed: they can be seen in between the three previous groups. They start with a predefined subset, then instances are added or deleted according to certain criterion.
- Fixed: these methods are a sub-family of mixed ones but, in this case, the final instance number is (as an input parameter of the algorithm) predefined from the outset.

1.3.1.2 Selection strategy

The keystone of the classification process is, forgive the repetition, classification boundaries. Decision boundaries are formed by instances of two or more different classes that are close to each other. Accordingly, instances can be either border points (close to boundaries) or central points[3] (far away from boundaries) (Wilson and Martinez, 1997). Figure 1.4 show an example of two dimensional data set with two classes and 50 instances. The instances found on the decision boundaries are called *border points*, while the others are called *central points*. Three groups are usually considered in the selection strategy:

- Condensation algorithms: attempt to retain border points, i.e. instances close to the decision boundaries. They commonly achieve high reduction rates. The problem with these methods, is that they are highly affected by noisy instances (Jankowski and Grochowski, 2004).

[3]Some authors, such as Liu and Motoda (2002), consider some other types of points such as critical points and prototypes, although these have been omitted from the taxonomy that is explained here.

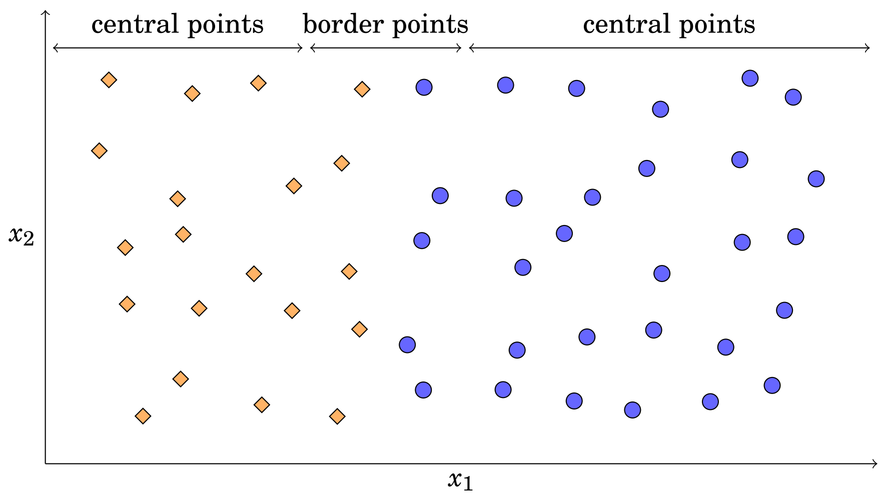


FIGURE 1.4. Artificial data set with 50 instances, two features (x_1 and x_2) and two classes (diamond and circle). The decision boundary is the area where both classes come together.

- Edition algorithms: work in the opposite direction, removing border points. They delete the instances that are not in agreement with their neighbours. They are not interested in reduction, but in noise elimination. As a result, their reduction rates are lower than condensation algorithms.

- Hybrid algorithms: as the name suggests, they are somewhere between the above techniques, and their aim is to find the smallest and the most accurate subset of instances. They remove both central and border instances.

Recently, a new approach that will not fit under any of the previous categories has emerged: *rank methods* (Rico-Juan and Iñesta, 2012). These methods sort instances by their importance (i.e. their usefulness for the classification process), after which, a subset of the best instances is selected (Valero-Mas et al., 2016).

1.3.1.3 Search Evaluation

Instance selection methods can be grouped according to the strategy used for selecting instances: either wrappers or filters (Olvera-López et al., 2010).

- Wrapper: the decision either to select or to delete an instance is obtained by a classifier, usually the kNN.

- Filter: the decision is made by using some heuristics or rules and is not based on a classifier.

1.3.2 Computational complexity

As previously stated, instance selection serves to reduce the size of a data set. The complexity of traditional instance selection algorithms is the main problem in any analysis (García-Osorio et al., 2010; Silva et al., 2016). As Table 1.3 shows, the computational complexity of the vast majority of instance selection algorithms is, at least, log-linear. In consequence, a possible solution to manage increasingly large data sets is their reduction with instance selection methods. Unfortunately, they are also affected by high computational complexity. Hence, some approaches have recently emerged that seek to overcome this problem. These different approaches are explained below.

1.3.2.1 Scaling-up approaches

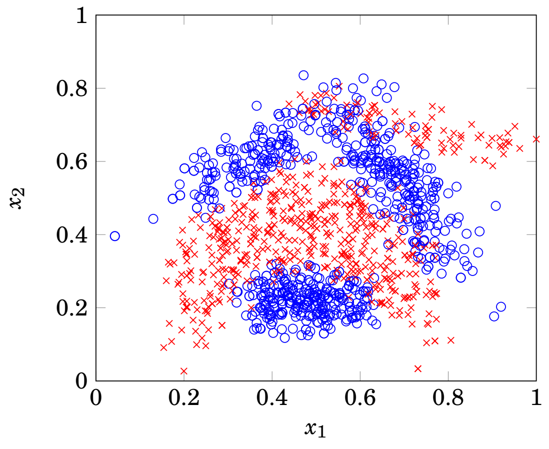
Over the last few years, different approximations have been used to try to adapt instance selection methods to big/huge data sets. The very first proposal was stratification, used by Cano et al. (2005a) to boost evolutionary instance selection methods. Their idea consists of splitting the original data set into disjoint strata (groups or sets of instances) with the same class distribution as the original one. The scaling-up benefits can be tuned by means of varying the size of each stratum. Moreover, the stratification process is suitable for boosting any other method. An improved version of the previous method was presented by de Haro-García and García-Pedrajas (2009). The beginning of the process is the same: to split the whole data set into disjoint sets. After the first batch of sets have been processed, the selected instances by the algorithm are joined, and the process starts again.

A more novel and remarkable approach (because of its performance) was proposed by García-Osorio et al. (2010). The process is performed in a predefined number of rounds r. In each round, a partition splits the whole data set into different disjoint subsets, also called bins. As in the previous approaches, an instance selection algorithm is performed over every single bin. The algorithm updates an array of votes by increasing them by one if the instance has been selected. After performing a predefined number of rounds, the array of votes is used to determine, by means of a threshold, which instances should be either selected or removed.

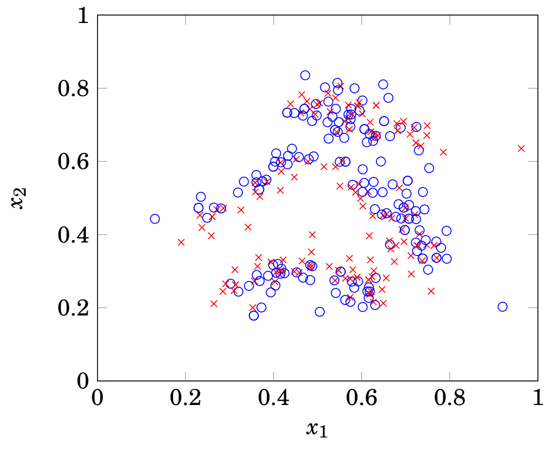
Other works, such as (Angiulli and Folino, 2007), have focused on developing a distributed method for computing a consistent subset of very large data sets.

1.3.3 Most common methods

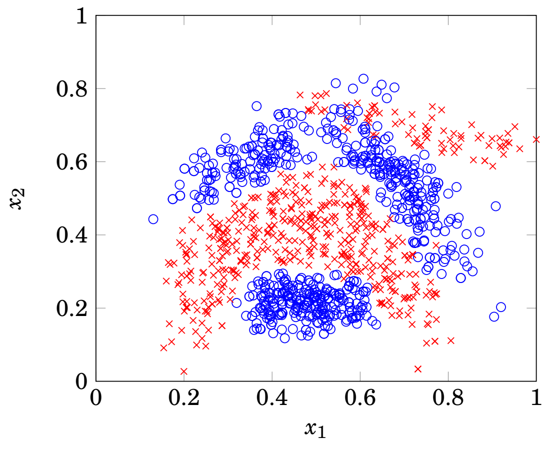
It has been noted in the current chapter that a great number of instance selection algorithms already exist and many others are presented every year. The most influential instance selection algorithms according to García et al. (2016) are depicted below: Condensed Nearest Neighbour (CNN), Edited Nearest Neighbour (ENN), Decremental Reduction Optimization (DROP) and Iterative Case Filtering (ICF). An application of the aforementioned methods to a subsample of the banana data set shows the selected subsets in Figure 1.5.



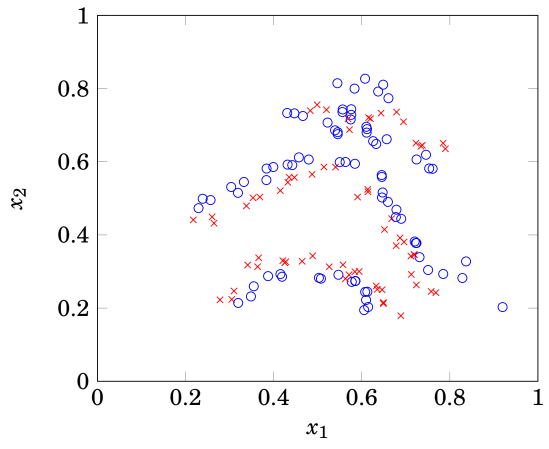
(a) Banana data set: 1 326 instances



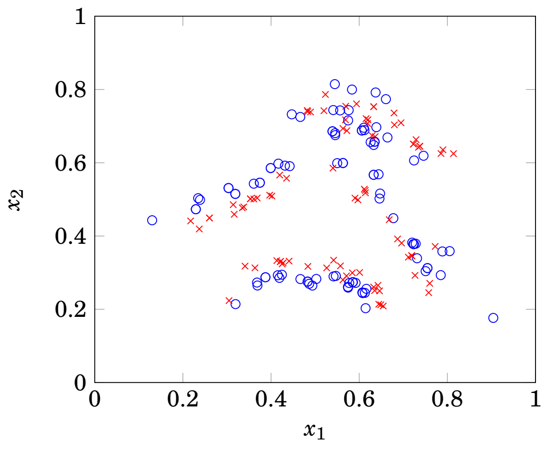
(b) CNN: 307 instances



(c) ENN: 1 168 instances



(d) DROP3: 144 instances



(e) ICF: 176 instances

FIGURE 1.5. Subsample of Banana data set filtered with the most influential instance selection methods according to García et al. (2016): CNN, ENN, DROP3 and ICF.

1.3.3.1 Condensed Nearest neighbour

The algorithm of Hart (1968), *Condensed Nearest Neighbours* (CNN) is considered the first formal proposal of instance selection for the nearest neighbour rule. The concept of consistency with respect to the training set is important in this algorithm, and is defined as follows: given a non-empty set X ($X \neq \emptyset$), a subset S of X ($S \subseteq X$) is consistent with respect to X if, using the subset S as a training set, the nearest neighbour rule can correctly classify all the instances in X. Following this definition of consistency, if we consider the set X as the training set, a condensed subset should have the properties of being consistent and should, ideally, be smaller than X.

Algorithm 1 shows the structure of the method. It starts with a data set, S, initially with only one randomly selected instance (alternatively, S could have one randomly selected instance per class in the data set). Then, it attempts to classify all the instances of X by using the instances in S, according to the nearest neighbour rule. If it is successful, the algorithm proceeds with the next instance, otherwise the misclassified instance is added to S and the verification of the correct classification of X starts from the beginning once again. It will eventually terminate, returning S as a selected data set.

Algorithm 1: Condensed Nearest Neighbour (CNN)

```
  Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$
  Output: The set of selected instances $S \subseteq X$
1 $S = \{\mathbf{x}_1\}$
2 foreach $\mathbf{x} \in X$ do
3     if $\mathbf{x}$ is misclassified using $S$ then
4         Add $\mathbf{x}$ to $S$
5         Restart
6 return $S$
```

1.3.3.2 Edited Nearest Neighbour

The first proposal for editing data sets was presented by Wilson (1972) with the name of *Edited Nearest Neighbour* (ENN). It is a decremental method, thus it starts with the whole data set X, and each instance is removed, if it is not well classified by its k nearest neighbours. The number of nearest neighbours, k, is a parameter of the algorithm. In the original paper, k was set to 3.

Algorithm 2 shows its pseudocode. ENN removes noisy as well as border instances, achieving neater decision boundaries. Moreover, central instances are unaffected by the editing process. The goal of this algorithm is not the reduction of data set, but to improve the accuracy of the selected subset. Due to its cleaning capabilities, it has been used by many other algorithms for noise filtering (e.g. DROP3, ICF. . .).

Algorithm 2: Edited Nearest Neighbours (ENN)

```
  Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, the number of nearest neighbours $k$
  Output: The set of selected instances $S \subseteq X$
1 $S = X$
2 foreach $\mathbf{x} \in S$ do
3     if $\mathbf{x}$ is misclassified using its $k$ nearest neighbours then
4         Remove $\mathbf{x}$ to $S$
5 return $S$
```

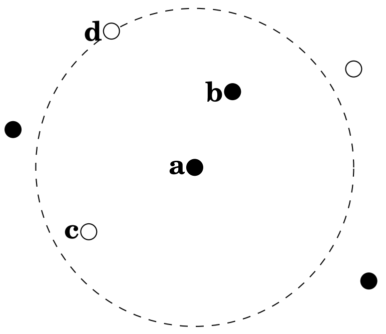


Figure 1.6: Representation of nearest neighbour and associate relations in a two dimensional space: each point represents an instance, there are two different classes (black and white), and $k = 3$. The nearest neighbours of **a** are $\{\mathbf{b}, \mathbf{c}, \mathbf{d}\}$, so **a** is an associate for $\mathbf{b}, \mathbf{c}$, and **d**.

1.3.3.3 Decremental Reduction Optimization Procedure

The DROP (Decremental Reduction Optimization Procedure) family of algorithms (Wilson and Martinez, 2000) comprises some of the best instance selection methods for classification (Brighton and Mellish, 2002; Olvera-López et al., 2009b; Pérez-Benítez et al., 2015). The instance removal criterion is based on two concepts: *associates* and nearest neighbours. The relation of associate is the opposite of nearest neighbour: an instance **p** that has **q** as one of its nearest neighbours is referred to as an associate of **q**. The set of nearest neighbours of one instance is called neighbourhood. The set of associates for each instance is a list with all instances that have that particular instance in their neighbourhood. Figure 1.6 shows a two dimensional data set with two classes (black and white points). The k nearest neighbours of **a**, for $k = 3$, are $\{\mathbf{b}, \mathbf{c}, \mathbf{d}\}$. This means that **a** is an associate of the instances of $\mathbf{b}, \mathbf{c}$ and **d** .

The pseudocode of DROP3 is described in Algorithm 3. It begins with a noise-filter (similar to ENN), after which, the instances are sorted in order of the distance to their nearest enemy. The lists of nearest neighbours and associates are calculated for each instance. Then, on the main loop of the algorithm, for each instance **x**, `with` contains the number of associates of **x** that are correctly classified when **x** is kept in the data set, whereas `without` contains the number of associates that are correctly classified when **x** is removed from the data set. If `without` is greater than or equal to `with`, the instance **x** is removed, because its elimination will not influence the classification of its associates. If **x** is removed, all of its associates need to update their neighbour list.

Algorithm 3: Decremental Reduction Optimization Procedure 3 (DROP3)

```
Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, the number of nearest neighbours $k$
Output: The set of selected instances $S \subseteq X$
1  Noise filtering: remove any instance in $X$ misclassified by its $k$ neighbours
2  $S = X$
3  Sort instances in $S$ by the distance to their nearest enemy
4  foreach instance $\mathbf{x} \in S$ do
5      Find $\mathbf{x}.N_{1...k+1}$, the $k+1$ nearest neighbours of $\mathbf{x}$ in $S$
6      Add $\mathbf{x}$ to each of its neighbour's list of associates
7  foreach instance $\mathbf{x} \in S$ do
8      Let with = # of associates of $\mathbf{x}$ correctly classified by $\mathbf{x}$ as a neighbour
9      Let without = # of associates of $\mathbf{x}$ correctly classified without $\mathbf{x}$
10     if without $\geq$ with then
11         Remove $\mathbf{x}$ from $S$
12         foreach associate $\mathbf{a}$ of $\mathbf{x}$ do
13             Remove $\mathbf{x}$ from $\mathbf{a}$'s list of nearest neighbour
14             Find a new nearest neighbour for $\mathbf{a}$
15             Add $\mathbf{a}$ to its new neighbour's list of associates
16 return $S$
```

1.3.3.4 Iterative Case Filtering

The selection rule of the Iterative Case Filtering algorithm (Brighton and Mellish, 2002), or ICF for short, uses two concepts: *coverage* and *reachable*. These two concepts are closely related to the neighbourhood and associate lists used by the DROP algorithms. The coverage of an instance is its neighbourhood but, instead of considering a fixed number of neighbours, k, all instances closer than its closest enemy are within its coverage set[4]. The reachable set of an instance is the set of all instances for which that particular instance is within their coverage set. Figure 1.7 represents, in a two dimensional space, the previous concept. The example is formed of six instances (points) that belong to two different classes (black and white). The dashed circle centred in **a** is the boundary of its local set, **c** is the nearest enemy of **a**, and the distance between both instances defines the radius of the local set of **a**.

The deletion rule is as follows: if the cardinality of the reachable set of an instance (its set of associates) is bigger than its coverage (its neighbourhood), the instance is removed from the data set. So, if another object generalizes the information of that instance, the algorithm will remove

[4]The local or coverage set is formed by the group of instances included in the largest hypersphere centred on an instance such that all of them are of the same class (Leyva et al., 2015).

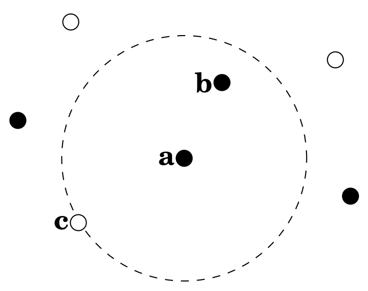


Figure 1.7: Representation of the local set in a two dimensional space: each point represents an instance, and there are two different classes (black and white). As the nearest enemy of **a** is **c**, the local set of **a** is composed of **a** and **b**: `LocalSet`($\mathbf{a}$) = $\{\mathbf{a},\mathbf{b}\}$.

it. The ICF algorithm begins with a noise-filtering stage that addresses the drawbacks of noisy data sets, in the same way as DROP3.

There are two stages in the ICF: *i*) noise filter, and *ii*) selection process (see Algorithm 4). First of all, it removes noisy instances from the original data set. Then, both the `coverage` and the `reachable` sets are calculated for each instance. On the main loop, the method checks the cardinality of `reachable` and `coverage` (for each instance). If one instance has |`reachable`| > |`coverage`|, it is marked for removal; once they have been evaluated, those marked for removal are deleted. This process continues until no further instance will be removed.

Algorithm 4: Iterative Case Filtering (ICF)

```
   Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, the number of nearest neighbours $k$
   Output: The set of selected instances $S \subseteq X$
1  $S = X$
2  Noise filtering: remove any instance in $S$ misclassified by its $k$ neighbours
3  repeat
4      foreach instance $\mathbf{x} \in S$ do
5          Compute coverage($\mathbf{x}$)
6          Compute reachable($\mathbf{x}$)
7      progress = False
8      foreach instance $\mathbf{x} \in S$ do
9          if |reachable($\mathbf{x}$)| > |coverage($\mathbf{x}$)| then
10             Flag $\mathbf{x}$ for removal
11             progress = True
12     foreach instance $\mathbf{x} \in S$ do
13         if $\mathbf{x}$ flagged for removal then
14             $S = S - \{\mathbf{x}\}$
15 until not progress
16 return $S$
```

1.3.4 Big data

In recent years, the massive growth in the volume of databases has led to the coining of the new term: *big data*. The definition of the new term is not clear, although Laney (2001) described it as the opportunities and difficulties that appear, as data volumes and variety and processing speeds increase. Another possible, and common, definition for *big data* is the difficulties and problems that emerge when the amount of data for processing exceeds the capabilities, memory and/or time, of a given system (Minelli et al., 2012).

Big data faces the problems associated with these types of data sets at various levels: firstly, we need implementations that, with regard to the computational complexity of the algorithms, are scalable and that run in linear time; at the level of methodologies, we are looking for a means of designing algorithms that can be executed in parallel on groups of computers, a task that is suited to *MapReduce* (Dean and Ghemawat, 2008); and, finally, at a technological level, we seek *frameworks* that provide a series of APIs and data structures that facilitate the work of implementing algorithms, for which purpose Spark (Zaharia et al., 2010) and Hadoop (White, 2009) have proven their worth.

Efficient methods are needed to process increasingly massive data sets, and an intuitive solution to cope with them is their size reduction. Instance selection has shown itself to be effective for this task, by reducing the size of the data sets while preserving their predictive capabilities. The problem that emerges at this point, as previously explained, is the high computational complexity that these methods have.

Recently, some studies have focused on instance reduction for *big data*, both on instance selection (Triguero et al., 2015) and on instance generation (Triguero et al., 2014). However, as García et al. (2016) remarked, more scalable methods are required for instance selection with the aim of tackling the current size of data sets.

1.4 Experimental methodology

Instance selection algorithms serve to reduce the size of data sets and to select the most representative possible subset. The task must be considered as a multi-objective problem: on the one hand, reduction and, on the other, accuracy. Both objectives, nonetheless, are usually in opposite directions (Leyva et al., 2015). This section presents the most common methodology used in the instance selection literature.

1.4.1 Model validation

Estimation of the accuracy of a predictive model (classifier or regressor) when using the selected subset is necessary for the evaluation of instance selection algorithms. If the accuracy of the model is to be properly estimated, then an estimation method with low bias and low variance (Kohavi, 1995) is necessary. Some of the most common estimation methods are presented here; the reason

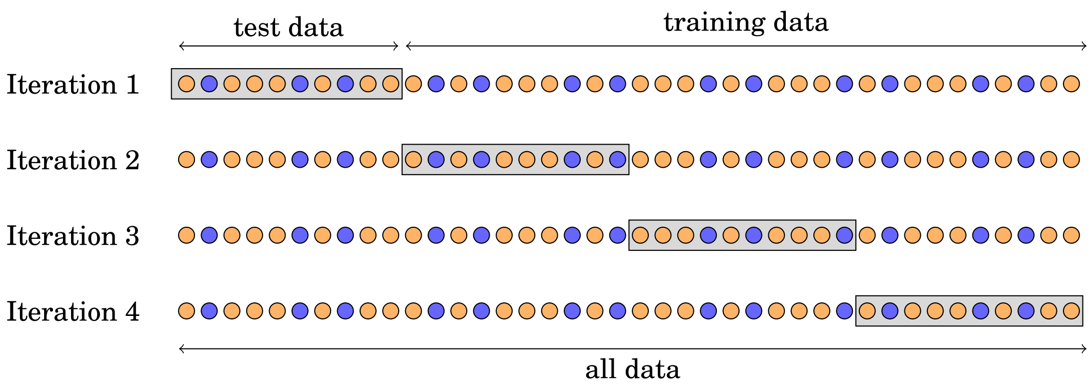


FIGURE 1.8. Diagram of k-fold cross-validation with $k = 4$. Each dot represents an instance and the colour defines the class.

why there are so many methods is because all of them fail under certain conditions (Schaffer, 1994).

1.4.1.1 Holdout

Holdout estimation, or test sample estimation, is performed in a simple manner by splitting the original data set into two disjoint subsets: a training set and a test (or holdout) set. A common configuration for this method is to use 2/3 of the original data set for training, and the remaining 1/3 for testing. The main problem with this method is that the data may not be properly used for training, because one third of the original data set is missing.

1.4.1.2 Cross-validation

Commonly referred to as k-fold cross-validation, or rotation estimation, this method splits the original data set into k disjoint sets (or *folds*) of approximately equal size. The learner is trained k times, using $k-1$ folds for training, and the remaining fold is used for testing. Training and testing sets are interchanged throughout the execution as can be seen in Figure 1.8.

A complete cross-validation would require all possible combinations to be tested, which is too expensive to apply in practice, so a number of 10 folds is commonly used (McLachlan et al., 2005).

1.4.2 Performance measures

When researchers wish to analyse an instance selection method, three measures are typically taken into account: accuracy, compression and computational complexity. Despite the fact that an *ideal* method would maximize accuracy and compression, as quickly as possible, all these goals often work in opposing directions (Leyva et al., 2015). All of these measures are briefly discussed below.

Notation	**Name**	**Example**
$\mathcal{O}(1)$	Constant	Determine whether a number is even or odd
$\mathcal{O}(\log n)$	Logarithmic	Find an item in a sorted vector of size n by using binary search
$\mathcal{O}(n)$	Linear	Compute the arithmetic mean of a vector of size n
$\mathcal{O}(n \log n)$	Loglinear	An average case of sorting a vector of size n by using quicksort
$\mathcal{O}(n^2)$	Quadratic	Compute the 1 nearest neighbour of a data set with n instances

TABLE 1.4. Summary of common computational complexities expressed in "Big $\mathcal{O}$" notation.

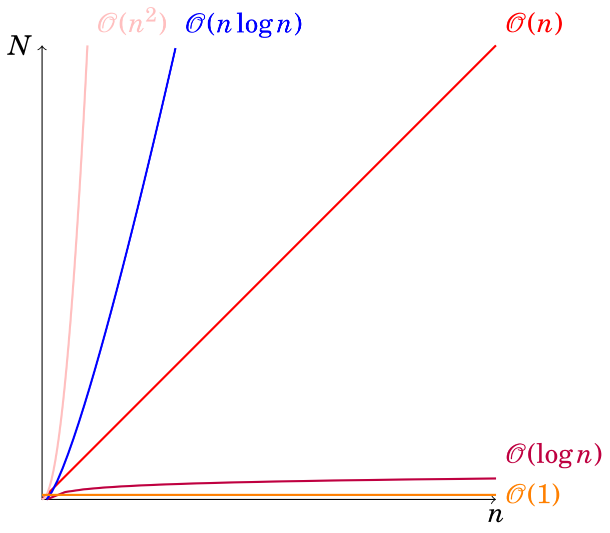


FIGURE 1.9. Number of operations according to the computational complexity. N is the number of operations and n the size of the input data set.

1.4.2.1 Computational complexity

Computational complexity is usually expressed in "Big $\mathcal{O}$" notation. It represents the response (in time) of the algorithm to changes in the input size. It is an asymptotic notation that facilitates a comparison of the different growth rates of various methods. It is also a means of showing the increased time that the algorithm requires when the data sets become larger.

Table 1.4 shows a brief list of common computational complexities expressed in the stated notation. Figure 1.9 offers a graphical representation of the number of operations that correspond to different computational complexities as the data sets grow in size.

		Predicted condition	
		Positive prediction	Negative prediction
Actual condition	Positive class	True positive (TP)	False negative (FN)
	Negative class	False positive (FP)	True negative (TN)

TABLE 1.5. Confusion matrix coloured according to positive/negative prediction and positive/negative condition.

1.4.2.2 Compression

One key aspect of instance selection algorithms is their capability to reduce data sets, in other words: their ability to distinguish the most relevant instances (Valero-Mas et al., 2016). Let us consider the retention rate as the number of instances retained by the algorithm ($|S|$) divided by the number of instances of the original data set ($|X|$),

$$m = \frac{|S|}{|X|} \tag{1.1}$$

the compression rate can be defined as $1 - m$.

The higher the compression, the lower the number of instances selected by the algorithm. Unfortunately, higher compression rates typically yield low accuracy selected subsets.

1.4.2.3 Accuracy

The most common metric for measuring accuracy is the rate of correctly classified instances divided by the total number of instances:

$$\text{accuracy} = \frac{\text{number of correctly labelled instances}}{\text{total number of instances}} \tag{1.2}$$

In spite of the fact that accuracy is a well-known measure, it does not take into account asymmetric costs. In many real world situations, the proportion of instances between classes is not symmetrical: there are many more instances of one class than the other. For example, in clinical diagnosis there are usually by far fewer instances of sick individuals than healthy ones. In these situations, other metrics are more appropriate, such as: F_1 score (Baeza Yates and Neto, 1999), and Geometric Mean (Barandela et al., 2003).

All of them are supported by a confusion matrix: a tabular representation of the hits and misses of the learner as shown in Table 1.5.

By using the confusion matrix, several rates can be defined. The Geometric Mean, or *G mean* for short, is defined as:

$$G\ mean = \sqrt{\text{specificity} \times \text{recall}} \tag{1.3}$$

where

$$\text{specificity} = \frac{TN}{TN + FP} \tag{1.4}$$

$$\text{recall} = \frac{TP}{TP + FN} \tag{1.5}$$

F_1 score (F-measure or F-score) is the Harmonic mean of *precision* and *recall*:

$$F_1 \text{ measure} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \tag{1.6}$$

where

$$\text{precision} = \frac{TP}{TP + FP} \tag{1.7}$$

1.4.3 Statistical comparisons

Statistical tests have become an essential tool for comparing different methods with the aim of determining whether one method (or more) is significantly better than the others (Derrac et al., 2011). Commonly, experiments used to check whether one method is better than another involve several data sets. The results of methods for the different data sets are the observations, which are compared by means of statistical tests[5]. The tutorial proposed by Derrac et al. (2011) was followed in this section.

According to the capability of tests to compare two or more methods, statistical tests can be sorted into two different groups: pairwise (one vs. one) and multiple comparisons (all vs. all).

1.4.3.1 Pairwise comparisons

These comparators are the simplest ones, only able to compare two different algorithms.

- The Sign test: begins by separately counting the wins and losses. These counters are used in inferential statistics with a two-tailed binomial test. The null hypothesis states that if each of the two algorithms wins on approximately $n/2$ out of n datasets then both algorithms are equivalent. By using the z test, it can be determined whether one algorithm is significantly better than the other. A specific definition would be as follows: if the number of wins of one algorithm is, at least, $n/2 + 1.96 \cdot \sqrt{n}/2$, then that algorithm is significantly better (at a confidence level of 0.05) than the other.

[5]The statistical tests explained and used in this thesis are non-parametric or distribution-free tests.

- The Wilcoxon signed rank test: more powerful and therefore preferable to the previous Sign Test. It starts by computing the differences between the scores of both algorithms (d_i) and takes no account of a pair of scores, if the difference between both scores is zero. These differences are ranked according to their absolute values and, in case of a tie, both ranks are summed up and divided by two. So, let R^+ be the sum of ranks when the first algorithm is better than the second and let R^- be the opposite.

$$R^+ = \sum_{d_i>0} \text{rank}(d_i) + \frac{1}{2} \sum_{d_i=0} \text{rank}(d_i) \tag{1.8}$$

$$R^- = \sum_{d_i<0} \text{rank}(d_i) + \frac{1}{2} \sum_{d_i=0} \text{rank}(d_i) \tag{1.9}$$

The result of the test is calculated by comparing the minimum value between R^+ and R^- ($T = \min(R^+, R^-)$) and the Wilcoxon distribution for n degrees of freedom. So, one algorithm will outperform the other, if T is less than or equal to the value of the Wilcoxon distribution for n degrees of freedom.

1.4.3.2 Multiple comparisons

When more than two algorithms are compared, the previously explained methods are no longer useful. There are other specifically designed methods to tackle these situations. In $1 \times N$ comparisons, one method is taken as the control method, and the other methods are compared against it. Moreover, $N \times N$ comparisons consider all possible combinations between all methods at the same time.

- Average ranks: rather than a statistical comparison itself, average ranks is included here because it is commonly used in combination with the other tests described below. Average ranks are calculated as follows: the results of the methods are ordered according to the measure of interest. A value of 1 is assigned to the best method, the value 2 to the second best, and so on. In the case of a tie, values of the ranks are added up and divided by the number of methods that have tied. Once the ranking of each data set and algorithm has been calculated, the average for each method is computed. The closer the ranking is to one, the better the method.

- The Friedman Test: a nonparametric procedure with similarities to ANOVA (ANalysis Of VAriance). The null hypothesis is that the medians of the samples are equal. The test begins with a calculation of the average ranks explained above. The null hypothesis states that all algorithms perform similarly, if the ranks are equal. The Friedman statistic F_f is computed as:

$$F_f = \frac{12n}{k(k+1)}\left[\sum_j R_j^2 - \frac{k(k+1)^2}{4}\right] \tag{1.10}$$

where n is the number of data sets, k is the number of models to be compared, and R_j is the average rank of the model j. F_f must be compared with a χ^2 distribution with $k-1$ degrees of freedom[6].

- Iman-Davenport's Test (Iman and Davenport, 1980): uses a modified statistic to avoid the undesired conservative effect of the Friedman test. The statistic is computed as

$$F_{ID} = \frac{(n-1)F_j}{n(k-1)-F_j} \tag{1.11}$$

  F_{ID} must be compared with F distribution with $k-1$ and $(k-1)(N-1)$ degrees of freedom.

1.4.3.3 Post-hoc procedures

The methods explained above are able to detect significant differences over all of the methods, however, they are unable to compare two methods by themselves properly. This drawback is the reason for the widespread use of post-hoc procedures.

A family of hypotheses can be defined for the purpose of drawing a comparison between one control method and some others. Post-hoc procedures offer a p-value to determine whether or not the hypothesis can be rejected.

For each nonparametric test, a conversion of the rankings is defined by using a normal approximation. Equation 1.12 shows the z computation for the Friedman test.

$$z = (R_i - R_j)/\sqrt{\frac{k(k+1)}{6n}} \tag{1.12}$$

where R_i and R_j are the average ranks of the algorithms that are compared.

[6]When n and k are large enough, Derrac et al. (2011) proposed $n > 10$ and $k > 5$, but exact critical values must be used for a smaller number of n and k (Sheskin, 2003).

Instance-based learning algorithms suffer from several problems.

Aha et al. (1991)

CHAPTER 2

MOTIVATION AND GOALS

Having introduced the theoretical background of the thesis in the preceding chapter, the rationale for this work is described below. The main goal of this thesis is the design of new methods and their improvement, so as to apply instance selection algorithms in under-explored areas, such as regression problems and huge data sets. All the chapters that are referenced hereinafter are from Part II – Publications.

- Despite the fact that instance selection for classification has been broadly researched over the last decades, instance selection methods for regression task has not aroused as much interest. The difficulties associated with this task are the main reasons. Chapters 1 and 3 present new instance selection methods designed specifically for regression.

- In the same way that the combination (ensemble) of either multiple classifiers or regressors offers better performances than those methods by themselves (Kuncheva, 2004), the idea of merging instance selection methods for regression is presented and tested in Chapter 2.

- As previously outlined, the computational complexity of instance selection methods means that they are unable to be used with big or huge data sets. Although recent works have been developed to scale up instance selection methods, all of them are based on the divide-and-conquer idea. Chapter 4 addresses the problem of instance selection on huge data sets from a new point of view. The use of locality sensitive hashing, LSH for short (Leskovec et al., 2014), means data sets may be processed extremely quickly in one pass. The new method is of linear complexity in relation to the number of instances.

Any sufficiently advanced technology is indistinguishable from magic.

Arthur C. Clarke

Chapter 3

Discussion of results

The most valuable aspect of research is communication and dissemination. The research performed during this thesis is no exception and has yielded valuable results in the form of journal papers, congress communications, and other informal communications. All of these contributions are listed below, however only journal papers are compiled as chapters in Part II of the present thesis.

3.1 Journal papers

1. Instance selection for regression by discretization.

   Authors: Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César Ignacio García-Osorio.

   Published in: Expert Systems With Applications (Q1).

   Year: 2016.

