A Pareto Front Approach for Feature Selection

Enguerran Grandchamp¹, Mohamed Abadi² and Olivier Alata³

¹Laboratoire LAMIA, Université des Antilles, Campus de Fouillole, 97157 Pointe-à-Pitre Guadeloupe, France
²Institut XLIM-SIC, UMR CNRS 6172, Université de Poitiers, BP 30179, 8692 Futuroscope-Chasseneuil Cedex, France
³Lab. Hubert Curien, UMR CNRS 5516, Univ. Jean Monnet Saint-Etienne, Univ. Lyon, 42000, Saint-Etienne, France

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Abstract: This article deals with the multi-objective aspect of an hybrid algorithm that we propose to solve the feature subset selection problem. The hybrid aspect is due to the sequence of a filter and a wrapper method. The filter method reduces the exploration space by keeping subsets having good internal properties and the wrapper method chooses among the remaining subsets with a classification performances criterion. In the filter step, the subsets are evaluated in a multi-objective way to ensure diversity within the subsets. The evaluation is based on the mutual information to estimate the dependency between features and classes and the redundancy between features within the same subset. We kept the non-dominated (Pareto optimal) subsets for the second step. In the wrapper step, the selection is made according to the stability of the subsets regarding classification performances during learning stage on a set of classifiers to avoid the specialization of the selected subsets for a given classifiers. The proposed hybrid approach is experimented on a variety of reference data sets and compared to the classical feature selection methods FSDD and mRMR. The resulting algorithm outperforms these algorithms.

1 INTRODUCTION

Feature Selection (FS) is an active topic of interest. A large number of algorithms have been proposed. The basic idea is to select a subset from a large set of features. FS is a branch of the Dimension Reduction problem (Hilario, 2008). FS is an important task in many fields such as text characterization, image research, bioinformatics, color image processing, data mining, etc. The aim is to select relevant features for knowledge interpretation or representation, computation time reduction and overall improvement in performance (such as classification accuracy).

The relevancy of the features can have different definitions depending on the application: in knowledge interpretation or representation, the size reduction and the semantic and/or the diversity of the selected features are important in order to keep in a lower dimension the topological structure of the information; for classification applications, relevancy is directly linked to a good rate in learning or classification; in protein biomarkers identification, the reduction of the feature subset size and its stability when applying different learning sets are more important than classification performances. The relevancy is linked to the quality, the complexity, the diversity or the performance of the feature subset.

Different approaches have been developed to select a subset of features. They differ by their research method to explore the subsets, their criterion for comparing and ranking them and their selection process.

We design a hybrid method to combine the advantages of both filter and wrapper approaches: a fast (filter) way to select diversified subsets (multi-objective) having good internal properties (filter) and a final selection based on performances (wrapper). The stability criterion avoid specializing the subsets to a given classifiers.

After a general presentation of the main exploration methods, the fitness functions and selection processes are presented in section 2. Section 3 presents the multi-objective principle. Then in section 4, we present the hybrid method and the criterions. In section 5, some formalism is given concerning the criterion, the non-domination principle and the algorithm. The algorithm is given in section 6. The experiments on benchmarking database, classification and segmentation applications are given in section 7. Finally, section 8 gives conclusions and perspectives of the work.
2 THE FEATURE SELECTION PROBLEM

Many papers have been published on the modeling and the description (Somol, 2010) of feature selection problem. We summarize the main ideas implemented in the different feature selection approaches. Categorization is done according to Exploration methods (Sun, 2010):

- Greedy methods based on sequential approaches such as Sequential Forward Selection (SFS) and Sequential Backward Selection (SBS).
- Sequential Forward Floating Selection (SFFS) and Sequential Backward Floating Selection (SBFS).
- Genetic Algorithms (GA)

Fitness functions:

- A quality measure evaluated on each features separately: Dependency, entropy, relief-f, distance measures, statistical measures and more recently probabilistic measures based on the estimation of Mutual Information (Peng, 2005); or directly on the subset: correlation, redundancy, Information Criteria, for example.
- A performance measure: the good classification rate or error rate during the learning step.
- A complexity measure: the cardinality of the subset, the complexity of the classifiers.

Selection processes:

- A single candidate selection for sequential approaches: maximization (classification rate, relevancy, etc.) or minimization (error rate, correlation, etc.) of the criterion.
- Multiple candidates for evolutionary approaches

The main used evaluation is based on their performances in a classification context.

