Efficient Feature Selection via Analysis of Relevance and Redundancy

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Abstract

Feature selection is applied to reduce the number of features in many applications where data has hundreds or thousands of features. Existing feature selection methods mainly focus on finding relevant features. In this paper, we show that feature relevance alone is insufficient for efficient feature selection of high-dimensional data. We define feature redundancy and propose to perform explicit redundancy analysis in feature selection. A new framework is introduced that decouples relevance analysis and redundancy analysis. We develop a correlation-based method for relevance and redundancy analysis, and conduct an empirical study of its efficiency and effectiveness comparing with representative methods.

Keywords: supervised learning, feature selection, relevance, redundancy, high dimensionality

1. Introduction

In classic supervised learning, one is given a training set of labeled fixed-length feature vectors (instances). An instance is typically described as an assignment of values $f = (f_1, ..., f_N)$ to a set of features $F = (F_1, ..., F_N)$ and one of l possible classes $c_1, ..., c_l$ to the class label C. The task is to induce a hypothesis (classifier) that accurately predicts the labels of novel instances. The learning of the classifier is inherently determined by the feature-values. In theory, more features should provide more discriminating power, but in practice, with a limited amount of training data, excessive features will not only significantly slow down the learning process, but also cause the classifier to over-fit the training data as irrelevant or redundant features may confuse the learning algorithm.

Feature selection has been an active and fruitful field of research and development for decades in statistical pattern recognition (Mitra et al., 2002), machine learning (Liu et al., 2002b; Robnik-Sikonja and Kononenko, 2003), data mining (Kim et al., 2000; Dash et al., 2002) and statistics (Hastie et al., 2001; Miller, 2002). It has proven in both theory and practice effective in enhancing learning efficiency, increasing predictive accuracy, and reducing complexity of learned results (Almuallim and Dietterich, 1994; Koller and Sahami, 1996; Blum and Langley, 1997). Let *G* be some subset of *F* and f_G be the value vector of *G*. In general, the goal of feature selection can be formalized as selecting a minimum subset *G* such that $\mathbf{P}(C | G = f_G)$ is equal or as close as possible to $\mathbf{P}(C | F = f)$, where $\mathbf{P}(C | G = f_G)$ is the probability distribution of different classes given the feature values in *G* and $\mathbf{P}(C | F = f)$ is the original distribution given the feature values in *F* (Koller and Sahami, 1996). We call such a minimum subset an *optimal* subset, illustrated by the example below.

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Example 1 (Optimal subset) Let features $F_1, ..., F_5$ be Boolean. The target concept is $C = g(F_1, F_2)$ where g is a Boolean function. With $F_2 = \overline{F_3}$ and $F_4 = \overline{F_5}$, there are only eight possible instances. In order to determine the target concept, F_1 is indispensable; one of F_2 and F_3 can be disposed of (note that C can also be determined by $g(F_1, \overline{F_3})$), but we must have one of them; both F_4 and F_5 can be discarded. Either $\{F_1, F_2\}$ or $\{F_1, F_3\}$ is an optimal subset. The goal of feature selection is to find either of them.

In the presence of hundreds or thousands of features, researchers notice (Yang and Pederson, 1997; Xing et al., 2001) that it is common that a large number of features are not informative because they are either irrelevant or redundant with respect to the class concept. In other words, learning can be achieved more efficiently and effectively with just relevant and non-redundant features. However, the number of possible feature subsets grows exponentially with the increase of dimensionality. Finding an optimal subset is usually intractable (Kohavi and John, 1997) and many problems related to feature selection have been shown to be NP-hard (Blum and Rivest, 1992).

Researchers have studied various aspects of feature selection. One of the key aspects is to measure the *goodness* of a feature subset in determining an optimal one (Liu and Motoda, 1998). Different feature selection methods can be broadly categorized into the *wrapper* model (Kohavi and John, 1997; Kim et al., 2000) and the *filter* model (Liu and Setiono, 1996; Liu et al., 2002b; Hall, 2000; Yu and Liu, 2003). The wrapper model uses the predictive accuracy of a predetermined learning algorithm to determine the goodness of the selected subsets. These methods are computationally expensive for data with a large number of features (Kohavi and John, 1997). The filter model separates feature selection from classifier learning and selects feature subsets that are independent of any learning algorithm. It relies on various measures of the general characteristics of the training data such as distance, information, dependency, and consistency (Liu and Motoda, 1998). Search is another key problem in feature selection. To balance the tradeoff of result optimality and computational efficiency, different search strategies such as complete, heuristic, and random search have been studied to generate candidate feature subsets for evaluation (Blum and Langley, 1997; Dash and Liu, 2003). According to the availability of class labels, there are feature selection methods for supervised learning (Dash and Liu, 1997; Yu and Liu, 2003) as well as for unsupervised *learning* (Kim et al., 2000; Dash et al., 2002). Feature selection has found success in many applications like text categorization (Yang and Pederson, 1997; Forman, 2003), image retrieval (Swets and Weng, 1995; Dy et al., 2003), genomic microarray analysis (Xing et al., 2001; Yu and Liu, 2004), customer relationship management (Ng and Liu, 2000), and intrusion detection (Lee et al., 2000).

Despite the impressive achievements in the current field of feature selection, we observe great challenges arising from domains such as genomic microarray analysis and text categorization where data may contain tens of thousands of features (Yu and Liu, 2004; Forman, 2003). First of all, the nature of high dimensionality of data can cause the so-called problem of "curse of dimensionality" (Hastie et al., 2001). Secondly, high-dimensional data often contains many redundant features. Both theoretical analysis and empirical evidence show that along with irrelevant features, redundant features also affect the speed and accuracy of learning algorithms and thus should be eliminated as well (Koller and Sahami, 1996; Kohavi and John, 1997; Hall, 2000). Existing feature selection methods mainly exploit two approaches: individual (feature) evaluation and subset evaluation (Blum and Langley, 1997; Guyon and Elisseeff, 2003). Methods of individual evaluation rank features according to their importance in differentiating instances of different classes and can only remove irrelevant features as redundant features likely have similar rankings. Methods of subset evaluation search for a minimum subset of features that satisfies some goodness measure and can remove

irrelevant features as well as redundant ones. However, among existing heuristic search strategies for subset evaluation, even greedy sequential search which reduces the search space from $O(2^N)$ to $O(N^2)$ can become very inefficient for high-dimensional data. The limitations of existing research clearly suggest that we should pursue a different framework of feature selection that allows efficient analysis of both feature relevance and redundancy for high-dimensional data.