2. Instance selection for regression: Adapting DROP.

   Authors: Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César Ignacio García-Osorio.

   Published in: Neurocomputing (Q1).

   Year: 2016.

3. Fusion of instance selection methods in regression tasks.

   Authors: Álvar Arnaiz-González, Marcin Blachnik, Mirosław Kordos, César García-Osorio.

Published in: Information Fusion (Q1).

Year: 2016.

4. Instance selection of linear complexity for big data.

   Authors: Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César García-Osorio.

   Published in: Knowledge-Based Systems (Q1).

   Year: 2016.

3.2 Non-indexed journals and other communications

1. MR-DIS: Democratic Instance Selection for big data by MapReduce.

   Authors: Álvar Arnaiz-González, Alejandro González-Rogel, José F. Díez-Pastor, Carlos López-Nozal

   Published in: Progress in Artificial Intelligence.

   Year: 2017.

2. MR-DIS – a scalable instance selection algorithm using MapReduce on Spark.

   Authors: Álvar Arnaiz-González, Alejandro González-Rogel, Carlos López-Nozal.

   Published in: ERCIM News.

   Year: 2017.

3. Study of instance selection methods (poster).

   Authors: Álvar Arnaiz-González.

   Presented in: INIT/AERFAI 2017 – Summer School on Machine Learning.

   Year: 2017.

3.3 Conference papers

1. Selección de instancias en regresión mediante discretización (Instance selection for regression by means of discretization).

   Authors: Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César Ignacio García-Osorio.

   Published in: ESTYLF 2014 – XVII Congreso Español Sobre Tecnologías y Lógica Fuzzy.

   Year: 2014.

2. LSH-IS: Un nuevo algoritmo de selección de instancias de complejidad lineal para grandes conjuntos de datos (LSH-IS: A new instance selection algorithm of linear complexity for huge data sets).

   Authors: Álvar Arnaiz-González, José F. Díez-Pastor, César Ignacio García-Osorio, Juan J. Rodríguez.

   Published in: CAEPIA 2015 – XVI Conferencia de la Asociación Española para la Inteligencia Artificial.

   Year: 2015.

3. Enfoque MapReduce para el democratizado de métodos de selección de instancias (MapReduce approach for the democratization of instance selection algorithms).

   Authors: Alejandro González-Rogel, Álvar Arnaiz-González, Carlos López Nozal, José F. Díez-Pastor.

   Published in: CAEPIA 2016 – XVII Conferencia de la Asociación Española para la Inteligencia Artificial.

   Year: 2016.

3.4 Source code repository

In science, it is important to be able to reproduce studies made by other researchers. As Collberg and Proebsting (2016) said: "*Reproducibility* is a cornerstone of the scientific process". With this in mind, the source code of the different algorithms designed and developed for the thesis are publicly available at the GitHub repository on: `https://github.com/alvarag/`.

It is impossible to compile a list of the most significant achievements in the past decade without offending or alienating half of my readership. I will leave this task to the main judge – time.

Kuncheva (2004)

Chapter 4 Conclusions

A study of instance selection methods is presented in this thesis. Their contributions can be grouped into two main problems: classification and regression. A summary of the chief contributions are listed below.

4.1 Regression

The lack of instance selection methods for regression (Kordos and Blachnik, 2012) sparked my initial interest in this task. The first idea to address this gap was discretization, which consists in transforming the continuous output variable into discrete counterparts. The proposal was tested as a noise filter against two state-of-the-art instance selection methods for noise reduction, both of which were prepared to process regression problems. The results showed a very good performance on noise identification, accuracy and compression. Moreover, the proposed meta-model can not only be used for noise filtering, but for adapting any other instance selection classification algorithm.

The DROP family, presented by Wilson and Martinez (2000), contains some of the best instance selection techniques and is now considered a standard for instance-based learning (García et al., 2016). Hence, our aim was to adapt these methods for regression, to test whether the adaptation inherits the same beneficial behaviour in regression. Two different approaches addressed the adaptation and both were empirically tested. The results were competitive and, additionally, the robustness of the method in the presence of noise was assessed.

Finally, the combination of several instance selection methods for regression was evaluated. A bagging-like process was presented and evaluated against different algorithms. The experimental study concluded that the combination gave better results than the method by itself, i.e. this study upheld the 'ensemble' thesis.

4.2 Classification

Given the aforementioned computational complexity of the traditional instance selection methods, a couple of new algorithms for huge data sets were proposed. The proposal is able to cope with vast amounts of data due to its linear complexity in relation to the number of instances. The new methods are not only faster than state-of-the-art algorithms, but they are also competitive in terms of accuracy. One of the proposed algorithms is able to process instances *on fly*, with no need to fit the whole data set into the memory, which makes it specially suitable for *big data* environments.

The problems that emerge with *big data* are diverse. We have centred on the lack of instance selection methods that are able to cope with *big data*. We focused on of the most popular methods, the Spark framework, which bases its performance on the MapReduce model (Dean and Ghemawat, 2008). With this in mind, we designed and implemented a parallel version of one instance selection method called Democratic Instance Selection (DIS) by following the MapReduce model. The results were satisfying and the method was tested in a *big data* environment by using the *Cloud Dataproc*[1] Google services.

[1]Main page of Google Cloud Dataproc available on `https://cloud.google.com/dataproc/`.

Anyone who has never made a mistake
has never tried anything new.

Albert Einstein

Chapter 5

Future lines

Instance selection is a research topic of great interest nowadays, as is evident from the numerous papers on the topic, frequently published in scientific journals. Researchers are engaged with both lines of investigation that form the central focus of this thesis: instance selection for regression (Song et al., 2017) and instance selection for big data (Si et al., 2017). As a result, the future lines of the research are twofold: on the one hand, to improve current instance selection methods for regression; and, on the other hand, to research new methods and to develop them so that they are able to manage extremely large data sets.

5.1 Regression

Three journal papers on instance selection for regression are compiled in this thesis. However there is still a lot of room for improvement, mainly related with the complexity of the methods. All of the algorithms that were implemented are based on traditional instance selection classification algorithms, so their complexity is at least exponential, $\mathcal{O}(n^2)$. The reduction of their complexity is a pressing topic and urgently required, due to the fast growth of real data sets. This is particularly important for industrial applications, as Kordos and Blachnik (2012) has noted, because there are massive regression data sets, which require faster and more effective reduction techniques.

5.2 Big data

In accordance with *big data* environments, the design and study of new methods (or the improvement of existing ones) are essential. Data sets are getting larger and larger, as previously explained, but there are still only a few instance selection methods capable of dealing with them. Even though some data reduction techniques of low complexity have emerged in recent

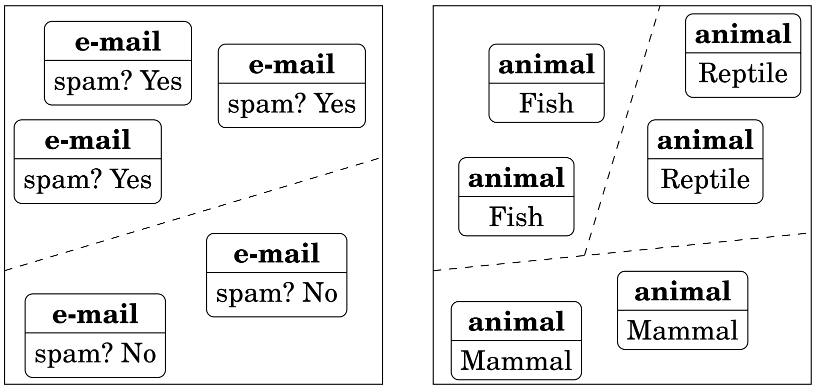


Figure 5.1: Visual examples of single-label data sets: binary on the left and multi-class on the right. Dashed lines represent the boundaries between classes.

years (Olvera-López et al., 2009a; Silva et al., 2016), their implementation into *big data* frameworks are not available. This means they can neither be used on real-world data sets, nor compared with the few existing implementations.

5.3 Multi-label

There is a new topic where the usefulness of instance selection is starting to become apparent: multi-label learning. In the same way as single-label classification seeks to assign a label to an instance for which the label is unknown, multi-label classification presents a similar task. The difference between them is that instances have a collection of labels, known as labelset, rather than only one. This peculiarity implies a much more difficult task, because there are hidden relationships between labels that must be taken into account. So far, there are only a couple of works in which instance selection has been used for multi-label data sets (Charte et al., 2014; Kanj et al., 2016). For this reason, my ongoing research is an attempt to design new instance-selection methods that are capable of processing multi-label data sets. Figure 5.1 shows a couple of examples of single-label data sets, with two (binary) and more classes. Figure 5.2 shows an example of a multi-label data set.

The work on this topic during the last year has already borne fruit, as a result the following couple of papers were submitted to indexed journals. The reviewers' answer of the first paper has not yet arrived. In regard to the second one, it is currently being reviewed.

- "Binary relevance approach for multi-label instance selection".
- "The extension of local sets to multi-label classification provides good instance selection methods".

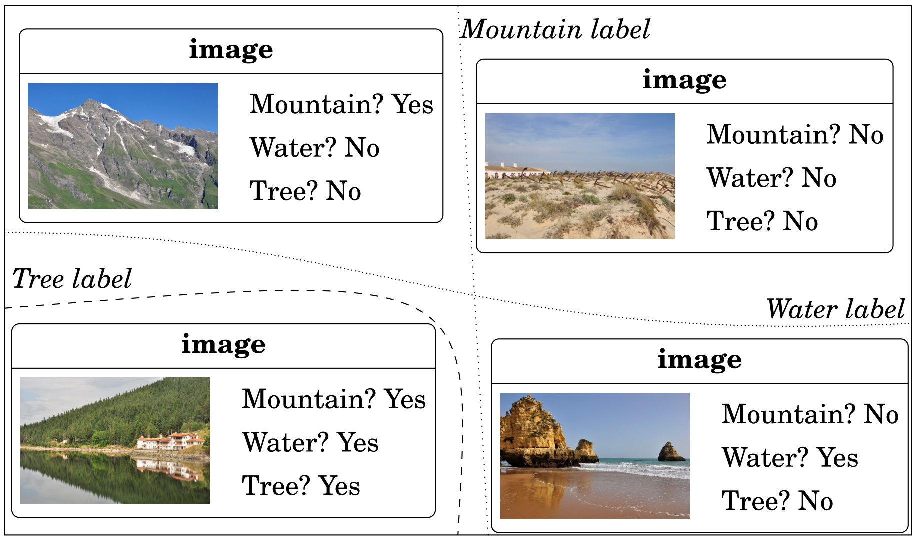


Figure 5.2: Visual example of a multi-label data set and its boundaries. Each of the four pictures is an instance and there are three classes: mountain, water, and tree. Dashed and dotted lines represent the boundaries between individual classes.

5.4 Multi-target regression

A topic closely related to multi-label is multi-target regression. Whereas each instance in multi-label learning has a set of labels, each instance in multi-target data sets has a set of numeric values (Appice and Džeroski, 2007). In other words, the aim of Multi-target regression is the simultaneous prediction of multiple target variables for each instance (Spyromitros-Xioufis et al., 2012).

There are many real-world problems to which multi-target regression can be applied. The typical example from the environmental sciences involves the prediction of the distribution structure of species in an environment (Demšar et al., 2006). Other areas where multi-target regression is commonly used are bio-informatics and medicine, among others (Appice and Džeroski, 2007). As in multi-label, instance selection for multi-target regression is yet to be researched.

Part II

Publications

Simple rules survive.

Devroye et al. (1996)

Chapter 1

Instance selection for regression by discretization

This journal paper presents the idea of using the discretization process with the aim of adapting instance selection algorithms for classification to regression. The meta-model process is presented, so that any instance selection method can be used. The concept in the paper is an adaptation of the Wilson Edition algorithm (ENN (Wilson, 1972)) that is tested against two instance selection methods for regression: MI (Guillen et al., 2010) and RegENN (Kordos and Blachnik, 2012). Both methods are noise filters, so the experiments were carried out by adding artificial noise. In addition to their comparison in terms of accuracy and compression (conventional instance selection measures), their identification of noise instances is also evaluated by considering a binary problem.

Authors: Álvar Arnaiz-González, Jose-Francisco Díez-Pastor, Juan José Rodríguez-Diez, César Ignacio García-Osorio
Type: Journal
Published in: Expert Systems with Applications 54: 340 – 350
Year: 2016
Reference: Arnaiz-González et al. (2016b)

Instance selection for regression by discretization

Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César García-Osorio

University of Burgos, Spain

Abstract

An important step in building expert and intelligent systems is to obtain the knowledge that they will use. This knowledge can be obtained from experts or, nowadays more often, from machine learning processes applied to large volumes of data. However, for some of these learning processes, if the volume of data is large, the knowledge extraction phase is very slow (or even impossible). Moreover, often the origin of the data sets used for learning are measure processes in which the collected data can contain errors, so the presence of noise in the data is inevitable. It is in such environments where an initial step of noise filtering and reduction of data set size plays a fundamental role. For both tasks, instance selection emerges as a possible solution that has proved to be useful in various fields. In this paper we focus mainly on instance selection for noise removal. In addition, in contrast to most of the existing methods, which applied instance selection to classification tasks (discrete prediction), the proposed approach is used to obtain instance selection methods for regression tasks (prediction of continuous values). The different nature of the value to predict poses an extra difficulty that explains the low number of articles on the subject of instance selection for regression.

More specifically the idea used in this article to adapt to regression problems "classic" instance-selection algorithms for classification is as simple as the discretization of the numerical output variable. In the experimentation, the proposed method is compared with much more sophisticated methods, specifically designed for regression, and shows to be very competitive.

The main contributions of the paper include: *i*) a simple way to adapt to regression instance selection algorithms for classification, *ii*) the use of this approach to adapt a popular noise filter called ENN (edited nearest neighbour), and *iii*) the comparison of this noise filter against two other specifically designed for regression, showing to be very competitive despite its simplicity.

Keywords: instance selection, regression, mutual information, noise filtering, class noise

Email addresses: `alvarag@ubu.es` (Álvar Arnaiz-González), `jfdpastor@ubu.es` (José F. Díez-Pastor), `jjrodriguez@ubu.es` (Juan J. Rodríguez), `cgosorio@ubu.es` (César García-Osorio)

1. Introduction

Automatic supervised learning begins with a dataset of instances or examples, each of which is composed of input-output pairs. The learning problem consists in determining the relation between the input and the output values. When the output is a nominal or discrete value, the task is one of classification, as opposed to regression in which the value to predict is a continuous, numerical and non-discrete value.

The problem of using a finite set of examples to learn the relation between the values of the dependent and independent variables is not unique to Machine Learning, but is also a classic problem of statistics and pattern recognition. There are many real applications in which a solution to this problem would be of interest, among which figure image processing [45, 56], speech recognition [53], genome sequencing [22], industrial processes [25], fraud detection [38], and software engineering [49], finances [51], to mention only a few.

Regardless of the dataset that is analysed, the presence of noise in the real-world applications is common [16, 41, 46, 60], besides reduce learning abilities of models [61] and their elimination is by no means a clear cut process [20]. Various methods have been proposed for their detection and elimination that follow various approaches. This paper centres on the selection of instances, which has been widely studied, focusing above all on classification. The problem has not been studied as much in relation to regression datasets, among other reasons because of the complexity of this type of dataset [34]. While in classification, the number of classes or values to be predicted is usually very low (the simplest example would be binary problems), the output variable in regression is continuous, such that the number of possible values to predict is unlimited [35]. This paper seeks to apply all the algorithms conceived for classification purposes to regression problems, on the basis of a meta-model.

The main contributions of the paper are:

- An approach for adapting to regression instance selection method initially designed for regression. It makes available a wide-range of instance selection methods for regression to researchers.
- The proposed approach was used to adapt ENN [57] (edited nearest neighbour) to regression.
- The performance of the new model was compared against two state-of-the-art noise filters for regression [23, 35].

This article has the following structure: first, the instance selection process for classification is explained and the problems involved in applying this technique to regression are analysed. Then, the proposed method, consisting of the discretization of the numerical variable, is presented in the section 3. In section 4, the results of the experimentation are analysed, and in the final section, the conclusions are extracted and future lines of work are suggested.

2. Instance-selection methods

Instance-based learners, also called lazy learners, are very effective, despite its simplicity [10] and nowadays are still frequently used in experimental studies in Machine

Learning [40]. However, these methods suffer from various disadvantages [33]. They are very sensitive to the presence of noise in the training data [43]. In addition, few algorithms are able to generate results within a reasonable time span when using large-sized datasets that need to be processed these days [35].

According to [30], instance selection serves two purposes: to reduce noise and to eliminate outliers in the datasets (noise filters); and, to reduce the complexity of instance-based learning algorithms [1] (condensing algorithms), with the intention of reducing the number of examples in the training set.

[35] explained that industries require expert and intelligent systems to optimize their processes. Datasets in industries are huge and require techniques able to reduce their complexity before building the prediction models. Moreover, instance selection has been used not only in industrial processes, below we described some other fields of application:

- Steel industry: We have found two works [36, 35] in which authors found necessary to reduce the size of datasets due to the great number of samples that are available in steel processes. Whereas [36] tried to reduce the size as previous stage of clustering, [35] used neural networks after instance selection process.

- Stock markets: in stock market analysis, [32] developed a new genetic instance selection method to reduce the complexity of induced solutions. They used the direction of change (increase or decrease of the stock index from one day to the next) in the daily Korea stock price index. Stock markets are complex and noisy, thus the instance selection method proposed gave the chance to improve the performance of artificial neural networks.

- Bankruptcy prediction: financial institutions need accurate bankruptcy prediction models, since is essential for their risk management. In [2] the combination of instance and feature selection was tested with the aim to improve, using genetic algorithms, the performance of case-base reasoning (CBR).

- Computer vision. A challenging problem in computer vision is the recognition of traffic signs (TSR) because in autonomous vehicles it has a crucial impact on driver safety. [13] used a genetic algorithm for feature and instance selection over a benchmark of TSR, as opposed to [2], they performed instance and feature selection separately. They addressed the trade-off between accuracy, data set size reduction and time spent during the selection process, which is always present.

- Time series. The domains where time-series classification is used are wide, including finance, networking, medicine, astronomy, robotic, chemistry and industry [31]. Therefore the use of instance selection techniques for this problem is already under investigation [11, 23].

2.1. Instance selection for classification

Instance-selection algorithms are intended to reduce the complexity of the learning algorithms by reducing the number of examples, they extract the most significant and discard those that do not provide valuable information [19], for example, the outliers and the examples introduced as a consequence of noise in the measurement process.

The literature contains a large number of instance-selection algorithms designed for classification purposes and new ones continue to appear. An up-to-date taxonomy may be found in [17].

The need for instance selection becomes obvious when the datasets used in real life are examined. Attempts to train a classifier, for example, on the basis of millions of instances can be a difficult, even an insurmountable task. The selection of instances therefore appears to be a good alternative, to reduce the complexity of the sample, enabling its subsequent treatment.

The term "instance selection" brings together a range of procedures and algorithms that are intended for the selection of a representative subset of the initial training dataset [32]. A first classification of these techniques is usually done using as criteria the purpose of their application, dividing them into two large groups: editing (or noise filtering), and condensation algorithms.

2.1.1. Edition techniques

Noise filtering techniques attempt to eliminate the erroneously labelled instances from the training set and, at the same time, they attempt to clear possible overlaps between regions of different classes. In other words, their principal objective is to achieve compact and homogeneous groups; one of such techniques is the *Wilson's editing algorithm* [57]. If an instance is badly classified on the basis of the rule k-NN, it will basically eliminate that instance from the training set (Algorithm 1).

Algorithm 1: Wilson's editing algorithm (ENN)

```
Data: Training set $\{X, Y\} = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, number of neighbours $k$ to
      consider, and $\delta_{kNN}(\mathbf{x}_i)$, the majority class of the $k$ nearest neighbours.
Result: Edited set $S \subseteq \{X, Y\}$
1 $S = \{X, Y\}$
2 foreach $\mathbf{x}_i, y_i \in S$ do
3     Find $\mathbf{x}.N_{1...k}$, the $k$ nearest neighbours of $\mathbf{x}_i$ in $X - \{\mathbf{x}_i\}$
4     if $\delta_{kNN}(\mathbf{x}_i) \neq y_i$ then remove $\mathbf{x}_i, y_i$ from $S$
  end
5 return $S$
```

2.1.2. Condensation techniques

One of the problems that arises when real-world datasets are analysed is the large number of examples that they contain, making the learning process computationally costly and preventing the use of certain algorithms on certain datasets. This condition is even more evident with algorithms based on neighbourhood criteria. The search for the neighbourhood of each instance grows in a significant way along with the size of the dataset. An obvious alternative that will counter this size-related problem and accelerate calculation of the nearest neighbour, in addition to the various efficient algorithms described in the literature, consists in reducing the number of instances in the training set, but trying not to increase the classification error.

In general, the objective of any condensation technique consists in removing all those instances from the training set that have no explicit influence on obtaining a classification result that is equal or very similar to the result obtained with the training set. The principal difference betweeen the different condensation techniques centres on the method used for the correct estimation of the instances that are and are not necessary.

The family of condensation techniques can be divided into selection and replacement schemes, depending on the form in which the instances are obtained from the condensed set. Algorithms that belong to the first group select instances in the original set, creating a condensed set that is a proper subset of the original training set. In the case of techniques with replacement strategies, the instance members of the condensed set are "constructed" on the basis of the examples in the original set through the use of a transformation function, so that these instances that are generated will not necessarily coincide with the original examples.

2.2. Instance selection for regression

Few studies have been conducted on the application of instance-selection techniques to datasets with a numerical and non-discrete output variable and there are few algorithms that are specifically designed for that purpose [50]. As previously mentioned, one of the reasons why instance selection for regression has not been the subject of many studies is its complexity [35]. While the problem in classification is to determine the boundaries between classes, and the number of these is finite, in regression, it is necessary to predict the value of the output variable, and this is continuous and with an arbitrary number of values. This research area is of interest for several reasons: *i*) there are datasets with a large number of instances that can not as yet be correctly analysed because of their size, *ii*) if it is possible to eliminate or reduce the noise, the results obtained with the predictors can be improved, *iii*) there are still few studies in the area.

Despite the difficulty, some instance selection algorithms have emerged that are able to deal with numeric class. [1] presented a new method (k-SN: k surrounding neighbours) for function prediction in lazy learning algorithms, it could be considered a first proposal of this kind of algorithm in regression task. A few years later, [52] presented a genetic algorithm for outlier detection and feature selection in linear regression models. More recently, [5], also following a genetic approach, addressed the problem in the framework of MOEL (multiobjective evolutionary learning) of fuzzy rule-based systems (FRBs [28]). Regarding time series prediction, [23] presented a new method based on mutual information for outlier detection achieving good results in both artificial and real datasets (a detailed description is given in section 2.2.1). Afterwards, the same approach was generalized for dataset reduction in time series [50]. Finally, some other authors have focused their efforts on adapting instance selection methods to regression that were initially designed for classification. In [35] CNN and ENN were adapted to work with regression problems (more details are given in section 2.2.2), and in [44] the method Class Conditional Instance Selection (CCIS) [42] is adapted to reduce the variance in genetic fuzzy systems (GFSs) [3]. Recently, ensembles of instance selection has revealed its benefits in classification [21]. The adaptation of ensembles of instance selection to regression was made by [8] who combined their own algorithms using bagging, achieving better performance and higher compression.

In this paper, we have conducted an experimental study in which the proposed method have been tested against two state of the art instance selection algorithms for regression.

2.2.1. Instance Selection Using Mutual Information

The use of mutual information (MI) for feature selection, based on the k-nearest neighbours, was presented by [29]. Later on, it has been used for instance selection giving good results for filtering, with emphasis in noise reduction [23]. Algorithm 2 shows the pseudo code, where n is the number of instances of the original dataset, α is a threshold that indicates the difference of the MI to select or discard an instance and k is the number of neighbours of the neighbourhood. The α value determines the specificity of the algorithm and must be set manually.

Algorithm 2: Algorithm based on mutual information

```
Data: Training set $\{X, Y\} = \{(\mathbf{x}_1, y_1, \dots \mathbf{x}_n, y_n\}$, the number $k$ of neighbours
Result: Edited set $S \subseteq \{X, Y\}$
1  $S = \varnothing$
2  for $i = 1 \dots n$ do
3      Calculate NN[$\mathbf{x}_i, j$], the $k$ nearest neighbours ($j = 1 \dots k$) in the input space
   end
4  for $i = 1 \dots n$ do
5      Calculate the value of mutual information $I(X, Y)_i$ when $\mathbf{x}_i$ is eliminated from $X$
   end
6  Normalize $I(X, Y)_i$ in $[0, 1]$
7  for $i = 1 \dots n$ do
8      $Cdiff = 0$
9      for $j = 1 \dots k$ do
10         $diff = I(X, Y)_i - I(X, Y)_{NN[\mathbf{x}_i, j]}$
11         if $diff > \alpha$ then $Cdiff = Cdiff + 1$
       end
12     if $Cdiff < k$ then add $\mathbf{x}_i, y_i$ to $S$
   end
13 return $S$
```

The mutual information of two variables (i.e. the value of attributes of two instances) is a quantity that measures their dependency, in other words, how much the uncertainty in the value of a variable can be reduced by knowing the value of the other, that is, it quantifies the amount of information that the variables share [50]. It may be defined as

$$I(X, Y) = \int \mu_{X,Y}(x, y) \log(\mu_{x,y}(x, y)/(\mu_X(x)\mu_Y(y)))dxdy$$

where $\mu_Y(y)$ is defined as $\int \mu_{X,Y}(x, y)dx$ using the joint-density function $\mu_{X,Y}$. But in [23], the mutual information is estimated on the basis of the nearest neighbours, defining the space $Z = \{X, Y\}$ and using the maximum norm (although any other norm could have been used) for each pair of points $z = (x, y)$ y $z' = (x', y')$.

$$||z - z'|| = \max\{||x - x'||, ||y - y'||\} \quad (1)$$

The distance from one point z_i to its k-th nearest neighbours is expressed as $\epsilon(i)$, while

$\epsilon_x(i)$ and $\epsilon_y(i)$ represent the distances between the same points projected onto subspaces X and Y, respectively. Having defined the above, $n_x(i)$ is defined as the number of points x_j at a distance from x_i which is strictly inferior to $\epsilon(i)$, and the same may be said of $n_y(i)$. And the formula for the calculation of mutual information is defined as

$$\hat{I}_1(X,Y) = \psi(k) - \frac{1}{N}\sum_{i=1}^{N}[\psi(n_x(i)+1) + \psi(n_y(i)+1)] + \psi(N)$$

where ψ is the digamma function

$$\psi(t) = \frac{\Gamma'(t)}{\Gamma(t)} = \frac{d}{dt}\ln\Gamma(t)$$

with

$$\Gamma(t) = \int_0^\infty u^{t-1}e^{-u}\mathrm{d}u \tag{2}$$

The digamma Function $\Gamma(t)$ satisfies the recurrence relation $\psi(x+1) = \psi(x)+1/x$ which starts with $\psi(1) = 0.57721...$ the Euler-Mascheroni constant.

2.2.2. Instance Selection Using Threshold

Unlike classification tasks which have a discrete class, instance selection algorithms for regression can not determine, using only the target value, if an instance is needed or not. [35] use an adaptive threshold to compare the output attribute value with its neighbourhood and determine if it belongs to the same *class*. This concept is similar to *soft-class* used by [37], but the novelty of this approach is that the threshold is adaptive to the standard deviation of its neighbours.

In Algorithm 3 we show the pseudo code, where $\texttt{Model}(T\backslash\mathbf{x}_i, \mathbf{x}_i)$ gives the target value calculated by a regressor trained using T without $\mathbf{x}_i$; R contains the k-nearest neighbours of the instance $\mathbf{x}_i$ on the subset T. The threshold θ is a multiple of the standard deviation of the outputs of the instances in R, whose value depends on the parameter α that is given as parameter to the algorithm. The α value determines the performance of the algorithm, if its value is large, an instance will be considered as noise, and therefore removed from the dataset, only if its output value is very different from the predicted by the model trained with its neighbourhood. If it is small, to keep the instance in the dataset, its output value must be very similar to the value predicted by the model.

3. Instance selection by means of discretization

The idea that we propose in this article is the possibility of applying to regression datasets, instance selection methods designed for classification tasks. To do so, the output variable is previously discretized in such a way that the dataset is turned into a classification problem. Having completed the selection of instances, the numerical value of the output variable is recovered for the selected instances.

This proposal is presented in Algorithm 4, and can be considered a meta-algorithm, as it allows to use in regression any previously existing classification method for instance selection, for example:

Algorithm 3: RegENN: Edited Nearest Neighbour for regression using a threshold

```
  Data: Training set $T = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$, parameter $\alpha$ to control how the
        threshold is calculated from the standard deviation, the number of
        neighbours $k$ to train the model
  Result: Instance set $S \subseteq T$
1 for $i = 1...n$ do
2     $\bar{Y}(\mathbf{x}_i) = \texttt{Model}(T \backslash \mathbf{x}_i, \mathbf{x}_i)$
3     $R = \texttt{kNN}(T, \mathbf{x}_i)$
4     $\theta = \alpha \cdot std\big(Y(X_R)\big)$
5     if $|Y(\mathbf{x}_i) - \bar{Y}(\mathbf{x}_i)| > \theta$ then
6         $T \leftarrow T \backslash \mathbf{x}_i$
      end
  end
7 $S \leftarrow T$
  return $S$
```

- Edition: ENN [57], ENRBF [30], RNGE [47], etc.
- Condensation: CNN [27], MSS [6], POP [48], ICF [10], DROP [58], ATISA [12], etc.

Algorithm 4: Proposed meta-model based on discretization of the output variable

```
  Data: Training set $\{X, Y\} = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$, Discretization algorithm and
        all the parameter that it needs
  Result: Instance set $S \subseteq \{X, Y\}$
1 $Y_D$ = Discretization of the numerical target $Y$
2 Apply classification-based instance selection algorithm over $\{X, Y_D\}$ to obtain
  subset $S$
3 Restore the numerical value of the output variable in $S$
  return $S$
```

3.1. Main features of the proposed method

The main advantages of the proposed method are its simplicity and its adaptability. The method is simple since the discretization stage is quite straightforward. On the other hand, it can be easily applied to any instance selection algorithm for classification, no changes are needed in the algorithms as they are used as black boxes and the discretization is completely independent of the chosen algorithm.

The keystone of our proposal is the discretization stage since it decisively influences instance selection. Traditionally, algorithms of discretization have been applied to input variables and divided into two families: supervised, when the output variable is taken into account, and unsupervised (or class-blind), when the output variable is not taken into account. In the proposal, the discretization is applied to the output variable, so only unsupervised algorithms can be used.

The method based on threshold (see Algorithm 3) has a totally different approach to the adaptation to regression of instance selection methods for classification. The decision to consider an instance 'out of class' is a local decision, which considers the neighbourhood of the instance to calculate a 'soft' class around the average output value of its neighbours (being the radius of this class a magnitude calculated from the standard deviation of the output values of its neighbours). In contrast, our method makes a global discretization of the output variable for the whole dataset, which makes it easier, faster and more general, since it is not necessary to modified the implementation of the adapted instance selection algorithm.

Compared with the method based on mutual information, our method, besides showing better performance (see the experimental study below), is much faster, as there is not need to compute the complex calculations of mutual information.

4. Experimental Study

In the experimental study, we have followed the methodology used by [23], adding noise to the original datasets to assess the performance of the algorithms as a filter noise.

4.1. Datasets

In the experiments, 29 datasets from the Keel repository [4] have been used. Table 1 shows some of the characteristics of these datasets: number of attributes and instances, and *root mean squared error* (RMSE) achieved by the regressors (using cross-validation): *k*NN (*k* nearest neighbours), RBF (radial basis function networks) and REPTree (reduced error-pruning tree) [59].

The only transformation performed on the datasets has been the normalization of all the attributes, excluding the output variable, to ensure that attributes with high variance do not distort the results of nearest neighbours calculations.

4.2. Experimental Setup

With the intention of evaluating the capability of the proposed model, it was compared with the techniques presented by [23] and [35]. Their methods are referred to as MI and RegENN in the following section. We have not considered any evolutionary algorithms because they are very time-consuming. The methods are presented as noise filters. As Guillen et al. the output variable was modified, by adding or subtracting a random value between its minimum and maximum values.

With the aim of evaluating the performance of the algorithms as noise filters, the selection process was evaluated as f it were a binary classification problem. After filtering, the resultant dataset returned by the algorithms was evaluated [16], counting how many actual and noisy instances were retained, to fill a confusion matrix (see the Table 2). The confusion matrix give us four rates:

- True positive (TP): an instance whose output value has been modified is correctly classified as noise.
- False positive (FP): an unmodified instance is classified as noise.
- True negative (TN): an unmodified instance is correctly classified as not modified.

Table 1: Datasets for experiments. The RMSE column shows the *root mean squared error* achieved by kNN regressor, radial basis function network regressor (RBF) and regressor tree (REPTree).

Dataset	**# Insts.**	**# Attrs**	**RMSE**		
			kNN	**RBF**	**REPTree**
machineCPU	209	6	73.3861	54.9182	74.1478
baseball	337	16	681.9675	694.5271	784.2473
dee	365	6	0.4136	0.4024	0.4886
autoMPG8	392	7	2.9245	2.6252	3.2893
autoMPG6	392	5	2.7766	2.9610	3.2841
ele-1	495	2	647.7872	637.9696	709.1737
stock	950	9	0.7816	1.0196	1.1843
laser	993	4	10.2126	7.4007	14.0605
concrete	1030	8	9.3890	7.2785	7.4055
treasury	1049	15	0.2423	0.2265	0.3214
mortgage	1049	15	0.1917	0.1063	0.2562
ele-2	1056	4	271.1403	123.7133	185.0631
friedman	1200	5	1.7855	1.5425	2.7496
wizmir	1461	9	1.7195	1.1542	1.7374
wankara	1609	9	1.9401	1.2973	2.0441
plastic	1650	2	1.6412	1.5113	1.7518
quake	2178	3	0.1954	0.1887	0.1887
ANACALT	4052	7	0.1188	0.1889	0.0709
abalone	4177	8	2.2223	2.0983	2.3359
delta-ail	7129	5	0.0002	0.0002	0.0002
compactiv	8192	21	3.0811	3.5825	3.2458
puma32h	8192	32	0.0273	0.0232	0.0089
delta-elv	9517	6	0.0015	0.0014	0.0015
ailerons	13750	40	0.0002	0.0002	0.0002
pole	14998	26	8.2376	16.7730	7.1492
elevators	16599	18	0.0036	0.0022	0.0036
california	20640	8	61915.5979	62456.4909	58826.3442
house	22784	16	38444.1767	38512.3930	38854.6220
mv	40768	10	1.8591	0.6156	0.3047

Table 2: Confusion matrix of the noise filter.

Predicted	**Actual**	
	Noise	No noise
Noise	TP	FP
No noise	FN	TN

- False negative (FN): an instance whose output value has been modified is wrongly classified as not modified.

Over the confusion matrix we calculated F_1 *score* [55]. This measure is the harmonic mean of precision and recall:

$$F_1 = 2 \cdot \frac{\texttt{precision} \cdot \texttt{recall}}{\texttt{precision} + \texttt{recall}} \tag{3}$$

where $\texttt{precision} = TP/(TP + FP)$ and $\texttt{recall} = TP/(TP + FN)$.

And *G mean* [39]:

$$Gmean = \sqrt{\texttt{specifity} \cdot \texttt{recall}} \tag{4}$$

where $\texttt{specifity} = TN/(TN + FP)$.

