



# A review of unsupervised feature selection methods

Saúl Solorio-Fernández<sup>1</sup> · J. Ariel Carrasco-Ochoa<sup>1</sup> · José Fco. Martínez-Trinidad<sup>1</sup>

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## Abstract

In recent years, unsupervised feature selection methods have raised considerable interest in many research areas; this is mainly due to their ability to identify and select relevant features without needing class label information. In this paper, we provide a comprehensive and structured review of the most relevant and recent unsupervised feature selection methods reported in the literature. We present a taxonomy of these methods and describe the main characteristics and the fundamental ideas they are based on. Additionally, we summarized the advantages and disadvantages of the general lines in which we have categorized the methods analyzed in this review. Moreover, an experimental comparison among the most representative methods of each approach is also presented. Finally, we discuss some important open challenges in this research area.

**Keywords** Unsupervised learning · Dimensionality reduction · Unsupervised feature selection · Feature selection for clustering

## 1 Introduction

Feature selection (Liu and Motoda 1998, 2007; Guyon et al. 2003) (also known as attribute selection) appears in different areas such as pattern recognition (Tou and González 1974; Theodoridis and Koutroumbas 2008a), machine learning (Kotsiantis 2011; Hall 1999), data mining (García et al. 2015; Chakrabarti et al. 2008) and statistical analysis (Webb 2003; Friedman et al. 2001). In all these areas, often the objects<sup>1</sup> under study include in their description irrelevant and redundant features (Ritter 2015), which can significantly affect the analysis of the data, resulting in biases or even incorrect models (Zhao and Liu 2011). Feature selection is the process of selecting the most useful features for building models in

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<sup>1</sup> Also called instances, observations or samples; commonly represented as vectors.

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✉ Saúl Solorio-Fernández  
sausolofer@inaoep.mx

J. Ariel Carrasco-Ochoa  
ariel@inaoep.mx

José Fco. Martínez-Trinidad  
fmartine@inaoep.mx

<sup>1</sup> Computer Sciences Department, Instituto Nacional de Astrofísica, Óptica y Electrónica, Luis Enrique Erro # 1, Tonantzintla, 72840 Puebla, Mexico

tasks like classification, regression or clustering. Moreover, feature selection not only reduces the dimensionality of the data facilitating their visualization and understanding; but also it commonly leads to more compact models with better generalization ability (Pal and Mitra 2004). All these characteristics make feature selection an interesting research area, wherein the last decades, numerous feature selection methods have been introduced.

According to the information available in the datasets, feature selection methods can be classified as supervised (Kotsiantis 2011; Tang et al. 2014), semi-supervised (Sheikhpour et al. 2017) and unsupervised (Alelyani et al. 2013). The former require a set of labeled data (supervised dataset) in order to identify and select relevant features; this label, assigned to each object in the dataset, can be a category, an ordered value or a real value (depending on the specific task). Semi-supervised methods only require that some objects be labeled. On the other hand, Unsupervised Feature Selection (UFS) methods (Dy and Brodley 2004; Alelyani et al. 2013; Fowlkes et al. 1988) do not require a supervised dataset.

Over the last decades, many feature selection methods have been proposed, most of them developed for supervised classification tasks (Tang et al. 2014). However, due to the technological development raised in the last years, as well as the vast amount of unlabeled data generated in different applications such as text mining (Feldman and Sanger 2006; Bharti and kumar Singh 2014; Forman 2003), bioinformatics (Saeys et al. 2007), image retrieval (Yasmin et al. 2014; Swets and Weng 1995), social media (Zafarani et al. 2014; Tang and Liu 2014) and intrusion detection (Ahmed et al. 2016; Lee et al. 2000; Agrawal and Agrawal 2015; Ambusaidi et al. 2015), to name a few; UFS methods have gained significant interest in the scientific community. Moreover, according to (Guyon et al. 2003; Nijima and Okuno 2009; Devakumari and Thangavel 2010), UFS methods have two important advantages. (1) they are unbiased and perform well when prior knowledge is not available, and (2) they can reduce the risk of data overfitting in contrast to supervised feature selection methods that may be unable to deal with a new class of data.

In the same way as in supervised and semi-supervised feature selection, according to the strategy used for selecting features, Unsupervised Feature Selection methods can be divided into three main approaches (Alelyani et al. 2013; Dong and Liu 2018):

- Filter methods select the most relevant features through the data itself, i.e., features are evaluated based on intrinsic properties of the data, without using any clustering algorithm that could guide the search of relevant features. The main characteristic of filter methods is their speed and scalability.
- Wrapper methods evaluate feature subsets using the results of a specific clustering algorithm. Methods developed under this approach are characterized by finding features subsets that contribute to improving the quality of the results of the clustering algorithm used for the selection. However, the main disadvantage of wrapper methods is that they usually have a high computational cost, and they are limited to be used in conjunction with a particular clustering algorithm.
- Hybrid methods try to exploit the qualities of both approaches, filter, and wrapper, trying to have a good compromise between efficiency (computational effort) and effectiveness (quality in the associated objective task when using the selected features).

Currently, in the literature we can find some reviews about feature selection (Cai et al. 2018; Sheikhpour et al. 2017; Miao and Niu 2016; Li et al. 2016; Ang et al. 2016; Chandrashekar and Sahin 2014; Vergara and Estévez 2014; Kotsiantis 2011; Liu et al. 2005; Yu 2005). Nevertheless, all of them are focused either on supervised/semi-supervised feature selection, or feature selection in general; while some reviews concentrate on describing feature selection applied to specific domains (Lee et al. 2017; Bharti and kumar Singh 2014; Lazar et al. 2012;

Mugunthadevi et al. 2011; Saeys et al. 2007). As far we know, the most similar work to our review is presented in Alelyani et al. (2013), where feature selection for clustering is reviewed. However, in Alelyani et al. (2013) only a few relevant methods of the state-of-the-art are mentioned; and mainly focusing on feature selection methods designed exclusively for specific domains, such as text data, streaming data, and link data. In our paper, we focus on Unsupervised Feature Selection (UFS). We intend to provide a big picture over UFS methods throughout a comprehensive and structured review of the most relevant (most referenced) and recent works of the state-of-the-art; describing their main characteristics and the fundamental ideas these methods are based on. Furthermore, in our review, we present a taxonomy of reviewed UFS methods; classifying them according to their approach, type, and subtype, and pointing out the major advantages and disadvantages of these general lines. Additionally, we perform an experimental comparison, on standard public datasets among the most representative methods of each approach and conclude our review highlighting some open challenges in Unsupervised Feature Selection. To the best of our knowledge, this is the first comprehensive review in Unsupervised Feature Selection that provides a general perspective to the audience, practitioners and academics, about the most relevant and recent feature selection methods in this field of research.

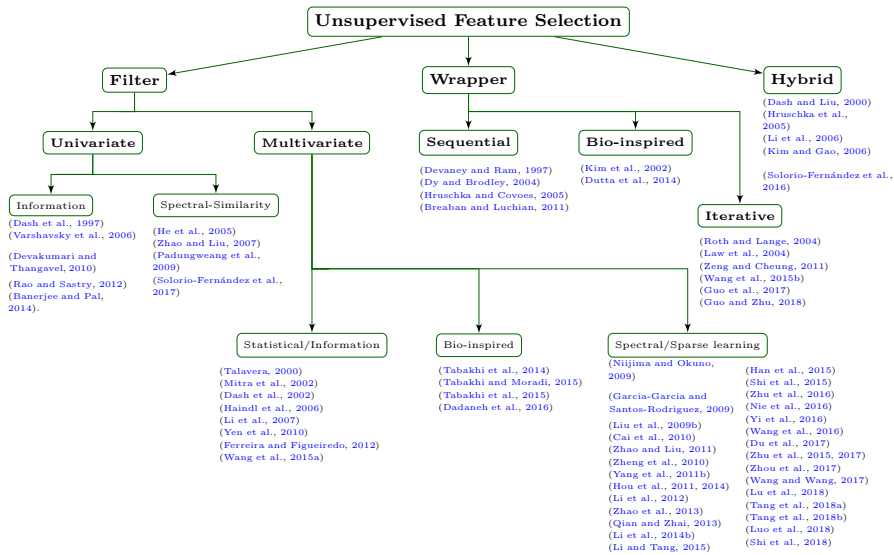
The structure of this paper is as follows: in Sect. 2, the main Unsupervised Feature Selection methods proposed in the literature are reviewed. An analysis and discussion of the UFS methods is presented in Sect. 3. In this section, the advantages, disadvantages, feature selection criteria, analysis of the performance evaluation, and the experimental comparison of the reviewed UFS methods are provided. Finally, in Sect. 4, our conclusions are exposed; pointing out some open challenges and research directions in Unsupervised Feature Selection.

## 2 Unsupervised feature selection methods

As we have commented in the previous section, Unsupervised Feature Selection (UFS) methods can be categorized according to the strategy used for selecting features as filter, wrapper, and hybrid methods. In this section, first, we organize the UFS methods reported in the literature into the taxonomy shown in Fig. 1. Then, we describe each one of these methods by focusing on their main characteristics and the ideas they are based on.

### 2.1 Filter approach

According to Alelyani et al. (2013), UFS methods based on the filter approach can be categorized as univariate and multivariate. The former, also known as ranking based UFS methods use some criteria to evaluate each feature in order to get an ordered list (ranking) of features, where the final feature subset is selected according to this order. Such methods can effectively identify and remove irrelevant features, but they are unable to remove redundant ones since they do not take into account possible dependencies among features. On the other hand, multivariate filter methods evaluate the relevance of the features jointly rather than individually. Multivariate methods can handle redundant and irrelevant features; thus, in many cases, the accuracy reached by learning algorithms using the subset of features selected by multivariate methods is better than the one achieved by using univariate methods (Tabakhi et al. 2015).



**Fig. 1** Taxonomy of unsupervised feature selection (UFS) methods

### 2.1.1 Univariate filter methods

Within the univariate filter methods, two main groups can be highlighted: methods that assess the relevancy of each feature based on Information Theory (Cover and Thomas 2006), and those methods that evaluate features based on Spectral Analysis (manifold learning) (Chung 1997; Luxburg 2007) using the similarities among objects. The former follow the idea of assessing the degree of dispersion of the data through measures such as entropy, divergence, mutual information, among others, to identify cluster structures in the data. On the other hand, methods based on Spectral Analysis—Similarity, also known as Spectral Feature Selection methods (Zhao and Liu 2011), follow the idea of modeling or identifying the local or global data structure using the eigen-system of Laplacian or normalized Laplacian matrices (Luxburg 2007) derived from an object similarity matrix.

**Information based methods** One of the first methods developed in this category was introduced in Dash et al. (1997), where the authors presented a new filter unsupervised feature selection method called SUD (Sequential backward selection method for Unsupervised Data). This filter method weighs features using a measure of entropy of similarities based on distance, which is defined as the total entropy induced from a similarity matrix  $W$ , where the elements of this matrix contain the similarity between pairs of objects in the dataset. The idea is to measure the entropy of the data based on the fact that when every pair of objects is very close or very far, the entropy is low, and it is high if most of the distances between pairs of objects are close to the average distance. Therefore, if the data has low entropy, there are well-defined cluster structures, while there are not when the entropy is high. The relevance of each feature is quantified using a leave-one-out sequential backward strategy jointly with the entropy measure above mentioned. The final result is a feature ranking ordered from the most to the least relevant feature.

