Review and Evaluation of Feature Selection Algorithms in Synthetic Problems

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Abstract: The main purpose of Feature Subset Selection is to find a reduced subset of attributes from a data set described by a feature set. The task of a *feature selection algorithm* (FSA) is to provide with a computational solution motivated by a certain definition of *relevance* or by a reliable evaluation measure. In this paper several fundamental algorithms are studied to assess their performance in a controlled experimental scenario. A measure to evaluate FSAs is devised that computes the degree of matching between the output given by a FSA and the known optimal solutions. An extensive experimental study on synthetic problems is carried out to assess the behaviour of the algorithms in terms of solution accuracy and size as a function of the relevance, irrelevance, redundancy and size of the data samples. The controlled experimental conditions facilitate the derivation of better-supported and meaningful conclusions.

Keywords: Feature Selection Algorithms; Empirical Evaluations; Attribute relevance and redundancy.

1 INTRODUCTION

The *feature selection* problem is ubiquitous in an inductive machine learning or data mining setting and its importance is beyond doubt. The main benefit of a correct selection is the improvement of the inductive learner, either in terms of learning speed, generalization capacity or simplicity of the induced model. On the other hand, there are the *scientific* benefits associated with a smaller number of features: a reduced measurement cost and hopefully a better understanding of the domain. A *feature selection algorithm* (FSA) is a computational solution that should be guided by a certain definition of *subset relevance*, although in many cases this definition is implicit or followed in a loose sense. This is so because, from the inductive learning perspective, the relevance of a feature may have several definitions depending on the precise objective that is looked for (Caruana and Freitag, 1994). Thus the need arises to count on common sense criteria that enables to adequately decide which algorithm to use (or *not* to use) in certain situations.

This work reviews the merits of several fundamental feature subset selection algorithms in the literature and assesses their performance in an artificial controlled experimental scenario. A *scoring measure* computes the degree of matching between the output given by the algorithm and the known optimal solution. This measure ranks the algorithms by taking into account the amount of relevance, irrelevance and redundancy on synthetic data sets of discrete features. Sample size effects are also studied.

The results illustrate the strong dependence on the particular conditions of the algorithm used, as well as on the amount of irrelevance and redundancy in the data set description, relative to the total number of features. This should prevent the use of a single algorithm specially when there is poor knowledge available about the structure of the solution. More importantly, it points in the direction of using principled combinations of algorithms for a more reliable assessment of feature subset performance.

The paper is organized as follows: we begin in Section 2 reviewing relevant related work. In section 3 we set a precise definition of the feature selection problem and briefly survey the main categorization of feature selection algorithms. We then provide an algorithmic description and

comment on several of the most widespread algorithms in section 4. The methodology and tools used for the empirical evaluation are covered in section 5. The experimental study, its results and a general advice to the data mining practitioner are developed in section 6. The paper ends with the conclusions and prospects for future work.

2 MOTIVATION AND RELATED WORK

Previous experimental work on feature selection algorithms for comparative purposes include Aha and Bankert (1995), Doak (1992), Jain and Zongker (1997), Kudo and Sklansky (1997) and Liu and Setiono (1998b). Some of these studies use artificially generated data sets, like the widespread *Parity*, *Led* or *Monks* problems (Thrun, 1991). Demonstrating improvement on synthetic data sets can be more convincing that doing so in typical scenarios where the true solution is completely unknown. However, there is a consistent lack of systematical experimental work using a common benchmark suite and equal experimental conditions. This hinders a wider exploitation of the power inherent in fully controlled experimental environments: the knowledge of the (set of) optimal solution(s), the possibility of injecting a desired amount of relevance, irrelevance and redundancy and the unlimited availability of data.

Another important issue is the way FSA performance is assessed. This is normally done by handing over the solution encountered by the FSA to a specific inducer (during of after the feature selection process takes place). Leaving aside the dependence on the particular inducer chosen, there is a much more critical aspect, namely, the relation between the performance as reported by the inducer and the true merits of the subset being evaluated. In this sense, it is our hypothesis that FSAs are very affected by finite sample sizes, which distort reliable assessments of subset relevance, even in the presence of a very sophisticated search algorithm (Reunanen, 2003). Therefore, sample size should also be a matter of study in a through experimental comparison. This problem is aggravated when using filter measures, since in this case the relation to true generalization ability (as expressed by the *Bayes error*) can be very loose (Ben-Bassat, 1982).

A further problem with traditional benchmarking data sets is the implicit assumption that the used data sets are actually *amenable* to feature selection. By this it is meant that performance benefits clearly from a good selection process (and less clearly or even worsens with a bad one). This criterion is not commonly found in similar experimental work. In summary, the rationale for using exclusively synthetic data sets is twofold:

1. Controlled studies can be developed by systematically varying chosen experimental conditions, thus facilitating the derivation of more meaningful conclusions.
2. Synthetic data sets allow full control of the experimental conditions, in terms of amount of relevance, irrelevance and redundancy, as well as sample size and problem difficulty. An added advantage is the knowledge of the set of optimal solutions, in which case the degree of closeness to any of these solutions can thus be assessed in a confident and automated way.

The procedure followed in this work consists in generating sample data sets from synthetic functions of a number of discrete relevant features. These sample data sets are then corrupted with irrelevant and/or redundant features and handed over to different FSAs to obtained a hypothesis. A *scoring measure* is used in order to compute the degree of matching between this hypothesis and the known optimal solution. The score takes into account the amount of relevance, irrelevance and redundancy in each suboptimal solution as yielded by an algorithm.

The main criticism associated with the use of artificial data is the likelihood that such a problem be found in real-world scenarios. In our opinion this issue is more than compensated by the mentioned advantages. A FSA that is not able to work properly in simple experimental conditions (like those developed in this work) is in strong suspect of being inadequate in general.

3 THE FEATURE SELECTION PROBLEM

Let X be the original set of features, with cardinality $|X| = n$. The *continuous* feature selection problem (also called Feature Weighing) refers to the assignment of weights w_i to each feature $x_i \in X$ in such a way that the order corresponding to its theoretical relevance is preserved. The *binary* feature selection problem (also called Feature Subset Selection) refers to the choice of a subset of features that jointly maximize a certain measure related to subset relevance. This can be carried out directly, as many FSAs do (Almuallim and Dietterich, 1991; Caruana and Freitag, 1994; Hall, 1999), or setting a *cut-point* in the output of the continuous problem solution. Although both types can be seen in an unified way (the latter case corresponds to the assignment of weights in $\{0, 1\}$), these are quite different problems that reflect different design objectives. In the continuous case, one is interested in keeping *all* the features but in using them *differentially* in the learning process. On the contrary, in the binary case one is interested in keeping just a *subset* of the features and (most likely) using them *equally* in the learning process.

A common instance of the feature selection problem can be formally stated as follows. Let J be a performance evaluation measure to be optimized (say to maximize) defined as $J : \mathcal{P}(X) \to \mathbb{R}^+ \cup \{0\}$. This function accounts for a general evaluation measure, that may or may not be inspired in a precise and previous definition of relevance. Let $c(x) \geq 0$ represent the *cost* of variable x (measurement cost, needed technical skill, etc) and call $c(X') = \sum_{x \in X'} c(x)$, for $X' \in \mathcal{P}(X)$. Let $C_X = c(X)$ be the cost of the whole feature set. It is assumed here that c is additive,

that is, $c(X' \cup X'') = c(X') + c(X'')$ (together with non-negativeness, this implies that c is monotone).