To achieve a better understanding of the effect of noise, we train the model on the distorted dataset and evaluate the learnt model using a clean dataset, following the experimental setup used in other works [9, 29, 60].

The experimental process was as follows (see Figure 1): beginning with the dataset with no noise, a cross-validation with 10 folds was performed, a percentage of noise was added to each of the training datasets and the regressor was trained with the dataset resulting from the filtering with the instance selection algorithm. In other words, the training is done over the training set from the instance-selection process, which was applied to the dataset after adding noise, and the test was performed on the original dataset. The process was set this way to ensure that the noise in the test phase would not distort the results of the regressor. At the same time, the aim was to test whether the noise filtering of the instance selection algorithm was sufficient so that a regressor trained with the filtered dataset achieve a good generalization. The noise configurations were tested at 10, 20, 30 and 40% adding or subtracting a random value to the target attribute (i.e. class noise).

The algorithms were implemented in *Weka* [24] and experimentation was done with the Weka experimenter, version 3.7.11. Radial basis function (RBF), k-Nearest Neighbours (kNN) and a tree-generation algorithm (REPTree, reduced error-pruning tree [59]) were used as regressors with the default values that appear in Weka, to ensure that any modification would not be advantageous to one method over another. We only changed the number of functions used by RBF because the default value is two, we increased to five as used by Guillen et al. in their experimentation. The initial centers for the functions are found using *KMeans* clustering algorithm. For kNN, with the aim of finding the best k value, we launched eleven experiments (from $k = 1$ to $k = 11$) over the 29

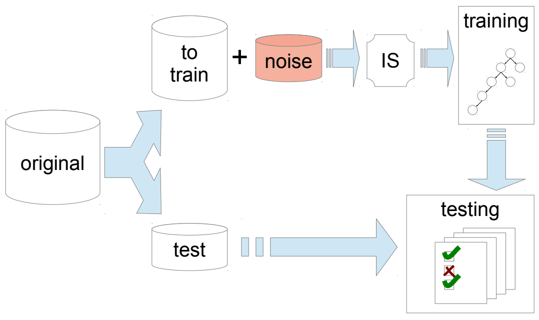


Figure 1: Configuration of the experiments.

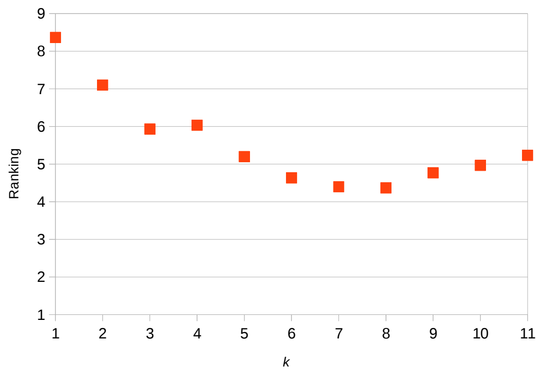


Figure 2: Average ranks over RMSE for regressor kNN varying k value from one to eleven. The best result was achieved for $k = 8$.

datasets (see Figure 2). The best results was achieved with ($k = 8$, in classification even values of k are discarded to avoid ties, but in regression this is not a problem).

The experiments were executed with the parameters recommended by authors:

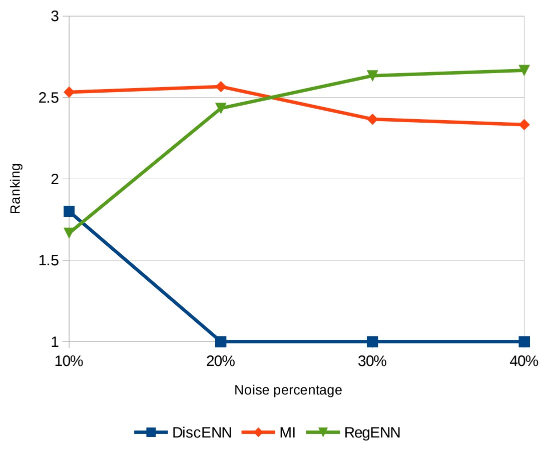
- Mutual Information (MI): $k = 6$ as number of nearest neighbours and $\alpha = 0.05$.
- ENN based on threshold (RegENN): $k = 9$ as number of nearest neighbours and $\alpha = 5$.

Given that these algorithms are designed to filter noise, the Wilson edition with $k = 9$ was used in the proposed meta-model, hereinafter DiscENN.

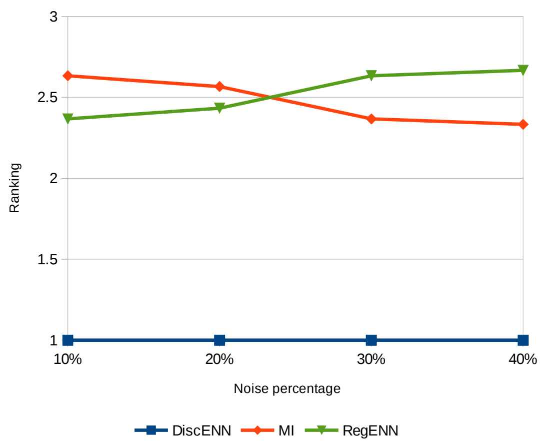
The unsupervised filter incorporated in Weka was used for discretization. The equal-width option was selected, so all bins in which the target attribute was split had the same size. The number of bins is selected from one to ten by the Weka filter using *leave-one-out cross-validation* to select the best way of separating the numerical output variable, i.e. the one that maximizes the entropy.

4.3. Results

Average ranks were used to compare the methods and were computed as follows: for each dataset, the methods were sorted from best to worst by assigning a rank of 1 to the



(a) F_1 score



(b) G *mean*

Figure 3: Average ranks over F_1 score (a) and G *mean* (b).

best, 2 to the second, and 3 to the third. Finally, the ranks of the different datasets were averaged for each instance selection method [14].

The *root mean squared error* (RMSE), the F_1 score and the G mean were used for the evaluation of the models.

Figure 3 presents the average rank over F_1 score and the G mean for the configuration tested. The margin between DiscENN and the others two methods enlarges as the noise rate increases.

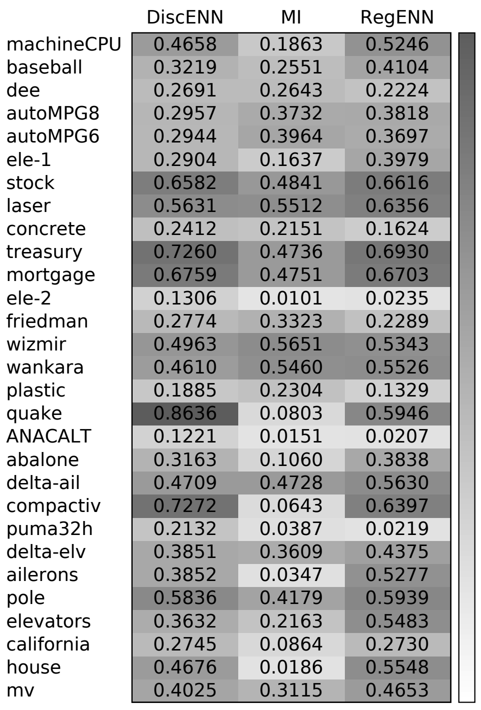
Figure 4 shows the *heatmaps* of F_1 scores for each dataset [16]. In these tables, each column is an instance selection method, each row is a dataset and in each cell the F_1 score is represented numerically and by means of a grayscale color. The darker the color, the higher the F_1 score. When noise percentage is low, i.e. 10%, the differences between instance selection algorithms is no clear. However, as noise increases the first column (DiscENN) darkens while the columns for the others methods lightens. The same representation is used in Figure 5 for the G *mean*. The results of the proposed method in these figures are better than the previous one, DiscENN achieved higher values for all levels of noise. For both F_1 score and G *mean*, the proposed method shows a much better behaviour than the other two methods when the noise level is higher than 10%.

To check if differences between the algorithms are statistically significant, Hochberg procedure [18] have been used.

As shown in Table 3, the proposed method is not the best for a noise level of 10%, but is not significantly worse than the best method, RegENN, for this level of noise. Note that RegENN is the only method that is not significantly worse than the method proposed for noise levels of 20% when RBF and REPTree are used as regressors.

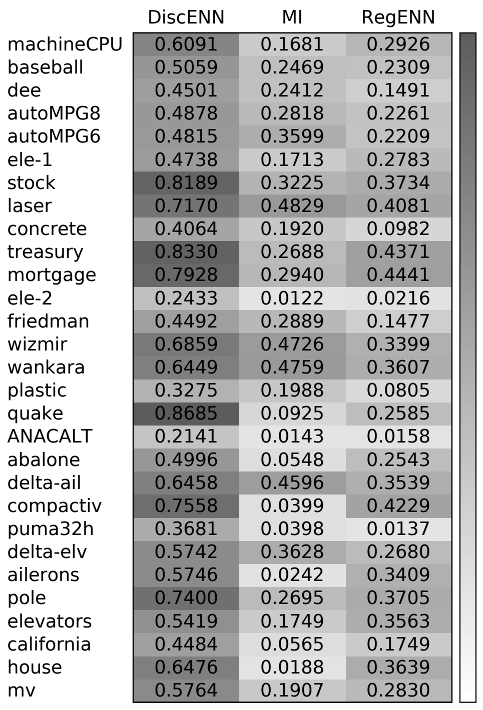
For noise levels of 20, 30 and 40%, the proposed method is always the best regardless of the regressor being used (kNN, RBF and REPTree). In the case of using kNN as regressor, the proposed method is a noise filter significantly better than the method based on MI and the RegENN method. As might be expected, in all cases, the noise filtering gets best results than to train the regressor directly to the noisy dataset.

As shown in Table 4, the proposed algorithm is the best method according to compression (i.e. it always achieves smaller datasets than the other methods) and differences



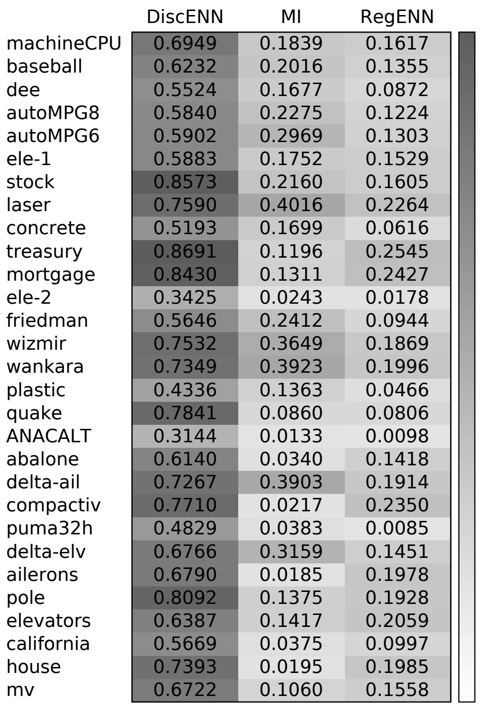
	DiscENN	MI	RegENN
machineCPU	0.4658	0.1863	0.5246
baseball	0.3219	0.2551	0.4104
dee	0.2691	0.2643	0.2224
autoMPG8	0.2957	0.3732	0.3818
autoMPG6	0.2944	0.3964	0.3697
ele-1	0.2904	0.1637	0.3979
stock	0.6582	0.4841	0.6616
laser	0.5631	0.5512	0.6356
concrete	0.2412	0.2151	0.1624
treasury	0.7260	0.4736	0.6930
mortgage	0.6759	0.4751	0.6703
ele-2	0.1306	0.0101	0.0235
friedman	0.2774	0.3323	0.2289
wizmir	0.4963	0.5651	0.5343
wankara	0.4610	0.5460	0.5526
plastic	0.1885	0.2304	0.1329
quake	0.8636	0.0803	0.5946
ANACALT	0.1221	0.0151	0.0207
abalone	0.3163	0.1060	0.3838
delta-ail	0.4709	0.4728	0.5630
compactiv	0.7272	0.0643	0.6397
puma32h	0.2132	0.0387	0.0219
delta-elv	0.3851	0.3609	0.4375
ailerons	0.3852	0.0347	0.5277
pole	0.5836	0.4179	0.5939
elevators	0.3632	0.2163	0.5483
california	0.2745	0.0864	0.2730
house	0.4676	0.0186	0.5548
mv	0.4025	0.3115	0.4653

(a) Noise 10%



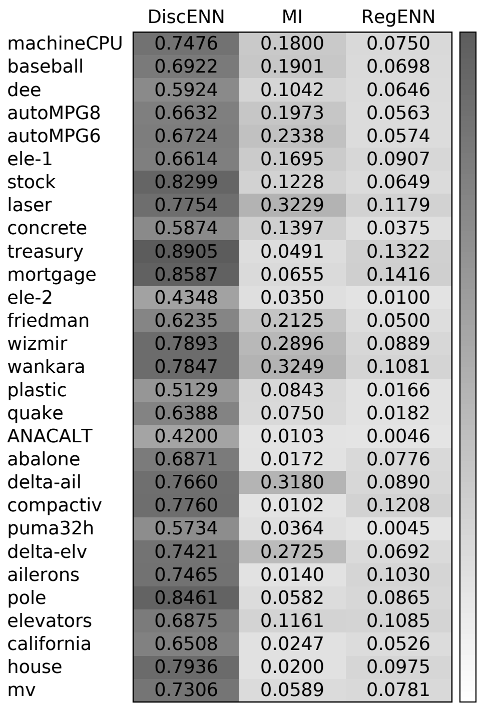
	DiscENN	MI	RegENN
machineCPU	0.6091	0.1681	0.2926
baseball	0.5059	0.2469	0.2309
dee	0.4501	0.2412	0.1491
autoMPG8	0.4878	0.2818	0.2261
autoMPG6	0.4815	0.3599	0.2209
ele-1	0.4738	0.1713	0.2783
stock	0.8189	0.3225	0.3734
laser	0.7170	0.4829	0.4081
concrete	0.4064	0.1920	0.0982
treasury	0.8330	0.2688	0.4371
mortgage	0.7928	0.2940	0.4441
ele-2	0.2433	0.0122	0.0216
friedman	0.4492	0.2889	0.1477
wizmir	0.6859	0.4726	0.3399
wankara	0.6449	0.4759	0.3607
plastic	0.3275	0.1988	0.0805
quake	0.8685	0.0925	0.2585
ANACALT	0.2141	0.0143	0.0158
abalone	0.4996	0.0548	0.2543
delta-ail	0.6458	0.4596	0.3539
compactiv	0.7558	0.0399	0.4229
puma32h	0.3681	0.0398	0.0137
delta-elv	0.5742	0.3628	0.2680
ailerons	0.5746	0.0242	0.3409
pole	0.7400	0.2695	0.3705
elevators	0.5419	0.1749	0.3563
california	0.4484	0.0565	0.1749
house	0.6476	0.0188	0.3639
mv	0.5764	0.1907	0.2830

(b) Noise 20%



	DiscENN	MI	RegENN
machineCPU	0.6949	0.1839	0.1617
baseball	0.6232	0.2016	0.1355
dee	0.5524	0.1677	0.0872
autoMPG8	0.5840	0.2275	0.1224
autoMPG6	0.5902	0.2969	0.1303
ele-1	0.5883	0.1752	0.1529
stock	0.8573	0.2160	0.1605
laser	0.7590	0.4016	0.2264
concrete	0.5193	0.1699	0.0616
treasury	0.8691	0.1196	0.2545
mortgage	0.8430	0.1311	0.2427
ele-2	0.3425	0.0243	0.0178
friedman	0.5646	0.2412	0.0944
wizmir	0.7532	0.3649	0.1869
wankara	0.7349	0.3923	0.1996
plastic	0.4336	0.1363	0.0466
quake	0.7841	0.0860	0.0806
ANACALT	0.3144	0.0133	0.0098
abalone	0.6140	0.0340	0.1418
delta-ail	0.7267	0.3903	0.1914
compactiv	0.7710	0.0217	0.2350
puma32h	0.4829	0.0383	0.0085
delta-elv	0.6766	0.3159	0.1451
ailerons	0.6790	0.0185	0.1978
pole	0.8092	0.1375	0.1928
elevators	0.6387	0.1417	0.2059
california	0.5669	0.0375	0.0997
house	0.7393	0.0195	0.1985
mv	0.6722	0.1060	0.1558

(c) Noise 30%



	DiscENN	MI	RegENN
machineCPU	0.7476	0.1800	0.0750
baseball	0.6922	0.1901	0.0698
dee	0.5924	0.1042	0.0646
autoMPG8	0.6632	0.1973	0.0563
autoMPG6	0.6724	0.2338	0.0574
ele-1	0.6614	0.1695	0.0907
stock	0.8299	0.1228	0.0649
laser	0.7754	0.3229	0.1179
concrete	0.5874	0.1397	0.0375
treasury	0.8905	0.0491	0.1322
mortgage	0.8587	0.0655	0.1416
ele-2	0.4348	0.0350	0.0100
friedman	0.6235	0.2125	0.0500
wizmir	0.7893	0.2896	0.0889
wankara	0.7847	0.3249	0.1081
plastic	0.5129	0.0843	0.0166
quake	0.6388	0.0750	0.0182
ANACALT	0.4200	0.0103	0.0046
abalone	0.6871	0.0172	0.0776
delta-ail	0.7660	0.3180	0.0890
compactiv	0.7760	0.0102	0.1208
puma32h	0.5734	0.0364	0.0045
delta-elv	0.7421	0.2725	0.0692
ailerons	0.7465	0.0140	0.1030
pole	0.8461	0.0582	0.0865
elevators	0.6875	0.1161	0.1085
california	0.6508	0.0247	0.0526
house	0.7936	0.0200	0.0975
mv	0.7306	0.0589	0.0781

(d) Noise 40%

Figure 4: F_1 score for each dataset. The darker the color is, the higher is the score (i.e. black color represents $F_1 = 1$ and white color $F_1 = 0$.

	DiscENN	MI	RegENN
machineCPU	0.8115	0.3888	0.6446
baseball	0.7291	0.4559	0.5214
dee	0.6624	0.4366	0.3616
autoMPG8	0.6939	0.5275	0.4950
autoMPG6	0.6948	0.5691	0.4838
ele-1	0.6907	0.3633	0.5103
stock	0.9398	0.5778	0.7061
laser	0.8654	0.6588	0.6933
concrete	0.6091	0.3891	0.2984
treasury	0.9208	0.5674	0.7318
mortgage	0.8880	0.5877	0.7116
ele-2	0.4318	0.0837	0.1269
friedman	0.6670	0.5081	0.3600
wizmir	0.8422	0.6840	0.6058
wankara	0.8328	0.6714	0.6186
plastic	0.5252	0.4387	0.2763
quake	0.9797	0.2324	0.6611
ANACALT	0.4058	0.1092	0.1242
abalone	0.7217	0.2500	0.4973
delta-ail	0.8368	0.6621	0.6393
compactiv	0.8019	0.1833	0.6947
puma32h	0.5211	0.1501	0.1055
delta-elv	0.7867	0.5690	0.5375
ailerons	0.7872	0.1355	0.6012
pole	0.8809	0.5771	0.6664
elevators	0.7690	0.3886	0.6292
california	0.6615	0.2152	0.4075
house	0.8385	0.0983	0.6430
mv	0.7853	0.4381	0.5507

(a) Noise 10%

	DiscENN	MI	RegENN
machineCPU	0.7937	0.3294	0.4287
baseball	0.7301	0.4004	0.3664
dee	0.6724	0.3824	0.2854
autoMPG8	0.7106	0.4171	0.3584
autoMPG6	0.7032	0.4908	0.3545
ele-1	0.6920	0.3312	0.4058
stock	0.9390	0.4433	0.4806
laser	0.8620	0.5753	0.5081
concrete	0.6071	0.3425	0.2277
treasury	0.9211	0.3956	0.5306
mortgage	0.8916	0.4201	0.5348
ele-2	0.4644	0.0857	0.1118
friedman	0.6591	0.4300	0.2830
wizmir	0.8495	0.5711	0.4535
wankara	0.8333	0.5739	0.4699
plastic	0.5159	0.3606	0.2082
quake	0.9481	0.2308	0.3866
ANACALT	0.4329	0.0938	0.0945
abalone	0.7202	0.1703	0.3834
delta-ail	0.8325	0.5750	0.4652
compactiv	0.7966	0.1429	0.5193
puma32h	0.5143	0.1463	0.0832
delta-elv	0.7878	0.5017	0.3945
ailerons	0.7883	0.1113	0.4537
pole	0.8813	0.4052	0.4798
elevators	0.7606	0.3212	0.4677
california	0.6577	0.1712	0.3113
house	0.8366	0.0981	0.4749
mv	0.7814	0.3256	0.4060

(b) Noise 20%

	DiscENN	MI	RegENN
machineCPU	0.7923	0.3299	0.3001
baseball	0.7283	0.3443	0.2703
dee	0.6696	0.3058	0.2142
autoMPG8	0.6906	0.3632	0.2563
autoMPG6	0.6930	0.4259	0.2655
ele-1	0.6841	0.3206	0.2887
stock	0.9208	0.3504	0.2958
laser	0.8362	0.5055	0.3579
concrete	0.5924	0.3123	0.1789
treasury	0.9116	0.2528	0.3825
mortgage	0.8918	0.2655	0.3722
ele-2	0.4768	0.1162	0.0973
friedman	0.6582	0.3785	0.2229
wizmir	0.8371	0.4768	0.3214
wankara	0.8272	0.4986	0.3333
plastic	0.4999	0.2789	0.1552
quake	0.8593	0.2157	0.2053
ANACALT	0.4418	0.0854	0.0713
abalone	0.7134	0.1322	0.2765
delta-ail	0.8205	0.5010	0.3255
compactiv	0.8013	0.1048	0.3651
puma32h	0.5037	0.1412	0.0655
delta-elv	0.7787	0.4437	0.2799
ailerons	0.7820	0.0968	0.3314
pole	0.8786	0.2732	0.3271
elevators	0.7443	0.2802	0.3390
california	0.6516	0.1384	0.2294
house	0.8321	0.0997	0.3324
mv	0.7761	0.2368	0.2906

(c) Noise 30%

	DiscENN	MI	RegENN
machineCPU	0.7872	0.3192	0.1995
baseball	0.7146	0.3279	0.1907
dee	0.6422	0.2360	0.1832
autoMPG8	0.6814	0.3324	0.1706
autoMPG6	0.6862	0.3680	0.1727
ele-1	0.6653	0.3085	0.2184
stock	0.8591	0.2573	0.1834
laser	0.8144	0.4400	0.2505
concrete	0.5705	0.2768	0.1385
treasury	0.9096	0.1587	0.2666
mortgage	0.8822	0.1841	0.2764
ele-2	0.4752	0.1358	0.0716
friedman	0.6400	0.3475	0.1603
wizmir	0.8244	0.4128	0.2158
wankara	0.8186	0.4420	0.2391
plastic	0.4706	0.2121	0.0916
quake	0.6873	0.1984	0.0958
ANACALT	0.4175	0.0729	0.0480
abalone	0.6991	0.0932	0.2011
delta-ail	0.8000	0.4372	0.2159
compactiv	0.8007	0.0716	0.2536
puma32h	0.4926	0.1367	0.0473
delta-elv	0.7683	0.4004	0.1894
ailerons	0.7747	0.0839	0.2331
pole	0.8735	0.1733	0.2127
elevators	0.7146	0.2495	0.2396
california	0.6418	0.1118	0.1644
house	0.8254	0.1006	0.2265
mv	0.7673	0.1743	0.2015

(d) Noise 40%

Figure 5: *G mean* for each dataset. The darker the color is, the higher is the score (i.e. black color represents $G = 1$ and white color $G = 0$.

Table 3: Average ranks and Hochberg procedure over RMSE. The ✖ means that the result of the algorithm is significantly worse than the best (the first of the ranking is highlighted in bold) at a confidence level of 0.95, we included NoFilter that shows the performance of the regressor trained over noisy datasets.

*k*NN

IS Alg.	**% noise**			
	10	**20**	**30**	**40**
DiscENN	2.172	**1.465**	**1.172**	**1.207**
MI	2.534	2.638 ✖	2.207 ✖	2.086 ✖
RegENN	**1.776**	2.224 ✖	3.965 ✖	3.965 ✖
NoFilter	3.517 ✖	3.672 ✖	2.655 ✖	2.741 ✖

RBF

IS Alg.	**% noise**			
	10	**20**	**30**	**40**
DiscENN	2.327	**1.672**	**1.431**	**1.465**
MI	2.483	2.603 ✖	2.707 ✖	2.758 ✖
RegENN	**1.983**	2.121	2.327 ✖	2.379 ✖
NoFilter	3.207 ✖	3.603 ✖	3.534 ✖	3.396 ✖

REPTree

IS Alg.	**% noise**			
	10	**20**	**30**	**40**
DiscENN	2.172	**1.638**	**1.431**	**1.396**
MI	2.621	2.862 ✖	2.810 ✖	2.931 ✖
RegENN	**2.000**	2.034	2.172 ✖	2.293 ✖
NoFilter	3.207 ✖	3.465 ✖	3.586 ✖	3.379 ✖

Table 4: Average ranks and Hochberg procedure over compression. The ✖ means that the result of the algorithm is worse than the best (the first of the ranking is highlighted in bold) at a confidence level of 0.95.

IS Alg.	**% noise**			
	10	**20**	**30**	**40**
DiscENN	**1.000**	**1.000**	**1.000**	**1.000**
MI	2.414 ✖	2.414 ✖	2.345 ✖	2.345 ✖
RegENN	2.586 ✖	2.586 ✖	2.655 ✖	2.655 ✖

are significant at a confidence level of 0.95.

Finally, with the aim to evaluate how well the instance selection works, average ranks over the three regressors were made. Table 5 shows the average ranks, the dashed line indicates that the difference between the first method and the others below the line is significant at a confidence level of 0.95. The table provides an indication of the performance of the different methods with different levels of noise: 10, 20, 30 and 40%. For all noise levels, the lowest error is achieved by RBF. When the noise level is only 10%, the selection done by RegENN outperforms the one done by DiscENN. However, as the noise level increases, the performance of the proposed method pays off, and the selection achieved by this method gives better results than the others. When the noise level is only 10%, the selection done by RegENN outperforms the one done by DiscENN. Also note that for noise levels of 30% and 40% the proposed method improves the results for all base regressor. As might be expected, kNN is the worst regressor in noisy environments, so it ranks low in all cases, however it is very noticeable that its rank improves remarkably when it is trained with the selection performed by the proposed method. This improvement is achieved even in the cases with high noise levels (30% and 40%), up to the point that it ranks second. Thus, the algorithm proposed in this paper allows to use regressors, which are not able to deal well with noise, in noisy environments.

5. Conclusions and future work

The construction of expert and intelligent systems requires the elicitation of the knowledge that they are going to use. Although in the past this required the intervention of experts in the subject matter of automation, today with the abundance of data, it is most frequent to obtain knowledge using data mining algorithms. However, there are two circumstances that may affect the use of these algorithms. On the one hand, some are very sensitive to noise. On the other hand, the presence of noise in the process of obtaining data is almost inevitable (for example, measurements in industrial environments).

Although there are numerous algorithms for instance selection in classification (the value to predict is discrete), it does not happen the same for problems in which the value to predict is continuous. The main contribution of this paper is a new approach to the problem of instance selection in regression. The approach is simple, even naive, the output variable is discretized to make use of an instance selection algorithm for classification. Besides simplicity, another major advantage of the method is that we now

Table 5: Average ranks and Hochberg procedure over RMSE for all regressors. The dashed line indicates the point at which the differences with regard to the first method were significant at a confidence level of 0.95. NoFilter shows the performance of the three regressors trained using noisy datasets.

Noise	**Algorithm**	**Rank**	**Noise**	**Algorithm**	**Rank**
	RBF RegENN	3.6379		RBF DiscENN	2.3793
	RBF DiscENN	3.9655		*k*NN DiscENN	3.2069
	RBF MI	4.5517		REP DiscENN	4.2759
	RBF (NoFilter)	5.5862		RBF RegENN	4.5690
	*k*NN RegENN	6.1897		RBF MI	4.9828
10 %	*k*NN DiscENN	6.2414	30 %	RBF (NoFilter)	6.1897
	REP RegENN	6.6552		REP RegENN	6.3448
	REP DiscENN	6.9655		REP MI	7.6552
	*k*NN MI	7.8448		*k*NN MI	8.5172
	REP MI	8.0345		REP (NoFilter)	8.7759
	REP (NoFilter)	8.9483		*k*NN (NoFilter)	9.2069
	*k*NN (NoFilter)	9.3793		*k*NN RegENN	11.8966
	RBF DiscENN	2.6897		RBF DiscENN	2.5172
	RBF RegENN	3.8966		*k*NN DiscENN	3.0517
	*k*NN DiscENN	4.3621		REP DiscENN	4.0172
	RBF MI	5.0690		RBF RegENN	4.6207
	REP DiscENN	5.1379		RBF MI	5.1207
20 %	RBF (NoFilter)	6.4138	40 %	RBF (NoFilter)	6.0517
	REP RegENN	6.7931		REP RegENN	6.6207
	*k*NN RegENN	7.6207		REP MI	7.7069
	REP MI	8.2414		REP (NoFilter)	8.3966
	*k*NN MI	8.4828		*k*NN MI	8.5000
	REP (NoFilter)	9.1897		*k*NN (NoFilter)	9.5000
	*k*NN (NoFilter)	10.1034		*k*NN RegENN	11.8966

have at our disposal all the algorithms of instance selection for classification existing in the literature. The utility of the approach has been proved experimentally, it offers competitive results when compare to the few existing methods of instance selection for noise removal in regression [23, 35], despite that the latter propose a more complex and sophisticated approaches to the problem. More specifically, its performance as a noise filter has been compared *i*) taking as reference the values of: the RMSE, the F_1 score, the *G mean* and the compression; *ii*) with different base regressors: k-nearest neighbours, RBF networks and REPTree, and *iii*) using 29 data set to which several levels of noise were added.

The main criticism that can be made to the proposal is the lack of theoretical justification. But the idea to address a continuous problem by means of a previous discretization step is a classical approach, perhaps the most representative example are the Rienmann sums to approximate the area under a curve and solve the problem of numerical integration. In any case, the discretization that is being done at the current implementation is too crude. We suspect that a discretization step more adjusted to the specific nature of the data could improve the method. The combination of results obtained with different discretizations could be beneficial as well (following a similar approach to the one used by ensemble methods). It may also be interesting to investigate whether the way in which the discretization is done affects the performance of the proposed approach. We hope to incorporate all these ideas in future research.

Another preprocessing operation that helps in the design of expert and intelligent systems is the selection of features [54, 7]. Some authors have successfully adapted to feature selection ideas originally designed for instance selection [26]. This makes us think that we too could do the same with our idea. In classification, simultaneous selection of instances and features has also proved to be beneficial [15], so perhaps our method can be also extended to this simultaneous selection. Finally, although our method has shown good results in a large set of standard datasets for benchmarking, it would be interesting to check its performance on specific domains, especially in industrial problems and in time series forecasting.

Acknowledgments

This work was supported by the project TIN2011-24046 of the Spanish Ministry of Economy and Competitiveness.

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If we had access to a classifier with perfect generalization performance, there would be no need to resort to ensemble techniques.

Polikar (2006)

CHAPTER 2

FUSION OF INSTANCE SELECTION METHODS IN REGRESSION TASKS

This journal paper presents the advantages of using a combination of instance selection methods in regression. The combination of multiple learners into an ensemble that has greater power than the sum of any one of its members is nothing new in itself. However, combinations of instance selection methods applied to regression tasks is a novel aspect that has not previously been tested.

Four instance selection methods, two edition algorithms and two condensation algorithms, were combined in homogeneous ensembles. Their superior performance supported the underlying principle of general ensembles: they work better than each method by itself alone

Authors: Álvar Arnaiz-González, Marcin Blachnik, Mirosław Kordos, César García-Osorio
Type: Journal
Published in: Information Fusion 30: 69 – 79
Year: 2016
Reference: Arnaiz-González et al. (2016)

Fusion of Instance Selection Methods in Regression Tasks[☆]

Álvar Arnaiz-González[a], Marcin Blachnik[b], Mirosław Kordos[c], César García-Osorio[a]

[a] *University of Burgos, Spain*
[b] *Silesian University of Technology, Poland*
[c] *University of Bielsko-Biala, Poland*

Abstract

Data pre-processing is a very important aspect of data mining. In this paper we discuss instance selection used for prediction algorithms, which is one of the pre-processing approaches. The purpose of instance selection is to improve the data quality by data size reduction and noise elimination.

Until recently, instance selection has been applied mainly to classification problems. Very few recent papers address instance selection for regression tasks.

This paper proposes fusion of instance selection algorithms for regression tasks to improve the selection performance. As the members of the ensemble two different families of instance selection methods are evaluated: one based on distance threshold and the other one on converting the regression task into a multiple class classification task.

Extensive experimental evaluation performed on the two regression versions of the Edited Nearest Neighbor (ENN) and Condensed Nearest Neighbor (CNN) methods showed that the best performance measured by the error value and data size reduction are in most cases obtained for the ensemble methods.

Keywords: instance selection, regression, ensemble models

1. Introduction

In real-world problems, we are often faced with regression tasks, aimed at predicting some real-value numbers. The quality of the prediction is often limited not by the learning algorithm, but by the quality of the data itself. There are various ways of improving the quality of the data on which the learning model is built. One of them is instance selection, in which we reject the training instances that are either not expected to improve or are expected to worsen prediction results.

In this paper, we use 'edited' or 'filtered' dataset interchangeably to refer to a dataset produced by an instance selection process.

Traditionally, instance selection methods are divided in two groups according to the approach used by algorithms to select an instance [29]:

[☆]This work was supported by the Project TIN2011-24046 of the Spanish Ministry of Economy and Competitiveness.

Email addresses: alvarag@ubu.es (Álvar Arnaiz-González), marcin.blachnik@polsl.pl (Marcin Blachnik), mkordos@ath.bielsko.pl (Mirosław Kordos), cgosorio@ubu.es (César García-Osorio)

- *Wrappers*: the algorithms of this family use the accuracy obtained by the classifier (usually the same that will be used after instance selection stage). Some of them are CNN [17], ENN [41], DROP1...5 [40], ICF [8], MSS [4]...
- *Filters*: as opposed to *wrappers*, the instance selection or rejection criterion is not based on a classifier. For example POP [32].

A large number of instance selection algorithms designed for classification tasks have been published in the scientific literature and new ones continue to appear. An up-to-date taxonomy can be found in [13].

However, two issues still require prompt attention: extending instance selection methodologies into regression tasks and applying the fusion of various sources to obtain better results. Regarding the first issue, we have already obtained some results in [21] and in this paper we propose a new approach based on the discretization of the output variable. The second issue has proven to be an effective approach in other domains [24], but to the best of our knowledge, no one has yet tried to apply ensembles to the combination of instance selection methods for regression.

The presence of noise is a common problem in Data Mining applications and noise filters are widely used to cope with this problem [35]. The usefulness and efficiency of instance selection methods for low quality and noisy data was confirmed in [23], which presented an experimental evaluation of several approaches to noise-resistant training of multilayer perceptron neural networks for classification and regression problems. Different noise reduction methods were evaluated with different noise levels in the data. For regression tasks, in most cases the solution that used the threshold-based ENN instance selection (in the following sections, we describe threshold-based ENN, short of Edited Nearest Neighbor, in detail) achieved the lowest mean-square error (MSE) on the test set for various levels of noise added to the data. The only exception was when the noise level was extremely high and for that case the lowest MSE was obtained by a combination of the threshold-based ENN with modification of the error function.