These different approaches lead to the separation of the methods in four families based on how to compare and rank the subsets:

- **Wrapper** methods use a machine learning algorithms during the exploration step to evaluate the candidate’s subsets and the corresponding classifier during the evaluation of the returned solution (test stage). It often gives the best performances but it is time consuming because of the training step on classifiers.
- **Filter** methods use an independent criterion to measure the quality of the feature subsets. These methods are the most popular because they considerably reduce the computation time.
- **Embedded** methods try to combine the advantages of both approaches. Nevertheless, the computation time still remain important.

- **Hybrid** methods use a sequence of **Filter** and **Wrapper** methods (Peng, 2005).

More details are given in the previous references and particularly in (Hilario, 2008) and (Somol, 2010) which are surveys of methods.

3 A MULTI OBJECTIVE APPROACH

Most of the time the exploration methods deal with a single criterion. However the use of only one characteristic to rank and select the subsets is insufficient in many cases. Authors then defined combinations of several criterions to integrate quality and performance. In practice, defining a combination of criterions is not an easy task. It depends on the application and often requires parameters to balance the different parts of the criterion. These criterions generally have opposite behaviors because increasing the performances often requires adding features which increase complexity.

In order to bypass this drawback, a multi-objective approach has been adopted in some studies (Hasan, 2010). A multi-objective approach try to simultaneously optimize several fitness functions during the exploration. However the criterions often have opposite behaviors leading to a set of non-dominated solutions called the Pareto set.

For the FS problem, the different approaches, deal with wrapper methods using GA as exploration method with a simple binary encoding and standard crossover and mutation. One of the objective is the cardinality of the subset and the other one a classification rate or error rate.

4 THE PROPOSED HYBRID APPROACH

4.1 Filter and Wrapper Combination

Hybrid methods are proposed in the literature (Cantu-Paz, 2004), (Peng, 2005), but the main objective of these works is to reduce the computation time. Indeed the criterion used in the wrapper step is the classifier performance in a mono-objective approach. The filter method is used to reduce the exploration space in a very high dimensional data set by evaluating the quality of the features in a mono-objective way: Kullback-Leibler distance between histograms of feature values; mRMR criterion; the relief criterion and; the relative certainty gain.
The way to select the subsets for the wrapper step represents the main differences between the approaches. In (Cantu-Paz, 2004) they select the features by fixing a threshold on the Kullback-Leiber distance; In (Peng, 2005), they keep subsets having a classification error under a given threshold.

As the number of features is reduced by the filter step, the wrapper step manages the retained features by the mean of a classical GA, or sequential forward and backward search with a classification accuracy criterion.

We propose a hybrid method by combining the Filter and Wrapper methods in two sequential steps. This approach improves the lack of diversity of the solutions returned by standard algorithms and reduces the dependency between subsets and classifiers. The computation time remains acceptable thanks to the use of a fast filter approach and a controlled exploration of Pareto solutions during the first step. These procedures coupled with a multi-objective approach with two quality objectives allow keeping diversity. All the selected subsets using the Pareto front are evaluated during the wrapper step.

We prefer a stability criterion to select the final subsets instead of raw performances regarding one classifier, in order to keep performances and independence between subsets and classifiers.

Indeed, we are looking for diversified subsets in the filter step in order to have different kinds of solutions to be evaluated during the wrapper step to increase the probability to reach stable ones. In this way, the building of the Pareto front seems to be the more appropriate choice.

### 4.2 Criterion and Diversity

The second stage of some previous approaches maintains a kind of diversity by the crossover step and the mutation step of a GA. On the other hand, the selection of the first pool of features by the filter step is done using a single criterion which restricts the explored subsets. Indeed, the evaluation of the subsets is done in a single way which leads to reject subsets having good properties according to another criterion. This is particularly the case for single criterions which are composed of multiple parts (mRMR for example, composed of Redundancy and Relevance). In this context, solution having very low redundancy or very high relevance could be rejected by the selection process if the resulting aggregation function has a low evaluation. To increase the diversity of the selected subsets our filter step explores the space in a multi-objective way with two quality objectives and a complexity objective.