In Varshavsky et al. (2006) another information-based UFS method called SVD-Entropy was proposed. The basic idea is to select those features that best represent the data, measuring the entropy of the original data matrix through its singular values (Alter and Alter 2000). This entropy varies between 0 and 1, in such a way that when the entropy is low (close to zero), well-formed clusters are generated, since the spectrum of the data matrix is not uniformly distributed; by contrast, when the entropy is high, the spectrum<sup>2</sup> is uniformly distributed, and the cluster structure is not well-defined. Through a leave-one-out comparison, the contribution of each feature to the entropy (CE) is evaluated, and the features are sorted according to their respective CE values. In this work, three different ways of selecting a final feature subset were presented: simple ranking, forward selection, and backward elimination. The first strategy consists in selecting the first  $d$  features from the ranking. The forward selection, on the other hand, starts choosing the first feature according to the highest CE, then the CE values of the remaining set of features are recalculated and the second feature according to the highest CE value is selected, this procedure continues until selecting  $d$  features. The backward elimination is similar to the forward selection, with the difference that it begins with the whole set of features and removes that feature with lowest CE value in each iteration until reaching the pre-specified number of features. Two more recent works based on this same idea were introduced in Devakumari and Thangavel (2010) and Banerjee and Pal (2014), where the authors propose to solve some drawbacks of SVD-Entropy. In Devakumari and Thangavel (2010) an Adaptive Floating Search which alleviates the weaknesses of forward/backward selection searches used in SVD-Entropy was proposed. Meanwhile, in Banerjee and Pal (2014), the inability of SVD-Entropy to distinguish features with a constant value was addressed. Furthermore, in the last, an extension to the supervised case was also proposed.

Another unsupervised univariate filter method that ranks features using information theory was proposed in Rao and Sastry (2012). In this method, the aim is weighting each feature using the concept of Representation Entropy (Devijver and Kittler 1982). Representation Entropy is a measure of information compression in a dataset, and it is computed from the entropy of eigenvalues of the covariance matrix of the data. Representation Entropy ranges from 0 to 1, where 1 represents the maximum compression, and 0 is the minimum one. In Rao and Sastry (2012), as in the previous methods, features are scored using a leave-one-out strategy, i.e., the importance of a particular feature in the dataset will depend on the increase in the value of the Entropy (CE value) of the dataset calculated without that particular feature. In this way, it is possible to obtain a feature ranking sorted from the most relevant feature (that one with the highest CE value) to the least one.

**Spectral-similarity based methods** One of the most referenced and relevant univariate filter UFS methods based on Spectral Feature Selection is Laplacian Score (LS) (He et al. 2005). In Laplacian Score, the importance of a feature is evaluated by its variance and its power of locality preserving (He and Niyogi 2004). This method assigns high weights to those features that most preserve the predefined graph structure (manifold structure) represented by the Laplacian matrix. This idea comes from the observation that two objects are probably related to the same cluster if they are close to each other; in such a way that those features that take similar values for close objects, and dissimilar values for the far away ones are the most relevant. An extension of the Laplacian Score called Laplacian++ was proposed in Padungweang et al. (2009), where the idea is to evaluate the features based on the global topology instead of the local topology.

<sup>2</sup> The set composed by the square of the singular values of the data matrix.

Another univariate filter method in this category is SPEC (SPECtrum decomposition) (Zhao and Liu 2007). SPEC evaluates the relevance of a feature by its consistency with the structure of the graph induced from the similarities among objects. This method consists of three steps: (1) building the object similarity matrix  $W$  as well as its graph representation. (2) evaluating features using the eigensystem of the graph by measuring the consistency between each feature and those nontrivial eigenvectors of the Laplacian matrix. And (3), ranking features in descending order in term of their feature relevance (consistency). According to Zhao and Liu (2011), SPEC is a generalization of Laplacian Score.

Finally, a recent univariate unsupervised spectral feature selection method developed to be applied over mixed data (De Leon and Chough 2013) called USFSM (Unsupervised Spectral Feature Selection Method for mixed data) was introduced in Solorio-Fernández et al. (2017). USFSM assess features by analyzing the changes in the spectrum distribution (spectral gaps) of the first non-trivial eigenvalues of the Normalized Laplacian matrix when each feature is excluded from the whole set of features separately. Features are sorted in descending order according to their respective spectral gaps values.

## 2.1.2 Multivariate filter methods

Multivariate filter methods can be divided into three main groups: Statistical/Information, Bio-inspired, and Spectral/Sparse Learning based methods. The former, as its name suggests, includes UFS methods that perform the selection using statistical and/or information theory measures such as variance-covariance, linear correlation, entropy, mutual information, among others. The second group, on the other hand, includes UFS methods that use stochastic search strategies based on the swarm intelligence paradigm (Beni and Wang 1993; Dorigo and Gambardella 1997) for finding a good subset of features, which satisfies some criterion of quality. Finally, the third group includes those UFS methods based on Spectral Analysis (Zhao and Liu 2011) or on a combination of Spectral Analysis and Sparse Learning (El Ghaoui et al. 2011). It is noteworthy that some authors (Chandrashekar and Sahin 2014; Ang et al. 2016) often call these last methods as *embedded* because feature selection is achieved as part of the learning process, commonly through the optimization of a constrained regression model. However, in this study, we prefer to categorize them as filter multivariate, since in addition to jointly evaluate features, the primary objective is to perform feature selection (or ranking) rather than finding the cluster labels. Moreover, we think that embedded methods could be considered as a sub-category inside the main approaches (i.e., filter, wrapper, and hybrid), not hindering the possibility of having embedded methods in the three approaches.

**Statistical/information based methods** One of the most representative and referenced works in this category is FSFS (Feature Selection using Feature Similarity) (Mitra et al. 2002). In this work, the authors introduced a statistical measure of dependency/similarity to reduce feature redundancy; this measure called Maximal Information Compression Index (MICI) is based on the variance-covariance between features. The idea of this method is partitioning the original set of features into clusters, such that those features in the same cluster are highly similar, while those in different clusters are dissimilar. Feature clustering is done iteratively based on the  $k$ NN principle as follows: In each iteration, FSFS computes the  $k$ -nearest features of each feature (using MICI). Then, the feature with the most compact subset of  $k$ -nearest features (determined by the distance to its farthest feature among the  $k$ -nearest) is selected, and its  $k$  nearest features are discarded. This procedure is repeated for the remaining features until all of them are either picked or discarded. Following a similar idea, in Li et al. (2007) a hierarchical method called Mitra's + AIF that removes both redundant

and irrelevant features was proposed. This method uses the algorithm developed in Mitra et al. (2002) to remove redundant features. Subsequently, an exponential entropy measure is used to sort the features according to their relevance. Afterward, from the feature ranking obtained in the previous step, a relevant-non-redundant feature subset is selected using the fuzzy evaluation index FFEI (Pal et al. 2000) in combination with a forward selection search.

Other two multivariate filter methods based on statistical measures were proposed in Haindl et al. (2006) and Ferreira and Figueiredo (2012) respectively. In Haindl et al. (2006), the idea is to evaluate all mutual correlations for all feature pairs. Then, the feature with the largest average mutual correlation with all other features is removed, and the process is repeated for the remaining features until a number of features, previously specified by the user, is reached. Meanwhile, in Ferreira and Figueiredo (2012), a filter supervised/unsupervised feature selection method called RRFs (Relevance Redundancy Feature Selection), which selects features in two steps was proposed. In this method, first, the features are sorted according to a relevance measure (variance for the unsupervised version and the Fisher's Ratio or mutual information for the supervised one). Then, in the second step, following the order generated in the previous step, the features are evaluated using a feature similarity measure to quantify the redundancy between them. Afterward, the first  $p$  features with the lowest redundancy are selected.

Following the idea of using statistical measures for feature selection, in Talavera (2000) a multivariate filter method based on a dependency measure was introduced. This method, unlike the previous ones, proposes that in the absence of classes, the relevant features are those that are highly correlated with others; and those features having low correlation with other features are not likely to play an important role in the clustering process (irrelevant features). This conjecture is based on the observation that cohesive and distinct clusters tend to capture feature inter-correlations (Fisher 1987). Therefore, the idea is to evaluate each individual feature  $f_i$  through the dependency measure above mentioned. Afterward, the  $p$  features with the highest dependency are selected.

Another multivariate statistical-based filter method was introduced in Yen et al. (2010). In this work, the objective is to remove redundant features using the concept of minimization of the feature dependency. The idea is to find independent features (relevant) by choosing a set of coefficients such that the linear dependency of features (expressed by the error vector  $E$ ) could be close to zero. At each iteration, the feature with the largest absolute coefficients (that one with the smallest  $\|E\|^2$ ) is removed, and the effect of its removal is updated. This process is iterated until all the remaining error vectors  $E$  are smaller than a threshold fixed by the user. Another statistical-based method with a similar idea called MPMR (feature selection based on Maximum Projection and Minimum Redundancy) was proposed in Wang et al. (2015a). In this work, a new criterion called maximum projection and minimum redundancy feature selection was introduced. The idea is to select a feature subset such that all original features are projected into a feature subspace (applying a linear transformation) with minimum reconstruction error. Moreover, in this work, with the aim of maintaining low redundancy, a term for quantifying the redundancy among features (redundancy rate using the Pearson correlation coefficient) was added.

Finally in Dash et al. (2002) a multivariate information-based method similar to Dash et al. (1997) was introduced. In this method, as in Dash et al. (1997), the basic idea is to select features using a measure of entropy of similarities based on distance. The main difference between (Dash et al. 1997) and (Dash et al. 2002) is that in Dash et al. (2002) some weighing parameters for the entropy measure were added, and the entropy measure was reformulated as an exponential function instead of a logarithmic function. Additionally, the authors select a subset of features using a forward selection search.



**Bio-inspired methods** Recently, several bio-inspired unsupervised feature selection methods based on the swarm intelligence paradigm (Beni and Wang 1993; Dorigo and Gambardella 1997) have been proposed. In Tabakhi et al. (2014), one of the first methods based on this idea called UFSACO (Unsupervised Feature Selection based on Ant Colony Optimization) was introduced. The main objective is to select feature subsets with low similarity among features (low redundancy). In this work, the search space is represented as a complete undirected graph; where the nodes represent the features and the weights of the edges represent the similarities between features. This similarity is computed using the cosine similarity function. The authors follow the idea that if two features are similar, then these features are redundant. Each node in the graph has a *desirability* value called pheromone, which is updated by agents (ants) in function of its current value, a pre-specified decay rate, and the number of times that a given feature has been selected by an agent. The agents traverse the graph iteratively preferring high pheromone values and low similarities until a pre-specified stop criterion (number of iterations) is reached. Finally, those features with the highest pheromone value are selected. Thus, it is expected to pick feature subsets with low redundancy. Other later methods based on the same idea are MGSACO (Microarray Gene Selection based on Ant Colony Optimization) (Tabakhi et al. 2015), RR-FSACO (Relevance-Redundancy Feature Selection based on ACO) (Tabakhi and Moradi 2015), and UPFS (Unsupervised Probabilistic Feature Selection using ant colony optimization) (Dadaneh et al. 2016). In both MGSACO and RR-FSACO, in addition to quantifying the feature redundancy as in the previous method, they also measure the relevance of each feature through its variance (Theodoridis and Koutroumbas 2008b). Therefore, the main objective of all these methods is to select features that minimize redundancy and at the same time maximize relevance. Meanwhile, UPFS, the idea is to pick non-redundant features, but using the Pearson's correlation instead of the cosine similarity.