Definition 1 (Feature Subset Selection) *The selection of an optimal feature subset ("Feature Subset Selection") is either of two scenarios:*

(1) Fix $C_0 \leq C_X$. Find the $X' \in \mathcal{P}(X)$ of maximum $J(X')$ among those that fulfill $c(X') \leq C_0$.

(2) Fix $J_0 \geq 0$. Find the $X' \in \mathcal{P}(X)$ of minimum $c(X')$ among those that fulfill $J(X') \geq J_0$.

If the costs are unknown, a meaningful choice is obtained by setting $c(x) = 1$ for all $x \in X$. Then $c(X') = |X'|$ and c can be interpreted as the *complexity* of the solution. In this case, (1) amounts to finding the subset with highest J among those having a maximum pre-specified size. In scenario (2), it amounts to finding the smallest subset among those having a minimum pre-specified performance (as measured by J). Only with these restrictions, an optimal subset of features need not exist; if it does, is not necessarily unique. In scenario (1), a solution always exists by defining $c(\emptyset) = 0$ and $J(\emptyset)$ to be the value of J with no features. In case (2), if there is no solution, an adequate policy may be to set $J_0 = \epsilon J(X), \epsilon > 0$, and progressively lower the value of ϵ. If there is more than one solution (of equal performance and cost, by definition) one is usually interested in them all. We shall speak of a FSA of *Type 1* (resp. *Type 2*) when it has been designed to solve the first (resp. second) scenario in Def. 1. If the FSA can be used in both scenarios, we shall speak of a *general-type* algorithm. In addition, if one has no control whatsoever, we shall speak of a *free-type* algorithm.

We shall use the notation $S(X')$ to indicate the subsample of S described by the features in $X' \subseteq X$ only.

4 FEATURE SUBSET SELECTION ALGORITHMS

The relationship between a FSA and the inductive learning method used to infer a model can take three main forms: *filter*, *wrapper* or *embedded*, which we call the *mode*:

Embedded Mode: The inducer has its own FSA (either explicit or implicit). The methods to induce logical conjunctions (Vere, 1975; Winston, 1975), decision trees or artificial neural networks are examples of this embedding.

Filter Mode: If feature selection takes place before the induction step, the former can be seen as a filter (of non-useful features). In a general sense it can be seen as a particular case of the embedded mode in which feature selection is used as a pre-processing. The filter mode is then independent of the inducer that evaluates the model after the feature selection process.

Wrapper Mode: Here the relationship is taken the other way around: the FSA uses the learning algorithm as a subroutine (John et al., 1994). The argument in favor of this mode is to *equal the bias* of the FSA and the inducer that will be used later to assess the goodness of the model. A main disadvantage is the computational burden that comes from calling the inducer to evaluate each and every subset of considered features.

In what follows several of the currently most widespread FSAs in machine learning are described and briefly commented on. General-purpose search algorithms, as genetic algorithms, are excluded from the review. None of the algorithms allow the specification of costs in the features. Most of them can work in filter or wrapper mode. The *feature weighing* algorithm RELIEF has been included, both in the review and in the experimental comparison, as a complement. This is so because it can also be used to select a subset of features, although a way of getting a subset out of the weights has to be devised. In the following we assume again that the evaluation measure J is to be maximized.

4.1 Algorithm LVF

LVF (Las Vegas Filter) (Liu and Setiono, 1998a) is a type 2 algorithm that repeatedly generates random subsets and computes the *consistency* of the sample: an *inconsistency* in X' and S is defined as two instances in S that are equal when considering only the features in X' and that belong to different classes. The aim is to find the *minimum* subset of features leading to zero inconsistencies. The *inconsistency count* of an instance $A \in S$ is defined as:

$$IC_{X'}(A) = X'(A) - \max_k X'_k(A) \tag{1}$$

where $X'(A)$ is the number of instances in S equal to A using only the features in X' and $X'_k(A)$ is the number of instances in S of class k equal to A using only the features in X' (Liu and Setiono, 1998b). The *inconsistency rate* of a feature subset in a sample S is then:

$$IR(X') = \frac{\sum_{A \in S} IC_{X'}(A)}{|S|} \tag{2}$$

This is a monotonic measure, in the sense

$$X_1 \subset X_2 \Rightarrow IR(X_1) \geq IR(X_2)$$

The evaluation measure is then $J(X') = \frac{1}{IR(X')+1} \in (0, 1]$ that can be evaluated in $O(|S|)$ time using a hash table.

LVF is described as Algorithm 1. It has been found to be particularly efficient for data sets having redundant features (Dash et al., 1997). Arguably its main advantage may be that it quickly reduces the number of features in the initial stages with certain confidence (Dash and Liu, 1998; Dash et al., 2000); however, many poor solution subsets are analyzed, wasting computing resources.

4.2 Algorithm LVI

LVI (Las Vegas Incremental) is also a type 2 algorithm and an evolution of LVI. It is based on the grounds that it is not necessary to use the whole sample S in order to

```
Input:
  max − the maximum number of iterations
  J − evaluation measure
  S(X) − a sample S described by X, |X| = n
Output:
  L − all equivalent solutions found

L := []      // L stores equally good sets
Best := X    // Initialize best solution
J0 := J(S(X)) // minimum allowed value of J
repeat max times
   X' := Random_SubSet(Best)
   if J(S(X')) ≥ J0 then
      if |X'| < |Best| then
         Best := X'
         L := [X']          // L is reinitialized
      else
         if |X'| = |Best| then
            L := append(L, X')
         end
      end
   end
end
```

Algorithm 1: LVF (Las Vegas Filter).

```
Input:
  max − the maximum number of iterations
  J − evaluation measure
  S(X) − a sample S described by X, |X| = n
  p − initial percentage
Output:
  X' − solution found

S0 := portion(S,p) // Initial portion
S1 := S \ S0
J0 := J(S(X))      // Minimum allowed value of J
repeat forever
   X' := LVF (max, J, S0(X))
   if J(S1(X')) ≥ J0 then stop
   else
      C := {x ∈ S1(X') making S1(X') inconsistent}
      S0 := S0 ∪ C
      S1 := S1 \ C
   end
end
```

Algorithm 2: LVI (Las Vegas Incremental).

evaluate the measure J, which for this algorithm is again *consistency* (Liu and Setiono, 1998b). The algorithm is described as Algorithm 2. It departs from a portion S_0 of S; if LVF finds a sufficiently good solution in S_0 then LVI halts. Otherwise the set of instances in $S \setminus S_0$ making S_1 inconsistent is added to S_0, this new portion is handed over to LVF and the process is iterated. Intuitively, the portion cannot be too small or too big. If it is too small, after the first iteration many inconsistencies will be found and added to the current portion, which will hence be very similar to S. If it is too big, the computational savings will be modest. The authors suggest $p = 10\%$ or a value proportional to the number of features. In Liu and Motoda (1998) it is reported experimentally that LVI adequately chooses relevant features, but may fail for noisy data sets, in which case the algorithm it is shown to consider irrelevant features. Probably LVI is more sensible to noise than LVF in cases of small sample sizes.

```
Input:
  p − sampling percentage
  d − distance measure
  S(X) − a sample S described by X, |X| = n
Output:
  w − array of feature weights

let m := p|S|
initialize array w[] to zero
do m times
   I := Random_Instance (S)
   Inh := Near−Hit (I, S)
   Inm := Near−Miss (I, S)
   for each i ∈ [1..n] do
      w[i] := w[i] + di(I, Inm)/m − di(I, Inh)/m
   end
end
```

Algorithm 3: RELIEF.