This paper is structured as follows: Section 2 is a brief review of instance selection methods for classification; Section 3 explains the problems of applying them to regression tasks; Subsection 3.1 presents the threshold-based approach, while Subsection 3.2 suggests another idea based on numerical target discretization; Section 4 shows the possibility of applying the idea of ensembles to the instance selection paradigm. Then, in Section 5 an experimental study is performed to compare both approaches and the improvements achieved when they are used within an ensemble, and how, in this case, we can outperform the regressor trained with the whole dataset. Finally, Section 6 summarizes the most important conclusions, and Section 7 presents some future lines of research.

2. Instance Selection for Classification

In general, instance selection algorithms can be classified into three types: noise filters, condensation algorithms and prototype selection algorithms [19]. Noise filters remove instances that show extreme differences with their neighbors, as they are considered noise. In the Edited Nearest Neighbor (ENN) algorithm [41] used for classification tasks, an instance is removed if it belongs to a different class than that predicted by the k

Nearest Neighbors algorithm (kNN), using the k nearest neighbors of the instance of interest. The condensation methods serve to reduce the number of instances in the dataset by removing instances that are overly similar to their neighbors. The Condensed Nearest Neighbor algorithm (CNN) [17] removes the instances in classification problems that are correctly predicted by kNN, as it is assumed that they do not bring any new information to build the classifier. Prototype selection methods do not select relevant instances, but rather transform the whole dataset into a few instances, each covering an area corresponding to the Voronoi cell[1] defined by each instance. An example of such methods is Learning Vectors Quantization (LVQ) [20].

The decisions about instance selection or rejection are very straightforward in instance selection for classification problems. They are based on the classification results obtained with an algorithm that is almost always kNN. The instance can either belong to the same class or to another that is different from the majority of its neighbors. The difference between the predicted and the real class of the instance determines the decision on its acceptance/rejection.

3. Instance Selection for Regression

There are very few papers that address the problem of instance selection for regression. The proposed methods fall into two categories: evolutionary-based and nearest neighbor-based (which includes our methods). The evolutionary based methods have very high computational cost, about 3 to 4 order of magnitude higher than the nearest neighbor-based methods for medium size datasets (according to the experiments and the data reported in [2]). For bigger datasets the difference is even larger, what makes the methods impractical in many applications.

However, we did not find in a literature any work on instance selection for regression tasks in a general setting, where the authors reported the improvements in terms of compression rate and classification accuracy even for a single arbitrary point, not to mention even the Pareto front, which we have examined in our work, so we were not able to use those methods for comparison.

Tolvi [39] presented the use of genetic algorithms for outlier detection. That approach does not rely on the dataset properties and purpose, so it can be used both for classification and regression problems. However they presented the results of only two very small datasets (35 instances with 2 features and 21 instances with 3 features).

In [2] Antoneli et al. also presented a genetic approach using quite complex multiobjective evolutionary algorithms with up to 300,000 evaluations of the fitness function.

In [15] Guillen et al. presented the use of mutual information for instance selection in time series prediction. Their idea was similar to k-NN based prediction, thus they determined the nearest neighbors of a given point and then instead of using k-NN to predict the output value, they calculated the mutual information (MI) between that point and each of their neighbors. Then they considered the loss of MI with respect to its neighbors in so that if the loss was similar to the vectors near the examined vector, this

[1]A Voronoi diagram (also known as Thiessen polygons or Dirichlet tessellation) is a geometrical construction to partition the Euclidean space. It divides the space into several polygons, Voronoi cells, each of them associated with a point, the seed. Each Voronoi cell defines a region of the space closer to its seed than to any other point, that is, the division is made according to the nearest neighbor rule [3].

vector was included in the filtered dataset. They evaluated their methods on artificially generated data with one and two input features. Later on, Stojanović et. al [37] extended the previous idea to instance selection in time series prediction.

In [33] a Class Conditional Instance Selection for Regression (CCISR) is proposed. The method is based on CCIS for classification [27]. CCIS builds two graphs: one for the nearest neighbors of the same class as a given instance and another for other class instances. Then a scoring function based on the distances in graphs is used to evaluate the instances. In the regression version (CCISR), instead of using only the nearest instances to construct these graphs, the neighborhood is defined based on the probability density function of the examples. The authors provided results on several real-world datasets for fuzzy rule based systems in terms of MSE and the number of extracted rules.

In the following subsections, we present our approaches two instance selection for regression.

3.1. Threshold-based Instance Selection for Regression

Instance selection methods developed for classification are based on the analysis of class labels of neighbor instances to determine the rejection/acceptance of a test instance. It usually takes the form of *if* statements where the condition of the *if* statement compares labels of the actual test instance with its neighbors. In the case of regression, label comparison is not possible since output values are not nominal but continuous. Thus, rather than labels, another quantity must be compared. An intuitive approach proposed in [21] is to use a similarity-based error measure such as:

$$Error = |Y_{real} - \bar{Y}_{predicted}| \tag{1}$$

and to compare the error to the predefined threshold, to determine whether the instance should be accepted or rejected:

$$\text{if } (Error > \theta) \text{ then } \ldots. \tag{2}$$

where (...), as the consequence of the if, can denote either instance acceptance or rejection, depending on a given algorithm. To improve the performance of this method, the threshold can depend on the local properties of the dataset. When the standard deviation of the adjacent cases (to the test case) is high, the condition should be less sensitive to the value of error shown in Equation (1). In other cases, when the local standard deviation is small, the condition should be more sensitive. This leads to the following modification of the previous formula:

$$\text{if } \big(Error > \alpha \cdot std(k)\big) \text{ then } \ldots \tag{3}$$

where $std(k)$ is the standard deviation of the outputs of the k-nearest neighbors of the instance.

This approach was used to adapt the ENN [41] and CNN [17] algorithms to meet the regression requirements. Moreover, it can also be easily introduced into other instance selection algorithms.

The pseudo-code of threshold-based regression ENN (T-ENN) is shown in Algorithm 1. It starts by iterating over the instances of the training set and in each iteration one instance x_i is examined, so it is temporally removed from the training set. Then, the remaining training set ($T \backslash x_i$) is used to predict the output value, $Y(x_i)$, of the instance x_i with kNN (line 2). If the error (defined as the difference between the predicted and the actual value) is greater than the predefined threshold θ, the instance x_i is marked for rejection. Otherwise, it is marked for acceptance. Then the instance x_i is returned to the original dataset and the procedure is repeated with all the other instances, one at a time. The new selected dataset consists of all the instances marked for acceptance. Thus, T-ENN tends to reject the outliers and can be used as a noise filter (like the ENN algorithm for classification, from which it is derived).

Algorithm 1: Edited Nearest Neighbor for regression using a threshold (T-ENN)

```
  Data: Training set $T = \{(\mathbf{x}_1, y_1), \ldots (\mathbf{x}_n, y_n)\}$, parameter $\alpha$ to control how the
        threshold is calculated from the standard deviation
  Result: Instance set $P \subseteq T$
1 for $i = 1...n$ do
2     $\bar{Y}(\mathbf{x}_i) = \texttt{Model}(T \backslash \mathbf{x}_i, \mathbf{x}_i)$
3     $S = \texttt{kNN}(T, \mathbf{x}_i)$
4     $\theta = \alpha \cdot std\big(Y(X_S)\big)$
5     if $|Y(\mathbf{x}_i) - \bar{Y}(\mathbf{x}_i)| > \theta$ then
6         $T \leftarrow T \backslash \mathbf{x}_i$
      end
  end
7 $P \leftarrow T$
  return $P$
```

In Algorithm 1, `Model` is the method used for prediction (any regression algorithm can be used), $Y(\mathbf{x}_i)$ is the actual target value of instance $\mathbf{x}_i$; $\texttt{Model}(T \backslash \mathbf{x}_i, \mathbf{x}_i)$ is the predicted value of the target output given by the model trained with dataset T without $\mathbf{x}_i$; and, S contains the k-nearest neighbors of the instance $\mathbf{x}_i$. The threshold θ is a multiple of the standard deviation of the outputs of the instances in S, the magnitude of this multiple depends on the parameter α that is given as input to the algorithm.

The pseudo-code of threshold-based regression CNN (T-CNN) is presented in Algorithm 2. Initially T-CNN starts with an empty dataset of selected instances. T-CNN uses a threshold θ defined in the same way as in T-ENN. The difference is that in the iteration when the remaining training set predicts the output value, $Y(\mathbf{x}_i)$, of the instance $\mathbf{x}_i$, the instance is marked for acceptance if the error is greater than the predefined threshold θ. As in T-ENN the new selected dataset consists of all the instances marked for acceptance. Instances are removed if they are too similar to their neighbors. Thus, the main purpose of T-CNN is to compress the dataset. However, the threshold θ for T-CNN must be much lower than for T-ENN. It is actually lower by about one order of magnitude. Generally, higher θ in T-ENN leads to the acceptance of more instances, while θ in T-CNN leads to the rejection of more instances.

Several parameters in both the T-CNN and the T-ENN algorithms can be tuned,as the θ value and various prediction methods (`Model`) can be used. We use kNN as a `Model` because of its simplicity and excellent performance with correctly selected parameters [22]. The most important parameter in kNN is the k value.

There are areas of naturally lower and higher densities in the data. In higher density

Algorithm 2: Condensed Nearest Neighbor for regression using a threshold (T-CNN)

```
Data: Training set $T = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$, parameter $\alpha$ to control how the
      threshold is calculated from the standard deviation
Result: Instance set $P \subseteq T$
1 $P = \varnothing$
2 $P \leftarrow P \cup \mathbf{x}_1$
3 for $i = 2...n$ do
4     $\bar{Y}(\mathbf{x}_i) = \mathtt{Model}(P, \mathbf{x}_i)$
5     $S = \mathtt{kNN}(T, \mathbf{x}_i)$
6     $\theta = \alpha \cdot std\big(Y(X_S)\big)$
7     if $|Y(\mathbf{x}_i) - \bar{Y}(\mathbf{x}_i)| > \theta$ then
8         $P \leftarrow P \cup \mathbf{x}_i$
9         $T \leftarrow T \backslash \mathbf{x}_i$
      end
  end
  return $P$
```

areas, even the slightest deviation from the value predicted by kNN can mean that an instance is an outlier and should be rejected by T-ENN. While in lower density areas, such deviations can be normal. For that purpose, we made the threshold θ proportional to the standard deviation of the output values of k-nearest neighbors of the instance.

3.2. Discretization-based Instance Selection for Regression

The other approach entails the direct usage of instance selection algorithms for classification tasks on regression datasets. For that purpose the output variable is first discretized and thus the problem is converted into a classification task. When instance selection is complete, the numerical value of the output variable is recovered for the selected instances.

This approach is a kind of meta-algorithm as it allows the use of the classification-based instance selection methods for different purposes: as noise filters (e.g. ENN [41], ENRBF [19], RNGE [36], . . .) or as data size reduction methods (e.g. CNN [17], MSS [4], POP [32], ICF [8], DROP [40], . . .).

The whole process is comprised of the following steps (see Algorithm 3):

1. Discretize the value of the numerical target variable of the training dataset.
2. Apply a classification-based instance selection algorithm to the discretized dataset to obtain the edited subset S.
3. Restore the numerical value of the target variable in S.

Discretization is the key step of this method, and it decisively influences instance selection, as the boundary between classes determines the instance selection or rejection in the edited dataset. Discretization algorithms can be divided into two families: supervised, when the class value is taken into account, and unsupervised (or class-blind), when the class value is not taken into account. Since it is the target attribute that is

Algorithm 3: The proposed meta-model based on discretization of the output variable

```
   Data: Training set ${X, Y} = {(\mathbf{x}_1, y_1), \ldots (\mathbf{x}_n, y_n)}$
   Result: Instance set $S \subseteq \{X, Y\}$
1  $Y_D$ = Discretization of the numerical target $Y$
2  Apply classification-based instance selection algorithm over $\{X, Y_D\}$ to obtain
   subset $S$
3  Restore the numerical value of the output variable in $S$
   return $S$
```

discretized, we must use the unsupervised algorithm. Two well-known unsupervised algorithms are equal-frequency and equal-width [12]. Nevertheless, this paper is not aimed at studying how discretization influences instance selection (and anyway this influence decreases when the method is used as the base block in the construction of an ensemble).

In the experiment section, we used two well-known instance selection methods for classification tasks: ENN and CNN. To adapt the meta-model to those methods, we replaced line 2 of Algorithm 3 by *Apply ENN* or *Apply CNN* respectively. The algorithms were selected in the experimental study, because we compared them to T-ENN and T-CNN threshold-based algorithms inspired by ENN and CNN respectively.

The discretization method used on the experiment was the Weka unsupervised filter invoked from RapidMiner. It optimizes the number of bins in the target variable by equal width binning using *leave-one-out* estimated entropy. The number of bins is varied in the bagging process up to a maximum value that is given as a parameter.

The details of the discretization process are given in Algorithm 4. Where b is the maximum number of bins to be created, T is the original dataset and D is the new dataset in which only the output variable was changed by discretizing its value. First of all, `LOWEstimatedEntropy` calculates the best entropy (the lowest one) trying different number of bins from 1 to the maximum value b. When the best number of bins is found, the function `CalcCutPoints` calculates cut points of the variable to be discretized, and finally, `DiscretizeClass` generates a new dataset D with all instances of the original dataset T but the original continuous output value is replaced by the class attribute obtained from the discretization process.

4. Information Fusion

The advantages of information fusion for instance selection comprise:

1. Improvement of results. As our experiments showed, in most cases (see Table 4), the ensemble methods allow for obtaining better results than single methods.
2. Better possibility of model parametrization. Without retraining the model, we are able to balance compression and prediction accuracy by changing only the acceptance threshold of the ensemble (this is how many ensemble members must vote the instance to make it finally accepted).
3. Possibility of process parallelization. Especially in case of big data, splitting the big dataset into many small subsets and performing the operations on the subsets

Algorithm 4: Equal-width binning using *leave-one-out* estimated entropy.

```
   Data: Training set $T = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$
   Maximum number of bins $b$
   Result: Discretized set $D = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$
1  $bestEntropy \leftarrow MAX\_VALUE$
2  for $i = 1...b$ do
3      $entropy =$ LOUEstimatedEntropy($T, i$)
4      if $entropy < bestEntropy$ then
5          $bestEntropy \leftarrow entropy$
6          $bestNumBins \leftarrow i$
       end
   end
7  $cutPoints =$ CalcCutPoints($T, i$)
8  $D =$ DiscretizeClass($T, cutPoints$)
   return $D$
```

on a computational cluster can accelerate the instance selection process, since the cost of ENN is O(n^2) and of CNN is O(n^3) [19].

The details of the first and second point are further discussed in the following subsections. Analysis of the third advantage is out of the scope of the paper.

4.1. Ensemble models

An ensemble (or committee) model is a predictive model composed of several simple models that work in parallel [34]. The final prediction of an ensemble is obtained by averaging the predictions of its member models.

The aim of ensemble methods is to combine several classifiers to obtain better predictive performance than could be obtained by any of them separately [31]. The idea behind the ensembles is that the combination of several weak-learners usually achieves better results than any of them alone [28]. Each member of the ensemble usually has areas in which it performs poorly and other areas in which it performs especially well. Given that poor performance areas differ for individuals, prediction averaging yields higher accuracy than that of any single model. To obtain this, each of the members contained in the ensemble has to be as different from the others as possible [9]. The diversity can be obtained in two different ways: by using heterogeneous classifiers and/or by training each member on a different subset of the dataset [42]. For example, if the prediction accuracy of each single model is 0.80 and the areas where different models make prediction errors are different, then averaging the single model predictions gives correct prediction in most cases. Only in the cases where the wrong prediction areas of most ensemble members overlap the final prediction will be incorrect. This is illustrated in the Figure 1.

An important aspect of ensembles is the strategy to combine the decisions of the different members. The purpose of this step is to amplify the correct decisions and shrink the incorrect ones. Many strategies can be followed. Frequently they can be grouped into: *i*) trainable vs. non-trainable combination rules or *ii*) combination rules that apply to class labels vs. to class-specific continuous outputs. A good analysis of committee models was presented in [31].

	Model 1	Model 2	Model 3	Model 4	Model 5	Voting
Instance 1	✓	✗	✓	✓	✗	✓
Instance 2	✓	✓	✗	✓	✗	✓
Instance 3	✓	✓	✓	✓	✓	✓
Instance 4	✓	✓	✗	✓	✓	✓
Instance 5	✗	✓	✓	✗	✓	✓
Instance 6	✓	✗	✓	✓	✓	✓
Instance 7	✓	✓	✗	✓	✓	✓
Instance 8	✗	✗	✗	✓	✗	✗
Instance 9	✓	✗	✓	✓	✓	✓
Instance 10	✓	✓	✓	✓	✗	✓
Instance 11	✓	✗	✓	✗	✓	✓
Instance 12	✓	✓	✓	✗	✓	✓
Instance 13	✓	✓	✗	✓	✓	✓
Instance 14	✓	✗	✓	✓	✓	✓
Instance 15	✗	✓	✓	✓	✗	✓
Instance 16	✗	✓	✓	✓	✗	✓
Instance 17	✗	✓	✗	✓	✓	✓
Instance 18	✓	✗	✓	✗	✓	✓
Instance 19	✗	✓	✓	✗	✓	✓
Instance 20	✗	✓	✗	✓	✓	✓
Result	**13**	**13**	**13**	**15**	**14**	**19**

Figure 1: Example of ensemble classifier. Where ✓ represents a correct prediction for a given instance by a given model and ✗ a wrong prediction. The last column represents the final prediction of the ensemble obtained by the five models voting. The result row at the bottom contains the number of correctly predicted instances by each model and by the ensemble.

One of the earliest ensemble algorithms is *bagging* (bootstrap aggregating) which, despite its simplicity, shows quite excellent performance [6]. In bagging each model is trained on a random subset of the original dataset to ensure diversity of the ensemble (of models). The subsets are obtained by drawing instances with replacement from the original dataset. Bagging selects different bootstrap subsets that are independent of one another. Thus, the models operating on the subsets can run in parallel, accelerating the bagging process.

4.2. Bagging for Instance Selection

We have extended the idea of bagging into instance selection [5]. Each individual instance selection algorithm within the ensemble returns an array of binary votes; one vote for each instance in the subset. A (positive) vote for each instance indicates that the instance has been selected by the algorithm. Then all the votes that a given instance received from each algorithm are summed. The importance of an instance in the training set is considered proportional to the number of accumulated votes. To perform the final instance selection, an accept/reject threshold is defined. The threshold determines the percentage of votes an instance must accumulate to be included in the resultant filtered dataset.

The pseudo-code for the Instance Selection Bagging is given in Algorithm 5. Where `ISAlg` is an instance selection algorithm, t is an integer that indicates the number of member-algorithms in the bagging, p is the percentage of instances from the original dataset that will be drawn into each subset and z is a threshold of votes to select or discard an instance. The function `Bootstrap`(T, p) returns the bootstrapped subset S_t by randomly drawing p percent instances of S, the function `CollectVotes`(P, v) adds the votes that a given instance receives from each member algorithm in P_t and the function SelectInstancesByVotes(T, v, z) returns the final selected dataset. To sum up, on each round the new bootstrapped subsets S_t is generated, and an instance selection algorithm is executed on the S_t return selected dataset P_t. The votes for the selected instances are added in v. And finally all the instances stored in each P_t, which altogether receives more than threshold z votes, are selected and stored in the dataset P.

Algorithm 5: ISBagging. Instance Selection Bagging

```
  Data: Training set $T = \{(\mathbf{x}_1, y_1), \dots (\mathbf{x}_n, y_n)\}$
  Instance selection algorithm ISAlg
  Number of member instance selection algorithms $t$
  Percent of instances in the bootstrapped training subsets $p$
  Threshold $z$
  Result: Instance set $P \subseteq T$
1 for $i = 1...t$ do
2     $S_t$ = Bootstrap$(T, p)$
3     $P_t$ = ISAlg$(S_t)$
4     $v$ = CollectVotes$(P_t, v)$
  end
5 $P$ = SelectInstancesByVotes$(T, v, z)$
  return $P$
```

Modifying the parameters of the model we can adjust the trade-off between the prediction accuracy and the dataset compression. In the approach based on data discretization and then transformation of regression task into multi-class classification task, the discretization method influences the results, for example by determining the different number of bins and the boundaries between them. It is also highly probable that the prediction of the data points, situated close to the boundaries, will be poor. The most important parameter is the percentage of ensemble members that must select the instance, to have the instance included in the final dataset. Changing this parameter gives more priority to accuracy or dataset size reduction.

In the Ensemble-CNN the problem may be that CNN usually has good compression. This means that a small subset of samples is selected by each individual algorithm. So, it is less likely that instances selected by different committee members will overlap. This observation may lead to the conclusion that Ensemble CNN provides a compression worse than pure CNN.

5. Experimental Evaluation

In the experimental evaluation we performed simulations to compare the eight instance selection methods for regression (four single methods and four ensembles) on 28 datasets.

5.1. Purpose and Scope

The purpose of the experimental evaluation was to assess how individual instance selection methods perform in terms of the accuracy obtained at a given compression level.

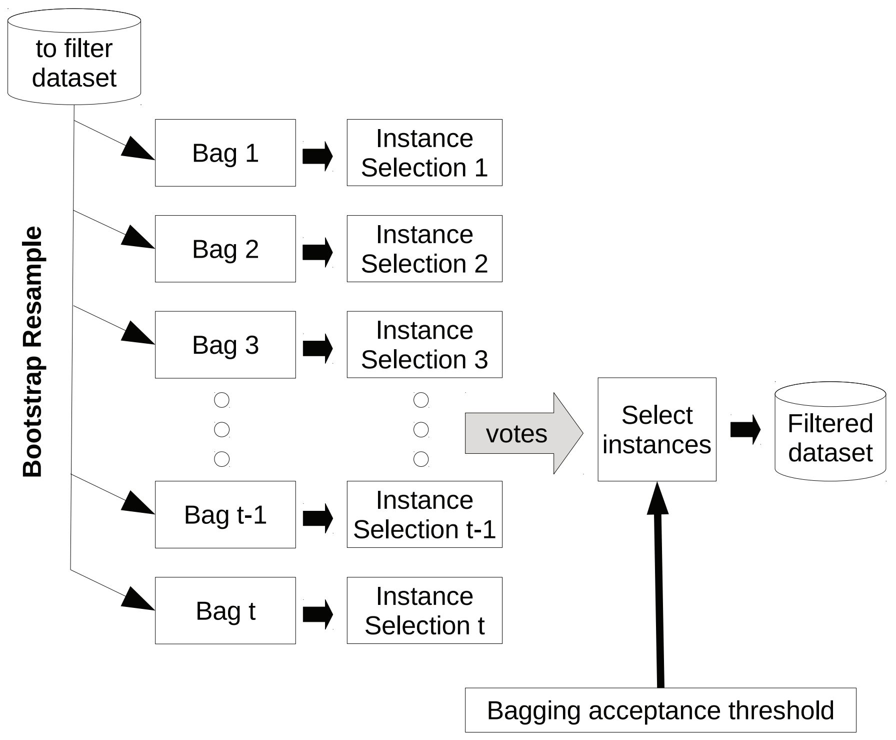


Figure 2: The process of bagging instance selection.

Based on the results, we hoped to provide recommendations for choosing the proper instance selection methods for regression problems. The evaluated instance selection methods were[2]:

- T-ENN: threshold-based ENN.
- T-CNN: threshold-based CNN.
- D-ENN: discretization-based ENN.
- D-CNN: discretization-based CNN.
- TE-ENN: ensemble of threshold-based ENN.
- TE-CNN: ensemble of threshold-based CNN.
- DE-ENN: ensemble of discretization-based ENN.
- DE-CNN: ensemble of discretization-based CNN.

[2]We also evaluated the CCISR method [33] (the adaption to regression of CCIS [27]) on some datasets. Because of very high computational time and memory demand, especially for bigger datasets, including CCISR in the full study was out of our resources. The results obtained with CCISR for the datasets: autoMPG6, autoMPG8, baseball, dee, ele-1, laser and machineCPU, confirm the general trend observed in the study; the use of CCISR within an ensemble generally improves the performance of the method used alone. The interested reader can check the folder `ccisr/Plots` in `http://prules.org/is/` where there are several plots showing the results with this method.

Based on the data of the experiment, we obtained a Pareto front representing the best accuracy for a given compression level for each of the evaluated methods and for each of the tested datasets. Pareto optimality is a state of allocation of resources or parametrization of the process (compression and accuracy) in which it is impossible to make any individual one better without making another one worse. The Pareto front is a set of parametrizations that are all Pareto optimal (compression is best for a given accuracy level and accuracy is best for a given compression level) [26]. The trade-off between accuracy and compression was adjusted to some parameters of the instance selection methods, as described in detail in the section below.

We performed the ranking of the methods over all the datasets, which allowed us to draw clear conclusions on the properties and the efficiency of each evaluated instance selection method.

5.2. Datasets

In the experiments, we used 28 regression datasets from the KEEL repository [1]. The datasets are summarized in Table 1, where a total number of attributes is given for each dataset: real (R), integer (I) and nominal (N) attributes and the number of instances.

5.3. Process and Environment

We implemented all instance selection methods in Java as RapidMiner plug-ins [18]. At the discretization stage, we used an unsupervised Weka filter [16] invoked from RapidMiner. This filter performs all the equal-width divisions of the target value from two intervals to the number of intervals passed as parameter, and then it selects the division with better estimated entropy. So the number of intervals (and hence classes) in the final discretization could be lower than the value passed to the filter.

The process started by loading one dataset and performing attribute standardization. Then, the whole process was run in a 10-fold cross-validation. The validation process of ensemble instance selection methods contained a bagging inside, and one of the proposed instance selection algorithms was used to build the members of the bagging ensemble. In the validation of non-ensemble methods, one of the instance selection algorithms was directly used. The bagging ensemble was set to 30 members, each of them was an instance selection algorithm which operated on a different subset of the training dataset. Each subset was created by randomly drawing instances without replacement from the training set. The number of instances in the subset was 80% of the instances in the training set. The final decision on accepting or rejecting each instance was then made. An instance was accepted if at least $z\%$ of the bagging members accepted the instance, otherwise it was rejected. Changing the $z\%$ parameter, we can change the behavior of the ensemble so that it prefers rather small resultant datasets (high compression), when z is close to 100%, or it prefers high prediction accuracy, for lower values of z.

The experiments were performed with various values of the following parameters of the algorithms:

- Number of k-nearest neighbors used by kNN: from 1 to 13 in steps of 2.
- Number of k-nearest neighbors used by instance selection algorithms: from 1 to 13 in steps of 2.
- Threshold controlled by α: from 0.1 to 1 in steps of 0.1.

Table 1: Datasets for experiments. The number of real (R), integer (I) and nominal (N) attributes are shown in last column.

Dataset	**Instances**	**Attributes**			
		Total	**R**	**I**	**N**
diabetes	43	2	2	0	0
machineCPU	209	6	0	6	0
baseball	337	16	2	14	0
dee	365	6	6	0	0
autoMPG8	392	7	2	5	0
autoMPG6	392	5	2	3	0
ele-1	495	2	1	1	0
forestFires	517	12	7	5	0
stock	950	9	9	0	0
laser	993	4	4	0	0
concrete	1030	8	7	1	0
treasury	1049	15	15	0	0
mortgage	1049	15	15	0	0
ele-2	1056	4	4	0	0
friedman	1200	5	5	0	0
wizmir	1461	9	9	0	0
wankara	1609	9	9	0	0
plastic	1650	2	2	0	0
quake	2178	3	2	1	0
ANACALT	4052	7	7	0	0
abalone	4177	8	7	1	0
compactiv	8192	21	21	0	0
tic	9822	85	0	85	0
ailerons	13750	40	36	4	0
pole	14998	26	26	0	0
elevators	16599	18	14	4	0
california	20640	8	3	5	0
house	22784	16	10	6	0

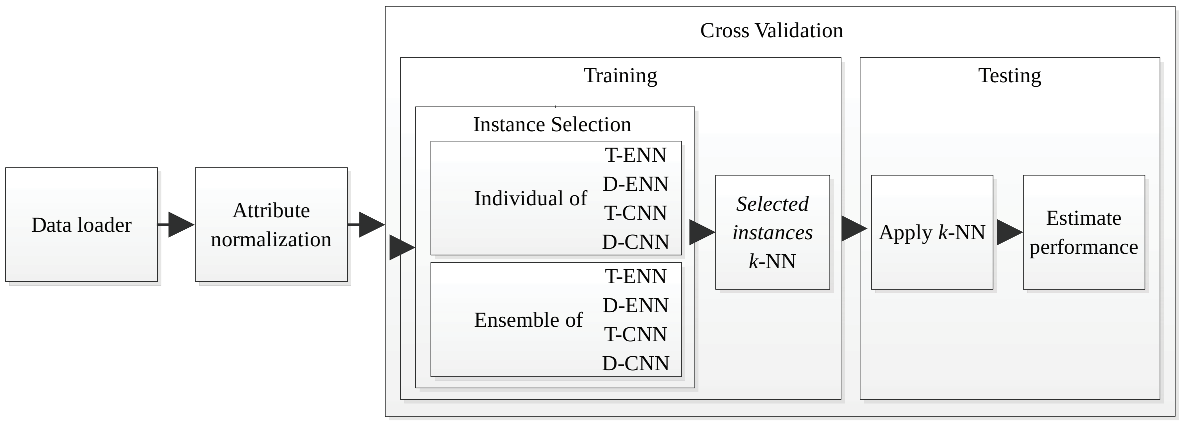


Figure 3: The experiment process setup.

- Maximum number of bins D: from 5 to 15 in steps of 1.
- Percentage of votes to select an instance z: from 0.1 to 0.9 in steps of 0.1.

The α parameter was only used for threshold algorithms, while the D parameter was only used for discretization based algorithms. The z parameter was used on the ensemble process.

It was shown in [22] that for most datasets (as well for regression as for classification) the optimal k in the kNN algorithm is about 9. However, the differences between k=5, k=9 and k=13 were only minimal. The biggest drop in accuracy was observed for the smallest values of k, especially when k was below 3. While k, being an even number, may not be the best choice for classification tasks, because of the high chance of a tie between two classes, it is fully acceptable for regression tasks. In our experiments in the kNN used for instance selection we used $k = [1, 3, 5, 7, 9, 11, 13]$. The choice of the optimal k in the kNN used for the final prediction depended on the compression ratio of the dataset obtained by instance selection.

After the instances were selected, they were used as the training set to predict the output of the test set instances using kNN with k varying from 1 to 13, evaluating the performance in terms of R^2 and compression. The process is presented in Figure 3.

5.4. Selected Detailed Results

In this section, we present graphical presentations of two kinds of results are shown: the detailed results for four selected datasets and the average results for all the 28 regression datasets The detailed results for the remaining datasets have similar properties as for the four selected, and they can be downloaded from the project website at `http://prules.org/is/`. The website also contains the RapidMiner process and the links to download our RapidMiner instance selection extension.

Figure 4 presents the Pareto fronts of the four selected datasets obtained with all the regression instance selection algorithms. The vertical axis shows prediction error, with larger values representing higher error and the horizontal axis shows compression with larger values representing weaker compression. BL-min and BL-max indicate the minimum and maximum baselines as the error values obtained by kNN on the original dataset (without any instance selection). BL-min is the lower and BL-max is the higher error obtained, while changing k in kNN from 1 to 13 (with step 2).

In the experiments we repeatedly changed the algorithm parameters, such as k in kNN used for instance selection, the threshold θ in T-ENN and T-CNN, the number of discretization bins in D-ENN and D-CNN and the threshold z in the ensemble methods. The Pareto plots were obtained by connecting the best points (with the lowest error for a given accuracy) for each algorithm.

We define the compression C_x as:

$$C_x = \frac{\#\_instances\_after\_selection}{\#\_instances\_before\_selection} \tag{4}$$

Thus, lower compression values mean stronger compression.

The accuracy can be defined in three ways; either *MSE* (mean square error), *RMSE* (root mean square error) or R^2 (the coefficient of determination) [11], among others. R^2 expresses the squared correlation between the predicted and the actual value. When the *RMSE* is small in relation to the variation in the data, the R^2 is close to 1. Since our data is standardized, choosing one of the accuracy representations only influences the result presentation to a very small degree. We use R^2 in the analysis of the results, because it is independent of the data standardization.

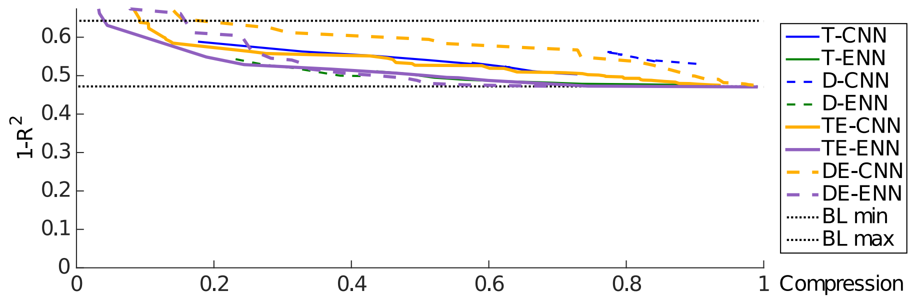
The four datasets presented in Figure 4 were chosen as examples from the 28 datasets on which we were running the experiments. Three of them show the typical tendency that is confirmed by the analysis in the next subsection: ensemble methods tends to perform better than single instance selection algorithms. While the last subfigure, for the Concrete dataset, shows that in some rare cases the single algorithms (here T-ENN and D-ENN) can also perform very well; even better than the ensembles. When compression equals one (no compression) then we have the performance of kNN.

In classification tasks, CNN removes most of the instances that are situated far from the class boundaries, because such instances are not required for correct classification. In big datasets over 90% of instances can be removed. In regression, on the other hand, the meaningful instances are located in the whole feature space and only those located very close to one another can be removed without the loss of prediction quality. As it can be seen from Figure 4, the CNN-based algorithms in regression tasks were unable to remove more than 20% of the instances without causing a noticeable increase in error. In the case of ENN, which removes outliers, the reduction rate in classification and regression can be comparable, because it depends on the degree of noise in the data and not on the prediction task. Thus on average in classification CNN removes more instances than ENN, while in regression, on the contrary, the ENN-based methods can provide better compression than the CNN-based (see the green and purple vs. blue and orange lines in Figure 4).

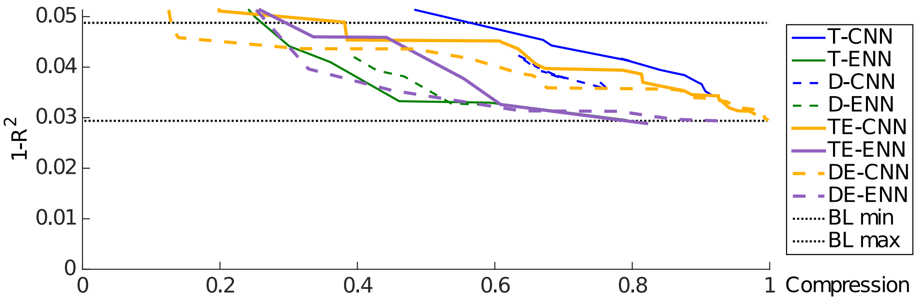
5.5. Aggregation of All Results

The graphical presentation shows the average of the final results over all the datasets, allowing us to notice the tendencies and the properties of particular instance selection algorithms.