The remainder of this paper is organized as follows. In Section 2, we review notions of feature relevance, identify the need for redundancy analysis, and provide a formal definition of feature redundancy. In Section 3, we analyze in detail the limitations of current approaches and propose a new framework of efficient feature selection. In Section 4, we describe correlation measures, and present a correlation-based method for efficient relevance and redundancy analysis under the new framework. Section 5 contains an empirical study of our method in terms of efficiency and effectiveness comparing with representative methods. Section 6 concludes this work and points out some future directions.

2. Feature Relevance and Feature Redundancy

Traditionally, feature selection research has focused on searching for relevant features. Although some recent work has pointed out the existence and effect of feature redundancy (Koller and Sahami, 1996; Kohavi and John, 1997; Hall, 2000), there is little work on explicit treatment of feature redundancy. In the following, we first present a classic notion of feature relevance and illustrate why it alone cannot handle feature redundancy, and then provide our formal definition of feature redundancy which paves the way for efficient elimination of redundant features.

2.1 Feature Relevance

Based on a review of previous definitions of feature relevance, John, Kohavi, and Pfleger classified features into three disjoint categories, namely, strongly relevant, weakly relevant, and irrelevant features (John et al., 1994). Let *F* be a full set of features, F_i a feature, and $S_i = F - \{F_i\}$. These categories of relevance can be formalized as follows.

Definition 1 (Strong relevance) A feature F_i is strongly relevant iff

$$\mathbf{P}(C \mid F_i, S_i) \neq \mathbf{P}(C \mid S_i) .$$

Definition 2 (Weak relevance) A feature F_i is weakly relevant iff

$$\mathbf{P}(C \mid F_i, S_i) = \mathbf{P}(C \mid S_i), \text{ and }$$

$$\exists S'_i \subset S_i$$
, such that $\mathbf{P}(C \mid F_i, S'_i) \neq \mathbf{P}(C \mid S'_i)$.

Corollary 1 (Irrelevance) A feature F_i is irrelevant iff

$$\forall S'_i \subseteq S_i, \mathbf{P}(C \mid F_i, S'_i) = \mathbf{P}(C \mid S'_i) .$$

Strong relevance of a feature indicates that the feature is always necessary for an optimal subset; it cannot be removed without affecting the original conditional class distribution. Weak relevance suggests that the feature is not always necessary but may become necessary for an optimal subset at certain conditions. Irrelevance (following Definitions 1 and 2) indicates that the feature is not necessary at all. According to these definitions, it is clear that in previous Example 1, feature F_1 is strongly relevant, F_2 , F_3 weakly relevant, and F_4 , F_5 irrelevant. An optimal subset should include all strongly relevant features, none of irrelevant features, and a subset of weakly relevant features. However, it is not given in the definitions which of weakly relevant features should be selected and which of them removed. Therefore, it is necessary to define feature redundancy among relevant features.

2.2 Defining Feature Redundancy

Notions of feature redundancy are normally in terms of feature correlation. It is widely accepted that two features are redundant to each other if their values are completely correlated (for example, features F_2 and F_3 in Example 1). In reality, it may not be so straightforward to determine feature redundancy when a feature is correlated (perhaps partially) with a set of features. We now formally define feature redundancy in order to devise an approach to explicitly identify and eliminate redundant features. Before we proceed, we first introduce the definition of a feature's Markov blanket given by Koller and Sahami (1996).

Definition 3 (Markov blanket) *Given a feature* F_i , *let* $M_i \subset F$ ($F_i \notin M_i$), M_i *is said to be a Markov blanket for* F_i *iff*

$$\mathbf{P}(F - M_i - \{F_i\}, C \mid F_i, M_i) = \mathbf{P}(F - M_i - \{F_i\}, C \mid M_i)$$

The Markov blanket condition requires that M_i subsume not only the information that F_i has about C, but also about all of the other features. It is pointed out in Koller and Sahami (1996) that an optimal subset can be obtained by a backward elimination procedure, known as *Markov blanket filtering*: let G be the current set of features (G = F in the beginning), at any phase, if there exists a Markov blanket for F_i within the current G, F_i is removed from G. It is proved that this process guarantees a feature removed in an earlier phase will still find a Markov blanket in any later phase, that is, removing a feature in a later phase will not render the previously removed features necessary to be included in the optimal subset. According to previous definitions of feature relevance, we can also prove that strongly relevant features cannot find any Markov blanket. Since irrelevant features should be removed anyway, we exclude them from our definition of redundant features.

Definition 4 (**Redundant feature**) Let G be the current set of features, a feature is redundant and hence should be removed from G iff it is weakly relevant and has a Markov blanket M_i within G.

From the property of Markov blanket, it is easy to see that a redundant feature removed earlier remains redundant when other features are removed. Figure 1 depicts the relationships between definitions of feature relevance and redundancy introduced so far. It shows that an entire feature set can be conceptually divided into four basic disjoint parts: irrelevant features (I), redundant features (II, part of weakly relevant features), weakly relevant but non-redundant features (III), and strongly relevant features (IV). An optimal subset essentially contains all the features in parts III and IV. It is worthy to point out that although parts II and III are disjoint, different partitions of them can result from the process of Markov blanket filtering. In previous Example 1, either of F_2 or F_3 , but not both, should be removed as a redundant feature.

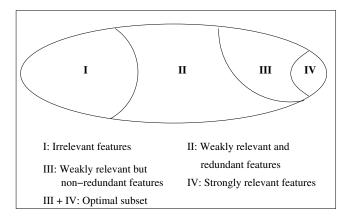


Figure 1: A view of feature relevance and redundancy.

3. Efficient Feature Selection via Relevance and Redundancy Analysis

We now review two major approaches in dealing with feature relevance and redundancy, analyze their limitations for high-dimensional data, and then propose a new framework of efficient feature selection based on relevance and redundancy analysis.