4.3 Algorithm RELIEF

RELIEF (Kira and Rendell, 1992) is a general-type algorithm that works exclusively in filter mode. The algorithm randomly chooses an instance $I \in S$ and finds its *near hit* and its *near miss*. The former is the closest instance to I among all the instances in the same class of I. The latter is the closest instance to I among all the instances in a different class. The underlying idea is that a feature is more relevant to I the more it separates I and its near miss, and the least it separates I and its near hit. The result is a weighed version of the original feature set. The algorithm for two classes is described as Algorithm 3.

When costs are just sizes, the algorithm can be used to simulate a type 1 scenario by iteratively checking the sequence of the first C_0 nested subsets in the order given by decreasing weights, calling the J measure, and returning that subset with the highest value of J. To simulate a type 2 scenario, the same sequence is checked looking for the first element in the sequence that yields a value of J not less than the chosen J_0. The more important advantage of RELIEF is the rapid assessment of irrelevant features with a principled approach; however it does not make a good discrimination among redundant features. The algorithm has been found to choose correlated features instead of relevant features (Dash et al., 1997), and therefore the optimal subset can be far from assured (Kira and Rendell, 1992). Some variants have been proposed to account for several classes (Kononenko, 1994), where the k more similar instances are selected and their averages computed.

4.4 Algorithms SFG/SBG

These two are classical general-type algorithms that may work in filter or wrapper mode. SFG (Sequential Forward Generation) iteratively adds features to an initial subset, trying to improve a measure J, always taking into account those features already selected. Consequently, an ordered list can also be obtained. SBG (Sequential Backward Generation) is the backward counterpart. They are jointly described as Algorithm 4. When the number of features is small, Doak (1992) reported that SBG tends to show better performance than SFG, most likely because SBG evaluates the contribution of all features from the onset. In addition, Aha and Bankert (1995) points out that SFG is preferable when the number of relevant features is (known to be) small; otherwise SBG should be used. Interestingly, it was also reported that SBG did not *always* have better performance than SFG, contrary to the conclusions in Doak (1992). Besides, SFG is faster in practice. The algorithms W-SFG and W-SBG (W for *wrapper*) use the accuracy of an inducer as evaluation measure.

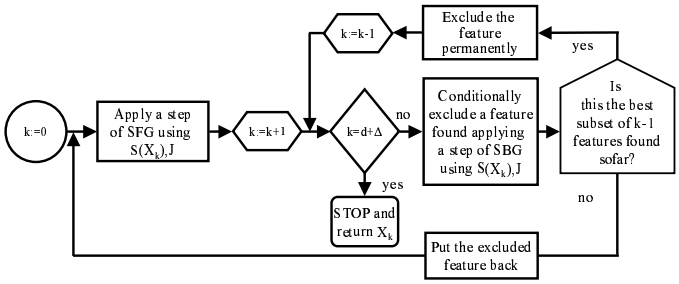
```
Input:
  S(X) − a sample S described by X, |X| = n
  J − evaluation measure
Output:
  X' − solution found

X' := ∅ /* Forward */ or X' := X /* Backward */
repeat
  x' := argmax{J(S(X' ∪ {x})) | x ∈ X \ X'}  /* Forward */
  x' := argmax{J(S(X' \ {x})) | x ∈ X'}  /* Backward */
  X' := X' ∪ {x'}  /* Forward */
  X' := X' \ {x'}  /* Backward */
until no improvement in J in last j steps
      or X' = X /*Forward*/ or X' = ∅ /*Backward*/
```

Algorithm 4: SBG/SFG (Sequential Backward/Forward Generation).

4.5 Algorithms SFFG/SFBG

These are free-type algorithms that may work in filter or wrapper mode. SFFG (Sequential Floating Forward Generation) (Pudil et al., 1994) is an exponential cost algorithm that operates in a sequential fashion, performing a forward step followed by a variable (and possibly null) number of backward ones. In essence, a feature is first unconditionally added and then features are removed as long as the generated subsets are the best among their respective size. The algorithm (described in Algorithm 5 as a flow-chart) is so-called because it has the characteristic of *floating* around a potentially good solution of the specified size. The backward counterpart SFBG performs a backward step followed by zero or more forward steps. These two algorithms have been found to be very effective in some situations (Jain and Zongker, 1997), and are among the most popular nowadays. Their main drawbacks are the computational cost, that may be unaffordable when the number of features nears the hundred (Bins and Draper, 2001) and the need to fix the size of the final desired subset.

Input:
$S(X)$ - a sample S described by $X, |X| = n$
J - evaluation measure
d - desired size of the solution
Δ - maximum deviation allowed with respect to d
Output:
solution of size $d \pm \Delta$



Algorithm 5: SFFG (Sequential Floating Forward Generation). The set X_k denotes the current solution (of size k); $S(X_k)$ is the sample described by the features in X_k only.

4.6 Algorithm QBB

The QBB (Quick Branch and Bound) algorithm (Dash and Liu, 1998) (described as Algorithm 7) is a type 1 algorithm. Actually it is a hybrid one, composed of LVF and ABB. The origin of ABB is in Branch & Bound (Narendra and Fukunaga, 1977), an optimal search algorithm. Given a threshold β (specified by the user), the search stops at each node the evaluation of which is lower than β, so that efferent branches are pruned. ABB (Automatic Branch & Bound) (Liu et al., 1998) is a variant having its bound as the inconsistency rate of the data when the full set of features is used (Algorithm 6). The basic idea of QBB consists in using LVF to find good starting points for ABB. It is expected that ABB can explore the remaining search space efficiently. The authors reported that QBB is, in general, more efficient than LVF or ABB in terms of average cost of execution and selected relevant features.

5 EMPIRICAL EVALUATION OF FSAs

The main question arising in a feature selection experimental design is: what are the aspects that we would like to evaluate of a FSA solution in a given data set? Certainly a *good* algorithm is one that maintains a well-balanced trade-off between small-sized and competitive solutions. To assess these two issues at the same time is a difficult un-

```
Input:
  S(X) - a sample S described by X, |X| = n
  J - evaluation measure (monotonic)
Output:
  L - all equivalent solutions found

procedure ABB (S(X): sample; var L': list of set)
  for each x in X do
    enqueue(Q, X \ {x}) // remove a feature at
                           a time
  end
  while not empty(Q) do
    X' := dequeue(Q)
    // X' is legitimate if it is not a subset of
       a pruned state
    if legitimate(X') and J(S(X')) ≥ J0 then
       L' := append(L', X')
       ABB(S(X'), L')
    end
  end
end

begin
   Q := ∅          // Queue of pending states
   L' := [X]       // List of solutions
   J0 := J(S(X)) // Minimum allowed value of J
   ABB (S(X), L') // Initial call to ABB
   k := smallest size of a subset in L'
   L := set of elements of L' of size k
end
```

Algorithm 6: ABB (Automatic Branch and Bound).

```
Input:
  max - the maximum number of iterations
  J - monotonic evaluation measure
  S(X) - a sample S described by X, |X| = n
Output:
  L - all equivalent solutions found

L_ABB := []
L_LVF := LVF (max, J, S(X))
for each X' ∈ L_LVF do
   L_ABB := concat(L_ABB, ABB(S(X'), J))
end
k := smallest size of a subset in L_ABB
L := set of elements of L_ABB of size k
```

Algorithm 7: QBB (Quick Branch and Bound).

dertaking in practice, given that their optimal relationship is user-dependent. In the present controlled experimental scenario, the task is greatly eased since the size and performance of the optimal solution is known in advance. The aim of the experiments is precisely to contrast the ability of the different FSAs to hit a solution with respect to relevance, irrelevance, redundancy and sample size.