**Spectral/sparse learning methods** Some multivariate methods based on Spectral Analysis derived from the SPEC and the Laplacian Score were introduced in Garcia-Garcia and Santos-Rodriguez (2009), Liu et al. (2009b), Nijima and Okuno (2009). In Garcia-Garcia and Santos-Rodriguez (2009), a feature selection method called mR-SP (minimum-Redundancy SPectral feature selection) that combines the SPEC ranking and the minimum redundancy optimality criterion (Peng et al. 2005) was proposed. The basic idea of this method is to add a way for controlling the feature redundancy in SPEC, by introducing an evaluation measure for quantifying the similarity of each pair of features through a modified cosine similarity function. While in Liu et al. (2009b) a method that combines the Laplacian Score with the distance entropy introduced in Dash et al. (2002) was developed. This method selects a feature subset (using the entropy measure) based on the ranking produced by the Laplacian Score. Likewise, in Nijima and Okuno (2009) a method called LLDA-RFE (Laplacian Linear Discriminant Analysis-based Recursive Feature Elimination) was proposed. This method extends the Linear Discriminant Analysis (LDA) (Fukunaga 1990) to the unsupervised case using the similarities among objects; this extension is called LLDA. The idea is to recursively remove features with the smallest absolute values of the discriminant vectors of the LLDA to identify features that potentially reveals clusters in the samples. According to the authors, LLDA-RFE is closely related to Laplacian Score; the main difference is that LLDA-RFE is a multivariate method, which allows selecting features that in combination contribute to discriminate.

Other multivariate feature selection methods that have received attention in the last years, due to their good performance and interpretability (Li et al. 2016), are those based on Spectral Analysis combined with Sparse Learning (El Ghaoui et al. 2011). Sparse Learning refers to those methods that seek a trade-off between some goodness-of-fit measure and the sparsity



(El Ghaoui et al. 2011) of the results. Examples of earlier methods based on this idea are: MCFS (Cai et al. 2010), MRSF (Zheng et al. 2010), UDFS (Yang et al. 2011b) NDFS (Li et al. 2012), JELSR (Hou et al. 2011, 2014), SPFS (Zhao et al. 2013), CGSSL (Li et al. 2014b), RUFs (Qian and Zhai 2013), and RSFS (Shi et al. 2015).

MCFS (Cai et al. 2010) and MRSF (Zheng et al. 2010) were among the earliest unsupervised multivariate spectral/sparse learning feature selection methods. MCFS (Multi-Cluster Feature Selection) consists of three steps: (1) spectral analysis, (2) sparse coefficient learning, and (3) feature selection. In the first step, spectral analysis (Luxburg 2007) is applied on the dataset to detect the cluster structure of the data. Then, in the second step, since the embedding clustering structure of the data is known, through of the first  $k$  eigenvectors of the Laplacian matrix, MCFS measures the importance of the features by a regression model with a  $l_1$ -norm regularization (Donoho and Tsaig 2008). Finally, in the third step, after solving the regression problem, MCFS selects  $d$  features based on the highest absolute values of the coefficients obtained through the regression problem. On the other hand, MRSF (Minimize the feature Redundancy for Spectral Feature selection) evaluates the features all together in order to eliminate redundant features. The idea is to formulate the feature selection problem as a multi-output regression problem (Friedman et al. 2001), and the selection is performed by enforcing the sparsity applying the norm  $l_{2,1}$  (Argyriou et al. 2008) instead of the  $l_1$ -norm. Moreover, in this work, an efficient algorithm based on the Nesterov's method (Liu et al. 2009a) for solving the regression problem was also proposed. The final feature subset is selected based on the values of a weighted  $W$  matrix.

Following a similar idea to MRFS, UDFS (Yang et al. 2011b) (Unsupervised Discriminative Feature Selection algorithm) performs feature selection by simultaneously exploiting discriminative information contained in the scatter matrices and feature correlations. This method proposes to address the feature selection problem taking into account the trace criterion (Fukunaga 1990) into the regression problem. Furthermore, UDFS adds some additional constraints to the regression problem and proposes an efficient algorithm to optimize it. UDFS ranks each feature according to the corresponding weight value in descending order, and the top-ranked features are selected. Another method that shares many common features with MRSF is JELSR (Joint Embedding Learning and Sparse Regression) (Hou et al. 2011). JELSR works with the same objective function as MRSF, and it only differs in the construction of the Laplacian graph, since in this work, locally linear approximation weight (Roweis and Saul 2000) is used to measure local similarity for building the Laplacian graph. A later generalization of JELSR was introduced in Hou et al. (2014), where instead of using the Laplacian graph to characterize the structure of high dimensional data and then apply regression, a unify embedding learning and sparse regression framework was proposed. Furthermore, in this work, a unified perspective for understanding and comparing many popular unsupervised feature selection methods was presented. A recent work related to JELSR is USFS (Wang et al. 2016) (Unsupervised Spectral Feature Selection with  $l_1$ -norm graph), where the idea is to use spectral clustering and a  $l_1$ -norm graph to select discriminative features. The main difference between USFS and JELSR is the way of building the Laplacian graph; JELSR uses locally linear approximation weights to construct the graph, while USFS adopts a new  $l_1$ -norm graph.

Another method related to the works described above is NDFS (Nonnegative Discriminative Feature Selection) (Li et al. 2012). NDFS like UDFS and MRFS, performs feature selection exploiting the discriminative information and feature correlations in a unified framework. First, NDFS uses Spectral Analysis to learn pseudo class labels (defined as non-negative real values). Then, a regression model with  $l_{2,1}$ -norm regularization (Argyriou et al. 2008) is formulated and optimized through a special solver also proposed in this work. According to

the authors, the main difference between NDFS and UDFS is that NDFS adds a non-negativity constraint to the regression problem, since removing this constraint NDFS becomes UDFS. The same authors proposed a later modification of NDFS in Li and Tang (2015), where a method called NSCR (Nonnegative Spectral analysis with Constrained Redundancy) was introduced. The main difference regarding NDFS is that NSCR adds a mechanism to explicitly control the redundancy. Following the idea of NDFS in Han et al. (2015), a method called FSLR (Feature subset with Sparsity and Low Redundancy) was proposed. FSLR employs Spectral Analysis to represent the data in a lower dimension and introduces a novel regularization term into the objective function with a non-negative constraint. Additionally, an iterative multiplicative algorithm to efficiently solve the constrained optimization problem was proposed. Another UFS method called CDL-FS (Couple Dictionary Learning Feature Selection) which uses a coupled analysis/synthesis dictionary instead of Spectral Analysis to learn pseudo class labels was proposed in Zhu et al. (2016). The general idea is to use a dictionary learning (Gu et al. 2014) in order to model the cluster structure of the data. Feature selection is achieved by imposing an  $l_{2,p}$ -norm ( $0 < p \leq 1$ ) regularization of the feature weight matrix on the dictionary learning model.

In Nie et al. (2016) a sparse learning based method called SOGFS (Structured Optimal Graph Feature Selection) which simultaneously performs feature selection and local structure learning, was proposed. SOGFS adaptively learns local manifold structure by introducing a similarity matrix in a sparse optimization model based on  $l_{2,1}$ -norm minimization on both loss function and regularization (Nie et al. 2010). Features are selected according to the corresponding weights once the proposed model has been optimized. Another sparse learning feature selection method named SPFS (Similarity Preserving Feature Selection) was introduced in Zhao et al. (2013). In this method, the idea is to select the  $d$  features that best preserve the similarity of the objects using multiple-output regression (Friedman et al. 2001) with an  $l_{2,1}$ -norm constraint. Additionally, in this work, the authors show the relationship between the proposed method and many other supervised and unsupervised feature selection methods of the state-of-the-art. The authors show that many existing feature evaluation criteria can be unified under a common formulation, where the relevance of features is quantified by measuring their capability in preserving the pairwise sample similarity specified by a predefined similarity matrix. Likewise, in Li et al. (2014b) another method called CGSSL (Clustering-Guided Sparse Structural Learning) was proposed. This work presents a general method for feature selection which jointly exploits nonnegative spectral analysis and structural learning with sparsity. The idea is to use the cluster indicators (learned with nonnegative spectral clustering) in a linear model to provide label information for the structural learning. Moreover, similar to the previous method, in this work, the authors show the relationships between the introduced method and several feature selection methods, including SPFS, MCFS, UDFS, and NDFS.

In order to address the problem of outliers or noise present in many datasets, in Qian and Zhai (2013) a filter method named RUFS (Robust Unsupervised Feature Selection) was proposed. The objective is to achieve both robust clustering and robust feature selection. Unlike the unsupervised feature selection methods above mentioned such as MCFS, UDFS, and NDFS, RUFS learns the pseudo cluster labels via local learning regularized robust non-negative matrix factorization (Kong et al. 2011). The idea is to learn the labels while feature selection is performed by means of a robust joint  $l_{2,1}$  norms minimization. In this work, the authors also proposed an iterative limited-memory BFGS (Liu and Nocedal 1989) algorithm for solving the optimization problem efficiently, and to make RUFS applicable on real-world applications. Following a similar idea to RUFS, in Du et al. (2017) a method called RUFSM (Robust Unsupervised Feature Selection via Matrix Factorization) was proposed. RUFSM

selects features by performing discriminative feature selection and robust clustering simultaneously using the  $l_{2,1}$ -norm. The main difference between RUFS and RUFSM is that the latter uses the cluster centers as objective concept rather than the pseudo labels of the data. Another method that addresses the problem of noisy features and outliers is RSFS (Robust Spectral learning framework for unsupervised Feature Selection) (Shi et al. 2015). RSFS selects features by applying a graph embedding step (using kernel regression) to efficiently learn the cluster structure, and sparse spectral regression to handle noise and outliers. The idea is to build the Laplacian graph taking into account a weight assigned to each object by local kernel regression and develop an efficient iterative algorithm in order to solve the optimization problem proposed.

In recent years, some works developed under Sparse Learning/Spectral analysis category but under a new perspective called *self-representation* of features, have been proposed. The assumption behind these methods is that each feature can be well approximated by a linear combination of relevant features and a coefficient matrix with sparsity constraints (which can be used as feature weights). RSR (Zhu et al. 2015) (Regularized Self-Representation model for unsupervised feature selection) was the first one on exploiting this idea. In this work, the authors argue that if a feature is important, then it will participate in the representation of most of the other features. The feature selection is done by the minimization of the self-representation error using the  $l_{2,1}$ -norm for the characterization of residuals, and the most representative features (those with high feature weights) are selected. In Zhu et al. (2017) an extended version of RSR was proposed, where the authors use the  $l_{2,p}$ -norm regularization instead of  $l_{2,1}$ -norm to select features with emphasis on small values for  $p$  ( $0 \leq p < 1$ ). Another method related to RSR is GRNSR (Graph Regularized Non-negative Self Representation) (Yi et al. 2016). Like RSR, GRNSR exploits the self-representation capability of the features, but with the difference that GRNSR also takes into account the geometrical structure of the data using a neighborhood weighted graph (low-rank representation graph). In GRNSR each feature is first represented by all other features through a non-negative linear combination. Then, a similarity matrix is constructed to uncover the local structure information of the objects and a Nonnegative Least Squares (NNLS) problem is formulated and considered as a new term in the final  $l_{2,1}$ -norm nonnegative constraint regression problem. Afterward, once the model (regression problem) has been optimized, the top  $d$  ranked features with the highest weights are selected.