The evaluation of the quality is based on the Mutual Information (MI) to separately measure the Dependency (D) and Redundancy (R) of the subsets. The theoretical interest for Mutual Information has been proved in (Peng, 2005). These two criterions measure both the individual quality of the selected features and the quality of the subset. The separate evaluation of these two measures (contrary to (Peng, 2005)) is important because a relevant subset is not necessarily a subset containing only significant attributes taken alone. Indeed the relevance of a subset may be due to combinations of features.

### 5 CRITERIONS

The criterions are based on the mutual information which is considered to be a good indicator to study the dependency between a feature and the classification and the redundancy between random features.

**Mutual Information**

Let $X$ and $Y$ be two random variables with discrete probability laws. The Mutual Information (MI) $I(X; Y)$ is defined by $P(X), P(Y)$ and $P(X, Y)$.

$$I(X; Y) = \sum_{y \in Y} \sum_{x \in X} p(x; y) \cdot \log \frac{p(x, y)}{p(x) \cdot p(y)}$$

with $\Omega_X$ and $\Omega_Y$ the sample spaces of $X$ and $Y$ respectively.

When $X$ and $Y$ are dependent, $I(X; Y)$ is high. $I(X; Y)$ is equal to zero when $X$ and $Y$ are independent.

**Selection criterion definition**

For each subset of features, we define the relevance expressed by the Dependency (D) which is the average MI between the variables of $S$ ($X$) taken separately and the class of the samples modeled by a discrete random variable called $c$ with sample space equal to the class labels:

$$D_S = \frac{1}{|S|} \sum_{X_i \in S} I(X_i; c)$$

$I(X_i; c)$ represents the MI between a variable and the classes. It translates how $X_i$ is useful to describe the classes.

The Dependency has to be maximized. However in order to have a homogenous expression of the objective we prefer to express the opposite of the Dependency (-D) to minimize each criterion.

The feature selection using only $D$ is not optimal because of redundancy between the variables.
Different ways exist to measure the redundancy and we use the one expressed in (Peng, 2005). It is based on the computation of the average MI between two variables \( (X_i;X_j)_{i,j=1,\ldots,m} \) belonging to the same subset \( S \) having \( m \) variables.

\[
R_S = \frac{1}{|S|^2} \sum_{X_i,X_j \in S} I(X_i;X_j) \quad (3)
\]

The redundancy must be minimized.

### 6 HYBRID AND MULTIOBJECTIVE ALGORITHM

#### 6.1 Principle

The novelty of our approach is that previous criterions are treated separately contrary to (Peng, 2005) and (Al-Ani, 2002) where criterions are combined to produce the mRMR (minimal-redondance-maximale-pertinence) criterions (ex. \( \max(D_i-R_i) \) or \( \max(D_i/R_i) \)). These mono-objective criterions didn’t ensure the simultaneous convergence of criterions (2) and (3) to their optimal value but lead to a trade-off between them.

We also keep the subset cardinality (L) which must be minimized as a third criterion.

The goal of a multi-objective optimization is to improve several criterions. When these criterions have opposite behaviors considering the research of a solution, we necessarily have to degrade at least one criterion to improve another one. This leads to different kind of solutions which are not necessarily comparable. If we don’t want to make a choice between solutions we must keep all solutions being better than any others on at least one criterion. This leads to the notion of domination which is essential to ensure diversity in the final sets.

Without loss of generality, we illustrate this notion in our particular case.

Following the previous section, each subset is evaluated with three values \( (f_1,f_2,f_3) = (-D,R,L) \).

- A subset \( S \) dominates a subset \( S_2 \) according to \( f_i \) if \( f_i(S) < f_i(S_2) \). \( i = 1, 2, \) or \( 3 \).
- A subset \( S \) dominates a subset \( S_2 \) if \( \forall i f_i(S) \leq f_i(S_2) \) and \( \exists i | f_i(S) < f_i(S_2) \).
- A subset \( S \) is not dominated if \( \nexists S_2 | S_2 \) dominates \( S \) ( \( \nexists S_2 | \forall i f_i(S_2) \leq f_i(S), \exists i f_i(S_2) < f_i(S) \) ).
- The set of all non dominated subsets is called the Pareto set.

The third criterion, which represents the complexity of the subset through its cardinality, allows keeping subsets with different size (for low number of features the redundancy may be better and for high number of features the dependency may be better). Nevertheless, even if we have one Pareto front for each possible subset size, there is no certainty to obtain at least one subset for each possible size. This could be an inconvenient for some applications. In such condition, the exploration step can deal with only the quality criterions and each intermediate Pareto front (corresponding to a specific size) could be kept. This approach called Multi Pareto Front (MF) is detailed in the next paragraph.