Relevance: Different families of problems are generated by varying the number of relevant features N_R. These are features that will have an influence on the output and whose role can not be assumed by any other subset.

Irrelevance: Irrelevant features are defined as those not having any influence on the output. Their values are generated at random for each example. For a problem with N_R relevant features, different numbers of irrelevant features N_I are added to the corresponding data sets (thus providing with several subproblems for each choice of N_R).

Redundancy: In this work, a redundancy exists when a feature can take the role of another. Following a parsimony principle, we are interested in the behaviour of the algorithms in front of this simplest case. If an algorithm fails to identify redundancy in this situation (something that is actually found in the experiments reported below), then this is interesting and something we should be aware of. This effect is obtained by choosing a relevant feature randomly and replicating it in the data set. For a problem with N_R relevant features, different numbers of redundant features $N_{R'}$ are added in a way analogous to the generation of irrelevant features.

Sample Size: number of instances $|S|$ of a data sample S. In these experiments, $|S| = \alpha k N_T c$, where α is a constant, k is a multiplying factor, N_T is the total number of features $(N_R + N_I + N_{R'})$ and c is the number of classes of the problem. This means that the sample size will depend linearly on the total number of features.

5.1 Evaluation of performance

We derive in this section a *scoring* measure to capture the degree to which a solution obtained by a FSA matches (one of) the correct solution(s). This criterion behaves as a *similarity* $s : \mathcal{P}(X) \times \mathcal{P}(X) \to [0, 1]$, between subsets of X in the data analysis sense (Chandon and Pinson, 1981), where $s(X_1, X_2) > s(X_1, X_3)$ indicates that X_2 is more similar to X_1 than X_3, and satisfying $s(X_1, X_2) = 1 \iff X_1 = X_2$ and $s(X_1, X_2) = s(X_2, X_1)$. Let us denote by X the total set of features, partitioned in $X = X_R \cup X_I \cup X_{R'}$, being $X_R, X_I, X_{R'}$ the subsets of relevant, irrelevant and redundant features of X, respectively and call $X^* \subseteq X$ any of the correct solutions (all and only relevant variables, no redundancy). Let us denote by $\mathcal{A}$ the feature subset selected by a FSA. The idea is to check how much $\mathcal{A}$ and X^* have in common.

Let us define $\mathcal{A}_R = X_R \cap \mathcal{A}$, $\mathcal{A}_I = X_I \cap \mathcal{A}$ and $\mathcal{A}_{R'} = X_{R'} \cap \mathcal{A}$. In general, we have $\mathcal{A}_T = X_T \cap \mathcal{A}$ (hereafter T stands for a subindex in $\{R, I, R'\}$). Since necessarily $\mathcal{A} \subseteq X$, we have that $\mathcal{A} = \mathcal{A}_R \cup \mathcal{A}_I \cup \mathcal{A}_{R'}$ is a partition of $\mathcal{A}$. The *score* $S_X(\mathcal{A}) : \mathcal{P}(X) \to [0, 1]$ is defined in terms of the similarity in that for all $\mathcal{A} \subseteq X, S_X(\mathcal{A}) = s(\mathcal{A}, X^*)$. Thus, $S_X(\mathcal{A}) > S_X(\mathcal{A}')$ indicates that $\mathcal{A}$ is more similar to X^* than $\mathcal{A}'$. The idea is to make a flexible measure, so that it can ponder each type of divergence (in relevance, irrelevance and redundancy) to the correct solution. To this end, a set of parameters is collected as $\alpha = \{\alpha_R, \alpha_I, \alpha_{R'}\}$ with $\alpha_T \geq 0$ and $\sum \alpha_T = 1$.

Intuitive Description. The criterion $S_X(\mathcal{A})$ penalizes three situations: (1) There are relevant features lacking in $\mathcal{A}$ (the solution is *incomplete*), (2) There are more than enough relevant features in $\mathcal{A}$ (the solution is *redundant*)

and (3) There are some irrelevant features in $\mathcal{A}$ (the solution is *incorrect*).

An order of importance and a weight will be assigned (via the α_T parameters), to each of these situations. The precedent point (3) is simple to model: if suffices to check whether $|\mathcal{A}_I| > 0$, being $\mathcal{A}$ the solution of the FSA. Relevance and redundancy are strongly related given that a feature is redundant or not depending on what other relevant features are present in $\mathcal{A}$. Notice then that the correct solution X^* is not unique, and all of them should be equally valid. To this end, the features are broken down in *equivalence classes*, where elements of the same class are redundant to each other (i.e., any correct solution must comprise only one feature of each equivalence class). Being A a feature set, we define a binary relation between two features $x_i, x_j \in A$ as: $x_i \sim x_j \iff x_i$ and x_j represent the same information. Clearly $\sim$ is an equivalence relation. Let $A/\sim$ be the quotient set of A under $\sim$; any correct solution must be of the same size than X_R and have one element in every subset of $(X_R \cup X_{R'})/\sim$.

Construction of the *score*. The set to be split in equivalence classes is formed by all the relevant features (redundant or not) chosen by a FSA. Define $\rho_{\mathcal{A}} = (\mathcal{A}_R \cup \mathcal{A}_{R'})/\sim$ *(equivalence classes in which the relevant and redundant features chosen by a FSA are split)*, $\rho_X = (X_R \cup X_{R'})/\sim$ *(same with respect to the original set of features)* and $\rho_{\mathcal{A}\subseteq X} = \{x \in \rho_X \mid \exists y \in \rho_{\mathcal{A}}, y \subseteq x\}$. For Q quotient set, let:

$$F(Q) = \sum_{x \in Q} (|x| - 1)$$

The idea is to express the *quotient* between the number of redundant features chosen by the FSA and the number it could have chosen, given the relevant features present in its solution. In the precedent notation, this is written (provided the denominator is not null):

$$\frac{F(\rho_{\mathcal{A}})}{F(\rho_{\mathcal{A}\subseteq X})}$$

Let us finally build the *score*, formed by three terms: relevance, irrelevance and redundancy. Defining:

$$I_{\mathcal{A}} = 1 - \frac{|\mathcal{A}_I|}{|X_I|}, \qquad R_{\mathcal{A}} = \frac{|\rho_{\mathcal{A}}|}{|X_R|},$$

$$R'_{\mathcal{A}} = \begin{cases} 0 & \text{if } F(\rho_{\mathcal{A}\subseteq X}) = 0 \\ \left(1 - \frac{F(\rho_{\mathcal{A}})}{F(\rho_{\mathcal{A}\subseteq X})}\right) & \text{otherwise.} \end{cases}$$

for any $\mathcal{A} \subseteq X$ the score is defined as $S_X(\mathcal{A}) = s(\mathcal{A}, X^*) = \alpha_R R_{\mathcal{A}} + \alpha_{R'} R'_{\mathcal{A}} + \alpha_I I_{\mathcal{A}}$. This score fulfills the two conditions (proof is given in the Appendix):