Other more recent methods also developed under *self-representation* perspective are SPNFSR (Zhou et al. 2017), LRSL (Wang and Wang 2017), DSRMR (Tang et al. 2018a),  $l_{2,1}$ -UFS (Tang et al. 2018b) and the proposed introduced in Lu et al. (2018). SPNFSR (Structure-Preserving Non-negative Feature Self-Representation),  $l_{2,1}$ -UFS ( $l_{2,1}$  based graph regularized UFS method) and DSRMR (Dual Self-Representation and Manifold Regularization) take into account both the self-representation and the structure-preserving ability of features by optimizing a model based on the  $l_{2,1}$ -norm. The general idea of these methods is to optimize a model (objective function) take into account three aspects: (1) the self-representation of features using the  $l_{2,1}$  norm. (2) the local manifold geometrical structure of the original data using a graph-based norm regularization term. And 3) a regularization term  $W$  to reflect the importance of each feature. The optimization problem is solved through an efficient iterative algorithm. At the final stage, each feature is sorted according to the corresponding  $W$  values in descending order and the top  $p$  ranked features are selected. For its part LRSL (Low-rank approximation and structure learning for unsupervised feature selection), unlike the previous methods, uses the Frobenius norm instead of  $l_{2,1}$ -norm. Finally, the method introduced in Lu et al. (2018) proposes an objective function for modeling the feature selection problem through a linear combination of all the features in the original feature space and considering

the local manifold structure of the data using an object similarity matrix. Then, once the model has converged, features are ordered according to the corresponding weights and the top  $p$  ranked features are selected.

Recently, some works that use Locally Linear Embedding (LLE) and non-convex sparse regularizers functions in sparse learning models have been proposed. In Luo et al. (2018), a novel unsupervised feature selection method that uses LLE (Roweis and Saul 2000) to model the manifold structure of the data was proposed. The idea is to characterize the intrinsic local geometric through an LLE graph-based instead of the typical pairwise similarity matrix jointly with a structure regularization term. For each feature, a feature-level reconstruction score based on the LLE graph is defined, and the final feature subset is selected according to this score. On the other hand, in Shi et al. (2018) a non-convex sparse learning model was proposed. The idea is to perform feature selection through an orthogonal-nonnegative constraint sparse regularized model using a new norm named  $\ell_{2,1-2}$ -norm defined as the difference of the  $\ell_{2,1}$  and the Frobenius norm. To solve the model efficiently, an iterative algorithm based on the Alternating Direction Method of Multipliers (ADMM) (Boyd et al. 2011) was also proposed.

## 2.2 Wrapper approach

UFS methods based on the wrapper approach can be divided into three broad categories according to the feature search strategy: sequential, bio-inspired, and iterative. In the former, features are added or removed sequentially. Methods based on sequential search are easy to implement and fast. On the other hand, bio-inspired methods try to incorporate randomness into the search process, aiming to escape from local optima. Finally, iterative methods address the unsupervised feature selection problem by casting it as an estimation problem and thus avoiding a combinatorial search.

### 2.2.1 Sequential methods

One of the most outstanding methods in this category was introduced in Dy and Brodley (2004). In this work, two feature selection criteria were evaluated: the criterion of Maximum Likelihood (ML) and the scatter separability criterion (trace criterion TR) (Fukunaga 1990). This method searches through the space of feature subsets, evaluating each candidate subset as follows: First, Expectation Maximization (EM) (Dempster et al. 1977) or  $k$ -means (MacQueen 1967) clustering algorithms are applied on the data described by each candidate subset. Then, the obtained clusters are evaluated with the ML or TR criteria. The method uses a forward selection search for generating subsets of features that will be evaluated as described above. The method ends when the change in the value of the used criterion is smaller than a given threshold.

In Breaban and Luchian (2011), a method that uses a new optimization criterion for, respectively, minimizing and maximizing the intra-cluster and inter-cluster inertias was proposed. The authors propose a function, unbiased w.r.t. the number of clusters and features, based minimization-maximization of the variance of scatter matrices obtained from the clusters built by the  $k$ -means clustering algorithm. This function assigns a ranking score to each partition that may be defined in the search space of all possible subsets of features and number of clusters. The criterion proposed in this method provides both a ranking of relevant features and an optimal partition.

A UFS method that uses a conceptual clustering algorithm for feature selection was proposed in Devaney and Ram (1997). In this work, the authors developed an unsupervised feature selection method based on a measure called *category utility*, which is used to measure the quality of the clusters found by the COBWEB hierarchical clustering algorithm (Fisher 1987). This method generates subsets of features with two search strategies: forward selection and backward elimination. Feature selection is performed running the COBWEB algorithm using the subset of features generated by the search strategy and evaluating the *category utility* for this feature subset. The process ends when no higher category utility score can be obtained in the backward or forward selection.

Finally, in Hruschka and Covoes (2005), a method for feature selection called SS-SFS (Simplified Silhouette Sequential Forward Selection) was proposed. This method selects a feature subset that provides the best quality according to the simplified silhouette criterion. In this method, a forward selection search is used for generating subsets of features. Each feature subset is used to cluster the data using the  $k$ -means clustering algorithm, and the quality of the feature subset is evaluated through the quality of the clusters measured with the simplified silhouette criterion. The feature subset that produces the best value of this criterion in the forward selection is selected.

### 2.2.2 Bio-inspired methods

A representative UFS method in this category was introduced in Kim et al. (2002), where an evolutionary local selection algorithm (ELSA) was proposed to search feature subsets as well as the number of clusters based on the  $k$ -means and Gaussian Mixture clustering algorithms. Each solution provided by the clustering algorithms is associated with a vector whose elements represent the quality of the evaluation criteria, which are based on the cohesion of the clusters, inter-class separation, and maximum likelihood. Those features that optimize the objective functions in the evaluation stage are selected.

Another method, also based on an evolutionary algorithm, was introduced in Dutta et al. (2014). In this work, feature selection is performed while the data are clustered using a multi-objective genetic algorithm (MOGA). This method proposes a multi-objective fitness function that minimizes the intra-cluster distance (uniformity) and maximizes the inter-cluster distance (separation). Each chromosome represents a solution, which is composed by a set of  $k$  cluster centroids (cluster center for continuous features and cluster mode for categorical features) described by a subset of features. The number of features used for each centroid in each chromosome is randomly generated, and the cluster centers and cluster modes of chromosomes in the initial population are created by generating random numbers, and feature values from the same feature domain, respectively. Then, for reassigning cluster centroids, MOGA uses the  $k$ -prototypes clustering algorithm (Huang 1997, 1998) which obtains its inputs from the initial population generated in the previous step. Afterward, the crossover, mutation, and substitution operators are applied, and the process is repeated until a pre-specified stop criterion is met. In the final stage, this method returns the feature subset that optimizes the fitness function jointly with the clusters that they produced.

### 2.2.3 Iterative

An outstanding method in this category was proposed in Law et al. (2004). The method proposes a strategy to cluster data and to perform feature selection simultaneously using the EM (Dempster et al. 1977) clustering algorithm. The idea is to estimate a set of weights (real

values in  $[0 - 1]$  called “*feature saliences*” (one for each feature) to quantify the relevance of each feature. This estimation is carried out by a modified EM algorithm derived for the task. The method returns the parameters of the density functions that model the components (clusters), as well as the set of *feature saliences* values. Then, the user can consider those *feature saliences* that best discriminate between different components (those with the highest values). Similar to the previous method, in Roth and Lange (2004) the authors perform feature selection and clustering simultaneously using a Gaussian mixture model (Figueiredo and Jain 2002). In this method, the idea is to optimize the Gaussian mixture model via the EM clustering algorithm, where the Maximization-step of this algorithm was reformulated as a  $l_1$ -constraint LASSO problem (Tibshirani 1996; Osborne et al. 2000). The method returns the clusters as well as the coefficients of the model; the coefficients indicate the relevance of each feature.

In more recent years, wrapper methods that use clustering algorithms for initialization or optimization of Sparse Learning models have been proposed, such is the case of the methods introduced in Zeng and Cheung (2011), Wang et al. (2015b), Guo et al. (2017), and Guo and Zhu (2018). In Zeng and Cheung (2011) a wrapper method called LLC-fs (Local Learning-based Clustering algorithm with feature selection) was proposed. In this method, it is assumed that the cluster indicator value at each point should be estimated by a ridge regression model. The authors propose to use the Local Learning-Based Clustering (LLC) framework (Wu and Schölkopf 2007) to formulate the final ridge regression model. Feature selection is done by introducing a binary feature selection vector  $\tau$  to the local discriminant function of the model. At the end, after the convergence, the output is the vector  $\tau$  along with a discretized cluster indicator matrix. In Wang et al. (2015b) a method called EUFS (Embedded Unsupervised Feature Selection), which directly embeds the feature selection in the clustering algorithm via Sparse Learning was proposed. In this work, a not convex sparse regression model using a loss function based on  $l_{2,1}$ -norm is introduced and optimized through an Alternating Direction Method of Multipliers (Boyd et al. 2011). EUFS uses the  $k$ -means clustering algorithm to initialize a pseudo cluster indicator matrix  $U$  and a latent feature matrix  $V$  (used for indicating feature weights) in the final model. Once the model has converged, the output is a feature ranking sorted according to the final values of the latent feature matrix along with the pseudo clusters indicators. A more recent work based on the same idea as the previous work was introduced in Guo et al. (2017). This method proposes the same objective function as EUFS and only differs in that the loss function of the final model uses the Frobenius-norm instead of  $l_{2,1}$ -norm, and the update of  $U$  and  $V$  is performed iteratively by the  $k$ -means clustering algorithm until convergence of the model. Moreover, in Guo and Zhu (2018), the first author of the last work proposed another wrapper method called DGUFS (Dependence Guided Unsupervised Feature Selection), which simultaneously performs feature selection and clustering<sup>3</sup> using a constraint model based on  $l_{2,0}$ -norm. The model is optimized using a modified algorithm based on the iterative Alternating Direction Method of Multipliers (Boyd et al. 2011).

### 2.3 Hybrids

In order to take advantage of the filter and wrapper approaches, hybrid methods, in a filter stage, the features are ranked or selected applying a measure based on intrinsic properties of the data. While, in a wrapper stage, certain feature subsets are evaluated for finding the

<sup>3</sup> Clustering can be made using the Constrained Boolean Matrix Factorization (CBMF) algorithm proposed by Li et al. (2014a) or employing eigendecomposition and exhaustive search.



best one, through a specific clustering algorithm. We can distinguish two types of hybrid methods: methods based on ranking and methods non-based on ranking of features. In this section, we described some methods of both types belonging to this approach.

In Dash and Liu (2000) one of the first based on ranking unsupervised hybrid feature selection methods was introduced. This method is based on the entropy measure proposed in Dash et al. (1997) (filter stage), jointly with the internal scatter separability criterion (Dy and Brodley 2004) (wrapper stage). In the filter stage, each feature, one by one, is removed from the whole set of features, and the entropy generated in the dataset after the elimination of the feature is computed. This produces a sorted list of features according to the degree of disorder that each feature generates when it was removed from the whole set of features. Once all features have been sorted, in the wrapper stage, a forward selection search is applied jointly with the  $k$ -means clustering algorithm in order to build clusters which are evaluated using the scatter separability criterion. This method selects the feature subset that reaches the highest value for the separability criterion.

Another hybrid method also based on feature ranking was proposed in Li et al. (2006). In this method, the authors combine an exponential entropy measure with the fuzzy evaluation index FFEI (Pal et al. 2000) for feature ranking and feature subset selection, respectively. The method employs sequential search considering subsets of features based on the generated ranking and using the fuzzy evaluation index as quality measure. In the wrapper stage, with the purpose of selecting even a smaller feature subset, the fuzzy-c-means algorithm and the scatter separability criterion (Dy and Brodley 2004) are used to select what the authors called a “compact” subset of features.