3.1 Existing Approaches in Dealing with Relevance and Redundancy

As mentioned earlier, there exist two major approaches in feature selection: *individual evaluation* and *subset evaluation*. Individual evaluation, also known as feature weighting/ranking (Blum and Langley, 1997; Guyon and Elisseeff, 2003), assesses individual features and assigns them weights according to their degrees of relevance. A subset of features is often selected from the top of a ranking list, which approximates the set of relevant features (II, III, and IV in Figure 1). With its linear time complexity in terms of dimensionality N, this approach is efficient for high-dimensional data. However, it is incapable of removing redundant features because redundant features likely have similar rankings. As long as features are deemed relevant to the class, they will all be selected even though many of them are highly correlated to each other. For high-dimensional data which may contain a large number of redundant features, this approach may produce results far from optimal.

Many feature selection methods take the subset evaluation approach which handles feature redundancy with feature relevance. The diagram in Figure 2 exhibits a traditional framework of feature selection via subset evaluation (Liu and Motoda, 1998). Subset generation produces candidate feature subsets based on a certain search strategy. Each candidate subset is evaluated by a certain evaluation measure and compared with the previous best one with respect to this measure. If a new subset turns out to be better, it replaces the previous best subset. The process of subset generation and evaluation is repeated until a given stopping criterion is satisfied. Distinguished from individual evaluation, evaluation measures used by this approach are defined against feature subsets, taking into account the existence and effect of redundant features. A feature subset selected by this approach approximates the optimal subset (parts III and IV in Figure 1). Many methods have proven effective to some extent in removing both irrelevant features and redundant features (John et al., 1994; Koller and Sahami, 1996; Bell and Wang, 2000; Hall, 2000). However, methods in this framework can suffer from an inevitable problem caused by searching through feature subsets required in the subset generation step. Although there exist various heuristic search strategies such as greedy sequential search, best-first search, and genetic algorithm (Liu and Motoda, 1998), most of them still incur time complexity $O(N^2)$, which prevents them from scaling well to data sets containing tens of thousands of features.

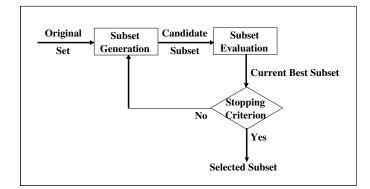


Figure 2: A traditional framework of feature selection.

3.2 A New Framework of Efficient Feature Selection

From previous discussions, it is clear that in order to eliminate redundant features, the state-of-theart feature selection methods have to rely on the approach of subset evaluation which *implicitly* handles feature redundancy with feature relevance. These methods can produce better results than methods without handling feature redundancy, but the high computational cost of the subset search makes them inefficient for high-dimensional data. Therefore, in our solution, we propose a new framework of feature selection which avoids implicitly handling feature redundancy and turns to efficient elimination of redundant features via *explicitly handling feature redundancy*.

Relevance definitions divide features into strongly relevant, weakly relevant, and irrelevant ones; redundancy definition further divides weakly relevant features into redundant and non-redundant ones. Our goal is to efficiently find the optimal subset (parts III and IV in Figure 1). We can achieve this goal through a new framework of feature selection (shown in Figure 3) composed of two steps: first, relevance analysis determines the subset of relevant features by removing irrelevant ones, and second, redundancy analysis determines and eliminates redundant features from relevant ones and thus produces the final subset. Its advantage over the traditional framework of subset evaluation lies in that by decoupling relevance and redundancy analysis, it circumvents subset search and allows a both efficient and effective way in finding a subset that approximates an optimal subset.

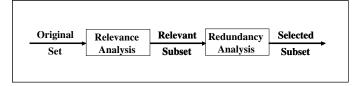


Figure 3: A new framework of feature selection.

It is sensible to use efficient heuristic methods to approximate the computation of relevant features and redundant features under our new framework for two reasons. On one hand, searching for an optimal subset based on the definitions of feature relevance and redundancy is combinatorial in nature. It is obvious that exhaustive or complete search is prohibitive with a large number of features. On the other hand, an optimal subset is defined based on the full population where the true data distribution is known. It is generally assumed (Mitchell, 1997; Miller, 2002) that a training data set is only a small portion of the full population, especially in a high-dimensional space. Therefore, it is not proper to search for an optimal subset from the training data as over-searching the training data can cause over-fitting (Jensen and Cohen, 2000). We next present our approximation method.

4. A Correlation Based Method

Correlation is widely used in machine learning and statistics for relevance analysis. In this section, we first introduce our choice of correlation measure in Section 4.1, then describe our correlationbased method for both relevance and redundancy analysis in Section 4.2, and present and analyze the algorithm in Section 4.3.

4.1 Correlation Measures

There exist broadly two types of measures for the correlation between two random variables: linear and non-linear. Of linear correlation, the most well known measure is *linear correlation coefficient*. For a pair of variables (X, Y), the linear correlation coefficient ρ is given by

$$\rho = \frac{\sum\limits_{i} (x_i - \overline{x_i})(y_i - \overline{y_i})}{\sqrt{\sum\limits_{i} (x_i - \overline{x_i})^2} \sqrt{\sum\limits_{i} (y_i - \overline{y_i})^2}} ,$$

where $\overline{x_i}$ is the mean of *X*, and $\overline{y_i}$ is the mean of *Y*. The value of ρ lies between -1 and 1, inclusive. If *X* and *Y* are completely correlated, ρ takes the value of 1 or -1; if *X* and *Y* are independent, ρ is zero. It is a symmetrical measure for two variables. Other measures in this category are basically variations of the above formula, such as *least square regression error* and *maximal information compression index* (Mitra et al., 2002). However, it is not safe to always assume linear correlation between features in the real world. Linear correlation measures may not be able to capture correlations that are not linear in nature. It can also be observed that linear correlation coefficient is not suitable for nominal data.