1. $S_X(\mathcal{A}) = 0 \iff \mathcal{A} = X_I$
2. $S_X(\mathcal{A}) = 1 \iff \mathcal{A} = X^*$

We can establish now the desired restrictions on the behavior of the score. From the more to the less severe: there are relevant features lacking, there are irrelevant features, and there is redundancy in the solution. This is reflected in the following conditions on the α_T:

1. Choosing an irrelevant feature is better than missing a relevant one: $\frac{\alpha_R}{|X_R|} > \frac{\alpha_I}{|X_I|}$
2. Choosing a redundant feature is better than choosing an irrelevant one: $\frac{\alpha_I}{|X_I|} > \frac{\alpha_{R'}}{|X_{R'}|}$

We also define $\alpha_T = 0$ if $|X_T| = 0$. Observe that the denominators are important for, say, expressing the fact that it is not the same choosing an irrelevant feature when there were only two that when there were three (in the latter case, there is an irrelevant feature that could have been chosen when it was not). In order to translate the previous inequalities into workable conditions, a parameter $\epsilon \in (0, 1]$ is introduced to express the precise relation between the α_T. Let $\underline{\alpha}_T = \frac{\alpha_T}{|X_T|}$. The following equations have to be satisfied, together with $\alpha_R + \alpha_I + \alpha_{R'} = 1$:

$$\beta_R \underline{\alpha}_R = \underline{\alpha}_I, \qquad \beta_I \underline{\alpha}_I = \underline{\alpha}_{R'}$$

for suitable chosen values of β_R and β_I. Reasonable settings are obtained by taking $\beta_R = \epsilon/2$ and $\beta_I = 2\epsilon/3$, though other settings are possible, depending on the evaluator's needs. With these values, at equal $|X_R|, |X_I|, |X_{R'}|$, α_R is at least twice more important than α_I (because of the $\epsilon/2$) and α_I is at least one and a half times more important than $\alpha_{R'}$. Specifically, the minimum values are attained for $\epsilon = 1$ (i.e., α_R counts twice α_I). For $\epsilon < 1$ the differences widen proportionally to the point that, for $\epsilon \approx 0$, only $\alpha_R R$ will practically count on the overall score.

6 EXPERIMENTAL EVALUATION

In the following sections we detail the experimental methodology and quantify the various parameters of the experiments. The basic idea consists on generating sample data sets using synthetic functions f with known relevant features. These data sets (of different sizes) are corrupted with irrelevant and/or redundant features and handed over to the different FSAs to obtained a hypothesis H. The divergence between the defined function f and the obtained hypothesis H will be evaluated by the *score* criterion (with $\epsilon = 1$). This experimental design is illustrated in Fig. 1.

6.1 Description of the FSAs used

Up to ten FSAs were used in the experiments. These are E-SFG, QBB, LVF, LVI, C-SBG, RELIEF, SFBG, SFFG, W-SBG, and W-SFG. The algorithms E-SFG, W-SFG are versions of SFG using entropy and the accuracy of a C4.5 inducer, respectively. The algorithms C-SBG, W-SBG are versions of SBG using consistency and the accuracy of a C4.5 inducer, respectively. Since RELIEF and E-SFG yield

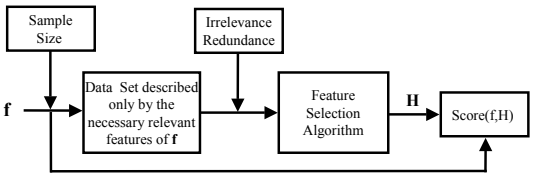


Figure 1: Flow-Chart of Experimental Design.

an ordered list of features x_i according to their weight w_i, an automatic filtering criterion is necessary to transform every solution into a subset of features. The procedure used here to determine a suitable cut point is simple: first the weights are sorted in decreasing order (with w_n the greatest weight, corresponding to the most relevant feature). Then those weights further than two variances from the mean are discarded (that is to say, with very high or very low weights). The idea is to look for the feature x_j such that $\frac{w_n - w_j}{w_n - w_1}\frac{j}{n}$ is maximum. Intuitively, this corresponds to obtaining the maximum weight with the lowest number of features. The cut point is then set between x_j and x_{j-1}.

6.2 Implementations of data families

A total of twelve families of data sets were generated studying three different problems and four instances of each, by varying the number of relevant features N_R. Let $x_1, \ldots, x_n$ be the relevant features of a problem f.

Parity: This is the classic problem where the output is $f(x_1, \cdots, x_n) = 1$ if the number of $x_i = 1$ is odd and $f(x_1, \cdots, x_n) = 0$ otherwise.

Disjunction: Here we have $f(x_1, \cdots, x_n) = 1$ if $(x_1 \wedge \cdots \wedge x_{n'}) \vee (x_{n'+1} \wedge \cdots \wedge x_n)$, with $n' = n\,div\,2$ (n even) and $n' = (n\,div\,2) + 1$ (n odd).

GMonks: This problem is a generalization of the classic *monks* problems (Thrun, 1991). In its original version, three independent problems were applied on sets of $n = 6$ features that take values of a discrete, finite and unordered set (nominal features). Here we have grouped the three problems in a single one computed on *each* chunk of 6 features. Let n be multiple of 6, $k = n\,div\,6$ and $b = 6(k'-1)+1$, for $1 \leq k' \leq k$. Let us denote for "1" the first value of a feature, for "2" the second, etc. The problems are the following:

1. $P1 : (x_b = x_{b+1}) \vee x_{b+4} = 1$
2. $P2$: two or more $x_i = 1$ in $x_b \cdots x_{b+5}$
3. $P3 : (x_{b+4} = 3 \wedge x_{b+3} = 1) \vee (x_{b+4} \neq 3 \wedge x_{b+1} \neq 2)$

For each chunk, the boolean condition $P2 \wedge \neg(P1 \wedge P3)$ is checked. If it is satisfied for $n_c\,div\,2$ or more chunks (being n_c the number of chunks) the function *Gmonks* is 1; otherwise, it is 0.

6.3 Experimental setup

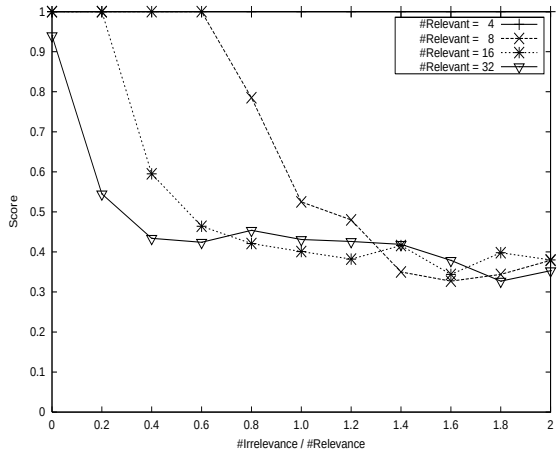
The experiments are divided in three main groups. The first group explores the relationship between *irrelevance vs. relevance*. The second one explores the relationship between *redundancy vs. relevance*. The last group is the study of the effect of different *sample sizes*. Each group uses three families of problems (*Parity*, *Disjunction* and *GMonks*) with four different instances for each one, varying the number of relevant features N_R, as indicated:

Relevance: The different numbers N_R vary for each problem, as follows: {4, 8, 16, 32} (for *Parity*), {5, 10, 15, 20} (for *Disjunction*) and {6, 12, 18, 24} (for *GMonks*).
Irrelevance: In these experiments, N_I runs from zero to twice the value of N_R. Specifically, $N_I \in \{(k \cdot N_R)/p, k = 0, 1, \ldots, 10\}$ (that is, eleven different experiments of irrelevance for each N_R). The value of p is chosen so that all the involved quantities are integer: $p = 4$ for *Parity*, $p = 5$ for *Disjunction* and $p = 6$ for *GMonks*.
Redundancy: Analogously to the generation of irrelevant features, we have $N_{R'}$ running from zero to twice the value of N_R (eleven experiments of irrelevance for each N_R).
Sample Size: Given the formula $|S| = \alpha k N_T c$ (see §5), different problems were generated considering $k \in \{0.25, 0.5, 0.75, 1.0, 1.25, 1.75, 2.0\}$, $N_T = N_R + N_I + N_{R'}$, $c = 2$ and $\alpha = 20$. The values of N_I and $N_{R'}$ were fixed as $N_I = N_{R'} = N_R\,div\,2$.