A more recent hybrid based on ranking unsupervised feature selection method was proposed in Solorio-Fernández et al. (2016). In this method, the authors combine spectral feature selection and the Calinski-Harabasz index (Calinski and Harabasz 1974) for selecting a relevant feature subset. The feature selection is divided into two stages: (1) Feature ranking and, (2) feature subset selection. In the first stage, the idea is to identify those features that preserve the data structure computing for each feature the Laplacian Score (He et al. 2005); this produces a feature ranking. After, in the second stage, taking advantage of the ranking generated in the previous stage and using forward or backward selection search, feature subsets are evaluated through a modified internal evaluation index called WNCH (Weighted Normalized Calinski-Harabasz index). The feature subset with the highest WNCH value is selected.

On the other hand, in Hruschka et al. (2005) a hybrid UFS method non-based on ranking called BFK that combines  $k$ -means and a Bayesian filter was introduced. This method, unlike all the above mentioned hybrid methods, begins with the wrapper stage, by running the  $k$ -means clustering algorithm on the dataset with a range of clusters specified by the user. The clusters are evaluated with the simplified silhouette criterion and the one with the highest value is selected. Subsequently, in the filter stage, using the concept of Markov blanket, a feature subset is selected through a Bayesian network, where each cluster represents a class, the nodes represent features, and the edges represent relationships between features.

Another hybrid method non-based on ranking that removes both irrelevant and redundant features was introduced in Kim and Gao (2006). This method performs feature selection in two steps: In the first step, a subset of features is founded by applying the least-square estimation (LSE)-based evaluation (Mao 2005). The second step works only with those features identified in the first step, and by using a Sequential Forward Selection search the best feature subset that maximizes the clustering performance (using a modified version of the EM clustering algorithm) is found.

Finally, It is worth noting that, in the literature, some hybrid unsupervised feature selection methods like (Jashki et al. 2009; Hu et al. 2009; Yang et al. 2011a; Yu 2011) designed specifically for handling data in specific domains also have been proposed. Likewise, there are other works such as those proposed in Hruschka et al. (2007), Luo and Xiong (2009) and Dash and Ong (2011), which solve the problem from another different perspective; performing feature selection assuming that a set of clusters can be modeled as being a set of different classes, where they can apply traditional supervised feature selection methods on data.

### 3 Analysis and discussion

In the previous section, Unsupervised Feature Selection methods were categorized and reviewed according to their approach, type, and subtype. In this section, some overall aspects, advantages, and disadvantages of the UFS methods described in Sect. 2 are discussed. Furthermore, in this section, an experimental evaluation of the most relevant and recent UFS methods of each category is carried out.

In Table 1, we summarize the general advantages and disadvantages of UFS methods belonging to the filter, wrapper, hybrid approaches, and in Table 2, we show the advantages and disadvantages of the described UFS methods regarding their type, subtype, and approach; in concordance to the taxonomy shown in Fig. 1. Moreover, in order to give more details about the UFS methods analyzed in this review, in Table 3, we show a summary of these methods. In this table, the reference, approach, type of method, as well as the datasets,<sup>4</sup> classifiers/clustering algorithms, and the validation measures used to assess the quality of the selection, are shown.

As we can see in Tables 1 and 2, in general, there is not a better UFS approach or method for all kind of data and domain, every approach has its own pros and cons. Nevertheless, from our literature study and from Tables 1, 2 and 3 we can highlight some important general characteristics of the different methods belonging to the different approaches and types.

In Table 3, we can see that there are only a few wrapper methods for Unsupervised Feature Selection, in contrast to filter methods. This is mainly because wrappers become less useful for high dimensionality problems, which makes them seldom used in practice. On the other hand, hybrid methods are preferred to wrapper ones, given their compromise between efficiency and quality of the selected feature subsets. However, there are also few hybrid methods for unsupervised feature selection reported in the literature. Conversely, the filter approach has received more attention. This is understandable given the technological advancement in the last years, and the vast amount of unlabeled data generated across many scientific disciplines, such as text mining, genomic analysis, social media, and intrusion detection, to name a few, where fast and scalable methods are needed. Unsupervised feature selection methods under the filter approach rely on general characteristics of data and evaluate features without involving any clustering algorithm; therefore, they do not have a bias to specific learning models. Besides, filter methods are easy to design, easy to be understood by other researchers, and they are usually very fast (Zhao 2010), which makes them attractive for high-dimensional data. Moreover, as we can see in the taxonomy of Fig. 1, there is an inclination to the development of filter methods based on Spectral Feature Selection and Sparse Learning. This last is mainly because these methods besides being fast, obtain good results in terms of the quality of the selected features.

<sup>4</sup> The number in parentheses denotes the number of datasets used for validation.

**Table 1** General advantages and disadvantages of UFS methods regarding their approach

Approach	Advantages	Disadvantages
Filter	Fast Scalable Independent of the clustering algorithm Parallelizable	Ignores interaction with clustering algorithms
Wrapper	Interact with the clustering algorithm to be used Can model feature dependencies	Risk of overfitting High computational cost
Hybrid	Interact with the clustering algorithm to be used Less time consuming than wrappers Can model feature dependencies	The selection is specific for the used clustering algorithm The selection is specific for the used clustering algorithm

**Table 2** Advantages and disadvantages of UFS methods regarding the type

Type/subtype of method	Approach	Advantages	Disadvantages
Univariate-information based	Filter	Solid theoretical background Information based measures can model linear and non-linear relationships Information based measures are unbiased regarding the dimensionality of the data	Ignore correlation among features
Univariate-spectral/similarity based	Filter	Solid theoretical background Provide a powerful framework for unsupervised feature selection	Ignore correlation among features
Multivariate-statistical/information based	Filter	Can model feature dependencies Less time consuming than wrapper methods	Slower than univariate methods Less scalable than univariate methods
Multivariate-bio-inspired	Filter	Less prone to local optima Model feature dependencies	Slower than univariate methods High memory requirements
Multivariate-spectral/sparse learning based	Filter	Solid theoretical background Handling redundant features	Slower than univariate methods Less scalable than univariate methods
Sequential	Wrapper	Simple to implement	Risk of overfitting Prone to local optima
Bio-inspired	Wrapper	Less prone to local optima Can model feature dependencies	Higher risk of overfitting than sequential based-methods High memory requirements
Iterative	Wrapper	Can model feature dependencies Feature selection and clustering are made simultaneously	Risk of overfitting
Based on ranking	Hybrid	Individual relevant features can be more easily identified and selected from the feature ranking	The filter and wrapper approaches can not be truly integrated with each other, which may lead to lower quality performance
Non-based on ranking	Hybrid	Can exploit other ideas that ranking-based methods cannot, for example, modeling feature dependency in the filter stage	Individual relevant features cannot be easily identified because there is no a ranking of features The filter and wrapper approaches cannot be truly integrated with each other, which may lead to lower quality performance

### 3.1 Criteria for determining relevant features

Unlike supervised and semi-supervised feature selection, Unsupervised Feature Selection is considered a much harder problem due to the difficulty of defining feature relevancy (Dy and Brodley 2004).<sup>5</sup> In this regard, from all UFS methods analyzed in our review, we have been able to identify three main criteria commonly used to determine relevant features. The first one consists in choosing those features that can best preserve the manifold structure of the original data; we can find examples of methods using this criterion in the Univariate and Multivariate Spectral/Sparse Learning-based methods belonging to the filter approach. The second criterion consists in seeking cluster indicators (considered as pseudo labels) through clustering algorithms and then transform the unsupervised feature selection into a supervised context; some examples of this kind of methods can be found in Multivariate Spectral/Sparse Learning-based methods of the filter, wrapper, and hybrid approaches. Finally, there is another criterion based on the analysis of correlation among features (feature dependency), where the objective consists in selecting a feature subset with the highest or lowest correlation among features. Some examples of this last criterion can be found in the Multivariate-Statistical based methods in the filter approach.

### 3.2 Criteria for determining redundant features

Feature correlation, besides to be used as a criterion for selecting relevant features, it is also used for defining feature redundancy. In general, in the literature of Unsupervised Feature Selection, we have identified two main approaches for quantifying redundancy of a particular subset of features: (1) quantifying redundancy without considering an objective concept, and (2) quantifying redundancy considering an objective concept. In the first case, the objective consists in measuring the degree of dependence, similarity, association or correlation (commonly by pairs) among the features by using statistical or information based measures. Some examples of methods under this approach are Mitra et al. (2002), Haindl et al. (2006), Garcia-Garcia and Santos-Rodriguez (2009), Yen et al. (2010), Zhao et al. (2013), Tabakhi et al. (2014), Tabakhi and Moradi (2015), Tabakhi et al. (2015), Han et al. (2015) and Li and Tang (2015). Meanwhile, in the second case, the aim is to quantify the relationship among features; considering further a specific task or objective concept for which these features could be considered redundant. This is commonly achieved by evaluating features jointly and using sparsity regularization in a constrained regression optimization model. Some examples of UFS methods using this last approach are Zheng et al. (2010), Cai et al. (2010), Zhao and Liu (2011), Hou et al. (2011) and Zhu et al. (2016).

### 3.3 Performance evaluation and datasets used for assessing UFS methods

Table 3 help us to appreciate that performance evaluation of Unsupervised Feature Selection methods has been done in different ways. Nevertheless, from the analysis made in this review, we can identify three main ways for evaluating the results of the UFS methods:

- Evaluation in terms of the quality of the selected features for a specific supervised/unsupervised classifier. This evaluation is the most widely used, and it has become

<sup>5</sup> Unlike supervised feature selection, which has class labels to guide the search for discriminative features, in UFS, we must define feature relevancy in the form of objective concepts.

the most accepted way for assessing Unsupervised Feature Selection methods. Within this type of evaluation, two standard ways are distinguished.

1. Evaluation using the *classification accuracy* or *error rate* of supervised classifiers such as *k*NN (Fix and Hodges 1951), SVM (Cortes and Vapnik 1995), and Naive Bayes (NB) (Maron 1961; John and Langley 1995), among others. From Table 3, we can see that this evaluation is commonly used by Spectral Feature Selection, Statistic-based, and Bio-inspired methods.
  2. Evaluation using the results of clustering algorithms such as *k*-means (MacQueen 1967), EM (Dempster et al. 1977), and COBWEB (Fisher 1987). For assessing the clustering quality, measures like *Normalized Mutual Information (NMI)* and *Clustering Accuracy (ACC)* are commonly used. Wrapper and hybrid UFS methods, as well as multivariate filter methods based on Sparse Learning and Spectral Feature Selection commonly use clustering algorithms to assess the quality of the selected features.
- Evaluation in terms of the redundancy of the selected features. This evaluation is used by those methods that consider the elimination of redundant features (Mitra et al. 2002; Li et al. 2007; Haindl et al. 2006; Yen et al. 2010; Wang et al. 2015a; Tabakhi et al. 2014; Garcia-Garcia and Santos-Rodriguez 2009; Li et al. 2012; Li and Tang 2015). For this evaluation, the *redundancy rate* (Zheng et al. 2010) and *Representation Entropy* (Devijver and Kittler 1982) are the most used redundancy measures.
  - Evaluation in terms of the correctness of the selected features. This evaluation consists in quantifying with a specific measure such as *precision*, *recall* or *F-measure* the amount of relevant features selected by an unsupervised feature selection method. Of course, this is commonly done using synthetic datasets, where the actual relevant features are known a priori, which usually is not possible for real-world datasets.

Regarding the datasets used for evaluation of UFS methods, from Table 3, it can be seen that at least half of the reviewed works use data from the well-known UCI machine learning repository<sup>6</sup> (Lichman 2013), which contains many kinds of datasets with different sizes in both, number of objects and features (including numeric, non-numeric and mixed). The other half of the reviewed works, especially those based on Spectral Analysis and Sparse Learning, mostly use datasets of high dimensionality, such as text, biological data, and images, among others. Likewise, we can observe in Table 3 that the number of datasets used to validate UFS methods ranges from 1 to 42, being seven the average. This indicates, from our point of view, that a more extensive empirical study using a large number of datasets is required to evaluate the actual performance of the UFS methods proposed in the literature.