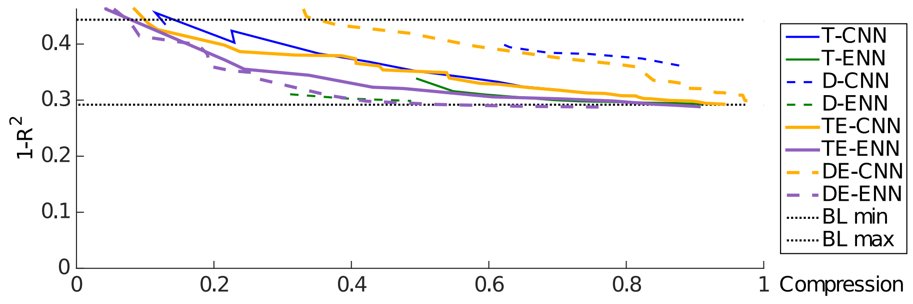
Figures 5 and 6 combine data reduction and prediction accuracy into a single performance measure called *benefit function* (BF). BF is computed using the following equation [25]:



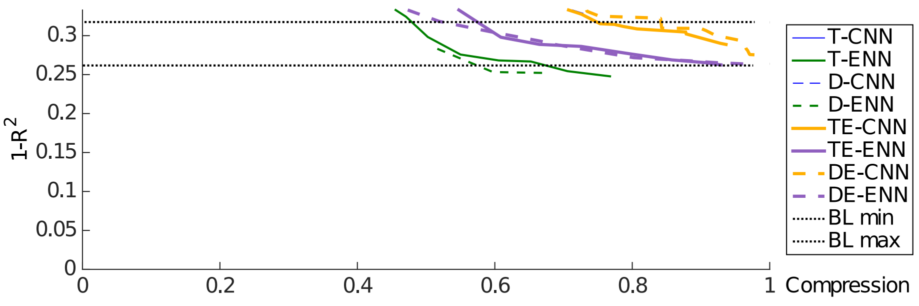
(a) House



(b) Wizmir



(c) Elevators



(d) Concrete

Figure 4: Error against compression for four datasets. Lower values in horizontal axis mean higher compression while lower values in vertical axis mean lower error. BL max represent the poorest precision of kNN on the entire original dataset, i.e. the worst k value, while BL min represents the better precision achieved with the best k. Each point of the plot represents the result of one specific configuration.

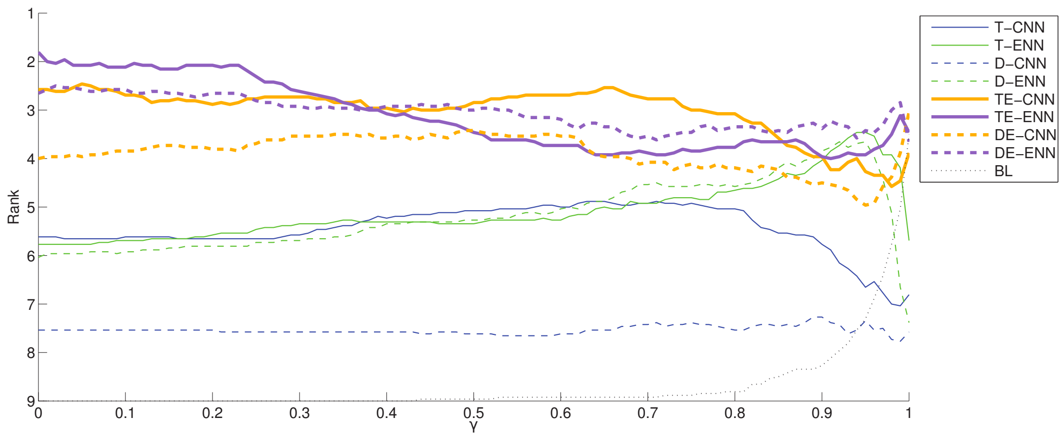


Figure 5: Ranking of all methods. The baseline (BL) represents the result of the kNN prediction on the original dataset.

$$BF = \gamma \cdot Accuracy + (1 - \gamma) \cdot Compression \tag{5}$$

where *Accuracy* is represented as the coefficient of determination (R^2) and *Compression* as the inverse of the Equation 4 ($1 - C_x$), where *gamma* is a parameter ($\gamma \in [0, 1]$) that allows trade-off balancing between data size reduction and prediction accuracy. Higher values of BF indicate better results for a given γ.

Figure 5 shows the ranking of all algorithms based on their benefit function for γ values within the interval $[0, 1]$.

Thin lines (colored in green and blue) show the results for methods with single instance selection algorithms, while thick lines (colored in orange and purple) show the results for bagging ensembles. The methods based on CNN algorithm are shown in blue and orange, and methods based on ENN in green and purple. We can see that even for $\gamma = 1$, that is, considering only the accuracy and not the compression, the best method is DE-CNN, outperforming all the others, including the baseline method. On the other hand, considering only the size-reduction of the filtered dataset, the best method is TE-ENN. For a better comprehension of the rankings, we zoomed it in for gamma values from 0.85 to 1 in Figure 6. The ensemble methods performed better than the individual methods for all the γ values, except T-ENN which surpassed the ensemble version TE-ENN for gamma values from 0.903 to 0.966.

In Table 2 we show the results of the Hochberg test [14] taking into account only the precision (that is for $\gamma = 1$), while in Table 3 we show the results taking into account only the compression (that is for $\gamma = 0$). The line in the middle of the tables indicates the statistical significance, i.e. the methods below the line are statistically worse, with a significance level of $\alpha = 0.05$, than the best method.

The graph in Figure 7 shows the percentage of datasets in which one method is the best option based on the benefit function. As can be seen, the chart is mainly filled by ensemble methods (on the top).

Figure 8 shows the average of the benefit function over all datasets for each of the proposed methods and the result of kNN prediction on the original dataset (BL).

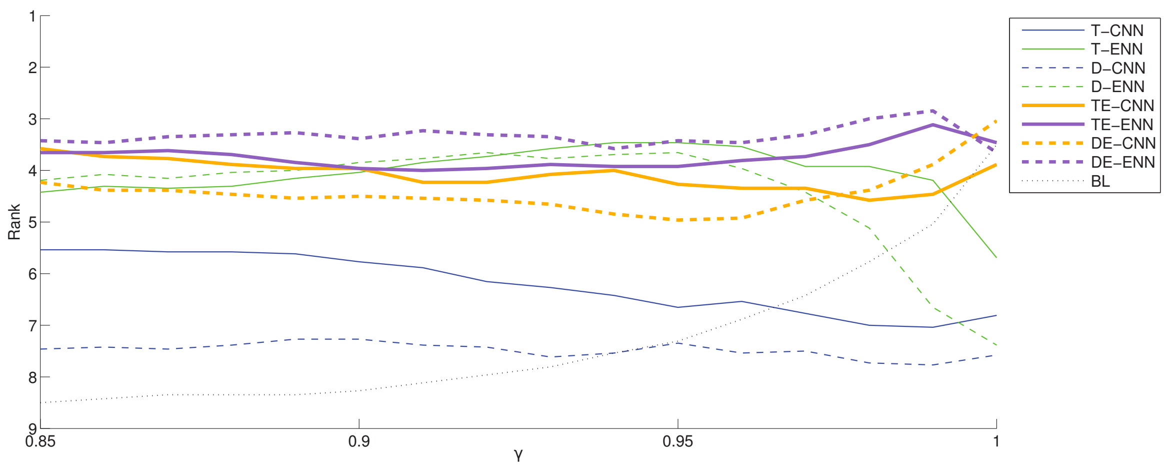


Figure 6: Zoom of the ranking for gamma values from 0.85 to 1. The baseline represents the result of the kNN prediction on the original dataset.

Table 2: Ranking and Hochberg procedure over precision. The methods considered statistically worse than the best method are below the line. The baseline represents the result of the kNN prediction on the original dataset.

IS algorithm	**Ranking**	p **Hoch.**
DE-CNN	3.04	
TE-ENN	3.46	0.577
Baseline	3.50	0.577
DE-ENN	3.65	0.577
TE-CNN	3.88	0.577
T-ENN	5.69	2.38E-3
T-CNN	6.80	4.17E-6
D-ENN	7.38	7.37E-8
D-CNN	7.57	1.84E-8

Table 3: Ranking and Hochberg procedure over compression. The methods considered statistically worse than the best method are below the line.

IS algorithm	**Ranking**	p **Hoch.**
TE-ENN	1.81	
TE-CNN	2.58	0.257
DE-ENN	2.65	0.257
DE-CNN	4.00	3.75E-3
T-CNN	5.62	8.34E-8
T-ENN	5.77	2.75E-8
D-ENN	6.04	2.84E-9
D-CNN	7.54	2.31E-16

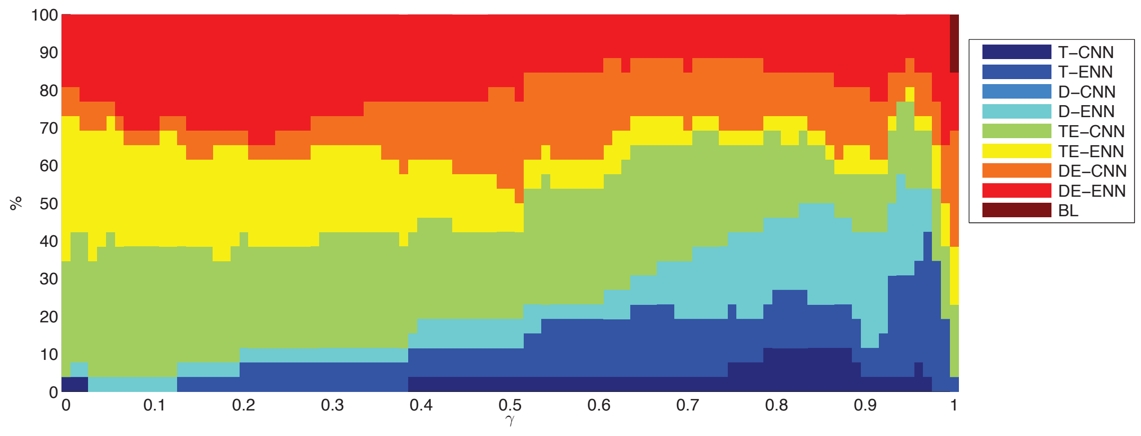


Figure 7: Percentage of datasets in which one method is the best based on the benefit function. Baseline (BL) represents the result of kNN prediction on the original dataset.

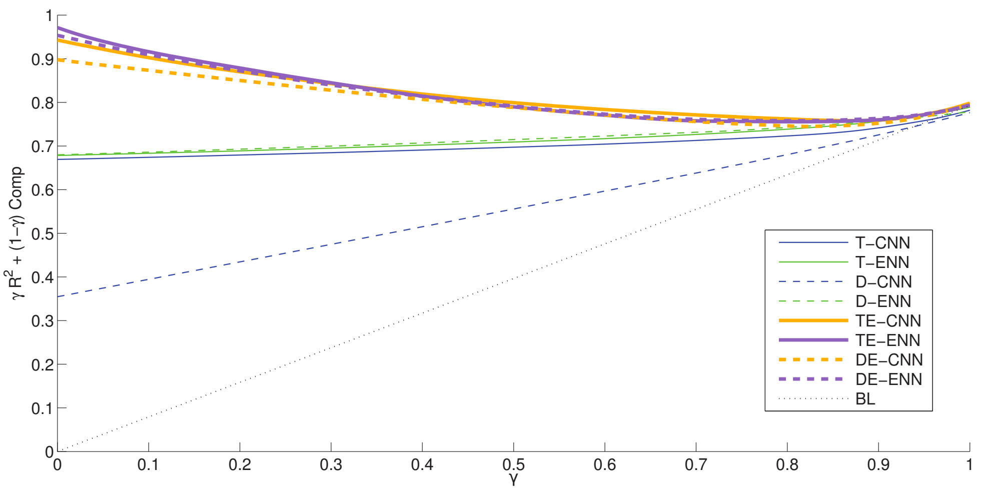


Figure 8: Average of benefit function for all datasets. Baseline (BL) represents the result of of kNN prediction on the original dataset.

Table 4: Comparison by Wilcoxon test: ensemble method against base method. The Table shows wins/losses (w/l), according to the benefit function, and the result of Wilcoxon test: ✓ indicates the ensemble method is better than the base method (for a confidence level of 95 %).

Algorithms	γ					
	0.0	**0.25**	**0.50**	**0.70**	**0.80**	**0.90**
TE-ENN vs. T-ENN	26 / 0 ✓	22 / 4 ✓	18 / 8 ✓	17 / 9 ✓	16 / 10 =	13 / 13 =
TE-CNN vs. T-CNN	25 / 1 ✓	26 / 0 ✓	25 / 1 ✓	25 / 1 ✓	23 / 3 ✓	21 / 5 ✓
DE-ENN vs. D-ENN	26 / 0 ✓	22 / 4 ✓	22 / 4 ✓	15 / 11 ✓	15 / 11 ✓	16 / 10 =
DE-CNN vs. D-CNN	26 / 0 ✓	26 / 0 ✓	25 / 1 ✓	25 / 1 ✓	24 / 2 ✓	24 / 2 ✓

The figures clearly show that the ensemble methods are at the top of the charts above the single algorithm methods. It is a bit surprising that for some datasets the errors do not increase in spite of the dataset being strongly compressed.

To summarize the benefits obtained from ensembles, we compared the ensemble methods to their base methods. Table 4 shows the results of this comparison for different values of γ for the benefit function. It also shows the wins/losses and the result of the Wilcoxon test. When the ensemble is significantly better than its base method, the results appear marked with ✓. When there is no significant differences, the character '=' is used. The reported γ values are 0.0, 0.1, 0.25, 0.5, 0.7, 0.8, 0.9 and 1.0. Usually more accuracy is desired rather than very high compression. For this reason we showed more γ values close to 1.

6. Conclusions

We discussed and tested some instances selection algorithms adapted to regression problems. The analysed algorithms are derived from two well known instance selection methods for classification, ENN and CNN, based on two different adaptation approaches.

We also compared them with one another and with their ensembles. As it could be expected, the best results were obtained for the ensembles. To the best of our knowledge this is the first time such a comparison is done for the methods of instance selection for regression problems.

Another advantage of combining instance selection algorithms into an ensemble is that the decision about the exact values of their parameters (number of nearest neighbors, number of discretization bins, α value) is less relevant, given that, in general, the ensembles give better results than the base method, even if the base method has its parameters specifically fine-tuned [10].

7. Future Work

The topic of our study was to evaluate the ensembles of instance selection algorithms. While working on that topic, also some other interesting issues appeared, which can be developed in the future works. In this section we shortly present these issues:

1. We extended to regression tasks and evaluated the ensembles of CNN and ENN — two of the base instance selection algorithms. It is likely that in an analogical way other instance selection algorithms known for classification tasks can be extended to regression using the same strategies proposed in this paper, as well, their adaptation can be combined in ensembles. It is worth examining how the regression extensions of particular instance selection methods perform and if any of them is especially well suited for regression tasks and for building ensembles.
2. Also two or more instance selection method can be used sequentially on the same data, what could help in simultaneously removing the noise (ENN) and reduce the dataset size (CNN) as in [38], or in parallel within one voting ensemble. In this case there would be no need to use bagging to differentiate the ensemble members, but different instance selection methods can provide the required diversity. This topic is however getting very complex, because of a high number of methods of different combinations that can be used, and the experimental evaluation will be able to comprise only several different combinations.
3. The way in which different levels of compression of the datasets affect the evolution of the error could be used as a measure of how ‘good’ the datasets are, and if we have enough samples in the dataset or if we should collect some more, or if collecting some more would entail any benefits. This is especially important in cases where collecting and labeling data is expensive.
4. The counterpart of instance selection in unsupervised learning is often called anomaly detection. The approach of combining several base methods within an ensemble could be also fruitful in the anomaly detection context. For example, as base methods Local Outlier Factor (LOF) [7] or Local Correlation Integral (LOCI) [30] could be used. The use of these methods within an ensemble could also lead to an increase in their performance and make them less sensitive to parameter tuning.

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Low-quality data will lead to low-quality mining results.

Han et al. (2011)

Chapter 3

Instance selection for regression: adapting DROP

This journal paper adapts the DROP family of instance selection methods for classification to regression. The DROP family was chosen, because it comprises some of the best instance selection methods to date. In particular, the focus of the paper is on the adaptation of the DROP2 and the DROP3 algorithms.

The keystone of this adaptation is its approach to the computation of the *with* and *without* variables that are used by the algorithm to decide whether or not an instance should be removed. The paper presents two different approaches to adapt DROP to regression. The usefulness and robustness of both approaches in the presence of noise is clearly demonstrated.

Authors: Álvar Arnaiz-González, Jose-Francisco Díez-Pastor, Juan José Rodríguez-Diez, César García-Osorio
Type: Journal
Published in: Neurocomputing 201: 66 – 81
Year: 2016
Reference: Arnaiz-González et al. (2016a)

Instance Selection for Regression: adapting DROP

Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César García-Osorio
University of Burgos, Spain

Abstract

Machine Learning has two central processes of interest that captivate the scientific community: classification and regression. Although instance selection for classification has shown its usefulness and has been researched in depth, instance selection for regression has not followed the same path and there are few published algorithms on the subject. In this paper, we propose that various adaptations of DROP, a well-known family of instance selection methods for classification, be applied to regression. Their behaviour is analysed using a broad range of datasets. The results are presented of the analysis of four new proposals for the reduction of dataset size, the effect on error when several classifiers are trained with the reduced dataset, and their robustness against noise. This last aspect is especially important, since in real life, it is frequent that the registered data be inexact and present distortions due to different causes: errors in the measurement tools, typos when writing results, existence of outliers and spurious readings, corruption in files, . . . When the datasets are small it is possible to manually correct this problems, but for big and huge datasets is better to have automatic methods to deal with these problems. In the experimental part, the proposed methods are found to be quite robust to noise.

Keywords: Machine Learning, regression, instance selection, DROP, noise filtering

1. Introduction

Automated Machine Learning is a discipline that is concerned with the design of algorithms for building models that are able to generalize the underlying behaviour of datasets composed of instances (also known as examples). It also covers the evaluation and the use of the models that are obtained. Depending on the nature of the datasets, learning processes can be divided into two groups: supervised, when there is a value that needs to be predicted (if the value is discrete, the learning process is called classification, if it is continuous, regression); and unsupervised, when the target is to discover the relations between instances (cluster analysis, outlier detection and association rule learning are some examples in this group) and the instances are a set of unlabeled values [26]. The present work centres on supervised learning, more specifically the task of regression.

Email addresses: alvarag@ubu.es (Álvar Arnaiz-González), jfdpastor@ubu.es (José F. Díez-Pastor), jjrodriguez@ubu.es (Juan J. Rodríguez), cgosorio@ubu.es (César García-Osorio)

Nowadays, a major challenge of Machine Learning algorithms is their application to increasingly massive datasets, such as insurance company data, banking transactions, telecommunications companies, financial markets and digital image processing... and more recently those needed in fields such as Bioinformatics [11]. One way to facilitate the learning process when applied to these huge datasets is the reduction of training dataset size by applying some instance selection techniques. Instance selection methods try to find a subset S in the same space as original training set T, such that $|S| < |T|$ and that, if S is used as a set to train a regressor, its predictive capability will be similar to T [28]. The reduction of the size of the training set accelerates the learning process, or the testing process in the case of instance-based learning (IBL) [7, 31]. But it also means that certain methods, which are not capable of working on very large datasets, can work with the selected subset to obtain an usable model [15].

The main contributions of the paper are:

- The proposal of new methods of instance selection for regression.
- The new methods were obtained by adapting to regression a method initially designed for classification using two approaches: one based on error accumulation and the other using an adaptive threshold.
- All methods have been evaluated following a multi-objective approach, where the two objectives of interest are: the reduction of the size of the selected subset, the increase of accuracy.
- Finally, the performance and robustness of the methods with noisy datasets have been measured.

This paper is structured in the following way: Section 2 begins with a description of instance selection, paying special attention to the DROP (Decremental Reduction Optimization Procedure) family of methods [40, 42]. In Section 3, the proposed approaches for adapting these methods to regression are explained. The experimental validation and discussion of the results may be found in Section 4, and the conclusions in Section 5. Finally, Section 6 summarizes the further work.

2. Instance selection

Instance selection is a technique that aims to reduce the size of the original training data, while retaining the predictive capability of the obtained models, or even improving them (if in the process of reducing the size, the noise instances may also be removed). It retains those examples in the filtered set that are relevant for the prediction of output variables, eliminating superfluous instances [33]. The elimination of instances is not always guided by the reduction of size, on occasions what is desired is to filter the noise out of the original dataset. Although the expectation is to obtain an accuracy equal to or better than the original dataset, in practice it is not usually achieved and a certain loss of accuracy is inevitable [9].

Depending on how the selected subset is constructed, these techniques may be classified as: incremental, decremental, and batch [40]. Incremental methods start with an empty set and continue adding instances to it. The order of the instances in the original set is important in these methods and will determine their effectiveness. A contrary approach is followed by the so-called decremental algorithms, which begins with the initial dataset and removes the instances that they consider “discardable”. Again, the order is important, but not as much as in the case of incremental algorithms, as the whole sample is there right from the start to take the decision. The batch methods mark the instances that are candidates to be eliminated, and once they have all been analysed, they are removed from the dataset. This technique ensures that the impact on the complete subset of the elimination of one instance is known [42].

There are a wide variety of instance selection methods for classification tasks [4, 7, 8, 21, 31, 34, 40, 41], as well as various surveys [14, 33] that present the state-of-the-art techniques. On the contrary, the selection of instances for regression problems has not been widely investigated [36], one of the reasons for that is its difficulty [25]. As the authors analysed in [6], there are two issues associated to regression task that makes it more complex: the rejection criterion (of an instance) and the class boundaries. In classification, many algorithms evaluate the utility of an instance according to the classification of its nearest neighbours. In regression, the correct or wrong classification of an instance according to its neighbours is not so straightforward. On the other hand, the correct identification of class boundaries in classification is the aim of many instance selection algorithms but, in regression, there are not boundaries in the strict sense of the term, which it makes harder to know which instances must be kept. In spite of its difficulty, the need for methods for this type of learning data has led to the appearance of some algorithms over recent years. Zhang [44] presented a new method (k-SN: k surrounding neighbours) for function prediction in lazy learning algorithms. Although, under a strict definition of the term, his method is not an instance selection method, it could be considered a first proposal of this kind of algorithm in regression task. Years later, Tolvi [38] presented a genetic algorithm [18] for outlier detection and feature selection in linear regression models. More recently, Antonelli et al. [3], also following a genetic approach, addressed the problem in the framework of MOEL (multiobjective evolutionary learning) of fuzzy rule-based systems (FRBs [22]). Regarding regression in time series, an interesting approach based on mutual information was introduced by Guillen et al. [20] for outlier detection achieving good results in both artificial and real time series. Afterwards, the same approach was generalized for dataset reduction in time series [37]. Finally, some other authors have focused their efforts on adapting instance selection methods to regression that were initially designed for classification. In [25] CNN and ENN are adapted to work with regression problems (as these methods are quite relevant for the work presented here, more details are given in next section), and in [36] the method Class Conditional Instance Selection (CCIS) [30] is adapted to reduce the variance in genetic fuzzy systems (GFSs) [1].

2.1. DROP algorithms

The family of methods known as DROPn (DROP1...5) [40] contains some of the methods that yield the best results in classification [8, 32, 35]. They belong to the category of decremental methods and the removal criteria is defined in terms of nearest neighbours and associates:

- *Nearest neighbours.* Given an instance $\mathbf{p}$, the nearest neighbours are those instances in the neighbourhood of $\mathbf{p}$. The expression $\mathbf{p}.N_{1,...k}$, or simply $\mathbf{p}.N$ denotes the list of k nearest neighbours of $\mathbf{p}$ ordered from closest to furthest.

- *Associates.* Those instances that have $\mathbf{p}$ as one of their k nearest neighbours are called associates of $\mathbf{p}$ and are denoted as $\mathbf{p}.A_{1,...a}$, where a is the number of associates of $\mathbf{p}$ that are considered. It is the inverse relation of nearest neighbours.

The differences between the variants of DROP methods [42] are as follows:

- DROP1 eliminates an instance $\mathbf{p}$ of S, if its associates in S are correctly classified without $\mathbf{p}$, that is, if the elimination of $\mathbf{p}$ does not affect the classification results.
- The DROP2 algorithm verifies the effect that causes the removal of an instance on the original sample[1]; in other words, DROP2 removes an instance $\mathbf{p}$ of S if the associates that $\mathbf{p}$ has in the original set, T, are correctly classified without $\mathbf{p}$. Before starting the selection, it sorts the instances in descending order from their distance to their *nearest enemy*[2]. In this way, instances are processed in an order that is the reverse of theirs distance to the class boundary, the furthest instance is processed first, then the second furthest, and so on.
- The DROP3 algorithm, applies a noise filter similar to Wilson editing or ENN [41] before starting the instance selection process. The filtering state removes all instances that are not correctly classified by their k nearest neighbours.
- DROP4 is identical to DROP3 but applies a slightly different noise filter, involving the removal of an instance only if it is misclassified by its k nearest neighbours and its removal does not mean that another instance is badly classified. This avoids the removal of too many instances in the the filtering stage.
- The DROP5 algorithm is similar to DROP2, but it begins to analyse the instances that are found close to its nearest enemy (those on the class boundary). To do so, it changes the initial order of processing from the shortest to the longest distance to its nearest enemy. Processing instances in this order has the effect of smoothing the class boundaries, the same effect that in DROP3 and DROP4 it is achieved with a noise filter, that is the why the filtering stage is not necessary in DROP5.

The reason behind the initial noise filtering of algorithms DROP3 to DROP5 becomes apparent after understanding the effect that noisy instances have on DROP1 and DROP2. Noisy instances have a profound impact on how instances are ordered at the beginning of these algorithms. A noise instance means that its neighbours are considered part of the class boundary, and they can be kept in the selected set that has been filtered even after the noisy instance has been removed [39].

In Algorithm 1 the pseudocode of DROP1 is shown, which is the foundation for the other DROP variants. The nearest neighbours and associates list are both built the same way in all variants of DROP. Then, instances are processed and the values of two variables, '`with`' and '`without`' are calculated. For each instance, the variable `with` counts how many of its associates are correctly classified when the instance is

[1]DROP3, DROP4 and DROP5 also verify the effect on the original sample.

[2]The nearest enemy of an instance is the closest instance of different class.

Algorithm 1: Decremental Reduction Optimization Procedure 1 (DROP1)

```
Input: Training set $T = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$
Output: Instance set $S \subseteq T$
1  Let $S = T$
2  foreach instance $\mathbf{x} \in S$ do
3      Find $\mathbf{x}.N_{1...k+1}$, the $k+1$ nearest neighbours of $\mathbf{x}$ in $S$
4      Add $\mathbf{x}$ to each of its neighbours' lists of associates
5  foreach instance $\mathbf{x} \in S$ do
6      Let with = # of associates of $\mathbf{x}$ classified correctly with $\mathbf{x}$ as a neighbour
7      Let without = # of associates of $\mathbf{x}$ classified correctly without $\mathbf{x}$ as a
       neighbour
8      if without $\geq$ with then
9          Remove $\mathbf{x}$ from $S$
10         foreach associate $\mathbf{a}$ of $\mathbf{x}$ do
11             Remove $\mathbf{x}$ from $\mathbf{a}$'s list of nearest neighbours
12             Find a new nearest neighbour for $\mathbf{a}$
13             Add $\mathbf{a}$ to its new neighbour's list of associates
14         foreach neighbour $\mathbf{n}$ of $\mathbf{x}$ do
15             Remove $\mathbf{x}$ from $\mathbf{n}$'s list of associates
16 return $S$
```

kept in the dataset, while the variable `without` records the count of correctly classified associates when the instance is removed from the dataset. If the value of `without` is greater than or equal to the value of `with` the instance is not helping in the classification of its associates, and hence, it can be removed from the dataset. When an instance is removed, it is necessary to update the nearest neighbours list of all its associates (a new nearest neighbour is needed). As shown in line 3, the nearest neighbours lists have actually $k + 1$ neighbours, this makes the calculation of the variable faster, since it is possible to postpone the search of a new nearest neighbour until the elimination of the instance effectively takes place.

DROP2 only differs from DROP1 because of the initial sorting done in DROP2, and because DROP2 eliminates lines 14 and 15. This modification means that DROP2 considers the whole initial dataset, instead of only the selected subset.

3. Proposed methods

In this section four new approaches to instance selection for regression are analysed. All of them are based on DROP but they change the way the values of `with` and `without` are calculated, which will determine the behaviour of the algorithms.

In classification, as we explained earlier, the calculation of `with` and `without` is straightforward. To cope with regression tasks, ie numeric class, we proposed two ideas: to compare the accumulated error that occurs when an instance is included and when it is discarded, and to use in regression an approximation to the concept of class used in classification (something like a *soft* class). Both ideas were used to adapt DROP2 and DROP3 to regression and the four resultant algorithms were tested in the experimental section.

3.1. DROP using error accumulation

As indicated in [42], algorithm DROP1 is identical to the RNN [17] method, with the exception that accuracy is tested on the edited set S instead of on the original set T. Thus, what we are trying to obtain with this adaptation for regression is that the removal of instance $\mathbf{x}$ only takes place if its elimination does not increase the prediction error of its associates. The idea consists in substituting the accounting of misclassified instances by the accumulation of the errors produced in the prediction of the output variables (the difference between the known value and the value given by the base regressor). For each instance $\mathbf{x}$ that is a candidate to be eliminated, its associates $\mathbf{a}$ are considered. The error from predicting the output variable is calculated for each associate $\mathbf{a}$ of $\mathbf{x}$ by means of a regressor trained with the nearest neighbours of $\mathbf{a}$ including $\mathbf{x}$ and the error if the instance $\mathbf{x}$ was not in the dataset (and another instance would therefore enter the set of nearest neighbours of $\mathbf{a}$). The errors of all associates of $\mathbf{x}$ are accumulated in `eWith` and `eWithout` respectively. Only the instance $\mathbf{x}$ will be removed, in case the accumulated error (the sum of the errors for each of their associates) that is obtained when it is excluded from the dataset is less than or equal to what is obtained when it is considered part of the dataset.

What has been explained above is presented in Algorithm 2, which we will refer to hereafter as DROP2-RE, where $Y(\mathbf{a})$ is the value of the output variable for instance $\mathbf{a}$ and $\texttt{Model}(\mathbf{a}.N \backslash \mathbf{x}, \mathbf{a})$ is the prediction for instance $\mathbf{a}$ given by a regressor trained with the nearest neighbours of $\mathbf{a}$ excluding the instance $\mathbf{x}$.

This first proposed method is based on DROP2, but without the initial sorting (in preliminary experiments the results with sorting were worse). DROP2 was selected as the base algorithm for this approach instead of DROP1, as the results of the latter were far from optimal in [19].

On the basis of DROP2, the second proposed method, DROP3 (referred to hereafter as DROP3-RE), is the result of including a noise filter at the beginning of Algorithm 2 and, subsequently, performing the initial sorting that characterizes DROP3. The noise filtering is done with the Wilson edition adapted to regression (RegENN shown in Algorithm 3) and the details of the sorting process are given in Section 3.2.1.

3.2. DROP using thresholding

In [25], the authors proposed an adaptation for regression of ENN [41] and CNN [21] instance selection algorithms that they called RegENN (see Algorithm 3) and RegCNN respectively. The first step they proposed was the need to find an alternative to the criterion of correct/incorrect prediction of a particular instance, through a measure that, on the basis of the numerical value of the output variable and a particular threshold, establishes whether that instance is far from the average of the output values of its neighbours (ie the instance has a different "*class*" than its neighbours). This concept of similarity, which allows an approximation to the concept of class in regression problems, is what in [27] is called *soft class* as opposed to the *hard class* of classification.

In Algorithm 3, $Y(\mathbf{x}_i)$ is the value of the output variable for instance $\mathbf{x}_i$, $\texttt{Model}(P \backslash \mathbf{x}_i, \mathbf{x}_i)$ is the prediction for instance $\mathbf{x}_i$ given by a regressor trained with the dataset P excluding

Algorithm 2: DROP2-RE: adaptation to regression of DROP2 by using error accumulation.

```
  Input: Training set $T = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$
  Output: Instance set $S \subseteq T$
1 Let $S = T$
2 foreach instance $\mathbf{x} \in S$ do
3     Find $\mathbf{x}.N_{1...k+1}$, the $k+1$ nearest neighbours of $\mathbf{x}$ in $S$
4     Add $\mathbf{x}$ to each of its lists of the associates of the neighbours
5 foreach instance $\mathbf{x} \in S$ do
6     Let eWith $= 0$
7     Let eWithout $= 0$
8     foreach associate $\mathbf{a}$ of $\mathbf{x}$ do
9         Add $|Y(\mathbf{a}) - \texttt{Model}(\mathbf{a}.N\backslash\mathbf{x}, \mathbf{a})|$ to eWithout
10        Add $|Y(\mathbf{a}) - \texttt{Model}(\mathbf{a}.N, \mathbf{a})|$ to eWith
11    if eWithout $\leq$ eWith then
12        Remove $\mathbf{x}$ from $S$
13        foreach associate $\mathbf{a}$ of $\mathbf{x}$ do
14            Remove $\mathbf{x}$ from $\mathbf{a}$ list of nearest neighbours
15            Find a new nearest neighbour for $\mathbf{a}$
16            Add $\mathbf{a}$ to its new neighbour's list of associates
17 return $S$
```

Algorithm 3: RegENN: adaptation to regression of Wilson filtering [25].

```
  Input: Training set $T = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$
  Output: Instance set $P \subseteq T$
1 $P \leftarrow T$
2 for $i = 1...n$ do
3     $\mathcal{N} = \texttt{kNN}(P, \mathbf{x}_i)$
4     $\theta_E = \alpha_E \cdot \mathrm{std}(Y(X_{\mathcal{N}}))$
5     if $|Y(\mathbf{x}_i) - \texttt{Model}(P\backslash\mathbf{x}_i, \mathbf{x}_i)| > \theta_E$ then
6         $P \leftarrow P\backslash\mathbf{x}_i$
7 return $P$
```

$\mathbf{x}_i$, $\mathcal{N}$ is the set of k nearest neighbours of $\mathbf{x}_i$, $\mathrm{std}(Y(X_\mathcal{N}))$ is the standard deviation of the output variable for the nearest neighbours of $\mathbf{x}_i$ and hence θ_E is the threshold for rejection/acceptance of instances calculated as the product of the standard deviation by a coefficient α_E. The parameter α_E makes it possible to adjust the radius of the *soft class* and therefore the specificity of the algorithm. Thus, an instance is removed from the set as long as the difference between the prediction given by a regressor trained with the dataset, without that instance, and the real value of the numerical output variable for that instance exceeds the threshold θ_E (in other words, if the prediction is outside its soft class). The value of θ_E is variable for each instance, as it is calculated for each of the instances. This characteristic allows the most appropriate radius to be adjusted to each instance according to its neighbourhood.