Among non-linear correlation measures, many measures are based on the information-theoretical concept of *entropy*, a measure of the uncertainty of a random variable. The entropy of a variable *X* is defined as

$$H(X) = -\sum_{i} P(x_i) \log_2(P(x_i)) ,$$

and the entropy of X after observing values of another variable Y is defined as

$$H(X|Y) = -\sum_{j} P(y_j) \sum_{i} P(x_i \mid y_j) \log_2(P(x_i \mid y_j)) ,$$

where $P(x_i)$ is the prior probabilities for all values of *X*, and $P(x_i | y_i)$ is the posterior probabilities of *X* given the values of *Y*. The amount by which the entropy of *X* decreases reflects additional

information about X provided by Y and is called *information gain* (Quinlan, 1993), given by

$$IG(X \mid Y) = H(X) - H(X \mid Y) .$$

According to this measure, feature *Y* is regarded more correlated to feature *X* than to feature *Z*, if IG(X | Y) > IG(Z | Y). It is easy to prove that information gain is a symmetrical measure. Symmetry is a desired property for a measure of correlations between features. It ensures that the order of two features ((*X*, *Y*) or (*Y*, *X*)) will not affect the value of the measure. Since information gain tends to favor features with more values, it should be normalized with their corresponding entropy. Therefore, we choose *symmetrical uncertainty* (Press et al., 1988), defined as

$$SU(X, Y) = 2\left[\frac{IG(X \mid Y)}{H(X) + H(Y)}\right]$$

It compensates for information gain's bias toward features with more values and restricts its values to the range [0,1]. A value of 1 indicates that knowing the values of either feature completely predicts the values of the other; a value of 0 indicates that X and Y are independent. In addition, it still treats a pair of features symmetrically. Entropy-based measures handle nominal or discrete features, and therefore continuous features need to be properly discretized (Liu et al., 2002a) in order to use entropy-based measures.

4.2 Efficient Relevance and Redundancy Analysis

Using symmetrical uncertainty (SU) as the correlation measure, we are ready to develop an approximation method for both relevance and redundancy analysis under our new framework introduced in Section 3.2. We first differentiate two types of correlation between features (including the class).

Definition 5 (*C*-correlation) The correlation between any feature F_i and the class *C* is called *C*-correlation, denoted by $SU_{i,c}$.

Definition 6 (*F*-correlation) The correlation between any pair of features F_i and F_j ($i \neq j$) is called *F*-correlation, denoted by $SU_{i,j}$.

Aiming to achieve high efficiency, we calculate *C*-correlation for each feature, and heuristically decide a feature F_i to be relevant if it is highly correlated with the class *C*, i.e., if $SU_{i,c} > \gamma$, where γ is a relevance threshold which can be determined by users. The selected relevant features are then subject to redundancy analysis. Similarly, we can evaluate the correlation between individual features for redundancy analysis without considering the correlation between various feature subsets. However, there are two difficulties in determining feature redundancy via pair-wise *F*-correlation calculation: (1) when two features are not completely correlated with each other, it may be hard to determine feature redundancy and which one to be removed; and (2) it may still require *F*-correlation calculation for a total of $\frac{N(N-1)}{2}$ pairs, which is inefficient for high-dimensional data. Below, we try to efficiently determine feature redundancy by substantially reducing the number of feature pairs evaluated for *F*-correlation.

In Section 2, we apply Markov blankets to *exactly* determine feature redundancy. When it comes to *approximately* determine feature redundancy, the key is to find approximate Markov blankets for the selected relevant features. We assume that a feature with a larger *C*-correlation value contains

by itself more information about the class than a feature with a smaller *C*-correlation value. We determine the existence of an approximate Markov blanket between a pair of correlated features F_i and F_j based on their *F*-correlation level $SU_{i,j}$ as follows. When $SU_{j,c} \ge SU_{i,c}$, we choose to evaluate whether feature F_j can form an approximate Markov blanket for feature F_i (instead of F_i for F_j) in order to maintain more information about the class. In addition, we heuristically use $SU_{i,c}$ as a threshold to determine whether the *F*-correlation $SU_{i,j}$ is strong or not. An approximate Markov blanket can be defined as follows.

Definition 7 (Approximate Markov blanket) For two relevant features F_i and F_j $(i \neq j)$, F_j forms an approximate Markov blanket for F_i iff $SU_{j,c} \ge SU_{i,c}$ and $SU_{i,j} \ge SU_{i,c}$.

Recall that Markov blanket filtering, a backward elimination procedure based on a feature's Markov blanket in the current set, guarantees that a redundant feature removed in an earlier phase will still find a Markov blanket in any later phase when another redundant feature is removed. It is easy to verify that this is not the case for backward elimination based on a feature's approximate Markov blanket in the current set. For instance, if F_j is the only feature that forms an approximate Markov blanket for F_i , and F_k forms an approximate Markov blanket for F_j , after removing F_j based on F_k will result in no approximate Markov blanket for F_i in the current set. However, we can avoid this situation by removing a feature only when it can find an approximate Markov blanket formed by a predominant feature, defined as follows.

Definition 8 (Predominant feature) A relevant feature is predominant iff it does not have any approximate Markov blanket in the current set.

Predominant features will not be removed at any stage. If a feature F_i is removed based on a predominant feature F_j in an earlier phase, it is guaranteed that it will still find an approximate Markov blanket (the same F_j) in any later phase when another feature is removed. To summarize, our method for redundancy analysis consists of (1) selecting a predominant feature, (2) removing all features for which it forms an approximate Markov blanket, and (3) iterating steps (1) and (2) until no more predominate features can be selected. An optimal subset can therefore be approximated by a set of predominant features.

4.3 Algorithm and Analysis

The approximation method for relevance and redundancy analysis presented before can be realized by an algorithm, named FCBF (Fast Correlation-Based Filter). It involves two connected steps: (1) selecting a subset of relevant features, and (2) selecting predominant features from relevant ones. As shown in Figure 4, for a data set *S* with *N* features and class *C*, the algorithm finds a set of predominant features S_{best} . In the first step (lines 2-7), it calculates the *SU* value for each feature, selects relevant features into S'_{list} based on a predefined threshold δ , and orders them in a descending order according to their *SU* values. In the second step (lines 8-18), it further processes the ordered list S'_{list} to select predominant features. A feature F_j that has already been determined to be a predominant feature can always be used to filter out other features for which F_j forms an approximate Markov blanket. Since the feature with the highest *C*-correlation does not have any approximate Markov blanket, it must be one of the predominant features. So the iteration starts from the first element in S'_{list} (line 8) and continues as follows. For all the remaining features (from the one right next to F_j to the last one in S'_{list}), if F_j happens to form an approximate Markov blanket

input: $S(F_1, F_2, ..., F_N, C)$ // a training data set // a predefined threshold output: S_{best} // a selected subset 1 begin 2 3 for i = 1 to N do begin calculate $SU_{i,c}$ for F_i ; if $(SU_{i,c} > \delta)$ 4 append F_i to S'_{list} ; 5 6 end: 7 order S'_{list} in descending $SU_{i,c}$ value; 8 $F_j = getFirstElement(S'_{list});$ 9 do begin 10 $F_i = getNextElement(S'_{list}, F_i);$ if $(F_i <> \text{NULL})$ 11 12 do begin 13 if $(SU_{i,j} \ge SU_{i,c})$ remove F_i from S'_{list} ; $F_i = getNextElement(S'_{list}, F_i)$; 14 15 end until ($F_i ==$ NULL); $F_j = getNextElement(S'_{list}, F_j)$; end until ($F_j ==$ NULL); 16 17 18 $S_{best} = S'_{list};$ 19 20 end;