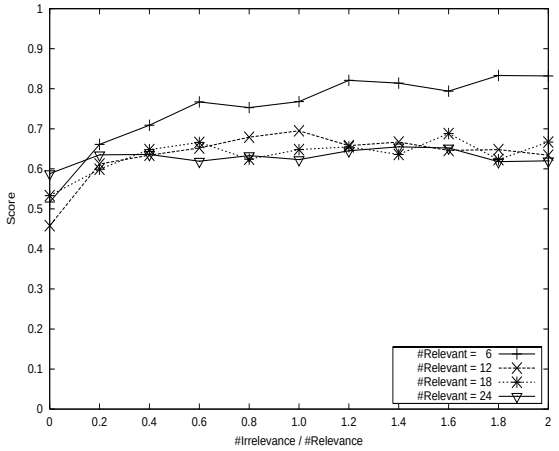
6.4 Discussion of the results

Due to space reasons, only a representative sample of the results is presented, in graphical form, in Figs. 2 and 3. In all the plots, each point represents the average of 10 independent runs with different random data samples. The Figs. 2(a) and (b) are examples of *irrelevance vs. relevance* for four instances of the problems, (c), (d) are examples of *redundancy vs. relevance* and (e), (f) of *sample size* experiments. In all cases, the horizontal axis represents the *ratios* between these particulars as explained above. The vertical axis represents the average results given by the score criterion.

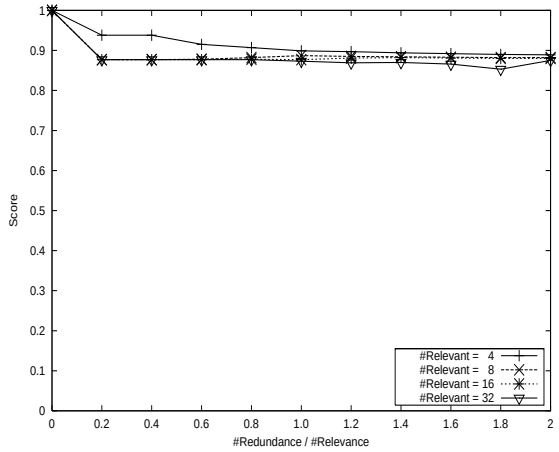
- In Fig. 2(a) the C-Sbg algorithm shows at first a good performance but clearly falls dramatically (below the 0.5 level from $N_I = N_R$ on) as the *irrelevance ratio* increases. Note that for $N_R = 4$ performance is perfect (the plot is on top of the graphic). In contrast, in Fig. 2(b) the Relief algorithm presents very similar and fairly good results for the four instances of the problem, being almost insensitive to the total number of features.
- In Fig. 2(c) the Lvf algorithm presents a very good and stable performance for the different problem instances of *Parity*. In contrast, in 2(d) Qbb tends to a poor general performance in the *Disjunction* problem when the total number of features increases.
- The plots in Figs. 2(e) and (f) show additional interesting results because we can appreciate the curse



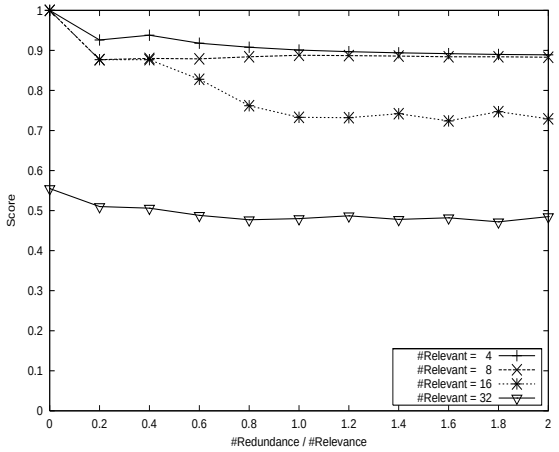
a. Irrelevance vs. Relevance
for *Parity* with C-SBG



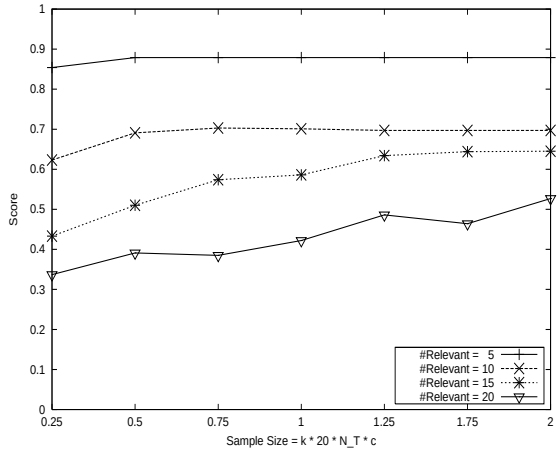
b. Irrelevance vs. Relevance
for *GMonks* with RELIEF



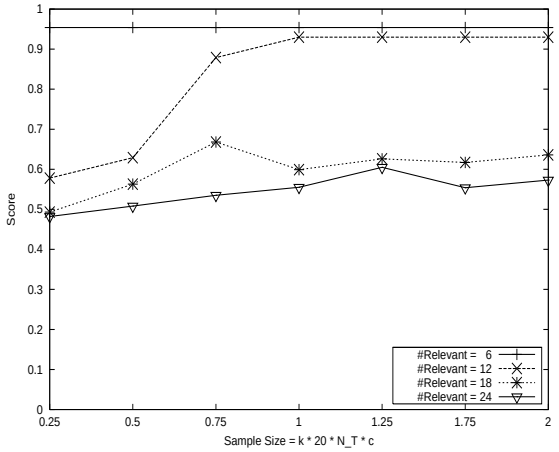
c. Redundance vs. Relevance
for *Parity* with LVF



d. Redundance vs. Relevance
for *Disjunction* with QBB



e. Sample Size
for *Disjunction* with LVI



f. Sample Size
for *Parity* with W-SBG

Figure 2: Selected results of the experiments: (a),(b) is *irrelevance* vs. *relevance*, (c),(d) are examples of *redundancy* vs. *relevance* and (e), (f) of *sample size* experiments. The horizontal axis is the *ratio* between these quantities. The vertical axis is the average result given by the *score* in 10 independent runs with different random data samples.

of dimensionality (Jain and Zongker, 1997). In these figures, LVI and W-SFG perform increasingly poorly (see the figure from top to bottom) with higher numbers of features, provided the number of examples is increased in a linear way. However, in general, as long as more examples are added, performance is better (left to right).