### 3.4 Experimental comparison

In order to make a comparison of the performance of the different approaches and categories of the UFS methods reviewed in this paper, we selected 15 of the most relevant and recent UFS methods (taking into account each approach and category) and we evaluated them on 15 datasets from the UCI machine learning repository (detailed information about the selected datasets is summarized in Table 4). The aim is to carry out an empirical comparison about the performance of these methods, regarding the quality of selected features and runtime, over different kind of data (numerical, non-numerical, and mixed data) and perform a further

<sup>6</sup> <https://archive.ics.uci.edu/ml/index.php>.



**Table 3** Summary of unsupervised feature selection methods

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Dash et al. (1997)	Filter	Univariate-entropy based	UCI machine learning repository (17)	C4.5 classifier	Error rate using tenfold cross-validation
Varshavsky et al. (2006)	Filter	Univariate-entropy based	Public available datasets (3)	QC	Averages of the Jaccard score of 100 runs of a clustering algorithm
Devakumari and Thangavel (2010)	Filter	Univariate-entropy based	UCI machine learning repository (5)	K-means	Objective function computed by K-means
Rao and Sastry (2012)	Filter	Univariate-entropy based	UCI machine learning repository (4)	C4.5 decision tree classifier	Error in classification and clustering using tenfold cross-validation
Banerjee and Pal (2014)	Filter	Univariate-entropy based	UCI machine learning repository (14)	K-means Fuzzy C-means	Sammon's error
Zhao and Liu (2007)	Filter	Univariate-spectral-similarity	Public available text and face image datasets (3)	INN (nearest neighbor) classifier	Cluster Preserving Index (CPI)
He et al. (2005)	Filter	Univariate-spectral-similarity	Iris	INN classifier	Error rate
Padungweang et al. (2009)	Filter	Univariate-spectral-similarity	PIE face data UCI machine learning repository (6)	K-means	Average of classification accuracy of 10 trials NMI and ACC
Solorio-Fernández et al. (2017)	Filter	Univariate-spectral-similarity	UCI machine learning repository (20)	5NN (nearest neighbor) classifier K-prototypes clustering algorithm Naive bayes, 3NN and SVM classifiers	Average of classification accuracy using tenfold cross validation NMI and ACC Classification accuracy using tenfold cross validation

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Mitra et al. (2002)	Filter	Multivariate-statistical based	UCI machine learning repository (9)	KNN (value of K not specified) and Bayes classifiers	Representation entropy, entropy, fuzzy evaluation index, and class separability Classification accuracy FFEI values
Li et al. (2007)	Filter	Multivariate-statistical/information-based	UCI machine learning repository (3)	3NN classifier	Classification accuracy FFEI values
			Synthetic datasets		Classification accuracy using tenfold cross validation
Haendl et al. (2006)	Filter	Multivariate-statistical based	UCI machine learning repository (2)	Naive Bayes classifier	Classification error using tenfold cross validation
			Emotional speech data collections (2)		
Talavera (2000)	Filter	Multivariate-statistical based	UCI machine learning repository (8)	COBWEB clustering algorithm	Average error rate of 5 replications using twofold cross validation
Ferreira and Figueiredo (2012)	Filter	Multivariate-statistical based	UCI machine learning repository (12)	SVM, Naive Bayes and 3NN classifiers	Average error rate for 10 runs with random train/test partitions of the datasets
			NIPS2003 challenge (5)		
			Microarray gene expression datasets (11)		
Yen et al. (2010)	Filter	Multivariate-statistical based	UCI machine learning repository (3)	None	Area under receiver operating characteristic (ROC) curve (AUC) versus the percent of features removed

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Wang et al. (2015a)	Filter	Multivariate-statistical based	ASU feature selection repository (6)	Not specified	NMI and ACC
Dash et al. (2002)	Filter	Multivariate-entropy based	Iris dataset	None	Redundancy rate Correctness of the selected features
Tabakhi et al. (2014)	Filter	Multivariate-bio-inspired	Synthetic datasets UCI machine learning repository (7)	SVM, decision trees, and Naive Bayes classifiers	Average error rate over 5 independent runs with random train/test partitions
Tabakhi and Moradi (2015)	Filter	Multivariate-bio-inspired	NIPS2003 challenge (2) UCI machine learning repository (9) Bioinformatics Research Group of Universidad Pablo de Olavide (1)	SVM, decision trees, and Naive Bayes classifiers	Average error rate over 5 independent runs with random train/test partitions
Tabakhi et al. (2015)	Filter	Multivariate-bio-inspired	NIPS2003 challenge (2) Microarray datasets from Universidad Pablo de Olavide (2) Gene expression model selector from Vanderbilt University (3)	SVM, Naive Bayes, and decision trees classifiers	Average error rate over 5 independent runs with random train/test partitions
Dadaneh et al. (2016)	Filter	Multivariate-bio-inspired	UCI machine learning repository (10)	SVM, Naive Bayes, and 1NN classifiers	Classification accuracy using tenfold cross validation
Nijima and Okuno (2009)	Filter	Multivariate-spectral	Public datasets of cancer microarrays (7)	Nearest mean classifier (NMC)	Average error rate over the 100 runs

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Garcia-Garcia and Santos-Rodriguez (2009)	Filter	Multivariate-spectral	Gene expression Profiles in human cancers challenge dataset (1)	Spectral clustering method	Clustering error
Liu et al. (2009b)	Filter	Multivariate-spectral	UCI machine learning repository (6)	K-means	Average clustering accuracy from 10 trials
Cai et al. (2010)	Filter	Multivariate-spectral-sparse learning	UCI machine learning repository (4)	K-means	NMI
Zheng et al. (2010)	Filter	Multivariate-spectral-sparse learning	Public high dimensional datasets (6)	INN classifier	Error rate using leave-one-out cross validation
Yang et al. (2011b)	Filter	Multivariate-spectral-sparse learning	Public benchmark datasets (6)	SVM classifier	Classification accuracy, Jaccard score
Hou et al. (2011), Hou et al. (2014)	Filter	Multivariate-spectral-sparse learning	Several public datasets, including images, voice and biological data	K-means	Redundancy rate NMI and ACC
Wang et al. (2016)	Filter	Multivariate-Spectral-Sparse learning	Public available datasets (5)	KNN classifier (value of K not specified) K-means	NMI and ACC Classification accuracy ACC
Li et al. (2012)	Filter	Multivariate-spectral-sparse learning	Public available datasets (8)	K-means	NMI and ACC

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Li and Tang (2015)	Filter	Multivariate-spectral-sparse learning	Public available image datasets (9)	K-means	NMI and ACC
Han et al. (2015)	Filter	Multivariate-spectral-sparse learning	Public available datasets (5)	K-means	Redundancy rate NMI
Zhu et al. (2016)	Filter	Multivariate-sparse learning	Public available datasets (6)	K-means	Purity F1-score NMI and ACC
Nie et al. (2016)	Filter	Multivariate-sparse learning	Public available datasets (8)	K-means	ACC
Zhao et al. (2013)	Filter	Multivariate-spectral-sparse learning	Public high dimensional datasets (8)	Linear SVM classifier	Classification accuracy
Li et al. (2014b)	Filter	Multivariate-spectral-sparse learning	Public benchmark datasets (12)	K-means	Jaccard score Redundancy rate NMI and ACC
Qian and Zhai (2013)	Filter	Multivariate-sparse learning	Benchmark real world datasets (6)	K-means	NMI and ACC
Du et al. (2017)	Filter	Multivariate-sparse learning	Public available datasets (6)	K-means	NMI and ACC
Zhu et al. (2015, 2017)	Filter	Multivariate-sparse learning	Synthetic and real-world datasets	K-means	NMI and ACC

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Shi et al. (2015)	Filter	Multivariate-sparse learning	Public available datasets (6)	K-means	NMI and ACC
Yi et al. (2016)	Filter	Multivariate-sparse learning	Standard face datasets (3)	5NN classifier	Classification accuracy
Zhou et al. (2017)	Filter	Multivariate-sparse learning	Public available benchmark datasets (6)	K-means	NMI and ACC
Wang and Wang (2017)	Filter	Multivariate-sparse learning	Public available datasets (12)	K-means	NMI and ACC
Tang et al. (2018a)	Filter	Multivariate-sparse learning	Public available datasets (10)	K-means	NMI and ACC
Tang et al. (2018b)	Filter	Multivariate-sparse learning	Public available datasets (10)	K-means	NMI and ACC
Lu et al. (2018)	Filter	Multivariate-sparse learning	Public available datasets (6)	K-means	NMI and ACC
Luo et al. (2018)	Filter	Multivariate-sparse learning	Public available datasets (8)	K-means	NMI and ACC
Shi et al. (2018)	Filter	Multivariate-sparse learning	Public available datasets (6)	K-means	NMI and ACC
Dy and Brodley (2004)	Wrapper	Sequential	Synthetic datasets (5)	EM and K-means	Class error rate
Breaban and Luchian (2011)	Wrapper	Sequential	UCI machine learning repository (3)	K-means	Bayes error
			synthetic datasets (40)		Precision and recall
			UCI machine learning repository (2)		Adjusted rand index
					Precision, recall, and F-measure



Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Devaney and Ram (1997)	Wrapper	Sequential	UCI machine learning repository (2)	COBWEB	Accuracy of predicting the class label of the previously unseen testing objects Class error
Hruschka and Covoes (2005)	Wrapper	Sequential	Synthetic datasets (1)	K-means	
Law et al. (2004)	Wrapper	Iterative	Bioinformatics datasets (6) Synthetic datasets (2)	EM	Error rates (using the ground truth labels) on the test data repeated 20 times
Roth and Lange (2004)	Wrapper	Iterative	UCI machine learning repository (4) USPS handwritten digits dataset (1)	EM	Stability of data partitions
Zeng and Cheung (2011)	Wrapper	Iterative	Stirling faces database (1) UCI machine learning repository (4)	None	ACC
Wang et al. (2015b)	Wrapper	Iterative	Public available benchmark datasets (6)	K-means	ACC and NMI
Guo et al. (2017)	Wrapper	Iterative	Public available benchmark datasets (6)	K-means	ACC
Guo and Zhu (2018)	Wrapper	Iterative	Public available benchmark datasets (6)	K-means	ACC and NMI
Kim et al. (2002)	Wrapper	Bio-inspired	Real datasets (1) Synthetic datasets (1)	K-means and EM	F-accuracy F-within and F-between

Table 3 continued

Literature	Approach	Type of method	Datasets used for validation	Classifier/clustering algorithm used for validation	Validation measure
Dutta et al. (2014)	Wrapper	Bio-inspired	UCI machine learning repository (4)	K-Prototypes	Davies–Bouldin index, C index, and Dunn index ACC
Dash and Liu (2000)	Hybrid	Based on ranking	Synthetic datasets (4) UCI machine learning repository (5)	K-means	Feature ranking Impurity
Li et al. (2006)	Hybrid	Based on ranking	Synthetic and real-world datasets from the UCI machine learning repository	3NN	Feature ranking
Solorio-Fernández et al. (2016)	Hybrid	Based on ranking	Synthetic datasets (20)	K-means	Classification accuracy using cross validation Jaccard index and global silhouette Retention and Run-time
Hruschka et al. (2005)	Hybrid	Non-based on ranking	UCI machine learning repository (22) Synthetic datasets (1) UCI machine learning repository (4)	K-means	Class error
Kim and Gao (2006)	Hybrid	Non-based on ranking	Synthetic datasets (2) UCI machine learning repository (2)	EM	Classification error using tenfold cross validation

analysis based on the experimental results. Specifically, in our experiments, we compared the following UFS methods:

- Filter
  - *Univariate*: SVD-Entropy (Varshavsky et al. 2006), Laplacian Score (LS) (He et al. 2005), SPEC (Zhao and Liu 2007), and USFSM (Solorio-Fernández et al. 2017).
  - *Multivariate*: FSFS (Mitra et al. 2002), RRFS (Ferreira and Figueiredo 2012), UDFS (Yang et al. 2011b), NDFS (Li et al. 2012), UFSACO (Tabakhi et al. 2014), MGSACO (Tabakhi et al. 2015), and DSRMR (Tang et al. 2018a).
- Wrapper
  - LLC-fs (Zeng and Cheung 2011) and DGUFS (Guo and Zhu 2018).
- Hybrid
  - Li et al. (2006) and WNCH-BE (Solorio-Fernández et al. 2016).
- All original features are adopted as the baseline in our experiments.