Figure 4: FCBF Algorithm.

for F_i (line 13), F_i will be removed from S'_{list} . After one round of filtering features based on F_j , the algorithm will take the remaining feature right next to F_j as the new reference (line 17) to repeat the filtering process. The algorithm stops until no more predominant features can be selected. Figure 5 illustrates how predominant features are selected with the rest features removed as redundant ones. In Figure 5, six features are selected as relevant ones and ranked according to their *C*-correlation values, with F_1 being the most relevant one. In the first round, F_1 is selected as a predominant feature, and F_2 and F_4 are removed based on F_1 . In the second round, F_3 is selected, and F_6 is removed based on F_3 . In the last round, F_5 is selected.

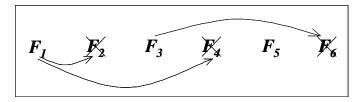


Figure 5: Selection of predominant features

We now analyze the time complexity of FCBF before an empirical study of its efficiency. As we can see from Figure 4, major computation of the algorithm involves SU values for C- and Fcorrelations, which has linear complexity in term of the number of instances in a data set. In terms of dimensionality N, to determine relevant features, the algorithm has linear complexity O(N); to determine predominant features from relevant ones (assuming all features are selected as relevant ones), it has a best-case complexity O(N) when only one feature is selected and all of the rest of the features are removed, and a worse-case complexity $O(N^2)$ when all features are selected. These time complexity results are comparable to subset evaluation based on greedy sequential search in which features are, one at a time, added to the current subset (i.e., sequential forward selection) or removed from the current subset (i.e., sequential backward elimination). However, in general cases when k(1 < k < N) features are selected, the number of evaluations performed by FCBF will typically be much less (and certainly never more) than the number of evaluations performed by greedy sequential search because features removed in each round are not considered in the next round and FCBF typically removes a large number of features (instead of only one by greedy sequential search) in each round. This makes FCBF substantially faster than algorithms of subset evaluation based on greedy sequential search, as will be demonstrated by the running time comparisons reported in Section 5. The more features removed in an earlier round, the faster FCBF is. Moreover, selecting a subset of relevant features in the first step can further improves its efficiency.

In summary, our method approximates relevance and redundancy analysis by selecting all predominant features and removing the rest features. It uses both C- and F-correlations to determine feature redundancy and combines sequential forward selection with elimination so that it not only circumvents full pair-wise F-correlation analysis but also achieves higher efficiency than pure sequential forward selection or backward elimination. However, our method is suboptimal due to the way C- and F-correlations are used for relevance and redundancy analysis and the approximates that it uses. It is fairly straightforward to improve the optimality of the results by considering different combinations of features in evaluating feature relevance and redundancy, which in turn increases time complexity. Another way to improve result optimality is to find better heuristics in determining a feature's approximate Markov blanket.

5. Empirical Study

In this section, we empirically evaluate the efficiency and effectiveness of our method by comparing FCBF with representative feature selection algorithms. We describe experimental setup in Section 5.1, discuss results on synthetic data and benchmark data in Sections 5.2 and 5.3 respectively, and summarize the findings in Section 5.4.

5.1 Experimental Setup

The efficiency of a feature selection algorithm can be directly measured by its running time over various data sets. As to effectiveness, a simple and direct evaluation criterion is how similar the selected subset and the optimal subset are, but it can only be measured over synthetic data for which we know beforehand which features are irrelevant or redundant. For real-world data, we often do not have such prior knowledge about the optimal subset, so we use the predictive accuracy on the selected subset of features as an indirect measure.

In terms of the above criteria, we limit our comparisons to the filter model as FCBF is a filter algorithm designed for high-dimensional data. We choose representative algorithms from both approaches (i.e., individual evaluation and subset evaluation). One algorithm, from individual evaluation, is ReliefF (Robnik-Sikonja and Kononenko, 2003) which searches for nearest neighbors of instances of different classes and weights features according to how well they differentiate instances of different classes. Another algorithm, from subset evaluation, is a variation of CFS (Hall, 2000),

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denoted by CFS-SF (Sequential Forward). CFS exploits best-first search based on some correlation measure which evaluates the goodness of a subset by considering the individual predictive ability of each feature and the degree of correlation between them. Sequential forward selection is used in CFS-SF as initial experiments show CFS-SF runs much faster to produce similar results than CFS. A third one, also from subset evaluation, is a variation of FOCUS (Almuallim and Dietterich, 1994), denoted by FOCUS-SF. FOCUS exhaustively examines all subsets of features, selecting the minimal subset that separates classes as consistently as the full set can. It is prohibitively costly even for data sets with moderate dimensionality. FOCUS-SF replaces exhaustive search in FOCUS with sequential forward selection. In our experiments, we heuristically set the relevance threshold γ to be the *SU* value of the $\lfloor N/\log N \rfloor$ th ranked feature for each data set. To test how the selection of threshold affects the performance of FCBF, we also include in our comparisons the results of FCBF with γ set to the default value 0. We use FCBF_(log) to represent a version of FCBF with the former setting, and FCBF₍₀₎ with the latter setting in the rest of the paper.

In addition to feature selection algorithms, we use two learning algorithms, NBC (Witten and Frank, 2000) and C4.5 (Quinlan, 1993), to evaluate the predictive accuracy on the selected subset of features. All these selected algorithms are from Weka's collection (Witten and Frank, 2000). FCBF is also implemented in Weka environment.