Figure 1: Pareto front evolution principle.

Figure 1 illustrate the evolution of the Pareto front projected in (-D,R) space. As the number of features increases the solutions in the Pareto front tend to decrease –D and R values. Figure 2 shows the same with in a real case using wineWhite database of the UCI.

Figure 2: Pareto front evolution for wineWhite UCI database.

#### 6.2 Filter Step: Multiobjective Exploration

For any optimization problem, a unique Pareto set exists for a given data set and the considered
criterions. In a multi-objective context, an exhaustive search, or an algorithm having asymptotic convergence properties such as Genetic algorithm, is classically required to find this set. Both are time consuming and sometimes too slow to reach the optimal Pareto set in a reasonable time. In practice, people build a sub-optimal Pareto front which is the Pareto front computed over the visited solutions. One of the main qualities of a search method is then its ability to provide solutions close to the ones of the optimal Pareto front. Our filter search method joins this ability and has been developed to approach the building of the optimal Pareto front.

The filter step uses a sequential forward search to explore the subset space adopting the following algorithm:

1. Let \( F = \{ F_i | i \in [1,M] \} \) be the complete set.
2. We start with all possible pairs of features \( V_2 = \{ (F_i, F_j) | i, j \in [1,M], i \not= j \} \).
3. Each subset \( S \) is evaluated with \((-D(S), R(S))\) criterions and the non-dominated subsets \((ND_k)\) are preserved. \( F_{k+1} \) is the Pareto front at iteration \( k \) \((F_k = ND_k)\).
4. At iteration \( k \), \( ND_k \) is the non dominated subsets of size \( k \) \((k>2)\) and \( F_k \) is the global Pareto Front \((F_k = U_{k \geq 2} ND_k)\).
5. We build \( V_{k+1} \) by adding to \( ND_k \) one new feature taken within the remaining features: \( V_{k+1} = \{ (S \cup F_i) | S \in ND_k, F_i \in F \} \). Each subset \( S \) in \( V_{k+1} \) is then evaluated with \((-D(S), R(S))\).
6. We build \( ND_{k+1} \) by retaining the non dominated subsets of size \( k+1 \) within \( V_{k+1} \). We note that \( ND_{k+1} \subseteq V_{k+1} \). This step is required because some subsets of \( V_{k+1} \) can be dominated by ones of \( F_k \) (opposite is impossible because each subset in \( V_{k+1} \) is greater than the ones in \( F_k \)).
7. The algorithm ends if \( k=M \).

This algorithm is called two Objectives Multi-Front Algorithm (2OMF) and the returned set of subsets is \( F_M = U_{k=1}^M ND_k \).

We can note that \( F_{k+1} \subseteq F_k \). Indeed, subsets of \( V_{k+1} \) couldn’t dominate subsets of \( F_k \) because these last ones have a lower size: \( \forall S_1 \in F_k, N(S_1) \leq k, \forall S_2 \in V_{k+1}, N(S_2) = k+1 \).

6.3 Wrapper Step: Stability Criterion

The wrapper step is used to rank the selected subsets and to select a subset considering the application. For this step, the exploration space has been sufficiently reduced during the filter step to allow an exhaustive evaluation of the remaining subsets \( ND_k \). A large majority of wrapper approaches deals with Feature Selection in terms of performances regarding a classifier, but few studies select subsets for their stability. Nevertheless, the stability is a topic of interest in studies dealing with high dimensional data and a small number of samples (Hilario, 2008). Moreover, wrapper methods can lead to good classification accuracy for a specific classifier but with poor generalization properties (Kalousis, 2007), (Peng, 2005) (i.e. over-fitting for one classifier and low performances for another one).

The stability is defined by (Somol, 2010) as being the quality of a subset to have the same performances with different training sets. Different stability indices can be used such as Hamming distance, correlation coefficients, Tanimoto distance, consistency index (simple, weighted or relative weighted) and Shannon entropy. In (Kuncheva, 2007) and, the stability is measured by running a wrapper scheme several times with a unique classifier and different learning sets (no cross-validation). The stability is based on an evaluation of the similarity between subsets returned by different runs. If the index is high the subset is selected. Otherwise the selection is based on the classification rate evaluation.