3.2.1. DROP2-RT

The threshold approach explained above was also used to adapt the DROP2 algorithm to regression (hereafter DROP2-RT), as shown in Algorithm 4. Where, as in the previous examples, $Y(\mathbf{a})$ is the value of the output variable for instance $\mathbf{a}$, $\mathtt{Model}(\mathbf{a}.N\backslash\mathbf{x}, \mathbf{a})$ is the prediction for instance $\mathbf{a}$ given by a regressor trained with the nearest neighbours of $\mathbf{a}$ excluding $\mathbf{x}$, and $\mathtt{Model}(\mathbf{a}.N, \mathbf{a})$ is the prediction of the output variable for instance $\mathbf{a}$ given by a regressor trained with all the nearest neighbours of instance $\mathbf{a}$ including $\mathbf{x}$.

The initial sorting stage of DROP2-RT is, like in DROP2, according to the distance to the closest enemy, but now the closest enemy of an instance $\mathbf{x}_i$ if defined as the instance $\mathbf{x}_j$ closest to $\mathbf{x}_i$ such that $|Y(\mathbf{x}_i) - Y(\mathbf{x}_j)| > \theta_D$. The previous sorting performed by DROP3-RE is of the same nature that is explained here.

3.2.2. DROP3-RT

DROP3-RT is similar to DROP2-RT but, as in DROP3, before the sorting stage, a noise filter is applied to the dataset. We used the Wilson edition adapted to regression (RegENN) shown in Algorithm 3 as the noise filter.

3.2.3. Combination of approaches

As shown in the experimental section, the use of error accumulation gets selected subsets with more accuracy whereas the use of threshold produces smaller selected subsets. For this reason, both ideas can be combined to get two new algorithm variants. In one of them instances are removed only if simultaneously $\mathtt{without} \geq \mathtt{with}$ and $\mathtt{eWithout} \leq \mathtt{eWith}$, this is the and-combination; in the other, instances are removed if any of the conditions are true, this is the or-combination. In the case of the and-combination the results were only a bit more accurate than DROPx-RE, but not significantly better. The or-combination shows results slightly worse than DROPx-RT, that is the worst method, again the difference was no statistically significant. As both algorithms are more complex, since more conditions need to be evaluated, we have not included in the paper a detailed study of these variants.

3.3. Similarities and differences between DROP and DROP-Rx

As explained earlier, the methods presented in this paper are based on the DROP family of instance selection methods for classification, whose basic structure consists in four steps: *i*) an initial ordering and/or filtering of the instances, *ii*) calculation of the

Algorithm 4: DROP2-RT: adaptation to regression of DROP2 using thresholding

```
Input: Training set $T = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$
Output: Instance set $S \subseteq T$
1  Let $S = T$
2  Sort the instances in $S$ by the distance to their nearest enemy
3  foreach instance $\mathbf{x} \in S$ do
4      Find $\mathbf{x}.N_{1...k+1}$, the $k+1$ nearest neighbours of $\mathbf{x}$ in $S$
5      Add $\mathbf{x}$ to each of its neighbours' lists of associates
6  foreach instance $\mathbf{x} \in S$ do
7      Let with $= 0$
8      Let without $= 0$
9      foreach $\mathbf{a}$ associate of $\mathbf{x}$ do
10         $\theta_D = \alpha_D \cdot \mathrm{std}(Y(\mathbf{a}.N))$
11         if $|Y(\mathbf{a}) - \texttt{Model}(\mathbf{a}.N \backslash \mathbf{x}, \mathbf{a})| \leq \theta_D$ then
12             Add 1 to without
13         if $|Y(\mathbf{a}) - \texttt{Model}(\mathbf{a}.N, \mathbf{a})| \leq \theta_D$ then
14             Add 1 to with
15     if without $\geq$ with then
16         Remove $\mathbf{x}$ from $S$
17         foreach associate $\mathbf{a}$ of $\mathbf{x}$ do
18             Remove $\mathbf{x}$ from $\mathbf{a}$ list of nearest neighbours
19             Find a new nearest neighbour for $\mathbf{a}$
20             Add $\mathbf{a}$ to its new neighbour's list of associates
21 return $S$
```

neighbours and associates of each instance, *iii*) calculation of the values of variable `with` and `without`, *iv*) using the values of these variables a decision is made of accepting or rejecting the instances as part of the selected subset.

The proposed methods use the neighbour and associate sets of each instance to calculate the values of variables `with` and `without` (or the variables `eWith` and `eWithout` with a similar role in the algorithm), as the methods on which they are based, and hence they have the same algorithmic complexity of the DROP family for classification.

The main difference is in how the variables `with` and `without` are calculated:

- Using Error accumulation: variables accumulate the error produced by the regressor (`Model`) on each of the instances, and therefore, they have real values.
- Using thresholding: variables are counters that increase their values depending on whether the difference of the regressor prediction (`Model`) and the actual value exceeds a threshold θ_D.

Besides the way these variables are calculated, the initial sorting and noise filtering of instances have had to be adapted to regression. Sorting was done as explained in Section 3.2.1, and for noise filtering, the algorithm RegENN (see Algorithm 3) has been used.

4. Experiments and results

This section evaluates the performance of the four methods proposed in the preceding section. They were compared between each other, against an instance selection algorithm for regression called RegCNN [25] and against the baseline of training the regressor without filtering. Finally, the robustness to noise of the new algorithms was tested.

4.1. Experimental setup

Experiments were performed using several datasets, several instance selection methods and several regressors. For each combination of these 3 elements, we applied a 10-fold cross validation [13]. The 10-fold cross validation was as following, each dataset was split into 10 subsets, the union of 9 of the subsets was reduced using instance selection and the resultant subset was used to train a regressor. The accuracy was calculated using the 10-th subset that was not used in the training phase.

Instance selection can be thought of as a multi-objective problem: on the one hand, it attempts to reduce the size of the resulting dataset and, on the other, to minimize the error [29]. Therefore, if we want a fair comparison of the results, considering accuracy only would not be the best approach. We have used the same idea as in [28] to combine both the retention rate and the error in a single index:

$$I_\omega = \omega \cdot \epsilon + (1 - \omega) \cdot m \tag{1}$$

where ϵ is the error (calculated as $1 - R^2$), ω is a value in the interval $[0, 1]$ that assigns greater importance to the accuracy or to the reduction of storage space, and m is the retention ratio, expressed as:

$$m = \frac{|S|}{|T|} \tag{2}$$

where, $|S|$ is the number of instances retained by the instance selection algorithm, and $|T|$ is the number of instances in the original dataset. The smaller the value of I_ω, the more favourable the results, as high values represent little reduction (higher retention ratio) and/or high error, however, lower values indicate greater reduction in the filtered dataset (lower retention ratio) and/or greater accuracy.

To measure the accuracy, we have chosen the correlation coefficient (R^2) [10] since its value is in the interval $[0, 1]$ and we can use it directly in the Equation 1.

4.2. Configurations

The experiments were performed in Weka [43], implementing the instance selection methods as Weka filters. The regressors used were:

- nearest neighbours (with $k = 8$).
- multilayer perceptron (trained with backpropagation with the following parameters: learning rate = 0.3, momentum = 0.2, number of hidden neurons = $\frac{\#attr+1}{2}$).
- REPTrees (with Weka default parameters).

Nevertheless, the exact regressors are not of extreme relevance to the study, as what we want to compare is the improvement or deterioration of the predictive ability when instance selection is applied.

The parameters of the instance selection methods were the following. The kNN nearest neighbour regressor was used as `Model`, with $k = 9$ (the value suggested in [25]). In the threshold-based methods (DROP2-RT and DROP3-RT), the value of α_D was 0.5 (the value that gave the best results in previous analyses). The best values of α_E were chosen after testing the values 1, 2, 3, 4 and 5. Table 1 shows the optimal values for the different adaptations to regression of DROP, the various regressors, and different levels of noise (see Section 4.5 for details of the analysis of robustness to noise).

Note that RegENN is a kind of noise filter so θ_E should be larger than the standard deviation of the output value of the neighbours, as only the outliers should be rejected, which is why α_E is bigger than 1, with $\alpha_E < 1$ the noise filtering would be too aggressive [25]. This is not the case for DROP algorithms and the value of α_D. If $\alpha_D > 1$, θ_D would be too large and it would be harder to detect the effect of removing an instance from the dataset (the conditions in lines 11 and 13 would almost always be false, the variables `with` and `without` would not be adapted, and the instances would be systematically removed from the dataset. In other words, the instance selection process would be too aggressive at removing instances).

RegCNN is influenced by two parameters α and k. With the aim to use reasonable values for these parameters, we first launched several experiments with different values: 0.25, 0.5, 0.75 and 1 for α; and 3, 5, 7 and 9 for k. The best results, for all regressors, were achieved using $\alpha = 0.25$. Whereas the optimal values for k depended on the regressor and the level of noise of the datasets, they are shown in Table 2.

4.3. Datasets

The datasets used for experimentation were obtained from the KEEL repository [2]. They are described in Table 3, which details the number of attributes, the number of

Table 1: Value of α_E which has achieved lower errors for the different regressors and noise levels (see Section 4.5 on noise tolerance).

Noise	**IS algorithm**	***k*NN**	**MLP**	**REPTree**
0 %	DROP3-RE	5	5	3
	DROP2-RT	4	2	1
	DROP3-RT	4	5	2
10 %	DROP3-RE	3	2	2
	DROP2-RT	3	5	2
	DROP3-RT	3	2	3
20 %	DROP3-RE	2	2	2
	DROP2-RT	3	1	3
	DROP3-RT	4	2	1
30 %	DROP3-RE	2	1	1
	DROP2-RT	1	3	5
	DROP3-RT	4	1	1

Table 2: Value of k for RegCNN which has achieved lower errors for the different regressors and noise levels (see Section 4.5 on noise tolerance).

Noise	***k*NN**	**MLP**	**REPTree**
0 %	9	9	9
10 %	3	7	3
20 %	9	7	9
30 %	7	7	7

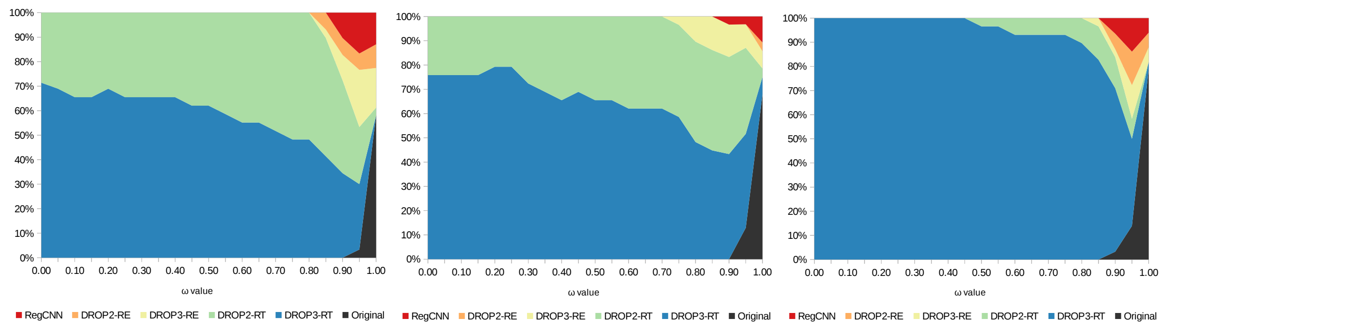
Table 3: Datasets used in the experiments

	Dataset	# attributes	# instances	Correlation coefficient		
				*k*NN	MLP	REPTree
1	MachineCPU	6	209	0.9335	0.9433	0.8127
2	Baseball	16	337	0.8291	0.7350	0.7775
3	DEE	6	365	0.9013	0.9061	0.8631
4	AutoMPG8	7	392	0.9276	0.9330	0.9133
5	AutoMPG6	5	392	0.9345	0.9277	0.9081
6	Ele-1	2	495	0.8321	0.8402	0.7969
7	Stock	9	950	0.9927	0.9864	0.9832
8	Laser	4	993	0.9725	0.9873	0.9527
9	Concrete	8	1 030	0.8296	0.9103	0.8978
10	Treasury	15	1 049	0.9974	0.9981	0.9955
11	Mortgage	15	1 049	0.9981	0.9995	0.9965
12	Ele-2	4	1 056	0.9904	0.9969	0.9950
13	Friedman	5	1 200	0.9425	0.9135	0.8495
14	Wizmir	9	1 461	0.9930	0.9967	0.9926
15	Wankara	9	1 609	0.9924	0.9964	0.9912
16	Plastic	2	1 650	0.8773	0.9024	0.8606
17	Quake	3	2 178	0.1074	0.0808	0.0699
18	ANACALT	7	4 052	0.9755	0.9890	0.9898
19	Abalone	8	4 177	0.7253	0.7516	0.6918
20	Delta-ail	5	7 129	0.8267	0.8314	0.8035
21	Compactiv	21	8 192	0.9860	0.9903	0.9839
22	Puma32h	32	8 192	0.4286	0.3200	0.9562
23	Delta-elv	6	9 517	0.7768	0.7913	0.7760
24	Ailerons	40	13 750	0.8966	0.8947	0.8728
25	Pole	26	14 998	0.9807	0.9491	0.9851
26	Elevators	18	16 599	0.8487	0.9499	0.8448
27	California	8	20 640	0.8438	0.8468	0.8612
28	House	16	22 784	0.6863	0.6736	0.6827
29	Mv	10	40 768	0.9853	0.9999	0.9995

instances and the correlation coefficient (R^2) [10] for the regressors used in the experiments: nearest neighbour (kNN), multilayer perceptron (MLP) and REPTree (Reduced Error-Pruning Tree) [43]. The only transformation performed on the data was the normalization of all the input attributes so that they appear in the range $[0, 1]$. This transformation is intended to prevent certain attributes with a lot of variance from distorting the results in the calculation of the nearest neighbour.

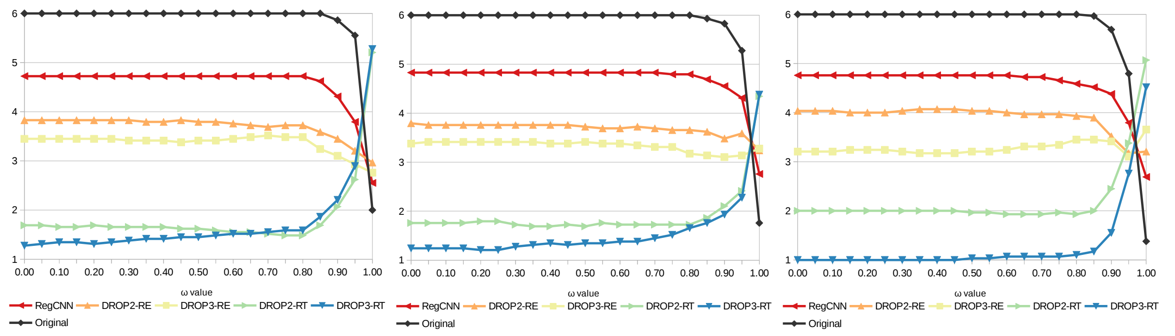
4.4. Results and discussion

In the experiments, besides the proposed methods, we have included the method RegCNN, a state-of-the-art method explained earlier, and the regressor trained with the unfiltered dataset. The obtained results are compared using the I_ω index for different values of ω.



(a) kNN (b) Multilayer Perceptron (c) REPTree

Figure 1: Comparison of the instance selection methods. In x axis the value of I_ω (see Eq. 1) is shown for ω values in the range [0, 1]. On the y axis, a percentage of datasets are represented in which a method is better than all the other approaches according to the evaluation index I_ω. The extreme left-hand-side of figures, ($\omega = 0$) corresponds to the results when only the reduction of the dataset is considered; the extreme right-hand-side, ($\omega = 1$) corresponds to the results for which only accuracy is considered of relevance and, on the middle ($\omega = 0.5$), the same relevance is given to accuracy and reduction. The method called 'Original' refers to the regressor trained with the original dataset.



(a) kNN (b) Multilayer Perceptron (c) REPTree

Figure 2: Comparison of average ranks for the instance selection methods (and the regressor without instance selection, shown as 'Original' in the legend) for all ω values in the range [0, 1] (axis x). Axis y plots the average rank (according to the evaluation index I_ω), low values are best, high values are worse.

Figure 1 shows the percentage of datasets for which a method is better than the rest. For $\omega = 1$, that is, considering accuracy alone, it is observed that the best value of the index is for the regressor trained with the original dataset (irrespective of the regressor). From that value, as greater importance is assigned to the reduction, the instance selection algorithms compete between each other. Thus, for $\omega < 1$, as the dataset reduction increases its weight in the index, DROP3-RT and DROP2-RT dominate the results for kNN and MLP, and DROP3-RT dominates for REPTree.

Average ranks [12] were used for comparing all the methods and were calculated in the following way: the results for each dataset were sorted according to their performance, assigning rank 1 to the best, rank 2 to the second best, and so on. In the case of a tie, the range is divided between all the tied methods. The average rank for each method is the mean value of all the datasets. Figure 2 shows the average ranks on the y axis plotted against the different values of ω on the x axis.

DROP3-RE for kNN and DROP2-RE for MLP and REPTree are the more conser-

Table 4: Average retention ratio (m). m is calculated as $|S|/|T|$, where $|S|$ is the number of instances retained by the instance selection algorithm, and $|T|$ is the number of instances in the original set.

IS algorithms	**Average m**
DROP2-RT	0.471
DROP3-RT	0.468
DROP2-RE	0.634
DROP3-RE	0.631
RegCNN	0.787

vative algorithms. If only accuracy is taken into account, these methods are the ones that comes closest to the result of the regressor trained on the original dataset. According to the ranking, RegCNN is in the middle between the regressor trained on the original dataset and the regressor trained with the selected subsets obtained with the proposed algorithms, again if compression is not taken into account. On the other hand, threshold-based approaches, DROP2-RT and DROP3-RT, yield good results for ω values lower than 0.9 or 0.95. Of these two, DROP3-RT is clearly better when the regressor is MLP or REPTree.

On the extreme left-hand-side of figures, ($\omega = 0$) corresponds to the results when considering only the reduction of the dataset; on the extreme right-hand-side, ($\omega = 1$) corresponds to the results for which only accuracy is considered of relevance. In each of these cases, the test of significance through the Hochberg procedure [23] has been calculated (Tables 5, 6, 7 and 8). The algorithm with best result (the one with lowest rank) is significantly better than the others when the value in column 'p Hoch.' is less than 0.1 (significance level: 0.9) or less than 0.05 (significance level: 0.95).

Since mean ranking only offers an order between the methods, Table 4 shows the average retention ratio of the different instance selection methods tested in the experiments. Whereas threshold methods have around 0.47 retention ratio, ie 53% of compression, methods based on error accumulation have around 0.63. On the other hand, RegCNN achieves the highest retention ratio, around 15% more than the most conservative of our algorithms (DROPx-RE). As it was expected, DROP2-Rx algorithms are more conservative than DROP3-Rx algorithms because DROP3-Rx algorithms have an initial filtering stage that reduces the dataset.

As explained in [24], instance selection techniques are computationally expensive. Both, CNN and DROP for classification, share a complexity of $\mathcal{O}(n^3)$, and the adaptation of these methods to regression inherits this complexity. If the average rank of the methods according to their filtering time is obtained for all datasets, RegCNN is the best and significant better than all DROPx-Rx. This can be explained by the fact that incremental methods are faster than decremental ones [42], also the calculations of DROP are more elaborated than those made in CNN. We have also compared the four proposed methods between each other. The fastest was DROP2-RE, this was expected since this method has not initial sorting, as DROP2-RT, nor initial noise filtering, as DROP3-Rx.

However, the aim of instance selection is to reduce the dataset that will be used to train. The reduction of training dataset implies, in lazy learning algorithms like kNN, the decrease in testing time. Whereas the training phase is executed only once and can be made batch, the speed in the testing phase is crucial because it is executed multiple times and, in many applications, the execution time should be as low as possible. If the methods are ranked according to their execution time in the testing phase for all datasets, DROP3-RT ranks the first followed by DROP3-RE and the others. Moreover the differences between DROP3-RT and DROP2-Rx, RegCNN and kNN are significant at 95% of confidence.

4.5. Noise tolerance

Real datasets contain noise [15] and their presence reduces the predictive capability of the learning algorithms. The instance selection methods may also be sensitive to the presence of noise and atypical values (*outliers*) [5]. In fact, in addition to the reduction of the training set, one of the great benefits that the selection methods present is their capability to reduce noise, and the elimination of outliers. Hence, it was considered of interest to perform a study of the robustness of these methods in the face of noise.

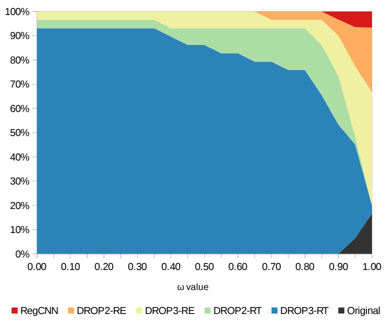
In classification, the characterization of the different types of noise, and how to introduce them in experimental validation have been investigated in depth (ie [45, 46]). On the contrary, in regression, what is considered noise and how to properly introduce it in the experimental validation is not that clear. In the experiments that were carried out, the noise was introduced by exchanging the output values of two randomly selected instances. This way, the distribution of the sample, both for the input variables and for the output variables was not modified.

Experiments were performed with 10%, 20% and 30% noise. Figures 3 and 4 show the robustness of the proposed methods. DROP3-RE performs an excellent task as a noise filter. For all the classifiers, the precision that is obtained was better when the filtered set was used than when the totality of the dataset was used. This behaviour was repeated as the noise that was introduced increased: 20% in figures 5 and 6, and 30% in figures 7 and 8.

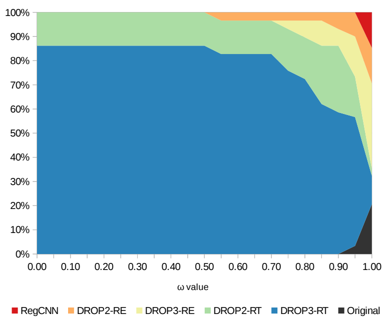
Besides, DROP2-RT, for levels of noise of 20% and 30%, showed poor behaviour when only accuracy was considered ($\omega = 1$), because as may be observed, the classifiers trained with the original noisy set yielded better values than when they were trained with the reduced set that was obtained by DROP2-RT. Nevertheless, this behaviour may be due to a more aggressive reduction of the dataset in DROP2-RT, because as may be seen from the figures, DROP2-RT is, together with DROP3-RT, the algorithm that shows the best behaviour, if we look only at the reduction of the datasets ($\omega = 0$). It is interesting to highlight that DROP3-RT for the values of $\omega \leq 0.9$ is the one which, in general, obtained better results, both for the original datasets and for the noisy datasets (DROP2-RT only appears to be at its same level for the k-NN classifier and for a noise of 10%).

As previously explained, Table 5 shows the ranking and the results of the Hochberg procedure for each of the methods taking into account only the reduction in size of the set of instances that were selected. Both in the original sets and in the tests completed with noise, DROP3-RT was, at a confidence level of 95%, significantly better than the error-based methods (DROP2-RE and DROP3-RE) and RegCNN. No significant differences were observed between DROP3-RT and DROP2-RT.

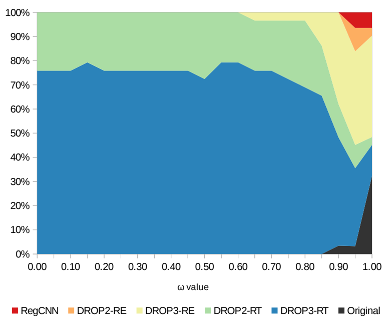
Tables 6, 7 and 8 show the ranking calculated over the accuracy ($\omega = 1$) of kNN, MLP and REPTree trained with the set returned by the instance selection algorithms. The result of training the regressor without previous filtering (Original) is included in



(a) kNN

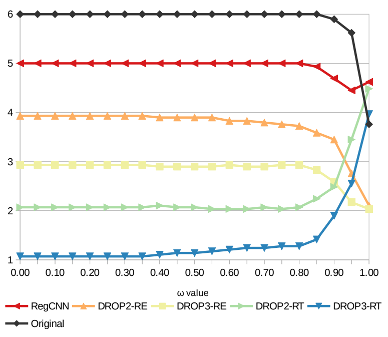


(b) Multilayer Perceptron

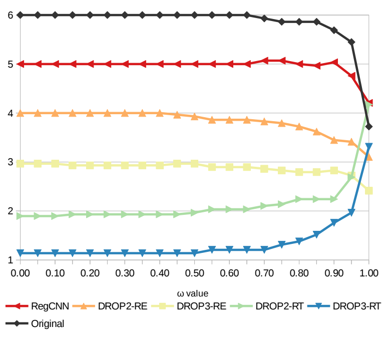


(c) REPTree

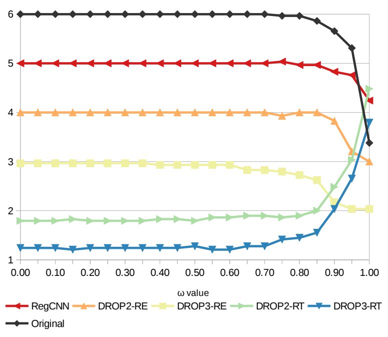
Figure 3: Experiments with a noise level of 10%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The y axis shows the percentage of datasets for which a method is better than the rest according to the evaluation index I_ω.



(a) kNN

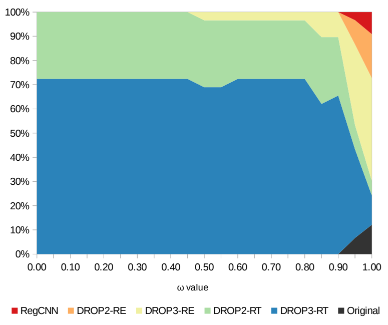


(b) Multilayer Perceptron

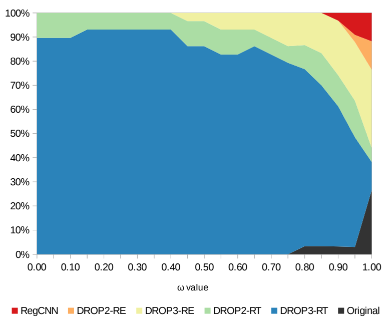


(c) REPTree

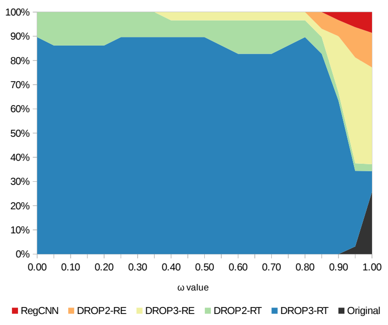
Figure 4: Experiments with a noise level of 10%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The y axis shows the average rank (according to the evaluation index I_ω), low values are better, high values are worse.



(a) kNN

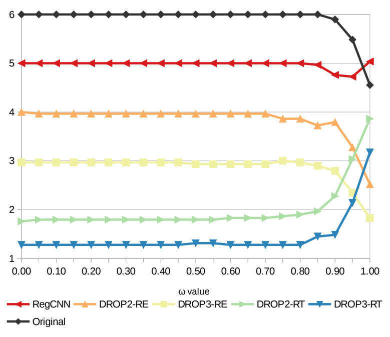


(b) Multilayer Perceptron

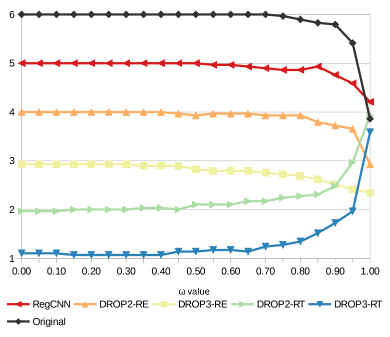


(c) REPTree

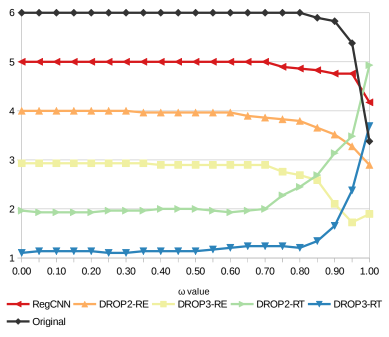
Figure 5: Experiments with a noise level of 20%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The y axis show the percentage of datasets for which a method is better than the rest according to the evaluation index I_ω.



(a) kNN

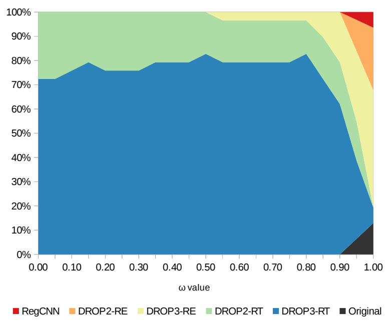


(b) Multilayer Perceptron

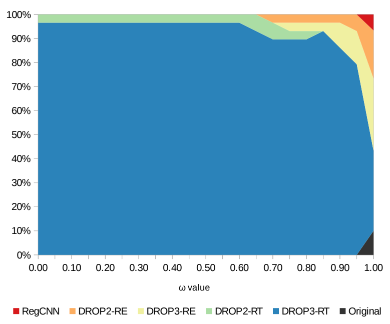


(c) REPTree

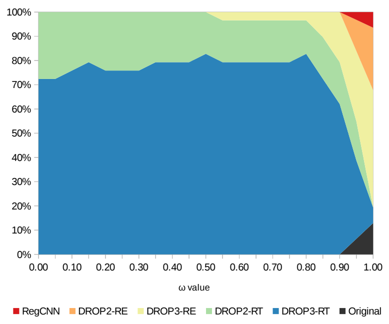
Figure 6: Experiments with a noise level of 20%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The y axis shows the average rank (according to the evaluation index I_ω), low values are better, high values are worse.



(a) kNN

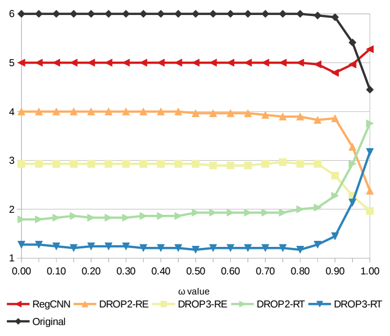


(b) Multilayer Perceptron

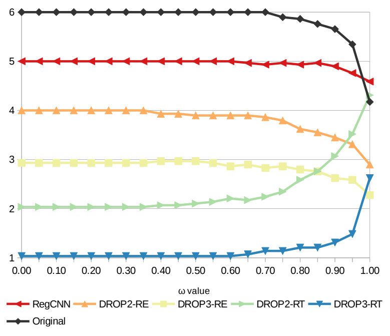


(c) REPTree

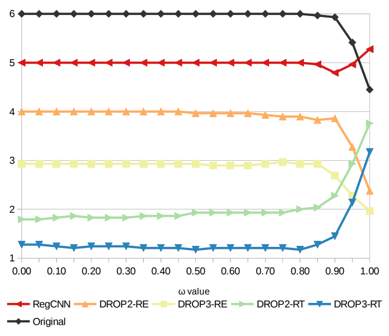
Figure 7: Experiments with a noise level of 30%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The y axis shows the percentage of datasets for which a method is better than the rest according to the evaluation index I_ω.



(a) kNN



(b) Multilayer Perceptron



(c) REPTree

Figure 8: Experiments with a noise level of 30%, the proposed methods are compared against RegCNN for all ω values in the range [0, 1] (axis x). The average rank (according to the evaluation index I_ω) is shown on the y axis, low values are better, high values are worse.

Table 5: Ranking and Hochberg procedure over compression.

Noise	**IS algorithm**	**Rank**	***p* Hoch.**
0 %	DROP3-RT	1.2931	
	DROP2-RT	1.7069	0.3189
	DROP3-RE	3.4483	4.1981E-7
	DROP2-RE	3.8276	3.1064E-9
	RegCNN	4.7241	5.6810E-16
10 %	DROP2-RT	1.4138	
	DROP3-RT	2.3793	0.0201
	DROP3-RE	2.6552	0.0056
	DROP2-RE	3.6896	1.2688E-7
	RegCNN	4.8621	4.0080E-16
20 %	DROP3-RT	1.2759	
	DROP2-RT	1.7586	0.2449
	DROP3-RE	2.9655	9.4338E-5
	DROP2-RE	3.9999	1.6078E-10
	RegCNN	5.0000	1.1978E-18
30 %	DROP3-RT	1.2759	
	DROP2-RT	1.7931	0.2129
	DROP3-RE	2.9310	1.3429E-4
	DROP2-RE	3.9999	1.6078E-10
	RegCNN	5.0000	1.1978E-18

Table 6: Ranking and Hochberg procedure over accuracy: *k*NN.

Noise	**IS algorithm**	**Ranking**	***p* Hoch.**
0 %	Original	2.0172	
	RegCNN	2.5862	0.2468
	DROP3-RE	2.8276	0.1981
	DROP2-RE	3.0172	0.1254
	DROP2-RT	5.2414	2.1177E-10
	DROP3-RT	5.3103	1.0224E-10
10 %	DROP3-RE	2.0517	
	DROP2-RE	2.1207	0.8884
	Original	3.7586	0.0010
	DROP3-RT	3.9655	2.9419E-4
	DROP2-RT	4.4827	2.9972E-6
	RegCNN	4.6207	8.5272E-7
20 %	DROP3-RE	1.8275	
	DROP2-RE	2.5172	0.1604
	DROP3-RT	3.1896	0.0111
	DROP2-RT	3.8793	8.8972E-5
	Original	4.5517	1.1777E-7
	RegCNN	5.0345	3.3478E-10
30 %	DROP3-RE	1.9655	
	DROP2-RE	2.3793	0.3996
	DROP3-RT	3.1724	0.0281
	DROP2-RT	3.7586	7.8769E-4
	Original	4.4482	1.7360E-6
	RegCNN	5.2759	8.0358E-11

the comparison. In the experiments without noise, the regressor trained with the original dataset was significantly better for MLP and REPTree, over a 95% confidence level, on the contrary, as noise was added, it was observed that the instance selection improved the results. For all levels of noise and all base regressors, DROP3-RE is the best method (see Tables 6, 7 and 8) and significantly better than Original (for a confidence level of 95%).

It can also be observed that the accuracy of RegCNN method decreases as the noise level increases. This is because it is an adaptation to regression of CNN which is very sensitive to noise in classification [42], as all condensation methods [29].

In all noise configurations, DROP3-Rx works better than the DROP2-Rx since the initial noise filtering allows the selection to be conducted on a cleaner set. With the aim of evaluating this behaviour we just compared our methods one vs. one by Wilcoxon test, ie DROP3-RT against DROP2-RT and DROP3-RE against DROP2-RE, the results of this comparison are shown in Table 9. On the table, ✓ means that DROP3-Rx is better than DROP2-Rx at a confidence level of 0.95, so we can conclude that DROP3-Rx has a better performance in noisy datasets than DROP2-Rx.

Table 7: Ranking and Hochberg procedure over accuracy: Multilayer Perceptron.

Noise	**IS algorithm**	**Ranking**	p **Hoch.**
0 %	Original	2.1724	
	RegCNN	2.8793	0.793
	DROP3-RE	3.4999	0.0051
	DROP2-RE	3.5172	0.0051
	DROP3-RT	4.5517	1.1990E-6
	DROP2-RT	4.5349	1.1990E-6
10 %	DROP3-RE	2.4310	
	DROP2-RE	3.1035	0.1711
	DROP3-RT	3.3449	0.1258
	Original	3.7241	0.0255
	DROP2-RT	4.1896	0.0014
	RegCNN	4.2069	0.0014
20 %	DROP3-RE	2.2759	
	DROP2-RE	2.9483	0.2328
	DROP3-RT	3.6034	0.0230
	Original	3.8621	0.0068
	DROP2-RT	3.9655	0.0043
	RegCNN	4.2586	5.6637E-4
30 %	DROP3-RE	2.3276	
	DROP3-RT	2.6724	0.4828
	DROP2-RE	2.9655	0.3883
	DROP2-RT	4.2069	3.9208E-4
	Original	4.2069	9.9208E-4
	RegCNN	4.6207	1.5253E-5

Table 8: Ranking and Hochberg procedure over accuracy: REPTree.