5.2 Results and Discussions on Synthetic Data

We use three synthetic data sets to illustrate the strengthes and limitations of FCBF and compare it with ReliefF, CFS-SF, and FOCUS-SF. The first data set is the widely used Corral data (John et al., 1994) which contains six Boolean features (A0, A1, B0, B1, I, R) and a Boolean class Y defined by $Y = (A0 \land A1) \lor (B0 \land B1)$. Features A0, A1, B0, and B1 are independent to each other, feature I is uniformly random, and feature R matches the class Y 75% of the time. It is obvious that an optimal subset includes A0, A1, B0, and B1. I is irrelevant, and R is redundant. The other two data sets, Corral-47 and Corral-46, are obtained by introducing more irrelevant features and redundant features to the original Corral data. As its name says, Corral-47 contains a total of 47 Boolean features including 5 original features A0, A1, B0, B1, and R, 14 irrelevant features, and 28 additional redundant features. Among the 14 irrelevant features, only two features are uniformly random and each of the remaining 12 is completely correlated with either of the two. Among the 28 additional redundant features, for each of A0, A1, B0, and B1, there are 7 features that are correlated with it at various levels. The ratios of non-matches are 0, 1/16, 2/16, ..., 6/16 respectively. Corral-46 is the same as Corral-47 except that it excludes R. Table 1 shows features selected by each algorithm. We use A0, A1, B0, B1 combined with subscripts $0, 1, \dots, 6$ to represent the newly introduced redundant features, with the value of the subscripts indicating the ratio of non-matches.

We can see that for Corral, all the algorithms in comparison remove the irrelevant feature I, but fail to remove the redundant feature R. FCBF_(log) misses three features due to the setting of an improper threshold. For Corral-47, these algorithm also remove all the irrelevant features, but fail to remove R. The difference is that FCBF_(log), FCBF₍₀₎, and CFS-SF successfully remove all the additional redundant features. For Corral-46, only FCBF_(log) and FCBF₍₀₎ find the optimal subset. In Corral-47 and Corral-46, the threshold in FCBF_(log) does not affect the selection results. These results suggest that when feature redundancy can only be identified based on feature subsets (e.g., the redundancy of R is defined by the subset of A0, A1, B0, and B1), FCBF may not successfully remove redundant features. This is a hard problem for most heuristic search algorithms as well.

	FCBF(log)	FCBF ₍₀₎	ReliefF	CFS-SF	FOCUS-SF
Corral	R A0	R A0 A1 B0	A0 B0 R B1	A0 A1 B0 B1	R
		<i>B</i> 1	A1	R	
Corral-47	R A0 A1 B0	R A0 A1 B0	R B11 A0 A00	A0 A1 B0 B1	A0 A1 A1 ₂ B0
	<i>B</i> 1	<i>B</i> 1	B1 B1 ₀ B0 B0 ₀	R	B1 R
			B02 A1 A10		
Corral-46	A0 A1 B0 B1	A0 A1 B0 B1	A0 A0 ₀ B1 ₁ B0	A0 A03 A04 A1	A0 A1 A13 A14
			B00 B1 B10 B02	A1 ₂ A1 ₄ B0 B0 ₀	B0 B1
			A1 A1 ₀	B1 B1 ₁	

Table 1: Features selected by each feature selection algorithm on synthetic data.

However, in high-dimensional data which often contains a large portion of irrelevant and/or redundant features (as in Corral-47 and Corral-46), FCBF can effectively remove redundant features. We next further verify its effectiveness as well as efficiency compared to other algorithms through various real-world data of high dimensionality.

5.3 Results and Discussions on Benchmark Data

In various machine learning domains, there are two forms of high-dimensional data. Traditionally, the dimensionality is usually thought high if data contains tens or hundreds of features. In this form of data, the number of instances is normally much larger than the dimensionality. In new domains such as text categorization and genomic microarray analysis, the dimensionality is in the order of thousands or even higher, and often greatly exceeds the number of instances. Therefore, we evaluate our method in comparison with others on high-dimensional data of both forms.

Title	Features	Instances	Classes
Lung-cancer	56	32	3
Promoters	57	106	2
Splice	60	3190	3
USCensus90	67	9338	3
CoIL2000	85	5822	2
Chemical	150	936	3
Musk2	166	6598	2
Arrhythmia	279	452	16
Isolet	617	1560	26
Multi-features	649	2000	10

5.3.1 UCI BENCHMARK DATA

Table 2: Summary of UCI benchmark data sets.

All together 10 data sets in the traditional form are selected from the UCI Machine Learning Repository¹ and the UCI KDD Archive.² These data sets contain various numbers of features, instances, and classes, as shown in Table 2. For each data set, we first run all the feature selection algo-

^{1.} http://www.ics.uci.edu/~mlearn/MLRepository.html

^{2.} http://kdd.ics.uci.edu

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rithms in comparison, and obtain the running time and selected features for each algorithm. For data sets containing features with continuous values, we apply the MDL discretization method (Fayyad and Irani, 1993) before applying FCBF, CFS-SF, and FOCUS-SF. For ReliefF, we use 5 neighbors and 30 instances throughout the experiments as suggested by Robnik-Sikonja and Kononenko (2003). We then apply NBC and C4.5 on both the original data set and each of the newly obtained data sets (with only selected features), and obtain overall accuracy of 10-fold cross-validation. All experiments were conducted on a Pentium IV PC with 1 GB RAM.

Table 3 records the running time for each feature selection algorithm. We can observe that $FCBF_{(0)}$ is consistently faster than CFS-SF and FOCUS-SF. The time savings from $FCBF_{(0)}$ become more obvious when the data dimensionality increases. In many cases especially compared with FOCUS-SF, the time savings are in degrees of magnitude. These results verify the superior computational efficiency of sequential forward selection with elimination applied by FCBF over greedy sequential search applied by CFS-SF and FOCUS-SF. Comparison between $FCBF_{(0)}$ and ReliefF shows that ReliefF is unexpectedly slow even though its time complexity is linear to dimensionality. The reason lies in that searching for nearest neighbors in ReliefF involves distance calculation which is more costly than the calculation of symmetrical uncertainty. When we compare $FCBF_{(0)}$ with $FCBF_{(log)}$, it is clear that the setting of a larger relevance threshold γ further speeds up FCBF.

Title	FCBF _(log)	FCBF ₍₀₎	ReliefF	CFS-SF	FOCUS-SF
Lung-cancer	0.001	0.02	0.09	0.05	0.08
Promoters	0.001	0.02	0.06	0.03	0.16
Splice	0.20	0.55	0.89	0.55	16.59
USCensus90	0.30	0.50	2.94	0.52	77.67
CoIL2000	0.25	0.50	4.25	1.98	143.94
Chemical	0.05	0.05	1.36	0.28	6.56
Musk2	0.53	0.88	9.55	4.84	85.78
Arrhythmia	0.06	0.08	1.19	0.78	13.70
Isolet	0.42	3.05	10.05	93.94	107.33
Multi-Features	1.19	19.42	11.42	71.00	67.56

Table 3: Running time (seconds) for each feature selection algorithm on UCI data.