A summary of the *complete* results is displayed in Fig. 3 for the ten algorithms, allowing for a comparison across all the sample datasets with respect to each studied particular. Specifically, Figs. 3(a), (c) and (d) show the average score of each algorithm for irrelevance, redundancy and sample size, respectively. Moreover, Figs. 3(b), (d) and (f) show the same average weighed by N_R, in such a way that more weight is assigned to more difficult problems (higher N_R). In each graphic there are two keys: the key to the left shows the algorithms ordered by *total* average performance, from top to bottom. The key to the right shows the algorithms ordered by average performance on the *last* abscissa value, also from top to bottom. In other words, the left list is topped by the algorithm that wins on average, while the right list is topped by the algorithm that ends on the lead. This is also useful to help reading the graphics.

- Fig. 3(a) shows that RELIEF ends up on the lead of the irrelevance vs. relevance problems, while SFFG shows the best average performance. The algorithm W-SFG is also well positioned.
- Fig. 3(c) shows the algorithms LVF and LVI, together with C-SBG, as the overall best. In fact, there is a bunch of algorithms that also includes the two *floating* and QBB showing a close performance. Note how RELIEF and the *wrappers* are very poor performers.
- Fig. 3(e) shows how the wrapper algorithms extract the most of the data when there is a shortage of it. Surprisingly, the backward wrapper is just fairly positioned on average. The SFFG algorithm is again quite good on average, together with C-SBG. However, all of the algorithms are quite close and show the same kind of dependency to the amount of available data. Note the general poor performance of E-SFG, most likely due to the fact that it is the only algorithm that computes its evaluation measure (entropy in this case) independently for each feature.

The weighed versions of the plots (Fig. 3 (b),(d) and (f)) do not seem to alter the picture very much. A closer look reveals that the differences between the algorithms have widened. Very interesting is the change for RELIEF, that takes the lead both on irrelevance and sample size, but not on redundancy.

6.5 General considerations

The results point to SFFG as the best algorithm on average in complete ignorance of the particulars of the data set, or whenever one is willing to use a single algorithm. However, in view of the reported results, a better strategy would be to run various algorithms in a *coupled* way (i.e., in different execution orders and piping the respective solutions) and observe the results. Specifically, we suggest to use RELIEF when one is interested in detecting *irrelevance*, LVF for detecting *redundancy* and W-SFG in presence of small sample size situations. In light of this, we conjecture that SFFG used in a wrapper fashion could be a better one-fits-all option for small to moderate size problems.
We would like to bring to attention the following points:

1. The wild differences in performance for different algorithms and data particulars: fixing an algorithm A and a problem P, performance of A is dramatically different for the various particulars considered (but in a consistent way in all instances of P). However, these results are coherent and scale quite well for increasing numbers of relevant features.

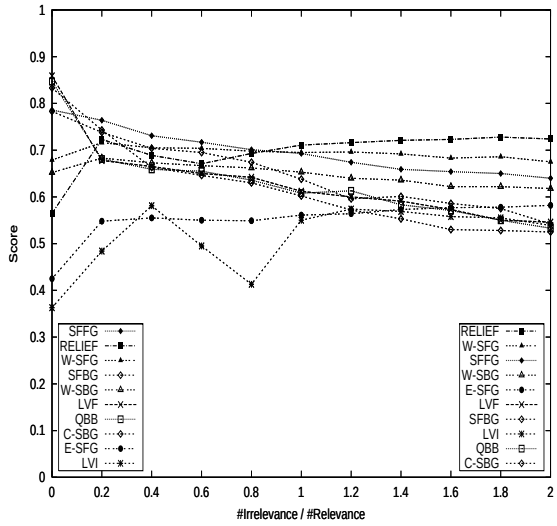
2. The *score* criterion seems to reliably capture what intuition tells about the quality of a solution at this simple level.

We would also like to emphasize the fact that the differences in the outcome yielded by the algorithms are not entirely due to their different approach to the problem. Rather, they are also attributable to the lack of a precise optimization goal, for example in the form described in Definition 1. Another good deal is the finite (and possibly very limited) sample size which, on the one hand, hinders the obtention of an accurate evaluation of relevance. On the other, the dependence on a specific sample reminds us that every evaluation of relevance in a feature subset should be regarded as the outcome of a *random variable*, different samples yielding different outcomes. In this vein, the use of *resampling* techniques like Random Forests (Breiman, 2001) is strongly recommended.

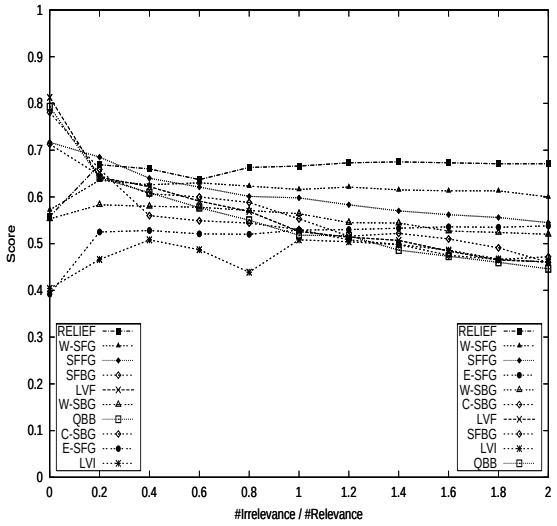
A final interesting point is the relation between the evaluation given by a specific inducer and the score. We were interested in ascertaining whether higher inducer evaluations imply higher scores. We next provide evidence that this need not be the case by means of a counterexample.

Conjecture: given a FSA and the solution it yields in a data set, we know this solution is suboptimal in the sense that better solutions may exist but are not found. However, we would expect the solution to be better (i.e. have a higher score) the better its performance is.

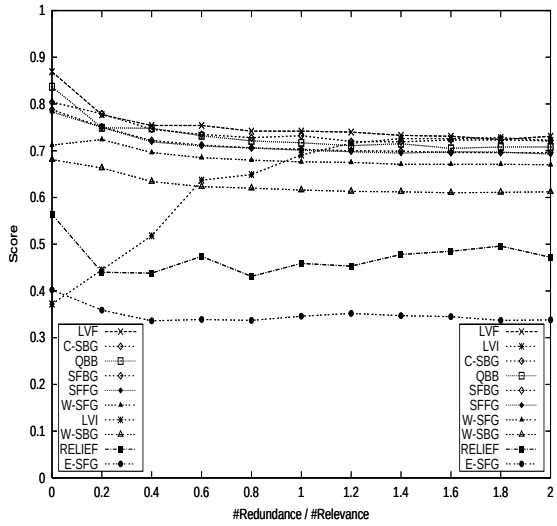
Experiment: we run W-SFG in 10 independent runs with different random data samples of size 600 using Naïve Bayes as inducer in an instance of the *GMonks* problem, described by $N_R = 24, N_{R'} = 12$ and $N_I = 24$ for $N_T = 60$. Table 1 shows the results: for each run, the final inducer performance is given, as well as the score of the solutions. Runs 5 and 8 correspond to very different solutions (number 5 being much better than number 8) that have almost the same inducer evaluation. Run 5 also has a lower evaluation than run 9, but a greater score.