Noise	**IS algorithm**	**Ranking**	***p* Hoch.**
0 %	Original	1.3793	
	RegCNN	2.7759	0.0045
	DROP2-RE	3.3103	1.6959E-4
	DROP3-RE	3.7414	4.5790E-6
	DROP3-RT	4.6207	1.6725E-10
	DROP2-RT	5.1724	5.7943E-14
10 %	DROP3-RE	2.0862	
	DROP2-RE	2.9655	0.0735
	Original	3.3793	0.0170
	DROP3-RT	3.8103	0.0013
	RegCNN	4.2414	4.6046E-5
	DROP2-RT	4.5172	3.7465E-6
20 %	DROP3-RE	1.9138	
	DROP2-RE	2.9310	0.0384
	Original	3.3793	0.0057
	DROP3-RT	3.7069	7.8769E-4
	RegCNN	4.1724	1.7128E-5
	DROP2-RT	4.8965	6.3515E-9
30 %	DROP3-RE	2.1379	
	DROP3-RT	3.1724	0.0352
	DROP2-RE	3.3103	0.0340
	Original	3.7069	0.0042
	DROP2-RT	4.1207	2.1775E-4
	RegCNN	4.5517	4.4838E-6

Table 9: Wilcoxon test over accuracy ($\omega = 1$) in noisy datasets. ✓ indicates that DROP3-Rx is better than DROP2-Rx at a confidence level of 95% and "-" means no significant difference.

Noise	**DROP3-RT vs DROP2-RT**	**DROP3-RE vs DROP2-RE**
10 %	✓	✓
20 %	✓	✓
30 %	✓	✓

4.6. Benefits of using the proposed methods

Some remarkable observations can be made from the results, in this section we discuss the main advantages and disadvantages of instance selection methods for regression. First, in contrast to instance selection for classification, the application of instance selection methods in regression are not able to improve the accuracy of the original dataset, neither the proposed methods nor RegCNN. Second, the different approaches proposed to cope with regression have different characteristics: error accumulation (DROPx-RE) achieves lower reduction and consequently more accuracy whilst thresholding (DROPx-RT) achieves better reduction rate and lower accuracy. RegCNN achieves a good accuracy at expense of the lowest retention rate. In addition, when RegCNN was applied over noisy datasets, the instance selection method was strongly penalised. Nevertheless, the methods proposed based on DROP dealt with noise in a better way, outperforming the accuracy achieved by the regressor trained over the whole noisy dataset. The robustness in noisy environments is due to the filtering noise stage of DROP3-Rx, as DROP3 for classification does.

5. Conclusions

In the paper, two new approaches have been introduced to adapt the family of DROP instance selection methods, so successfully used for classification, to regression. Using these approaches four new algorithms for instance selection for regression have been proposed. It is an interesting contribution given that currently there are no many instance selection methods for regression. The proposed methods have been subjected to benchmark testing, where they were compared against each other, against RegCNN, one of the few methods for this kind of Machine Learning task, and against the result obtained from a regressor trained with the original dataset. The regressors used were: a method based on instances (kNN), a multilayer perceptron, and a method for constructing regression trees (REPTree).

We have discussed two approaches to adapt the DROP algorithms: using the error for the calculation of the variables `with` and `without`, and using the concept of *soft class* defined by means of an adaptive threshold. The results are of interest as, although, in all methods, to a greater or lesser extent the predictive power is reduced, this reduction is low in comparison with the reduction of dataset size.

In addition, a comparison has been drawn with a dual approach of reduction and accuracy to see how both objectives are related, as greater importance is given to one rather than another. In this way, the best algorithms is DROP3-RE in most cases if accuracy is to be maximised, as these methods are designed to minimize the loss of predictive capability of the resulting dataset. On the one hand, if the aim is to minimize the size of the datasets after selection, the best method is DROP3-RT both in the experimentation with the original and with the noisy datasets.

A remarkable property of the proposed adaptations of DROP for regression is their robustness in the presence of noise. The experiments carried out with noise levels of 10%, 20% and 30% have shown that the proposed instance selection algorithms are not only able to reduce the size of the training dataset, but they are also able to reduce the noise and significantly improve the accuracy achieved by different regressors.

6. Future lines

New instance selection methods for classification are still emerging, the use of thresholding makes it possible to adapt them directly to regression task. In future works we intend to adapt other promising instance selection methods with this idea, as for example [29].

In addition, the ideas presented in the paper can be applied to other fields like, for example, feature selection. Feature selection is related with instance selection [16] but, unlike instance selection, algorithms try to find the best subset of features, not instances. The similarities between both techniques suggest that these ideas could be achieve good results too.

Acknowledgments

This work was partially supported by the Spanish Ministry of Economy and Competitiveness through project TIN2011-24046.

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Big data marks the beginning of a major transformation.

Mayer-Schönberger and Cukier (2013)

Chapter 4

Instance selection of linear complexity for big data

This journal paper presents a new instance selection method for classification with a remarkable characteristic: linear complexity in the number of instances. In the paper, two different algorithms are described: one is able to process instances in the *on-fly* mode (i.e. with no need for the whole data set to fit in the memory) and the other performs the task in two *passes*.

It is the concept of Local Sensitive Hashing (LSH) that makes linear complexity possible. These families of hashing functions have a particular feature, instead of avoiding collisions they attempt to place similar objects in the same bucket and different instances in other buckets.

Authors: Álvar Arnaiz-González, Jose-Francisco Díez-Pastor, Juan José Rodríguez-Diez, César García-Osorio
Type: Journal
Published in: Knowledge-Based Systems 107: 83-95
Year: 2016
Reference: Arnaiz-González et al. (2016c)

Instance selection of linear complexity for big data

Álvar Arnaiz-González, José F. Díez-Pastor, Juan J. Rodríguez, César García-Osorio

University of Burgos, Spain

Abstract

Over recent decades, database sizes have grown considerably. Larger sizes present new challenges, because machine learning algorithms are not prepared to process such large volumes of information. Instance selection methods can alleviate this problem when the size of the data set is medium to large. However, even these methods face similar problems with very large-to-massive data sets.

In this paper, two new algorithms with linear complexity for instance selection purposes are presented. Both algorithms use *locality-sensitive hashing* to find similarities between instances. While the complexity of conventional methods (usually quadratic, $\mathcal{O}(n^2)$, or log-linear, $\mathcal{O}(n \log n)$) means that they are unable to process large-sized data sets, the new proposal shows competitive results in terms of accuracy. Even more remarkably, it shortens execution time, as the proposal manages to reduce complexity and make it linear with respect to the data set size. The new proposal has been compared with some of the best known instance selection methods for testing and has also been evaluated on large data sets (up to a million instances).

Keywords: nearest neighbor, data reduction, instance selection, hashing, big data

1. Introduction

The k nearest neighbor classifier (kNN) [11], despite its age, is still widely used in machine learning problems [9, 17, 20]. Its simplicity, straightforward implementation and good performance in many domains means that it is still in use, despite of some of its flaws [37]. The kNN algorithm is included in the family of instance based learning, in particular within the *lazy learners*, as it does not build a classification model but just stores all the training set [8]. Its classification rule is simple: for each new instance, assign the class according to the majority vote of its k nearest neighbors in the training set, if $k = 1$, the algorithm only takes the nearest neighbor into account [45]. This feature means that it requires a lot of memory and processing time in the classification phase [48]. Traditionally, two paths have been followed to speed up the process: either accelerate the calculation of the closest neighbors [3, 4], or decrease training set size by strategically selecting only a small portion of instances or features [38].

Email addresses: alvarag@ubu.es (Álvar Arnaiz-González), jfdpastor@ubu.es (José F. Díez-Pastor), jjrodriguez@ubu.es (Juan J. Rodríguez), cgosorio@ubu.es (César García-Osorio)

Regarding the acceleration of algorithms, perhaps one of the most representative approaches is to approximate nearest neighbors, a broadly researched technique in which the nearest neighbor search is done over a sub-sample of the whole data set [56]. In this field, many algorithms have been proposed for approximate nearest neighbor problems [3, 4, 30, 34, 39].

The focus of this paper is on the second path, the reduction of data set size. The reason is that this reduction is beneficial for most methods rather than only those based on nearest neighbors. Although we will only consider the reduction of instances (instance selection) in this paper, the reduction could also be applied to attributes (feature selection), or even both at the same time [51]. The problem is that the fastest conventional instance selection algorithms have a computational complexity of at least $\mathcal{O}(n \log n)$ and others are of even greater complexity.

The need for rapid methods for instance selection is even more relevant nowadays, given the growing sizes of data sets in all fields of machine learning applications (such as medicine, marketing or finance [43]), and the fact that the most commonly used data mining algorithms for any data mining task were developed when the common databases contained at most a few thousands of records. Currently, millions of records are the most common scenario. So, most data mining algorithms find many serious difficulties in their application. Thus, a new term has emerged, "Big Data", in reference to those data sets that, by volume, variability and speed, make the application of classical algorithms difficult [44]. With regard to instance selection, the solutions that have appeared so far to deal with big data problems adopt the 'divide and conquer' approach [13, 22]. The algorithms proposed in the present paper offer a different approach, just a sequential but very quick and simple processing of each instance in the data set.

In particular, the major contribution of this paper is the use of Locality-Sensitive Hashing (LSH) to design two new algorithms, which offers two main advantages:

- Linear complexity: the use of LSH means a dramatic reduction in the execution time of the instance selection process. Moreover, these methods are able to deal with huge data sets due to their linear complexity.

- *On-the-fly* processing: one of the new methods is able to tackle the instances in one step. It is not necessary for all instances fit in memory: a characteristic that offers a remarkable advantage in relation to big data.

The paper is organized as follows: Section 2 presents the reduction techniques background, with special emphasis on the instance selection methods used in the experimental validation; Section 3 introduces the concept of *locality-sensitive hashing*, the basis of the proposed methods which are presented in Section 4; Section 5 presents and analyzes the results of the experiments and, finally, sections 6 and 7 set out the conclusions and future research, respectively.

2. Reduction techniques

Available data sets are progressively becoming larger in size. As a consequence, many systems have difficulties processing such data sets to obtain exploitable knowledge [23]. The high execution times and storage requirements of the current classification algorithms make them unusable when dealing with these huge data sets [28]. These problems can be decisive, if a lazy learning algorithm such as the nearest neighbor rule is used, and can even prevent results from being obtained. However, reducing the size of the data set by selecting a representative subset has two main advantages: it reduces the memory required to store the data and it accelerates the classification algorithms [19].

In the scientific literature, the term "reduction techniques" includes [61]: prototype generation [32]; prototype selection [52] (when the classifier is based on kNN); and (for other classifiers) instance selection [8]. While prototype generation replaces the original instances with new artificial ones, instance selection and prototype selection attempt to find a representative subset of the initial training set that does not lessen the predictive power of the algorithms trained with such a subset [45]. In the paper, prototype generation is not addressed, however a complete review on it can be found in [57].

2.1. Instance selection

The aforementioned term "instance selection" brings together different procedures and algorithms that target the selection of a representative subset of the initial training set. There are numerous instance selection methods for classification, a complete review of which may be found in [21]. Instance selection has also been applied to both regression [2, 33] and time series prediction [26, 55].

According to the order in which instances are processed, instance selection methods can be classified into five categories [21]. If they begin with an empty set and they add instances to the selected subset, by means of analyzing the instances in the training set, they are called incremental. The decremental methods, on the contrary, start with the original training data set and they remove those instances that are considered superfluous or unnecessary. Batch methods are those in which no instance is removed until all of them have been analyzed, instances are simply marked from removal if the algorithm determines that they are not needed, and at the end of the process only the unmarked instances are kept. Mixed algorithms start with a preselected set of instances. The process then decides either to add or to delete the instances. Finally, fixed methods are a sub-family of mixed ones, in which the number of additions and removals are the same. This approach allows them to maintain a fixed number of instances (more frequent in prototype generation).

Considering the type of selection, three categories may be distinguished. This criterion is mainly correlated with the points that they remove: either border points, central points, or otherwise. Condensation techniques try to retain border points. Their underlying idea is that internal points do not affect classification, because the boundaries between classes are the keystone of the classification process. Edition methods may be considered the opposite of condensation techniques, as their aim is to remove those instances that are not well-classified by their nearest neighbors. The edition process achieves smoother boundaries as well as noise removal. In the middle of those approaches are hybrid algorithms, which try to maintain or even to increase the accuracy capability of the data set, by removing both: internal and border points [21].

Evolutionary approaches for instance selection have shown remarkable results in both reduction and accuracy. A complete survey of them can be found in [16]. However, the main limitation of those methods is their computational complexity [36]. This drawback is the reason why they are not taken into account in this study, because the methods it proposes are oriented towards large data sets.

Table 1: Summary of state-of-the-art instance selection methods used in the experimental setup (taxonomy from [21]; computational complexity from [31] and authors' papers).

Strategy	Direction	Algorithm	Complexity	Year	Reference
Condensation	Incremental	CNN	$\mathcal{O}(n^3)$	1968	[27]
	Incremental	PSC	$\mathcal{O}(n \log n)$	2010	[46]
	Decremental	RNN	$\mathcal{O}(n^3)$	1972	[25]
	Decremental	MSS	$\mathcal{O}(n^2)$	2002	[6]
Hybrid	Decremental	DROP1-5	$\mathcal{O}(n^3)$	2000	[60]
	Batch	ICF	$\mathcal{O}(n^2)$	2002	[8]
	Batch	HMN-EI	$\mathcal{O}(n^2)$	2008	[41]
	Batch	LSBo	$\mathcal{O}(n^2)$	2015	[37]

In the remaining part of this section, we give further details of the most representative methods used in the experimental setup. A summary of the methods considered in the study can be seen in Table 1.

2.1.1. Condensation

The algorithm of Hart, *Condensed Nearest Neighbor* (CNN) [27] is considered the first formal proposal of instance selection for the nearest neighbor rule. The concept of training set consistency is important in this algorithm and is defined as follows: given a non empty set X ($X \neq \varnothing$), a subset S of X ($S \subseteq X$) is consistent with respect to X if, using the subset S as training set, the nearest neighbor rule can correctly classify all instances in X. Following this definition of consistency, if we consider the set X as the training set, a condensed subset should have the properties of being consistent and, ideally, smaller than X. After CNN appeared, other condensation methods emerged with the aim of decreasing the size of the condensed data set, e.g.: Reduced Nearest Neighbor (RNN) [25]. One of the latest is the Prototype Selection by Clustering (PSC) [46], which uses clustering to speed up the selection process. So, the use of clustering gives a high efficiency to PSC, if compared against state-of-the-art methods, and better accuracy than other clustering-based methods such as CLU [40].

In [6], the authors proposed a modification to the definition of a selective subset [54], for a better approximation to decision borders. The selective subset can be thought of as similar to the idea of the condensed algorithm of Hart, but applying a condition stronger than the condition of consistency. The aim is to find the selected instances in an easier way, which is less sensitive to the random initialization of S and the order of exploration of X in Harts' algorithm. The subset obtained in this way is called the selective subset (SS).

A subset S of the training set X is a *selective* subset (SS), if it satisfies the following conditions:

1. S is consistent (as in Harts' algorithm).
2. All instances in the original training set, X, are closer to a *selective neighbor* (a member of S) of the same class than to any instance of a different class in X.

Then, the authors present a greedy algorithm which attempts to find selective instances starting with those instances of the training set that are close to the decision boundary of the nearest neighbor classifier. The algorithm presented is an efficient alternative to the Selective algorithm [54] and it is usually able to select better instances (the ones closer to the boundaries).

2.1.2. Hybrid

One problem that arises when condensation methods are used is their noise sensitivity, while hybrid methods have specific mechanisms to make them more robust to noise [37].

The DROP (Decremental Reduction Optimization Procedure) [60] family of algorithms comprises some of the best instance selection methods for classification [8, 47, 50]. The instance removal criteria is based on two relations: *associates* and nearest neighbors. The relation of associate is the inverse of nearest neighbors: those instances **p** that have **q** as one of their nearest neighbors are called associates of **q**. The set of nearest neighbors of one instance is called the *neighborhood* of the instance. For all instances, its list of associates is a list with all instances that have that particular instance in their neighborhood.

Marchiori proposed a new graph-based representation of the data set called Hit Miss Networks (HMN) [41]. The graph has a directed edge from each instance to its nearest neighbor on the different classes, with one edge per class. The information in the graph was used to define three new hybrid algorithms: HMN-E, HMN-C and HMN-EI. A couple of years later, HMNs were used to define a new information-theoretic instance scoring method to define a new instance selection method called Class Conditional Nearest Neighbor (CCIS) [42]. According to [21], HMN-EI is able to achieve more accurate data sets than CCIS which is the reason why HMN-EI was used in experimental setup.

The local-set (LS) concept, proposed for the very first time in [7], is a powerful tool for some machine learning tasks, including instance selection. A local-set of an instance **x** contains all those instances which are closer to **x** than its nearest neighbor of different class, its *nearest enemy*. The selection rule of the Iterative Case Filtering algorithm (ICF) [7] uses local sets to build two sets: *coverage* and *reachability*. These two concepts are closely related to the neighborhood and associate list used in DROP algorithms. The coverage of an instance is its LS, that can be seen as a neighborhood of the instance that, instead of considering a fixed number k of neighbor, includes all instances closer to the instance than its closest enemy. The reachable set of an instance is its set of associates. The coverage set of an instance is its neighborhood. The deletion rule is as follows: an instance is removed from the data set if its reachable set (its set of associates) is bigger than its coverage (its 'neighborhood'). This rule means that the algorithm removes an instance if other object exists that generalizes its information. To address the problem of noisy data sets, both ICF and DROP3, begin with a noise-filter stage. Recently, Leyva et al [37] presented three new instance selection methods based on LSs. Their hybrid approach, which offers a good balance between reduction and accuracy, is called Local Set Border Selector (LSBo) and it uses a heuristic criterion: the instances in the boundaries between classes tend to have greater LSs. As is usual in hybrid methods, LSBo starts with a noise filtering algorithm which was presented in the same paper called LSSm.

2.2. Scaling up instance selection

The main drawback of instance selection methods is their complexity that is quadratic $\mathcal{O}(n^2)$, where n is the number of instances [22] or, at best, log-linear $\mathcal{O}(n \log n)$; thus, the majority of them are not applicable in data sets with hundreds or even many thousands of instances [15]. Table 1 summarizes the computational complexity of the instance selection methods used in the experimental section.

One approach to deal with massive data sets, is to divide the original problem into smaller subsets of instances; known as stratification. The underlying idea of these methods is to split the original data set into disjointed subsets, then an instance selection algorithm is applied to each subset [10, 13, 22, 24]. This approach is used in [22] where a method was proposed that addressed the splitting process, using Grand Tour [5] theory, to achieve linear complexity.

The problem known as big data refers to the challenges and difficulties that arise when huge amounts of data are processed. One way to accelerate instance selection methods and to be able to cope with massive data sets is adapt them to parallel environments [49]. To do so, the way that algorithms work has to be redesigned. The MapReduce paradigm offers a robust framework with which to process huge data sets over clusters of machines. Following up on this idea, a new proposal was presented recently by Triguero et al. [58].

3. Locality-sensitive hashing

The *locality-sensitive hashing* (*LSH*) is an efficient method for checking similarity between elements. It makes a particular use of *hash* functions that, unlike those used in other applications of hashing[1], seeks to allocate similar items to the same bucket with a high probability, and at the same time to greatly reduce the probability of assigning dissimilar items to the same bucket [35].

LSH use is common to increase the efficiency of nearest neighbors calculation [3, 21]. An indirect benefit of LSH for instance selection algorithms is the speeding up of nearest neighbor calculation, required in most of these sorts of algorithms. However, the complexity of the algorithms remain unchanged, since the loop nesting and structures of the algorithms remain the same. It is only the kNN step that is improved.

What we propose in this paper is a novel use of LSH, not merely as support for the calculation of nearest neighbors, but as an operation that defines the nature of the new instances selection algorithm. Basically, the idea is to make the instance selection on each of the buckets that will be obtained by LSH when applied to all instances. This process permits the selection of instances using a unique processing loop of the data set, thereby giving it linear complexity. So a reasonable question arises; when a classifier is trained with a selected subset obtained by this approach, will its prediction capabilities decrease? This article offers an experimental response to this question[2]. But before giving the details of our proposal, let us look at a brief introduction to the underlying theory of LSH.

[1]The aim of conventional cryptographic hash functions is to avoid the collision of items in the same bucket.

[2]In any case, note that even a certain degradation of classifier performance would be acceptable, if the new algorithm achieved a substantial acceleration or reduction in storage [9], it is often better to gain a quick approximation within a reasonable time than an optimal solution when it is too late to use it.

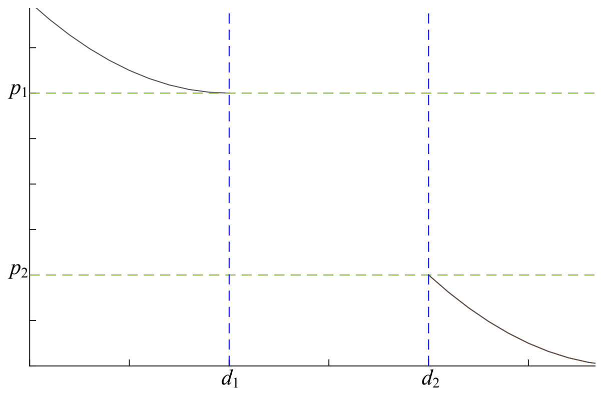


Figure 1: Expected behavior of the probabilities of a (d_1, d_2, p_1, p_2)-sensitive function. The function will assign the same value to two instances with a probability greater than p_1, if their distance is shorter than d_1. The function will assign the same value to two instances with a probability lower than p_2, if their distance is greater than d_2. For distances between d_2 and d_1, there is no restriction regarding that the values the function can assign to the instances.

3.1. Locality-sensitive functions

In this section we follow [35], to formally define the concept of local sensitivity and the process of amplifying a locality-sensitive family of functions.

Given a set of objects S and a distance measure D, a family of hash functions $\mathcal{H} = \{h : S \to U\}$ is said to be (d_1, d_2, p_1, p_2)-sensitive, if the following properties hold for all functions of h in the family $\mathcal{H}$:

- For all x, y in S, if $D(x, y) \leq d_1$, then the probability that $h(x) = h(y)$ is at least p_1.
- For all x, y in S, if $D(x, y) > d_2$, then the probability that $h(x) = h(y)$ is at most p_2.

In this definition, nothing refers to what happens when the distance of the objects is between d_1 and d_2 (see the representation in Figure 1). However, distances d_1 and d_2 can be as close as possible, but the cost will be that p_1 and p_2 are also closer. However, as shown below, it is possible to combine families of hash functions that separate the probabilities p_1 and p_2 without modifying the distances d_1 and d_2.

Given a (d_1, d_2, p_1, p_2)-sensitive family of hash functions $\mathcal{H}$, it is possible to obtain a new family $\mathcal{H}'$ using the following amplification operations

AND-construction The functions h in $\mathcal{H}'$ are obtained by combining a fixed number r of functions $\{h_1, h_2, \ldots, h_r\}$ in $\mathcal{H}$. Now, $h(x) = h(y)$, if and only if $h_i(x) = h_i(y)$ **for all** i. If the independence of functions in $\mathcal{H}$ can be guaranteed, the new family of functions $\mathcal{H}'$ will be $(d_1, d_2, (p_1)^r, (p_2)^r)$-sensitive.

OR-construction The functions h in $\mathcal{H}'$ are obtained by combining a fixed number b of functions $\{h_1, h_2, \ldots, h_b\}$ in $\mathcal{H}$. Now, $h(x) = h(y)$, if and only if $h_i(x) = h_i(y)$ **for any** i. If the independence of functions in $\mathcal{H}$ can be guaranteed, the new family of functions $\mathcal{H}'$ will be $(d_1, d_2, 1 - (1 - p_1)^b, 1 - (1 - p_2)^b)$-sensitive.

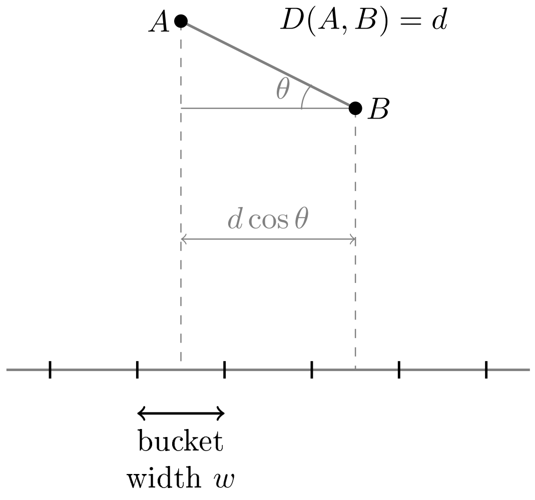


Figure 2: Two points (A, B) at distance $d \gg w$ have a small chance of being hashed to the same bucket.

The AND-construction decreases the probabilities and the OR-construction increases them. However, if r and b are properly chosen and with the chaining of constructions the probability p_1 may be brought closer to 1, while the probability p_2 will stay reasonably close to 0.

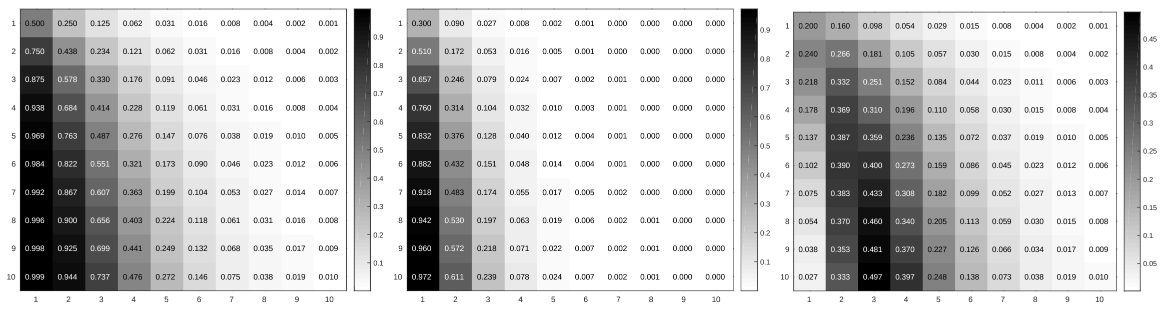
In the experimental setup, the hash functions in the base family were obtained using the following equation [12].

$$h_{\vec{a},b}(\vec{x}) = \left\lfloor \frac{\vec{a} \cdot \vec{x} + b}{w} \right\rfloor \tag{1}$$

where $\vec{a}$ is a random vector (Gaussian distribution with mean 0 and standard deviation 1), b is a random real value from the interval $[0, w]$ and w is the width of each bucket in the hash table.

This equation gives a $(w/2, 2w, 1/2, 1/3)$-sensitive family. The reason for these numbers is as follows (suppose, for simplicity, a 2-dimensional Euclidean space), if the distance d between two points is exactly $w/2$ (half the width of the buckets) the smallest probability for the two points falling in the same segment would happen for $\theta = 0$, and in this case the probability would be 0.5, since d is exactly $w/2$. For angles greater than 0, this probability will be even higher; in fact, it will be 1 for $\theta = 90$. And for shorter distances than $w/2$, the probability will equally increase. So the lower boundary for this probability is 1/2. If the distance d is exactly $2w$ (twice the width of the bucket), the only chance for both points to fall in the same bucket is that their distances, once projected in the segment, are lower than w, what means that $\cos\theta$ must be lower than 0.5, since the projected distance is $d\cos\theta$ and d is exactly $2w$. For θ in the interval 0 to 60, $\cos\theta$ is greater than 0.5, so the only chance of $\cos\theta$ being lower than 0.5 is that θ is in the interval $[60, 90]$, and the chance of that happening is at most 1/3. For distances greater than $2w$, the probabilities are even lower. So the upper boundary of this probability is 1/3. This reasoning is reflected in Figure 2.

By using the $(w/2, 2w, 1/2, 1/3)$-sensitive family previously described, we have computed the probabilities p_1 and p_2 for the AND-OR construction with a number of functions from 1 to 10. Figure 3 shows the probabilities p_1 (a) and p_2 (b) for the case of the



(a) p_1

	1	2	3	4	5	6	7	8	9	10
1	0.500	0.250	0.125	0.062	0.031	0.016	0.008	0.004	0.002	0.001
2	0.750	0.438	0.234	0.121	0.062	0.031	0.016	0.008	0.004	0.002
3	0.875	0.578	0.330	0.176	0.091	0.046	0.023	0.012	0.006	0.003
4	0.938	0.684	0.414	0.228	0.119	0.061	0.031	0.016	0.008	0.004
5	0.969	0.763	0.487	0.276	0.147	0.076	0.038	0.019	0.010	0.005
6	0.984	0.822	0.551	0.321	0.173	0.090	0.046	0.023	0.012	0.006
7	0.992	0.867	0.607	0.363	0.199	0.104	0.053	0.027	0.014	0.007
8	0.996	0.900	0.656	0.403	0.224	0.118	0.061	0.031	0.016	0.008
9	0.998	0.925	0.699	0.441	0.249	0.132	0.068	0.035	0.017	0.009
10	0.999	0.944	0.737	0.476	0.272	0.146	0.075	0.038	0.019	0.010

(b) p_2

	1	2	3	4	5	6	7	8	9	10
1	0.300	0.090	0.027	0.008	0.002	0.001	0.000	0.000	0.000	0.000
2	0.510	0.172	0.053	0.016	0.005	0.001	0.000	0.000	0.000	0.000
3	0.657	0.246	0.079	0.024	0.007	0.002	0.001	0.000	0.000	0.000
4	0.760	0.314	0.104	0.032	0.010	0.003	0.001	0.000	0.000	0.000
5	0.832	0.376	0.128	0.040	0.012	0.004	0.001	0.000	0.000	0.000
6	0.882	0.432	0.151	0.048	0.014	0.004	0.001	0.000	0.000	0.000
7	0.918	0.483	0.174	0.055	0.017	0.005	0.002	0.000	0.000	0.000
8	0.942	0.530	0.197	0.063	0.019	0.006	0.002	0.001	0.000	0.000
9	0.960	0.572	0.218	0.071	0.022	0.007	0.002	0.001	0.000	0.000
10	0.972	0.611	0.239	0.078	0.024	0.007	0.002	0.001	0.000	0.000

(c) $p_1 - p_2$

	1	2	3	4	5	6	7	8	9	10
1	0.200	0.160	0.098	0.054	0.029	0.015	0.008	0.004	0.002	0.001
2	0.240	0.266	0.181	0.105	0.057	0.030	0.015	0.008	0.004	0.002
3	0.218	0.332	0.251	0.152	0.084	0.044	0.023	0.011	0.006	0.003
4	0.178	0.369	0.310	0.196	0.110	0.058	0.030	0.015	0.008	0.004
5	0.137	0.387	0.359	0.236	0.135	0.072	0.037	0.019	0.010	0.005
6	0.102	0.390	0.400	0.273	0.159	0.086	0.045	0.023	0.012	0.006
7	0.075	0.383	0.433	0.308	0.182	0.099	0.052	0.027	0.013	0.007
8	0.054	0.370	0.460	0.340	0.205	0.113	0.059	0.030	0.015	0.008
9	0.038	0.353	0.481	0.370	0.227	0.126	0.066	0.034	0.017	0.009
10	0.027	0.333	0.497	0.397	0.248	0.138	0.073	0.038	0.019	0.010

Figure 3: Probabilities p_1 and p_2 and the difference between them. The darker the color the higher the value. Each cell gives the value for the chaining of an OR-construction (number of combined basic functions on the x-axis) after an AND-construction (on the y-axis the number of combined functions).

chaining of an OR-construction just after an AND-construction, and the difference between these two probabilities (c). The row number indicates the number of functions used in the AND-construction, while the column number indicates the number of functions used in the OR-construction.

4. New instance selection algorithms based on hashing

This section presents the algorithms proposed in this work: LSH-IS-S and LSH-IS-F. The first completes the selection process in a single pass, analyzing each instance consecutively. It processes instances in one pass, so not all instances need to fit in memory. The second performs two passes: in the initial one, it counts the instances in each bucket, in the second, it completes the instance selection with this information. The complexity of both algorithms is linear, $\mathcal{O}(n)$ (note that this is even true for the second algorithm, i.e. although two passes are performed).

Both algorithms can be seen as incremental methods, due to the fact that the selected data set is formed by successive additions to the empty set. However, the second one conforms more closely to batch processing because it analyzes the impact of the removal on the whole data set.

The main advantage of the presented methods is the drastic reduction in execution time. The experimental results show a significant difference when they are compared against state-of-the-art instance selection algorithms.

4.1. LSH-IS-S: One-pass processing

As shown in Algorithm 1, the inputs of the LSH-IS-S method are: a set of instances to select and a set of families of hash functions. The loop processes each instance $\mathbf{x}$ of X, using the function families to determine the bucket u to which the instance belongs[3]. If in the bucket u assigned to the instance there is no other instance of the same class of $\mathbf{x}$,

[3]The bucket identifier u given to an instance by a family $g \in \mathcal{G}$ can be thought of as the concatenation of all bucket identifiers given by the hash functions in g, since the function families in $\mathcal{G}$ are obtained by using an AND-construction on base functions obtained using Equation 1. The OR-construction is implemented in the foreach loop at line 3 of Algorithm 1.

x is selected and added to S and to the bucket u. The algorithm ends when all instances in X have been processed. Note that each instance is processed only once, which grants an extremely fast performance at the expense of not analyzing the instances that are selected in each bucket in detail. Instances are analyzed in sequence without needing information on other instances. This process means that the method may be used in a single-pass process, without requiring the whole dataset to fit in the memory.

Algorithm 1: LSH-IS-S – Instance selection algorithm by hashing in one pass.

```
  Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, set $\mathcal{G}$ of hash function families
  Output: The set of selected instances $S \subseteq X$
1 $S = \varnothing$
2 foreach instance $\mathbf{x} \in X$ do
3     foreach function family $g \in \mathcal{G}$ do
4         $u \leftarrow$ bucket assigned to $\mathbf{x}$ by family $g$
5         if there is no other instance of the same class of $\mathbf{x}$ in $u$ then
6             Add $\mathbf{x}$ to $S$
7             Add $\mathbf{x}$ to $u$
8 return $S$
```

4.2. LSH-IS-F: A more informed selection

The algorithm explained in the previous section is remarkably fast and allows instances to be processed as they arrive, in one pass. On the other hand, because of how it works, it is not using all information that may be relevant to decide which instances to choose. For example, the algorithm has no control over the number of instances of each class that go to each bucket, because once an instance of a class is selected, it discards other instances of the same class that may come later.

LSH-IS-F (see Algorithm 2) is an evolution of the LSH-IS-S. In this method, one-pass processing is replaced by a more informed selection. The first loop is similar to LSH-IS-S but, instead of directly selecting instances, it first records the bucket to which each instance belongs. When there is only one instance of a class, the instance is rejected, otherwise, if two or more instances of the same class are present, one of them is randomly chosen. The idea here is to give the algorithm some tolerance of the presence of noise in the input data set.