Table 4 records the number of features selected by each feature selection algorithm. We can see that all these algorithms achieve significant reduction of dimensionality by selecting only a small portion of the original features. $FCBF_{(log)}$ on average selects the smallest number of features.

Tables 5 and 6 show the 10-fold cross-validation accuracy of NBC and C4.5 respectively. For each data set, we conduct Student's paired two-tailed t-Test in order to evaluate the statistical significance of the difference between two averaged accuracy values: one resulted from $FCBF_{(log)}$ and the other resulted from one of $FCBF_{(0)}$, the full set, ReliefF, CFS-SF, and FOCUS-SF. Each value in a *p*-val column records the probability associated with the t-Test. The smaller the value, the more significant the difference of the two average values is. The last row (L/W/T) in each table summarizes over all data sets the losses/wins/ties in accuracy (at significance level 0.1) comparing various feature sets with those selected by $FCBF_{(log)}$. We can see that in general $FCBF_{(log)}$ achieves similar accuracy as $FCBF_{(0)}$. Therefore, the effectiveness of FCBF can be verified from the following two general trends: (1) $FCBF_{(log)}$ improves or maintains the accuracy of both NBC and C4.5, and the

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Title	FCBF(log)	FCBF ₍₀₎	ReliefF	CFS-SF	FOCUS-SF
Lung-cancer	4	6	5	8	4
Promoters	6	6	4	4	4
Splice	9	22	11	6	10
USCensus90	3	4	2	1	13
CoIL2000	3	5	12	10	29
Chemical	4	5	7	7	11
Musk2	2	2	2	10	11
Arrhythmia	5	12	25	25	24
Isolet	5	32	23	137	11
Multi-Features	27	130	14	87	7
Average	7	22	11	30	12

Table 4: Number of features selected by each feature selection algorithm on UCI data.

	FCBF _(log)	FCF	$3F_{(0)}$	Ful	Full Set		iefF	CFS	S-SF	FOCUS-SF	
Title	Acc	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val
Lung-cancer	83.33	86.67	0.34	78.33	0.34	84.17	0.85	86.67	0.34	87.5	0.46
Promoters	93.27	93.27	1	91.55	0.55	87.82	0.25	95.18	0.17	90.45	0.40
Splice	93.95	96.14	0.00 ⁺	95.52	0.00+	91.32	0.00^{-}	93.54	0.24	94.36	0.08 ⁺
USCensus90	97.94	97.88	0.19	93.49	0.00-	97.97	0.17	97.99	0.65	97.87	0.44
CoIL2000	93.94	93.92	0.34	78.68	0.00-	93.89	0.66	92.92	0.01^{-}	83.22	0.00-
Chemical	71.91	67.73	0.02^{-}	60.90	0.00-	71.26	0.77	70.51	0.35	66.35	0.00^{-}
Musk2	84.59	84.59	1	84.78	0.51	84.59	1	64.87	0.00^{-}	83.53	0.01-
Arrhythmia	67.48	65.73	0.45	60.88	0.01-	55.79	0.00-	69.05	0.45	69.06	0.56
Isolet	50.06	83.33	0.00+	84.10	0.00+	60.90	0.00+	87.31	0.00+	71.03	0.00+
Multi-feat	95.9	95.65	0.50	94.1	0.01 ⁻	67.65	0.00-	96.15	0.64	93.7	0.02^{-}
L/W/T	-	1/2	2/7	5/2/3		3/1/6		2/1/7		4/2/4	

Table 5: Accuracy of NBC on selected features for UCI data: Acc records 10-fold cross-validation accuracy rate (%) and *p*-Val records the probability associated with a paired two-tailed t-Test. The symbols "+" and "-" respectively identify statistically significant (at 0.1 level) wins or losses over FCBF_(log).

improvement is more pronounced for NBC; and (2) $FCBF_{(log)}$ can achieve similar or even higher accuracy compared with other algorithms.

5.3.2 NIPS BENCHMARK DATA

Three data sets with very high dimensionality but relatively few instances are selected from the NIPS 2003 feature selection benchmark data sets.³ All these data sets contain two classes and a large number of artificially introduced random features in addition to real features. A summary of the data sets is given in Table 7. For each data set, we conduct experiments following the same procedure as that used in UCI data. The results are shown in Tables 8, 9, 10, and 11.

From Table 8, we observe similar trends as those from UCI data except that (1) for Dexter and Dorothea data, CFS-SF did not produce running time results (hence, neither selected features nor

^{3.} http://clopinet.com/isabelle/Projects/NIPS2003/

	FCBF(log)	FCE	$BF_{(0)}$	Ful	Full Set		iefF	CFS	S-SF	FOCUS-SF	
Title	Acc	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val
Lung-cancer	86.67	86.67	1	80.83	0.17	84.17	0.34	84.17	0.34	84.17	0.34
Promoters	80.18	80.18	1	78.09	0.42	82.36	0.55	80.18	1	81.36	0.67
Splice	94.01	94.14	0.64	93.98	0.89	90.53	0.00^{-}	93.39	0.00^{-}	93.79	0.11
USCensus90	98.12	98.12	1	98.19	0.39	98.12	1	97.99	0.00^{-}	98.21	0.11
CoIL2000	94.02	94.02	1	93.87	0.12	94.02	1	94.02	1	93.97	0.39
Chemical	95.41	95.41	1	94.13	0.01-	95.94	0.14	95.94	0.14	95.31	0.86
Musk2	91.35	91.35	1	96.91	0.00+	88.00	0.00^{-}	95.79	0.00 ⁺	95.45	0.00^{+}
Arrhythmia	71.47	68.80	0.19	67.70	0.04-	69.02	0.07-	68.58	0.13	67.02	0.04-
Isolet	49.17	75.77	0.00^{+}	79.87	0.00+	59.10	0.00^{+}	81.35	0.00 ⁺	68.84	0.00^{+}
Multi-feat	92.45	93.65	0.04 ⁺	94.3	0.01 ⁺	78.65	0.00^{-}	94.7	0.00 ⁺	91.75	0.42
L/W/T	-	0/2	2/8	2/3/5		4/1/5		2/3/5		1/2/7	

Table 6: Accuracy of **C4.5** on selected features for **UCI** data: Acc records 10-fold cross-validation accuracy rate (%) and *p*-Val records the probability associated with a paired two-tailed t-Test. The symbols "+" and "-" respectively identify statistically significant (at 0.1 level) wins or losses over FCBF_(log).