Following the standard ways to assess UFS methods, we evaluate the UFS methods in terms of clustering and classification performance. For evaluating the clustering results, the commonly used clustering performance metrics ACC (Clustering Accuracy) and the NMI (Normalized Mutual Information) were applied over the partitions produced by the  $k$ -means clustering algorithm<sup>7</sup> on the selected features by each UFS method on each dataset. On the other hand, for evaluating the UFS methods in terms of classification performance, we used the well-known and broadly used SVM (Cortes and Vapnik 1995) classifier. For the evaluation, we applied stratified fivefold cross-validation, and the final classification performance is reported as the average accuracy over the five folds. For each fold, each UFS method is first applied on the training set (ignoring the class labels) to obtain a feature subset. Then, after training the classifier using the selected features, the respective test sets are used for assessing the classifier through its accuracy. Additionally, we evaluate the runtime spent by each UFS method for performing feature selection.

The SVM classifier and the  $k$ -means clustering algorithm used in our experiments were taken from the Weka data mining software tool (Hall et al. 2009), for SVM we used its default parameter values while the parameter  $k$  for  $k$ -means was set as the number of classes declared for each dataset. Likewise, for the different UFS methods analyzed in our experiments, we used the author's implementation, and the parameter values were fixed according to the recommendation of their respective authors. All experiments were run in Matlab® R2018a with Java 1.8, using a computer with an Intel Core i7-2600 3.40 GHz  $\times$  8 processor with 32 GB DDR4 RAM, running 64-bit Ubuntu 16.04 LTS (GNU/Linux 4.13.0-38 generic) operating system.

In our experiments, for those UFS methods that provide a feature ranking as output, or those that need as an input parameter the number of features to select, we set 40%, 50% and 60% of the ranked features for the first ones, and the same percentage of the whole set of features for the second ones, respectively. The best classification and clustering results in the different percents were reported as the final result for all the feature selection methods. Furthermore, in our experiments, the Friedman test (Friedman 1937) was used to make and evaluate the ranking of all the evaluated methods over all the datasets. It is important to mention that for all datasets, class labels were removed for feature selection and clustering, and for those UFS methods that can only process numerical features, the non-numerical

<sup>7</sup> In order to get more reliable results, we repeat the  $k$ -means algorithm ten times with different initial points and report the average clustering quality results.

**Table 4** Description of the used datasets taken from the UCI machine learning repository

#	Dataset	No. of objects	No. of features	No. of classes
1	Automobile	205	25	6
2	Breast-cancer	286	9	2
3	Heart-c	303	13	2
4	Heart-statlog	270	13	2
5	Hepatitis	155	19	2
6	Ionosphere	351	34	2
7	Liver-disorders	345	6	2
8	Lung cancer	32	56	3
9	Lymphography	148	18	4
10	Monks-problems-2-train	169	6	2
11	Sonar	208	60	2
12	Soybean	683	35	19
13	Wdbc	569	30	2
14	Wine	178	13	3
15	Zoo	101	17	7

features were transformed into numerical ones by mapping each categorical value into an integer value in the order of appearance of the dataset.

Tables 5, 6, 7 and 8 show the final results regarding classification (see Table 5), clustering (see Tables 6 and 7), and runtime (see Table 8) performance. In Tables 5, 6 and 7 the best method on average for each dataset appears in “bold”, and the last row of each table shows the average rank over all tested datasets.

Regarding the evaluation of the UFS methods in terms of supervised classification performance, from Table 5, it can be seen that UFS methods allow obtaining competitive or in some cases better classification performance than using all the features, but with fewer features. In this table, we can see that USFSM and NDFS obtained the best average ranking among those UFS methods in the filter approach; LLC-fs was the best in the wrapper approach, and the method proposed by Li et al. (2006) was the best in the hybrid approach.

On the other hand, regarding the evaluation of the UFS methods in terms of clustering performance, in Tables 6 and 7 we can see that among univariate methods, for both quality measures NMI and ACC, into the filter approach, the best results were obtained by SVD-entropy and LS methods among UFS univariate methods; meanwhile UDFS, NDFS, DSRMR, and UFSACO got the best results among the multivariate ones. Notice that most of above mentioned univariate and multivariate methods got even better results than those obtained when using all the features. The worst results in the filter approach were obtained by the multivariate statistical methods. In this case, in general, the methods in the wrapper and hybrid approaches obtained the worst results.

Regarding the runtime, from Table 8, we can see that the fastest UFS methods were those in the filter approach; LS and SPEC among univariate UFS methods, and FSFS, RRFS among multivariate UFS methods. While LLC-fs and LS-WNCH-BE were the fastest methods in the wrapper and hybrid approaches respectively. It also can be noted that the slowest methods were DSRMR, USFSM, and the hybrid method proposed in Li et al. (2006).

Finally, from the results shown in Tables 5, 6, 7 and 8, we can conclude the following:

**Table 5** Classification accuracy of the evaluated UFS methods using SVM

Dataset	Filter		Wrapper										Hybrid	Original		
	Univariate		Multivariate						LLC-fs							
	SVD-entropy	LS	SPEC	USFSM	FSFS	RRFS	UDFS	NDFS	UFSACO	MGSAO	DSRMR	DGUFs			Li et al.	LS-WNCH-BE
Automobile	0.498	0.478	0.478	0.595	0.659	0.668	0.507	0.566	0.678	0.668	0.561	0.517	0.683	<b>0.693</b>	0.673	<b>0.693</b>
Breast-cancer	0.710	<b>0.724</b>	0.703	0.696	0.717	0.692	0.706	0.710	0.713	0.696	0.699	0.703	0.713	0.678	0.685	0.685
Heart-c	0.822	0.818	0.835	<b>0.845</b>	0.792	0.802	0.815	0.812	0.785	0.818	0.809	0.802	0.759	0.819	0.815	0.832
Heart-statlog	0.830	0.778	0.826	0.763	0.778	0.826	0.778	0.822	0.833	0.796	0.830	0.804	0.807	0.793	0.726	<b>0.837</b>
Hepatitis	0.852	0.852	0.858	0.832	0.839	0.826	0.858	<b>0.871</b>	0.839	0.839	0.845	0.845	0.819	0.852	0.845	0.845
Ionosphere	0.866	0.832	0.789	0.889	0.852	0.866	0.869	0.880	0.889	0.866	0.886	0.866	<b>0.889</b>	0.874	0.852	0.883
Liver-disorders	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>	<b>0.580</b>
Lung-cancer	0.529	0.476	0.467	0.533	0.471	0.505	0.533	0.476	0.471	0.529	0.443	<b>0.538</b>	0.433	0.510	0.476	0.500
Lymphography	0.784	0.777	0.831	<b>0.845</b>	0.764	0.689	0.804	0.837	0.817	0.845	0.804	<b>0.845</b>	0.797	0.838	0.616	0.838
Monks-problems-2_train	<b>0.621</b>	<b>0.621</b>	0.598	<b>0.621</b>	0.610	0.598	<b>0.621</b>	0.610	<b>0.621</b>	0.598	0.610	0.610	<b>0.621</b>	<b>0.621</b>	<b>0.621</b>	0.604
Sonar	<b>0.798</b>	0.789	0.755	0.759	0.760	0.746	0.774	0.774	0.779	0.784	0.765	0.765	0.779	0.702	0.755	0.755
Soybean	0.871	0.880	0.892	0.898	0.898	0.862	0.873	0.868	0.889	0.921	0.896	0.925	0.902	0.912	<b>0.937</b>	0.928
Wdbc	0.944	0.952	0.965	0.952	0.958	0.963	0.951	0.967	0.965	0.961	0.956	0.975	0.972	0.949	0.935	<b>0.977</b>
Wine	0.955	0.955	0.955	0.949	0.933	0.921	0.926	0.966	0.938	0.944	0.938	0.972	0.938	0.910	0.961	<b>0.989</b>
Zoo	0.941	0.940	0.891	0.950	0.871	0.831	0.921	0.921	0.881	0.921	0.920	0.930	0.921	<b>0.960</b>	0.960	0.960
Average rank	<b>7.533</b>	<b>8.633</b>	<b>9.466</b>	<b>7.466</b>	<b>10.833</b>	<b>11.833</b>	<b>8.866</b>	<b>7.500</b>	<b>7.866</b>	<b>8.033</b>	<b>9.466</b>	<b>7.033</b>	<b>8.166</b>	<b>8.133</b>	<b>9.400</b>	<b>5.766</b>

**Table 6** ACC results of the evaluated UFS methods using *k*-means

Dataset	Filter		Wrapper										Hybrid	Original	
	Univariate		Multivariate						LLC-fs		Li et al. LS-WNCH-BE				
	SVD-entropy	LS	SPEC	USFSM	FSFS	RRFS	UDFS	NDFS	UFSACO	MGSAO		DSRMR			
Automobile	0.398	0.374	0.382	0.399	0.382	0.340	<b>0.403</b>	0.365	0.392	0.380	0.366	0.389	0.389	0.401	0.401
Breast-cancer	0.629	0.595	0.616	0.653	0.603	0.654	0.639	0.564	0.594	<b>0.655</b>	0.563	0.605	0.628	0.550	0.609
Heart-c	0.785	0.799	0.786	0.714	0.683	0.795	0.791	0.779	0.779	0.782	0.736	0.782	0.735	0.697	<b>0.809</b>
Heart-statlog	0.789	0.768	0.753	0.773	0.727	<b>0.796</b>	0.739	0.789	0.670	0.727	0.763	0.589	0.681	0.753	0.796
Hepatitis	0.746	0.725	0.768	0.733	0.726	0.701	0.645	0.645	0.667	0.672	0.761	0.726	0.644	<b>0.790</b>	0.675
Ionosphere	0.707	0.707	0.698	0.698	<b>0.726</b>	0.676	0.712	0.712	0.694	<b>0.726</b>	0.716	0.715	0.698	0.693	0.707
Liver-disorders	0.559	0.553	0.559	0.559	0.553	0.556	0.547	0.559	<b>0.578</b>	0.545	0.559	0.548	0.551	0.551	0.548
Lung-cancer	0.563	0.563	0.506	<b>0.600</b>	0.556	0.500	0.569	0.531	0.563	0.581	0.575	0.544	0.538	0.550	0.594
Lymphography	<b>0.546</b>	0.462	0.492	0.509	0.486	0.380	0.497	0.482	0.518	0.462	0.466	0.470	0.476	0.462	0.458
Monks-problems-2_train	0.559	<b>0.598</b>	0.546	0.538	0.538	0.568	0.541	0.579	<b>0.598</b>	0.579	<b>0.598</b>	0.559	0.544	0.530	0.543
Sonar	0.554	0.575	0.539	0.552	0.587	0.591	0.544	0.544	<b>0.625</b>	0.559	0.545	0.550	0.587	0.510	0.549
Soybean	0.597	0.601	0.616	0.589	0.383	0.414	0.620	<b>0.669</b>	0.542	0.529	0.558	0.467	0.378	0.493	0.472
Wdbc	0.928	0.930	0.940	0.936	0.953	<b>0.958</b>	0.924	0.927	0.938	0.924	0.903	0.935	0.914	0.921	0.928
Wine	0.957	0.957	0.936	0.912	0.916	0.935	0.957	<b>0.973</b>	0.943	0.908	0.942	0.933	0.927	0.892	0.949
Zoo	<b>0.893</b>	0.885	0.697	0.667	0.721	0.513	0.895	0.715	0.806	0.776	0.816	0.719	0.703	0.727	0.707
Average rank	<b>5.233</b>	<b>6.766</b>	<b>8.066</b>	<b>7.566</b>	<b>9.033</b>	<b>8.966</b>	<b>7.066</b>	<b>8.400</b>	<b>7.166</b>	<b>8.566</b>	<b>8.000</b>	<b>9.400</b>	<b>11.166</b>	<b>11.233</b>	<b>7.933</b>