In this paper, we investigate another kind of stability between different classifiers (each trained and evaluated with a cross-validation process). According to this kind of stability has been neglected in the literature. A subset is stable regarding classifiers if the performances obtained with different classifiers are close. The easiest way to compute the stability of a subset is to compute the amplitude of the classification rates obtained with several classifiers K-Nearest Neighbor (KNN), Linear Discriminant Analysis (LDA), Mahalanobis (Mah), Naive Bayes (NB), Simple Vector Machine (SVM) and Probabilistic Neural Network (PNN):

\[
A(S) = \max_{c \epsilon C} \{ R_c(S) \} - \min_{c \epsilon C} \{ R_c(S) \} \tag{4}
\]

Where \( S \) is the subset, \( C \) a set of classifiers and \( R_c(S) \) the classification rate obtained with the classifier \( c \) applied on the subset \( S \).

Finally, we identify the stable and successful subsets. Therefore, the selection of the interesting subsets is done in a two objectives way by maximizing the mean classification rate \((M(S))\) and by minimizing the amplitude \((A(S))\).

\[
M(S) = \text{mean}_{c \epsilon C} \{ R_c(S) \} \tag{5}
\]

7 RESULTS

In a first step we present the results obtained with the 2OMF algorithm. In a second step we compare the
2OMF method with two other existing feature selection methods: mRMR (Peng, 2005) and FSDD (Liang, 2008). Both are using filter criterions to select the features and then they evaluate the unique returned solution using classifiers. We choose mRMR method because it uses the same criterions as 2OMF but in a mono-objective way. We choose FSDD because it is a fast algorithm which converges to the optimal solution regarding a distance criterion. In both cases, it is interesting to project the solutions obtained with different filter steps in the space (performance, stability) of the wrapper step and to compare them with our pool of solutions. The comparison is done by means of the size and the stability of the subsets returned by each method and also the computational time of each method.

Each step uses UCI databases for validation and more particularly iris, TAE, abalone, PimaIndianDiabetes, wineRed, wineWhite, wine, imgSeg, ionosphere and landSat databases containing 4, 5, 7, 8, 11, 11, 13, 18, 34 and 36 features respectively. Figure 3 to 5 present some of the obtained results. The stability is computed after applying KNN, LDA, Mah, NB, and PNN classifiers.

7.1 2OMF Method Analysis

We analyse more precisely the results of the 2OMF algorithm after the second step of the algorithm. This step is based on the wrapper approach which sorts and then selects among the retained subsets during the filter step. We recall that the used criterion is the stability (in a two objectives way) when different classifiers are applied. In this space (mean rate, amplitude) we compute a new Pareto front composed of several solutions and we focus on them to select the most interesting ones.

b) (which is a zoomed part of the Figure 3 a), a lot of subsets dominates the complete set (purple star in the figure) even if they are not in the Pareto front: these subsets are within the red rectangle. All of these subsets have higher mean classification rate and lower amplitude than the complete set. They can also be interesting because some of them have lower number of features than the one in the Pareto Front and a quite good classification stability as it is better than the complete set stability. For the studied database, there are 21 subsets in the front (6 dominating complete set) and 73 subsets that dominate the complete set.

Figure 3 c) shows the histogram of the selected features computed using all subsets of the 2OMF wrapper Pareto Front. We note that quite every features are represented. In the same way Figure 3 d) gives the repartition of the size of the Pareto subsets in order to illustrate the diversity of the solutions. landSat database is composed of 36 features and some of the subsets in the Pareto front are composed of less than 10 features. A further analysis of the subset sizes is given in the next section.

Figure 4 shows the features used by the different Pareto solutions for the wine database. We remark that some features are not present (4 and 5) or underrepresented (2, 9) in the Pareto front and some are overrepresented (1, 7, 8, 11, 12). This suggests an individual quality evaluation of the features which could be studied later.
Figure 5. shows the min and max good classification rate after the wrapper step for each Pareto front solution for wine database. We remark a great diversity both in terms of good classification rate than in terms of standard deviation. In this view we are looking for solutions having a high classification rate and a low standard deviation (examples are given within the red circles).