		Features		Instances				
Title	Total	Real	Random	Total	Class 1	Class 2		
Arcene	10000	7000	3000	100	44	56		
Dexter	20000	9947	10053	300	150	150		
Dorothea	100000	50000	50000	800	78	722		

Table 7: Summary of NIPS benchmark data sets.

accuracy results) because the program ran out of memory after a period of considerably long time due to its quadratic space complexity; and (2) FCBF achieves tremendous time savings for this group of data sets, for instance, roughly 1 minute by FCBF_(log) versus 4.5 hours by FOCUS-SF in Dorothea data. Results in Table 9 show that all the algorithms in comparison can dramatically reduce the dimensionality for this group of data sets. In spite of its impressive efficiency and capability of dimensionality reduction, the effectiveness of FCBF can still be clearly revealed by the results in Tables 10 and 11. As we can see, FCBF either improves or maintains the accuracy of both NBC and C4.5 for all the three data sets. In addition, for each of the three data sets, the highest accuracy is achieved by applying NBC on the feature subset selected by FCBF.

Title	FCBF(log)	FCBF(0)	ReliefF	CFS-SF	FOCUS-SF
Arcene	0.42	0.75	9.16	1108.66	21.39
Dexter	1.80	2.63	45.43	N/A	928.78
Dorothea	68.95	393.80	349.27	N/A	16470.92

Table 8: Running time (seconds) for each feature selection algorithm on NIPS data.

Title	FCBF _(log)	FCBF ₀	ReliefF	CFS-SF	FOCUS-SF
Arcene	24	39	45	50	4
Dexter	35	35	71	N/A	23
Dorothea	50	96	137	N/A	21

Table 9: Number of features selected by each feature selection algorithm on NIPS data.

	FCBF _(log)	FCBF ₍₀₎		Full Set		ReliefF		CFS-SF		FOCUS-SF	
Title	Acc	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val
Arcene	91.0	93.0	0.34	69.0	0.00^{-}	69.0	0.02^{-}	92.0	0.68	59.0	0.00^{-}
Dexter	90.0	90.0	1	88.0	0.26	73.00	0.00^{-}	N/A	N/A	90.0	1
Dorothea	97.5	98.38	0.01 ⁺	90.25	0.00^{-}	94.38	0.00^{-}	N/A	N/A	95.25	0.00^{-}

Table 10: Accuracy of **NBC** on selected features for **NIPS** data: Acc records 10-fold crossvalidation accuracy rate (%) and *p*-Val records the probability associated with a paired two-tailed t-Test. The symbols "+" and "-" respectively identify statistically significant (at 0.1 level) wins or losses over FCBF_(log).

5.4 Summary

From the previous empirical study, we can conclude that FCBF can efficiently achieve high degree of dimensionality reduction and enhance or maintain predictive accuracy with selected features. Its proven efficiency and effectiveness compared with other algorithms through various synthetic and benchmark data sets suggest that FCBF is practical for feature selection of high-dimensional data. It is worthy to emphasize that feature subsets selected by FCBF are decoupled from the choice of learning algorithms. In other words, FCBF does not directly aim to increase the accuracy within affordable time, a wrapper algorithm based on an intended learning algorithm can be applied to the significantly reduced subset obtained from FCBF.

In FCBF, there is one parameter, the relevance threshold γ . As consistently shown from the benchmark data, different settings of γ affect the speed of FCBF. The closer γ is set to 1, the faster FCBF is. As shown from Corral-47 and Corral-46 as well as many of the benchmark data sets which may contain a large number of irrelevant and/or redundant features, speeding up the algorithm by

	FCBF(log)	FCBF(0)		Full Set		ReliefF		CFS-SF		FOCUS-SF	
Title	Acc	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val	Acc	<i>p</i> -Val
Arcene	83.0	82.0	0.76	76.0	0.17	65.0	0.04^{-}	79.0	0.40	75.0	0.26
Dexter	83.67	83.67	1	76.33	0.02^{-}	76.67	0.08-	N/A	N/A	90.00	0.01 ⁺
Dorothea	92.88	93.0	0.76	90.38	0.01-	93.38	0.68	N/A	N/A	96.5	0.00^{+}

Table 11: Accuracy of **C4.5** on selected features for **NIPS** data: Acc records 10-fold crossvalidation accuracy rate (%) and *p*-Val records the probability associated with a paired two-tailed t-Test. The symbols "+" and "-" respectively identify statistically significant (at 0.1 level) wins or losses over FCBF_(log).

setting γ to a reasonably large value does not sacrifice the goodness of the selected subsets. However, a close look at the accuracy of individual data sets in Tables 5 and 6 reveals that in certain cases (e.g., Isolet data), FCBF_(log) results in significantly reduced accuracy than FCBF₍₀₎ due to the setting of overly high threshold. Therefore, when we do not have prior knowledge about data, an easy and safe way of applying FCBF is to set γ to the default value 0.

6. Conclusions

In this paper, we have identified the need for explicit redundancy analysis in feature selection, provided a formal definition of feature redundancy, and investigated the relationship between feature relevance and redundancy. We have proposed a new framework of efficient feature selection via relevance and redundancy analysis, and a correlation-based method which uses *C*-correlation for relevance analysis and both *C*- and *F*-correlations for redundancy analysis. A new feature selection algorithm FCBF is implemented and evaluated through extensive experiments comparing with three representative feature selection algorithms. The feature selection results are further verified by two different learning algorithms. Our method demonstrates its efficiency and effectiveness for feature selection in supervised learning in domains where data contains many irrelevant and/or redundant features.

Some future works are planed along the following directions. First, since symmetrical uncertainty measure only handles nominal or discrete values, our current method requires continuous values be discretized, which opens the opportunity to investigate how different discretization methods affect the performance of FCBF. Second, it would be interesting to explore measures that can handle all types of values or ways of combining different measures under our framework of relevance and redundancy analysis. Another direction is to investigate how our method can be extended to deal with regression problems in which the class contains continuous values. Moreover, additional effort is needed to experiment our method on genomic microarray data for informative gene selection and investigate how small samples affect the performance of feature selection.

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