The execution time of this method is not much larger than in the previous method, since the number of buckets is much lower than the number of instances. Although, the differences in execution time increase with the increase in the number of OR functions.

4.3. Behavior of proposed methods

The aim of this section is to try to shed some light on the behavior of the new algorithms proposed in the paper. As previously stated, LSH-IS-S makes the selection of instances in one pass, selecting one instance of each class in each bucket. On the other hand, LSH-IS-F tries to avoid retaining noisy instances. The more informed selection criterion of LSH-IS-F allows it to remove instances that can be harmful for the classification.

Algorithm 2: LSH-IS-F – Instance selection algorithm by hashing with two passes.

```
   Input: A training set $X = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$, set $\mathcal{G}$ of hash function families
   Output: The set of selected instances $S \subseteq X$
1  $S = \varnothing$
2  foreach instance $\mathbf{x} \in X$ do
3      foreach function family $g \in \mathcal{G}$ do
4          $u \leftarrow$ bucket assigned to $\mathbf{x}$ by family $g$
5          Add $\mathbf{x}$ to $u$
6  foreach function family $g \in \mathcal{G}$ do
7      foreach bucket $u$ of $g$ do
8          foreach class $y$ with some instance in $u$ do
9              $I_y \leftarrow$ all instances of class $y$ in $u$
10             if $|I_y| > 1$ then
11                 Add to $S$ one random instance of $I_y$
12 return $S$
```

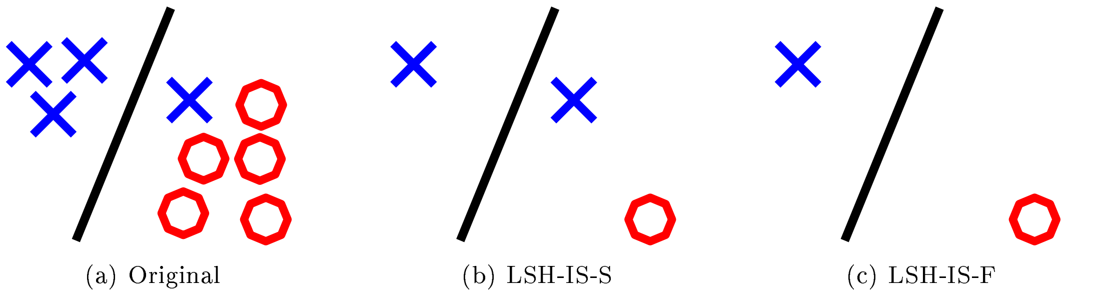
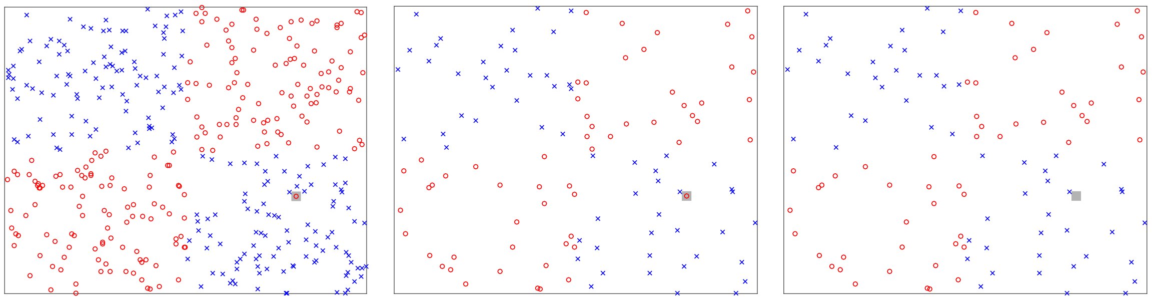


Figure 4: Example to illustrate the behavior of both algorithms. (a) Initial instances, two buckets are identified by LSH and the line shows the boundary. (b) Instances selected by LSH-IS-S. (c) Instances selected by LSH-IS-F.

In Figure 4 we show an example with nine instances: four of one class (crosses) and five of the other (circles). The LSH algorithm is using two buckets, the line represents the boundary between them. LSH-IS-S selects one instance of each class in each bucket (b), while LSH-IS-F does not select the instance of class cross because it is identified as noise.

Figure 5 illustrates the effect of the algorithms in the XOR data set [42] formed by 400 instances, 200 per class. An outlier was added and highlighted with a gray square. As indicated above, LSH-IS-S retains the instance, while LSH-IS-F removes it.

With the aim of illustrating the behavior of the proposed instance selection methods when the number of hash functions increases, we used the Banana data set. It has two numeric features and two classes, the size of the data set is 5300 instances (see Table 3). Figure 6(a) shows the original data set. Despite the fact that two clusters can be easily identified, a high overlap exists between the two classes in some regions [21]. Table 2 summarizes the number of instances selected by both algorithms when only one OR function is used and the number of AND functions changes. LSH-IS-F retains less



(a) Original (b) LSH-IS-S (c) LSH-IS-F

Figure 5: (a) Original XOR example, an outlier is highlighted in gray. (b) LSH-IS-S selection maintains the outlier. (c) LSH-IS-F removes the outlier.

Table 2: Number of Banana data set instances that the proposed algorithms retain by the number of AND functions.

Algorithm	Number of AND functions				
	2	4	6	8	10
LSH-IS-S	25	123	249	466	684
LSH-IS-F	24	110	225	423	627

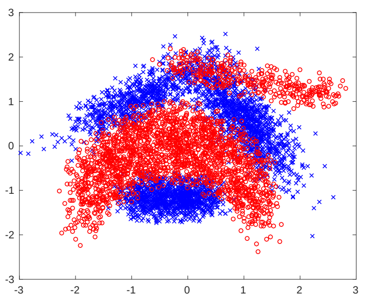
instances, because those instances of one class isolated in one bucket with instances of the other class are identfied as noise and therefore deleted.

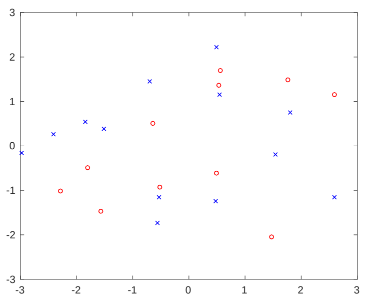
Figures 6 and 7 show the instances retained by both algorithms, LSH-IS-S and LSH-IS-F respectively, when only one OR function is used and different numbers of AND functions: 2, 4, 6, 8 and 10. The number of retained instances increases with the number of functions. This behavior is quite interesting, because it enables the user to choose whether more or fewer instances are retained, by varying the number of functions that are used.

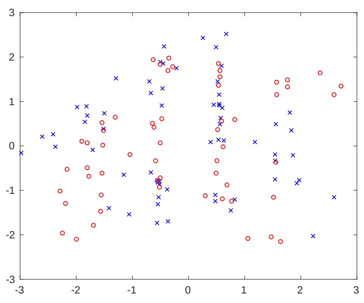
5. Experimental study

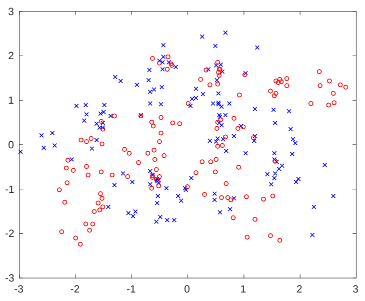
This section presents the experimental study performed to evaluate the new proposed methods. We compared them against seven well-known state-of-the-art instance selection algorithms in a study performed in Weka [62]. The instance selection methods included in the experiments were: CNN, ICF, MSS, DROP3, PSC, HMN-EI, LSBo and the two approaches based on hashing. The parameters selected for the algorithms were those recommended by the authors: the number of nearest neighbors used on ICF and DROP3 were set to $k = 3$, the number of clusters for PSC was set to $6r$ (where r is the number of classes of the data set). Evolutionary algorithms were not included in the experiments, due to their high computational cost.

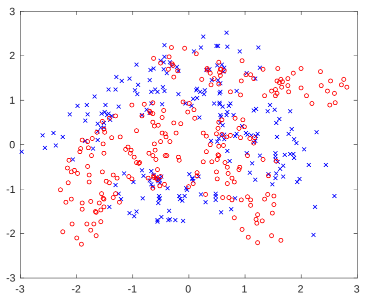
For the experiments, we used 30 data sets from the Keel repository [1] that have at least 1000 instances. Table 3 summarizes the data sets: name, number of features, number of instances and the accuracy given by two classifiers (using ten fold cross-validation): the nearest neighbor classifier with $k = 1$ and the J48, a classifier tree (the


(a) Banana (Orig.)


(b) LSH-IS-S: AND=2


(c) LSH-IS-S: AND=4


(d) LSH-IS-S: AND=6


(e) LSH-IS-S: AND=8

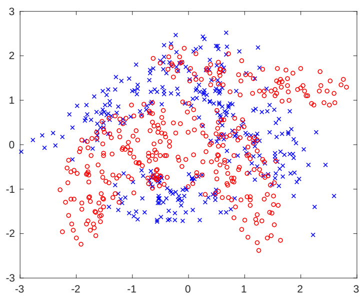
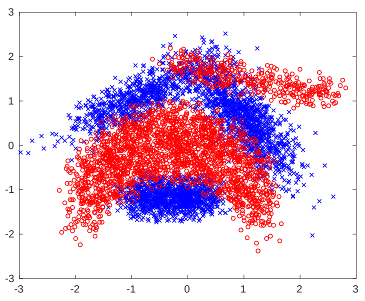
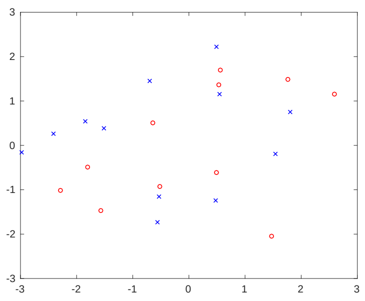
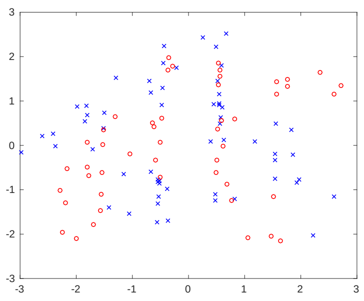
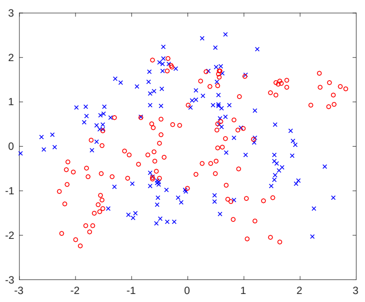

(f) LSH-IS-S: AND=10

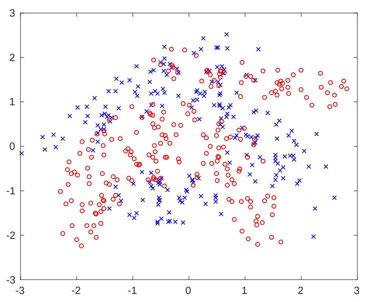
Figure 6: The number of instances selected by LSH-IS-S as the number of functions increases.


(a) Banana (Orig.)


(b) LSH-IS-F: AND=2


(c) LSH-IS-F: AND=4


(d) LSH-IS-F: AND=6


(e) LSH-IS-F: AND=8

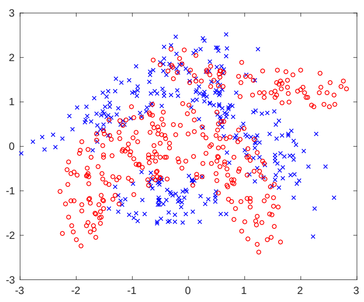

(f) LSH-IS-F: AND=10

Figure 7: The number of instances selected by LSH-IS-F as the number of functions increases.

Weka implementation of C4.5 [53]). The last five data sets are huge (below dashed line), with more than 299 000 instances, the traditional instance selection methods are unable to address them. The only transformation carried out was the normalization of all input features, to set their values at between 0 and 1.

We used the nearest neighbor classifier (1NN), as most instance selection methods have been designed for that classifier ($k = 1$ in kNN) [37, 51]. Moreover, we used the J48 classifier tree, to evaluate the extent to which the instances selected by the algorithms were suitable for training other classifiers.

As shown in Section 3, there are ways of combining the hash functions families that appear more promising than others (see Figure 3). However, it is unclear which of them will achieve the best results in combination with the proposed algorithms. Therefore, we conducted a study with 60 combinations: AND-constructions, combining between 1 to 10 hash functions, and OR-constructions, combining 1 to 6 functions, obtained by the previous AND-construction, avoiding constructions with too many functions and, consequently, reducing the computational cost.

The subsets selected by the algorithms were used to build a classifier (1NN), the average rank [14] of which was performed over the accuracy of all 60 combinations. Average ranks were calculated as follows: the results of the experiments were sorted, one for the best method, two for the second, and so on. In the case of a tie, values of the ranks were added up and divided into the number of methods that tied. When the ranking of each data set was calculated, the average for each method was computed. Better methods had rankings closer to one. The results of the rankings are shown in Figure 8. Each cell represents the ranking value for a specific combination of AND-OR-constructions, where the number of functions in the OR-constructions is shown by the x-axis and the number of functions in the AND-constructions is shown by the y-axis number. The darker the cell the higher its ranking (lower values are better). The best configuration is different for each algorithm:

- LSH-IS-S: the best configuration is one that uses OR-constructions of 6 functions obtained using an AND-construction on 10 functions of the base family (functions obtained using Equation 1).
- LSH-IS-F: the best results were obtained using OR-constructions of 5 functions obtained by combining by AND-construction 10 functions of the base family.

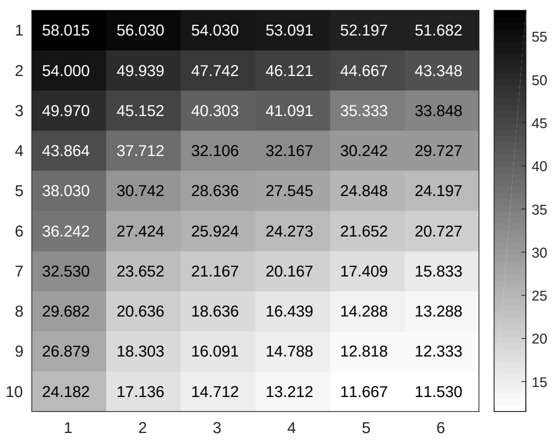
Figure 9 shows how the time execution increases, on average, for the proposed algorithms: LSH-IS-S (gray) and LSH-IS-F (black). The higher the number of AND functions, the bigger the gap between LSH-IS-S and LSH-IS-F. This behavior is explained because LSH-IS-F has one loop more than LSH-IS-S (see pseudocodes 1 and 2) that is used to go through all the buckets counting the number of instances of each class. The number of buckets searched increases with the number of hash functions.

Ten fold cross-validation was applied to the instance selection methods under study. The performances were as follows:

- accuracy achieved by 1NN and J48 classifiers trained with the selected subset;
- filtering time by instance selection;
- reduction achieved by instance selection methods (size of the selected subset).

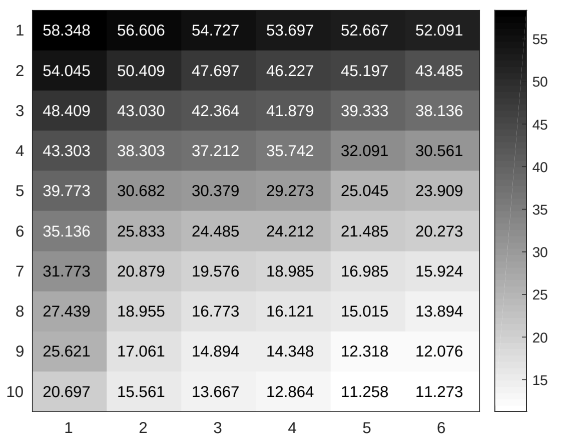
Table 3: Summary of data sets characteristics: name, number of features, number of instances and accuracy (1NN). Last five data sets, below dashed line, are huge problems.

	Data sets	# attributes		# instances	Accuracy	
		Continuous	Nominal		1NN	J48
1	German	7	13	1 000	72.90	71.80
2	Flare	0	11	1 066	73.26	73.55
3	Contraceptive	9	0	1 473	42.97	53.22
4	Yeast	8	0	1 484	52.22	56.74
5	Wine-quality-red	11	0	1 599	64.85	62.04
6	Car	0	6	1 728	93.52	92.36
7	Titanic	3	0	2 201	79.06	79.06
8	Segment	19	0	2 310	97.23	96.62
9	Splice	0	60	3 190	74.86	94.17
10	Chess	0	35	3 196	72.12	81.85
11	Abalone	7	1	4 174	19.84	20.72
12	Spam	0	57	4 597	91.04	92.97
13	Wine-quality-white	11	0	4 898	65.40	58.23
14	Banana	2	0	5 300	87.21	89.04
15	Phoneme	5	0	5 404	90.19	86.42
16	Page-blocks	10	0	5 472	95.91	97.09
17	Texture	40	0	5 500	99.04	93.13
18	Optdigits	63	0	5 620	98.61	90.69
19	Mushroom	0	22	5 644	100.00	100.00
20	Satimage	37	0	6 435	90.18	86.28
21	Marketing	13	0	6 876	28.74	31.06
22	Thyroid	21	0	7 200	92.35	99.71
23	Ring	20	0	7 400	75.11	90.95
24	Twonorm	20	0	7 400	94.81	85.12
25	Coil 2000	85	0	9 822	90.62	93.95
26	Penbased	16	0	10 992	99.39	96.53
27	Nursery	0	8	12 960	98.13	97.13
28	Magic	10	0	19 020	80.95	85.01
29	Letter	16	0	20 000	96.04	87.98
30	KR vs. K	0	6	28 058	73.05	56.58
31	Census	7	30	299 285	92.70	95.42
32	KDDCup99	33	7	494 021	99.95	99.95
33	CovType	54	0	581 012	94.48	94.64
34	KDDCup991M	33	7	1 000 000	99.98	99.98
35	Poker	5	5	1 025 010	50.61	68.25



	1	2	3	4	5	6
1	58.015	56.030	54.030	53.091	52.197	51.682
2	54.000	49.939	47.742	46.121	44.667	43.348
3	49.970	45.152	40.303	41.091	35.333	33.848
4	43.864	37.712	32.106	32.167	30.242	29.727
5	38.030	30.742	28.636	27.545	24.848	24.197
6	36.242	27.424	25.924	24.273	21.652	20.727
7	32.530	23.652	21.167	20.167	17.409	15.833
8	29.682	20.636	18.636	16.439	14.288	13.288
9	26.879	18.303	16.091	14.788	12.818	12.333
10	24.182	17.136	14.712	13.212	11.667	11.530

(a) LSH-IS-S



	1	2	3	4	5	6
1	58.348	56.606	54.727	53.697	52.667	52.091
2	54.045	50.409	47.697	46.227	45.197	43.485
3	48.409	43.030	42.364	41.879	39.333	38.136
4	43.303	38.303	37.212	35.742	32.091	30.561
5	39.773	30.682	30.379	29.273	25.045	23.909
6	35.136	25.833	24.485	24.212	21.485	20.273
7	31.773	20.879	19.576	18.985	16.985	15.924
8	27.439	18.955	16.773	16.121	15.015	13.894
9	25.621	17.061	14.894	14.348	12.318	12.076
10	20.697	15.561	13.667	12.864	11.258	11.273

(b) LSH-IS-F

Figure 8: Average rank over accuracy of the proposed methods for the different configurations of AND-OR constructions. The darker the cell, the higher the ranking (lower is better). Each cell represents an AND-OR-construction where the column is the number of functions in the OR-construction and the row is the number of functions in the AND-construction.

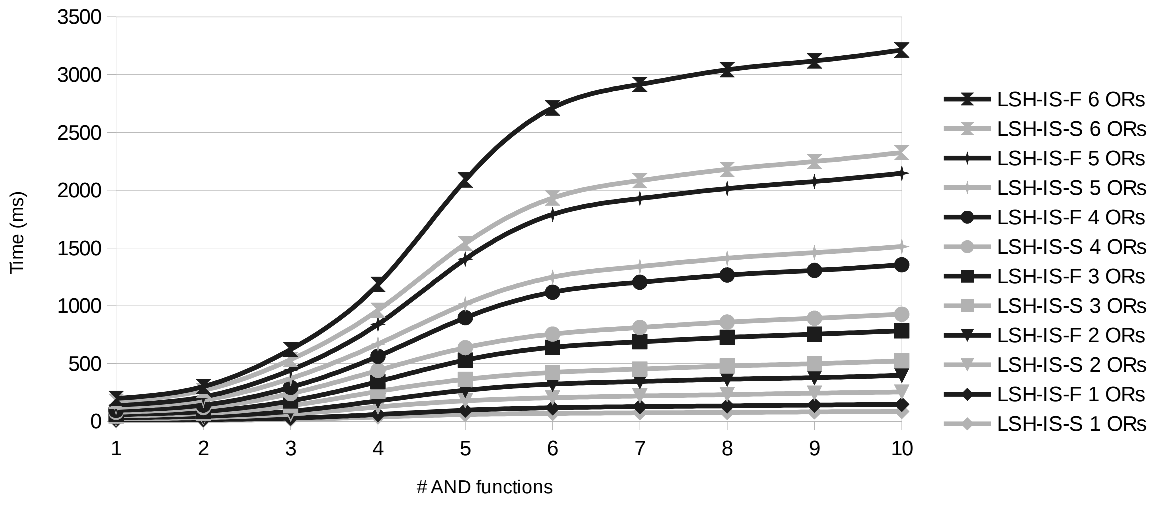


Figure 9: Average execution time of the proposed algorithms as the number of AND-functions increases. LSH-IS-S is represented in gray and LSH-IS-F in black with different lines and marks for the different numbers of OR-functions.

Table 4: Average ranks and Hochberg procedure over accuracy: 1NN.

Algorithm	Ranking	p Hoch.
HMN-EI	2.92	
LSBo	3.85	0.1869
LSH-IS-F	4.45	0.0602
MSS	4.58	0.0553
LSH-IS-S	4.98	0.0139
DROP3	5.03	0.0138
CNN	5.17	0.0088
ICF	5.75	0.0004
PSC	8.27	0.0000

Table 5: Average ranks and Hochberg procedure over accuracy: J48.

Algorithm	Ranking	p Hoch.
LSH-IS-F	3.63	
LSH-IS-S	3.88	0.7237
HMN-EI	4.10	0.7237
LSBo	4.57	0.5606
MSS	5.03	0.1909
CNN	5.28	0.0981
ICF	5.67	0.0242
DROP3	5.90	0.0094
PSC	6.93	0.0000

Table 6: Average ranks and Hochberg procedure over storage reduction, and average reduction rate.

Algorithm	Ranking	p Hoch.	Reduction rate
DROP3	1.67		0.896
ICF	3.10	0.0427	0.813
LSBo	3.70	0.0081	0.737
PSC	4.70	0.0001	0.762
CNN	5.43	0.0000	0.658
MSS	6.00	0.0000	0.665
HMN-EI	6.10	0.0000	0.577
LSH-IS-F	6.62	0.0000	0.455
LSH-IS-S	7.68	0.0000	0.405

According to the accuracy of 1NN classifier (see Table 4), the best four algorithms were HMN-EI followed by LSBo, LSH-IS-F and MSS. According to the Hochberg procedure [29], differences between them were not significant at a 0.05 significance level. However, differences between LSBo and the other methods were significant. When J48 was used as the classifier (see Table 5), the best six algorithms were LSH-IS-F followed by LSH-IS-S, HMN-EI, LSBo, MSS and CNN; the differences between them were not significant at 0.05. Furthermore, as can be seen, the least accurate model is PSC for both classifiers.

Table 6 shows the average ranks over compression. DROP3 is the best method at a 0.05 significance level. Furthermore, the average reduction rate for each method is also shown. The proposed methods are the most conservative, although, as previously stated, a higher compression could have been achieved using fewer functions in the LSH process.

The third relevant feature of instance selection methods is the time required by the algorithms to calculate the selected subset. Table 7 shows the average rank over execution time of the instance selection algorithms. The three fastest methods were LSH-IS-F, LSH-IS-S and PSC, between them differences were not significant at a 0.05 significance level. The differences were significant from MSS and the following methods; the slowest was

Table 7: Average ranks and Hochberg procedure over filtering time.

Algorithm	Ranking	p Hoch.
LSH-IS-F	1.53	
LSH-IS-S	1.57	0.9624
PSC	3.00	0.0761
MSS	4.20	0.0005
ICF	5.33	0.0000
LSBo	6.73	0.0000
HMN-EI	6.70	0.0000
DROP3	7.67	0.0000
CNN	8.27	0.0000

CNN. It is worth noting that PSC achieved, according to the significance tests, a really competitive execution time. Nevertheless the shortcoming of PSC was its poor accuracy, as it obtained the worst results of all of the methods under analysis, as noted in Tables 4 and 5.

It might be surprising that LSH-IS-F was faster than LSH-IS-S, because this contradicts Figure 9. The reason for this was the number of functions used by the algorithms; as commented on at the beginning of this section, LSH-IS-S was launched using 6 OR functions, while LSH-IS-F was launched with only 5.

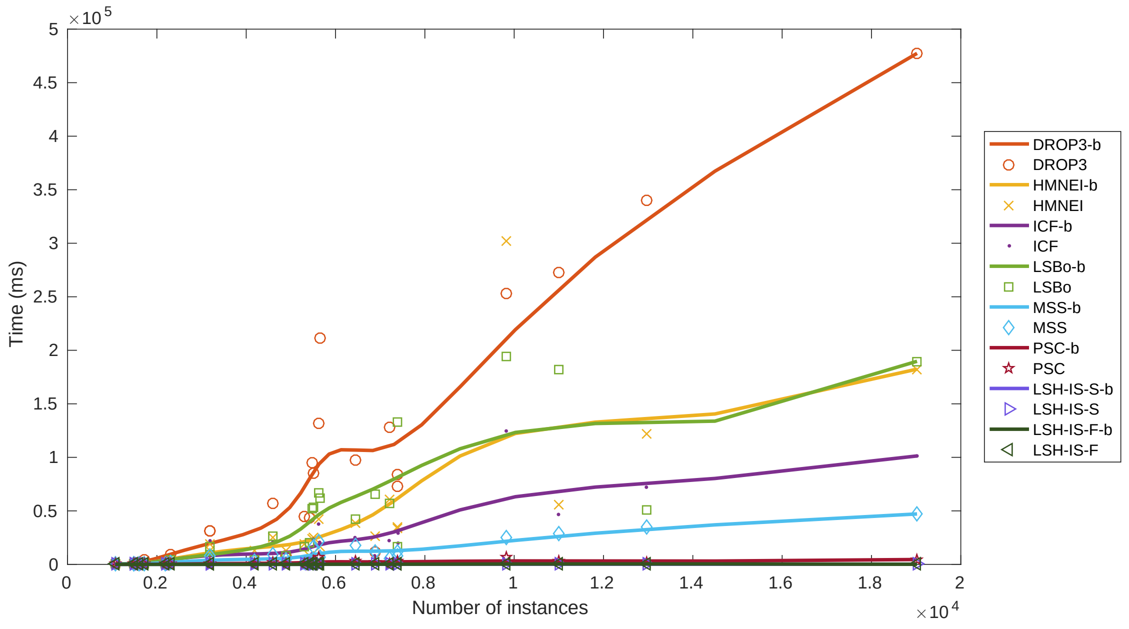
Figure 10 shows the filtering time as a function of the number of instances. The results obtained with the data sets of the experiments were used to draw these figures. Since there were no results available for all possible values of numbers of instances, the available results were used to draw Bezier lines and to show the general trend of the algorithms. Although other methods (CNN, HMN-EI, LSBo, DROP3, MSS and ICF) have an execution time that increases swiftly, our algorithms based on hashing are at the bottom of the figures together with PSC. However, in the logarithmic scale, the growth of PSC is visibly greater.

As a summary of the experimentation with medium size data sets, we can highlight that the proposed methods achieved competitive results in terms of accuracy. Considering the reduction rate, DROP3 achieved the maximum compression, while our methods were the worst in terms of compression. Finally, considering execution time, the methods presented in the paper were able to compute the selected subset much faster than the other algorithms in the state of the art. Exceptionally, PSC worked surprisingly fast, although slower than the speed of our proposals, and with the shortcoming of the poor accuracy when its selected subsets were used for training the classifiers.

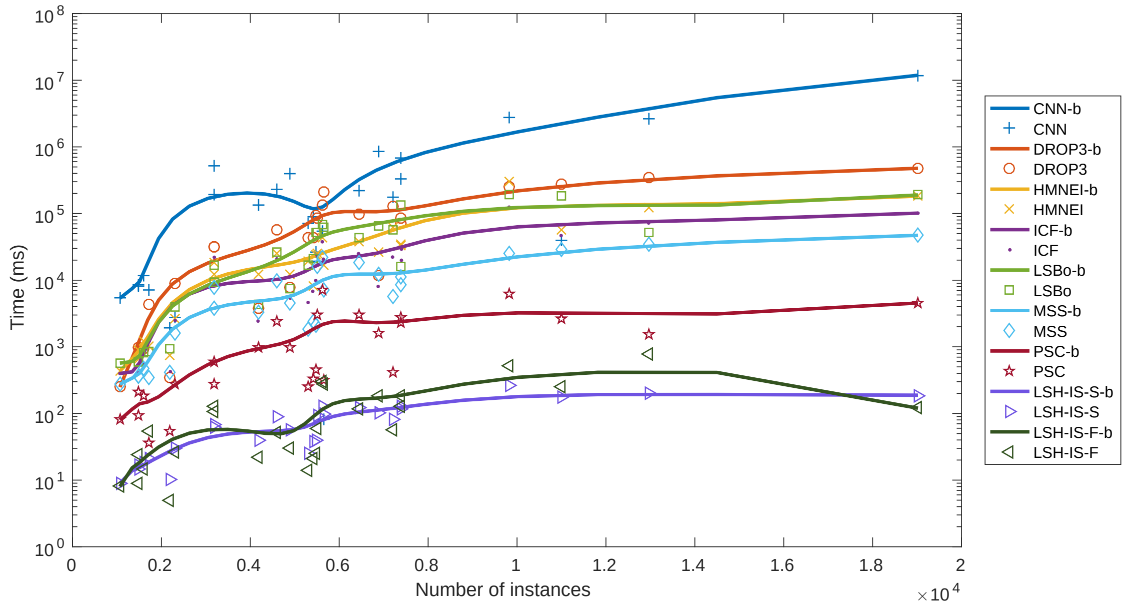
5.1. Huge problems

Due to the fact that instance selection methods are not able to face huge problems, the experimental study performed over Census, CovType, KDDCup99, KDDCup991M[4]

[4]We divided the original KDDCup 1999 data set into two sets with different number of instances: KDDCup99 has 10% of the original instances and KDDCup991M has a million.



(a) Linear scale



(b) Logarithmic scale

Figure 10: Computational cost of tested methods, in linear (a) and logarithmic scale (b) on the y axis. In (a) the CNN was not plotted because its growth was so high that it was not possible to appreciate the differences between the other methods. The dots are the results on the available data sets, lines (denoted by "-b" in the legend) are the Bezier lines built with these dots to show the general trend of the algorithms.

Table 8: Average ranks over accuracy for huge problems.

Algorithm	Ranking
LSH-IS-F	2.0
DIS.RNN	2.2
LSH-IS-S	2.6
DIS.DROP3	3.6
DIS.ICF	4.6

Table 9: Average ranks over storage reduction for huge problems.

Algorithm	Ranking
DIS.RNN	1.8
DIS.DROP3	2.4
LSH-IS-F	3.2
DIS.ICF	3.4
LSH-IS-S	4.2

and Poker (see Table 3), the algorithms proposed were tested against the Democratic Instance Selection (DIS) [22]. Although PSC showed a competitive results in terms of execution time, it was not included in the study of huge problems, because of its poor accuracy.

As in the previous experiments, ten fold cross-validation was performed on LSH-IS-S and LSH-IS-F in Weka. Testing error, using 1-NN classifier, and storage reduction were reported and compared against results published in [22]. Execution times were not compared because different implementations and machines would not have allowed a fair comparison.

The main conclusion of the experiments was that our methods can face huge problems. Results of average ranks over the accuracy are shown in Table 8. The accuracy of the methods under study is similar to DIS, though the most accurate method is LSH-IS-F. As in the medium size experiment, LSH-IS-F improved the accuracy with regard to LSH-IS-S. On the other hand, the Table 9 shows the average ranks over storage reduction. In terms of compression, the best method was DIS.RNN, as proved in medium size data sets, while the methods based on hashing were too conservative. However, the number of instances that they retain can be adjusted by the number of functions used. The success of the proposed methods is even more remarkable when compared against scalable approaches. The simple idea of using LSH overcomes the democratization methods and opens the way to their use in huge data sets and big data.

6. Conclusions

The paper has introduced a novel approach to the use of families of locality sensitive functions (LSH) for instance selection. Using this approach, two new algorithms of linear complexity have been designed. In one approach, the data are processed in one pass, which allows the algorithm to make the selection without requiring that the whole data set to fit in memory. The other approach needs two passes: one processes each instance of the data set, and the second processes the buckets of the families of hash functions. Their speed and low memory consumption mean that they are suitable for big data processing.

The experiments have shown that the strength of our methods is the speed, which is achieved through a small decrease in accuracy and, more remarkably, the reduction rate. Although the best methods according to accuracy differ depending on the classifier that is used, the proposed methods offer a competitive performance. Moreover, the reduction rate can be adjusted by increasing or by decreasing the number of hash functions that are used.

Furthermore, the proposed methods were evaluated on huge problems and compared against Democratic Instance Selection, a linear complexity method. Experimental results on accuracy showed how our methods outperformed DIS, even though our methods were conceptually much simpler.

7. Future work

In their current version, the way the algorithms make the instance selection is very simple and quite “naive”. The selected subset could be improved using additional information about the instances assigned to each bucket, and not just the count of instances of each class. A future research line could be to store additional information of the instances assigned to each bucket: for example, simple statistics such as the incremental average of instances in the bucket, or the percentage of instances of each class in the bucket. This information might mean that the instance selection process would be better informed, without excessively penalizing run-time. Although prototype generation has not been analyzed in the paper, the generation of a new instance, or group of them, for each bucket is one of the future lines of research. This idea can be developed using LSH-IS-F, seeking each of the buckets to build or to create a new set of instances, by selecting the medoids or centroids of the instances in the buckets.

According to [63], one of the most challenging problems in data mining research is mining data streams in extremely large databases. Accurate and fast processes able to work on stream are required, without any assumption that information can be stored in large databases and repeatedly accessed. One of the problems that arises in those environments is called *concept drift*, which appears when changes in the context take place. In the management of concept drift, three basic approaches can be distinguished: ensemble learning, instance weighting and instance selection [59]. A comparison of the proposed method in a streaming benchmark would be made to test whether LSH-IS-S can beat the state-of-the-art algorithms that are able to deal in streaming data [18].

Many more research approaches can be considered, but the principal one for us is to adapt the new methods to a big data environment. We are working on the adaptation of this idea to a MapReduce framework, which offers a robust environment to face up to the processing of huge data sets over clusters of machines [58].

Acknowledgements

Supported by the Research Projects TIN 2011-24046 and TIN 2015-67534-P from the Spanish Ministry of Economy and Competitiveness.

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