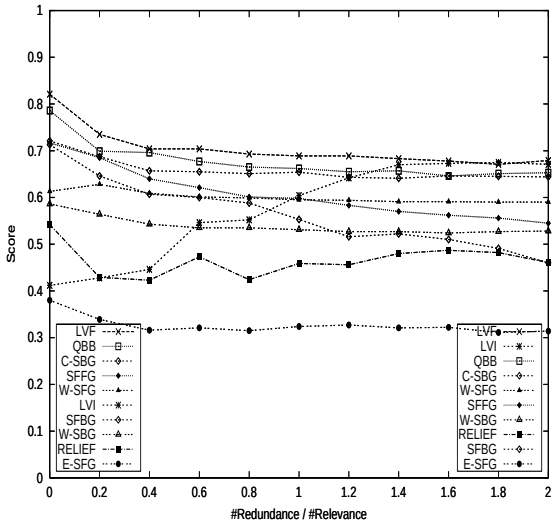
a. Irrelevance



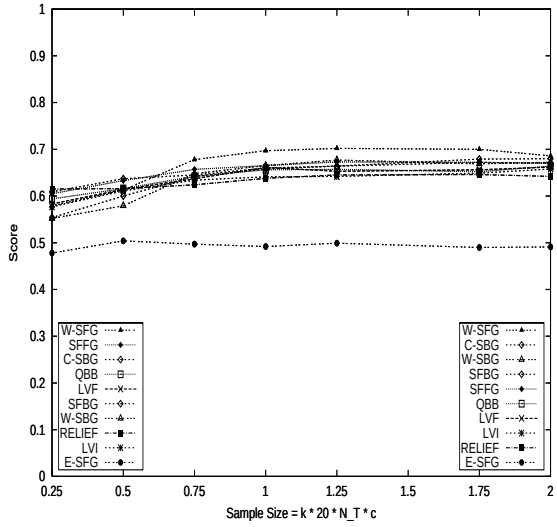
b. Irrelevance (weighed)



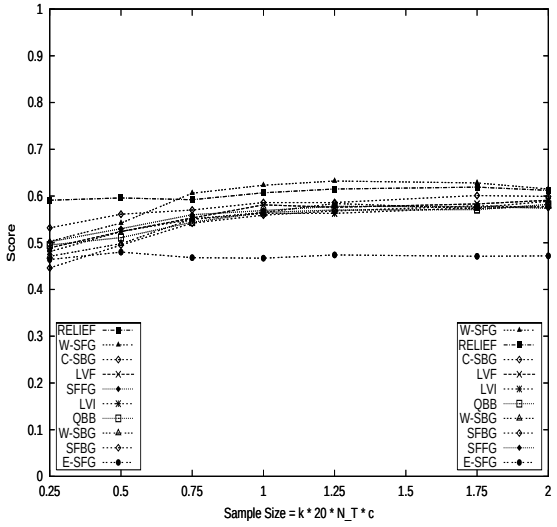
c. Redundance



d. Redundance (weighed)



e. Sample Size



f. Sample Size (weighed)

Figure 3: Results ordered by total average performance on the data sets (left inset) and by end performance (right inset). Figs. (b), (d) and (f) are weighed versions of (a), (c) and (e), respectively.

#	Naïve Bayes	score s	$\lvert\mathcal{A}_R \cup \mathcal{A}_{R'}\rvert$	$\lvert\mathcal{A}_I\rvert$
1	0.876	0.603	22	15
2	0.869	0.601	24	14
3	0.884	0.588	19	10
4	0.858	0.609	22	13
5	0.876	0.730	30	19
6	0.875	0.475	5	0
7	0.872	0.456	8	6
8	0.880	0.412	5	2
9	0.881	0.630	14	4
10	0.873	0.630	28	20

Table 1: Results of the experiment on variability.

This same experiment can be used to show the variability in the results as a function of the data sample. It can be seen that the numbers of relevant and redundant as well as irrelevant features depend very much on the sample. A look at the precise features chosen reveals that they are very different solutions (a fact that is also indicated by the score) that nonetheless give a similar evaluation by the inducer. Given the incremental nature of W-SFG, it can be deduced that classifier improvements where obtained by adding completely irrelevant features.

7 CONCLUSIONS

The task of a *feature selection algorithm* (FSA) is to provide with a computational solution to the feature selection problem motivated by a certain definition of *relevance* or, at least, by a performance evaluation measure. This algorithm should also be increasingly reliable with sample size and pursue the solution of a clearly stated optimization goal. The many algorithms proposed in the literature are based on quite different principles and loosely follow these recommendations, if at all. In this research, several fundamental algorithms have been studied to assess their performance in a controlled experimental scenario. A measure to evaluate FSAs has been devised that computes the degree of matching between the output given by a FSA and the known optimal solution. This measure takes into account the particulars of relevance, irrelevance, redundancy and size of synthetic data sets.

Our results illustrate the pitfall in relying in a single algorithm and sample data set, very specially when there is poor knowledge available about the structure of the solution or the sample data size is limited. The results also illustrate the strong dependence on the particular conditions in the data set description, namely the amount of irrelevance and redundancy relative to the total number of features. Finally, we have shown by a simple example how the evaluation of a feature subset can be misleading even when using a reliable inducer. All this points in the direction of using *hybrid* algorithms (or principled combinations of algorithms) as well as resampling for a more reliable assessment of feature subset performance.

This work can be extended in many ways, to carry up more general evaluations (considering richer forms of redundancy) and using other kinds of data (e.g., continuous data). A specific line of research is the corresponding extension of the scoring criterion.

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Appendix

Proposition. The score fulfills the two conditions:

a) $S_X(\mathcal{A}) = 0 \Longleftrightarrow \mathcal{A} = X_I$
b) $S_X(\mathcal{A}) = 1 \Longleftrightarrow \mathcal{A} = X^*$

Proof:
a) $\boxed{\Longleftarrow}$ Let $\mathcal{A} = X_I$. Then $S_X(\mathcal{A}) = S_X(X_I)$; since $\mathcal{A}_I = X_I \cap \mathcal{A} = X_I \cap X_I = X_I$, we have $I = 0$; since $\mathcal{A}_R = \mathcal{A}_{R'}$ we have $R = R' = 0$. Thus $S_X(X_I) = 0$.

$\boxed{\Longrightarrow}$ Suppose $S_X(\mathcal{A}) = 0$; since all terms that make up $S_X(\mathcal{A})$ are non-negative, it is necessary that all of them are zero. Now $R = 0$ implies $\mathcal{A}_R \cup \mathcal{A}_{R'} = \emptyset$, which implies $\mathcal{A}_R = \mathcal{A}_{R'} = \emptyset$; then $\mathcal{A} = \mathcal{A}_I$; thus $\mathcal{A} = \mathcal{A} \cap X_I$ and hence $\mathcal{A} \subseteq X_I$. Since I must be zero, $|\mathcal{A}_I| = |X_I|$ and therefore $\mathcal{A} = X_I$.

b) Suppose $\mathcal{A} = X^*$; then it can be checked that $R = R' = I = 1$ and thus $\alpha_R R_{\mathcal{A}} + \alpha_{R'} R'_{\mathcal{A}} + \alpha_I I_{\mathcal{A}} = \alpha_R + \alpha_{R'} + \alpha_I = 1$. Now this is the only way to achieve this value, since any other situation $\mathcal{A} \neq X^*$ leads to either R, R' or I to be less than 1.