**Table 7** NMI results of the evaluated UFS methods using  $k$ -means

Dataset	Filter		Wrapper										Hybrid	Original		
	Univariate		Multivariate								LLC-fs	DGUFS				
	SVD-entropy	LS	SPEC	USFSM	FSFS	RRFS	UDFS	NDFS	UFSACO	MGSAO					DSRMR	
Automobile	0.188	0.166	0.181	0.264	0.249	0.183	0.257	0.189	0.245	0.192	0.162	0.180	<b>0.266</b>	0.244	0.213	0.244
Breast-cancer	0.024	0.010	0.028	0.015	0.004	0.007	<b>0.031</b>	0.006	0.008	0.022	0.004	0.009	0.013	0.003	0.021	0.021
Heart-c	0.246	0.272	0.256	0.176	0.117	0.268	0.279	0.255	0.240	0.247	0.202	0.247	0.175	0.156	0.147	<b>0.292</b>
Heart-statlog	0.254	0.220	0.190	0.230	0.172	<b>0.270</b>	0.190	0.254	0.097	0.168	0.205	0.024	0.103	0.190	0.266	0.270
Hepatitis	0.126	0.130	0.192	0.157	0.106	0.107	0.072	0.071	0.056	0.100	0.177	0.077	0.094	<b>0.195</b>	0.107	0.107
Ionosphere	0.126	0.126	0.108	0.112	<b>0.183</b>	0.082	0.131	0.131	0.102	0.141	0.130	0.129	0.095	0.092	0.126	0.128
Liver-disorders	0.001	0.001	0.003	0.000	0.001	0.002	0.001	0.003	<b>0.010</b>	0.002	0.001	0.001	0.000	0.000	0.001	0.000
Lung-cancer	<b>0.282</b>	0.271	0.176	0.243	0.179	0.147	0.274	0.217	0.214	0.236	0.224	0.203	0.180	0.241	0.221	0.279
Lymphography	0.144	0.122	0.138	0.111	0.148	0.055	0.125	0.117	<b>0.185</b>	0.149	0.119	0.131	0.103	0.137	0.042	0.132
Monks-problems-2_train	0.002	<b>0.017</b>	0.008	0.003	0.004	0.008	0.012	0.007	<b>0.017</b>	0.007	<b>0.017</b>	0.003	0.012	0.001	0.001	0.006
Sonar	0.007	0.018	0.010	0.013	0.019	0.023	0.007	0.008	<b>0.042</b>	0.012	0.012	0.005	0.022	0.002	0.007	0.007
Soybean	0.711	0.695	0.724	0.700	0.495	0.481	0.707	<b>0.731</b>	0.612	0.625	0.663	0.577	0.487	0.607	0.645	0.593
Wdbc	0.625	0.619	0.660	0.641	0.719	<b>0.753</b>	0.611	0.605	0.686	0.611	0.538	0.672	0.579	0.581	0.584	0.611
Wine	0.846	0.846	0.783	0.743	0.697	0.800	0.835	<b>0.889</b>	0.798	0.706	0.815	0.787	0.760	0.704	0.808	0.835
Zoo	<b>0.882</b>	0.881	0.667	0.645	0.748	0.425	0.901	0.738	0.803	0.759	0.817	0.703	0.658	0.773	0.752	0.752
Average rank	<b>6.500</b>	<b>6.500</b>	<b>7.533</b>	<b>8.800</b>	<b>9.366</b>	<b>9.233</b>	<b>6.066</b>	<b>8.000</b>	<b>7.533</b>	<b>7.733</b>	<b>8.533</b>	<b>10.800</b>	<b>11.133</b>	<b>11.100</b>	<b>9.800</b>	<b>7.366</b>

**Table 8** Runtime of the evaluated UFS methods

Dataset	Filter		Wrapper										Hybrid		
	Univariate		Multivariate					Wrapper							
	SVD-entropy	LS	SPEC	USFSM	FSFS	RRFS	UDFS	NDFS	UFSACO	MGSAO	DSRMR	LLC-fs		DGUFS	Li et al.
Automobile	0.042	0.045	0.031	0.604	0.038	0.045	0.072	0.327	0.081	0.070	2.854	0.134	0.892	0.664	0.422
Breast-cancer	0.008	0.007	0.017	0.555	0.003	0.040	0.088	0.298	0.042	0.038	12.925	0.150	0.733	0.557	0.076
Heart-c	0.007	0.006	0.015	0.752	0.005	0.037	0.082	0.236	0.041	0.067	13.884	0.156	0.598	0.744	0.141
Heart-statlog	0.005	0.008	0.016	0.611	0.004	0.032	0.084	0.132	0.044	0.036	9.823	0.127	0.628	0.412	0.202
Hepatitis	0.010	0.005	0.006	0.173	0.006	0.027	0.050	0.129	0.034	0.039	4.639	0.062	0.290	0.342	0.084
Ionosphere	0.035	0.009	0.019	2.828	0.016	0.043	0.121	0.182	0.115	0.113	25.374	0.251	0.808	2.762	1.817
Liver-disorders	0.002	0.007	0.018	0.600	0.002	0.036	0.116	0.239	0.039	0.038	20.834	0.229	0.865	0.195	0.193
Lung-cancer	0.038	0.005	0.003	0.024	0.047	0.047	0.103	0.194	0.371	0.348	0.118	0.070	0.001	0.750	0.124
Lymphography	0.011	0.004	0.005	0.169	0.007	0.025	0.057	0.198	0.046	0.039	3.666	0.079	0.296	0.530	0.122
Monks-problems-2_train	0.002	0.007	0.008	0.087	0.002	0.021	0.047	0.174	0.031	0.026	5.018	0.078	0.350	0.160	0.323
Sonar	0.125	0.007	0.011	1.191	0.039	0.037	0.117	0.118	0.385	0.410	7.297	0.088	0.415	1.611	0.108
Soybean	0.048	0.019	0.120	20.191	0.021	0.092	0.403	0.468	0.165	0.167	451.395	0.716	2.117	5.483	0.857
Wdbc	0.061	0.015	0.049	10.462	0.015	0.059	0.223	0.238	0.101	0.112	220.122	0.456	1.702	2.920	0.415
Wine	0.006	0.005	0.006	0.180	0.004	0.019	0.050	0.087	0.023	0.026	14.511	0.057	0.320	0.452	0.352
Zoo	0.013	0.004	0.003	0.057	0.004	0.038	0.055	0.107	0.043	0.049	2.336	0.056	0.236	0.341	0.107
Average	<b>0.028</b>	<b>0.010</b>	<b>0.022</b>	<b>2.566</b>	<b>0.014</b>	<b>0.040</b>	<b>0.111</b>	<b>0.208</b>	<b>0.104</b>	<b>0.105</b>	<b>52.986</b>	<b>0.180</b>	<b>0.683</b>	<b>1.195</b>	<b>0.356</b>



1. The quality of the features selected by each UFS method depends to a large extent on the learning algorithm and the validation measure used. For example, we can observe that a useful feature subset for SVM might not be as good for  $k$ -means and vice versa.
2. The best results in both classification and clustering tasks were obtained by filter multivariate Spectral/Sparse Learning based methods. Conversely, the multivariate statistical based methods generally got the worst results in both classification and clustering tasks. Especially those methods that eliminate redundant features without first considering the elimination of irrelevant ones.
3. The quality of the results of clustering algorithms is better when feature selection is applied, while in tasks of supervised classification it is worse.
4. Filter methods are the fastest, specifically, statistical based methods. However, these filter methods usually provide the worst results in terms of quality.

## 4 Concluding remarks

Unsupervised Feature Selection methods have drawn interest in various research areas due to their ability to select features in unlabeled data (unsupervised datasets). This paper provides a review of the most relevant and recent UFS methods of the state-of-the-art. Additionally, we have introduced a taxonomy of UFS methods, and we have summarized the advantages and disadvantages of the general lines in which we have categorized the methods analyzed in this review. Moreover, an experimental comparison among the most representative methods of each approach was also presented.

In general, we observe that many researchers have devoted huge and fruitful efforts in developing methods under the filter approach. This because, commonly, filter methods have lower computational cost than wrappers and hybrids, which makes them suitable for high dimensionality datasets. Moreover, recent developments indicate that filter methods based on Spectral Feature Selection (Zhao and Liu 2011) and Sparse Learning (El Ghaoui et al. 2011) have increasingly been developed, particularly for their application on image, text, and biological data.

Regarding the main challenges and open problems in Unsupervised Feature Selection, we can mention the following:

- Based on the literature review, it was observed that most of the unsupervised feature selection methods (filter, wrapper or hybrids) require the specification of hyper-parameters such as the number of features, number of clusters or other parameters inherent to the feature selection technique used by each method. However, there is no such knowledge in practice, and most of the time it is impossible to know the best parameters values for each dataset. Therefore, the automatic selection of the best parameter values is an open problem.
- Scalability is another important challenge in feature selection, since many applications involve very large collections of objects and/or features. In the last few years, datasets with millions of features have been produced, and according to Bolón-Canedo et al. (2015) there is evidence that this number will increase, given the rapid advancements in computing and information technologies. Therefore, scalable methods are needed, since existing ones can not deal with a huge number of features.
- Stability of feature selection methods is the sensitivity of the selection toward data perturbation (Alelyani et al. 2011). According to Li et al. (2016), studying stability for Unsupervised Feature Selection is much more difficult than supervised methods because,

in Unsupervised Feature Selection, we do not have enough prior knowledge about the cluster structure of the data. Although some recent efforts for analyzing the stability of feature selection methods in the unsupervised contexts have been done (Alelyani 2013), there is a lot of work to do in this direction.

- Another important challenge in Unsupervised Feature Selection is regarding how to select relevant features in problems where data are described simultaneously by both numerical and non-numerical features (mixed data). Mixed data is very common, and it appears in many real-world problems. For example, in biomedical and health-care applications (Daniels and Normand 2005), socioeconomics and business (De Leon and Chough 2013), software cost estimations (Liu et al. 2013), etc. However, as we have seen in this review, most of the current methods (except those proposed in Solorio-Fernández et al. (2017) and Dutta et al. (2014)) have been designed only for numerical data. Therefore, there is a room for developing new Unsupervised Feature Selection methods for mixed data.

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