7.2 Comparison between 2OMF, mRMR and FSDD

We compare our algorithm with two well-known feature selection methods: mRMR and FSDD. Figure 6 displays the visited subsets using mRMR algorithm (blue) with their corresponding Pareto front (blue line) and using FSDD algorithm (black) with their corresponding Pareto front (black line). We observe that these subsets are not Pareto optimal when compared to the 2OMF subsets (green points). Moreover, few of them dominate the complete subset.

The same observation can be done for most of the databases. Indeed, in few databases we observe an mRMR subset that dominates the complete subset. A subset of mRMR and a subset of FSDD fall into the Pareto set only for TAE database and for iris.

The size of the corresponding subsets is also displayed near the subset as well as the complete set (purple star). We can observe that the subset size follows high variations: between 2 and 33 for the 2OMF Pareto front for ionosphere database and between 4 and 29 for the 2OMF Pareto front of the landSat database for example. The mean classification rate is also varying in a wide range: for

<table>
<thead>
<tr>
<th>Database</th>
<th>Method</th>
<th>Size</th>
<th>Mean</th>
<th>Var</th>
<th>KNN</th>
<th>Mah</th>
<th>NB</th>
<th>PNN</th>
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<td>Wine</td>
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<td>13</td>
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Table 1: Good classification rate and stability of interesting subsets (Bold faces indicate the best result(s)).
ionosphere database the mean rate is about 75.5% for a two features subset, 86% for a 5 features subset and 84% for a 10 features subset; for the landsat database the mean rate is about 82.5% for a 4 features subset and 85.5% for a 28 features subset.

We now focus on the good classification rate obtained for some interesting subsets. The table 1. shows subsets obtained with 2OMF, mRMR and FSDD methods. Information about the Pareto optimality is also given (Underlined size in table). In addition to this, we present whether a subset dominates the complete set (Green background color in table). The mRMR and FSDD subsets are chosen among the visited ones according to their mean rate value.

All the displayed subsets obtained with the 2OMF method are interesting because they have a low number of features and a better stability than the complete set. Nevertheless, some subsets have lowest number of features and others highest classification rates. For example, for the wine database, a subset with two features (features 2 and 7) have a higher mean rate and a lower amplitude than the complete set having 13 features. Moreover, it has a higher classification rates for 4 classifiers over 5. In the same way, for imgSeg database the number of features is divided by 2 with the 2OMF method.

Let us consider now the methods from the literature. For landsat database none of the visited subsets dominate the complete set for both mRMR and FSDD. Moreover, stable and successful subsets obtained with FSDD have a higher number of features than the ones obtained with 2OMF. Only one stable subset having low number of features is obtained with mRMR (8 features). However, it is dominated by the subset returned by 2OMF which has seven features (last line in the table). We always found a subset among 2OMF subsets having a lower number of features, a higher classification mean rate and a lower classification amplitude than the best subsets returned by mRMR and FSDD.

8 CONCLUSION

This paper presents a two steps algorithm for feature selection and studies its multi-objective aspect. The algorithm begins with a filter step to quickly select a first pool of subsets in a Multi-Objectives and Multi- Fronts way (2OMF). The subsets are evaluated using the Dependency (D) and the Redundancy (R) of the features. Then a second step based on a wrapper approach is applied to measure the performances of the subsets regarding several classifiers (KNN, LDA, Mah, NB, PNN). Then the selection of the interesting subsets is performed using the stability of the subsets which is evaluated with the mean and amplitude of the classification rates. From our experimentations, it is observed that the interesting subsets dominate the complete set regarding both objectives. The use of the stability to select the subsets leads to robust results which are very interesting for some applications such as in biology where the stability of the subsets is more important than its raw classification rate. The wrapper step is required because some subsets of the filter Pareto front could have a higher classification rate than the complete set for a given classifiers but not for another one. A selection of features only based on a filter method does not ensure that the selected subset will improve classification rates for a large set of classifiers.

The results are very convincing for all tested databases. The subsets obtained after applying our algorithm have lower number of features and better classification performances compare to the complete set of features. Moreover, the diversity of the final pool of subsets allows selecting a subset adapted to a specific application (good classification expected or reduction of a high number of features). We also compared the proposed algorithm with two feature-selection methods (mRMR and FSDD). It is observed that our method outperforms the other tested methods in almost all cases.

REFERENCES

A. Kalousis, J. Prados, and M. Hilario, "Stability of feature selection algorithms: A study on high-dimensional