Toward better feature weighting algorithms: a focus on Relief

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Abstract

Feature weighting algorithms try to solve a problem of great importance nowadays in machine learning: The search of a relevance measure for the features of a given domain. This relevance is primarily used for feature selection as feature weighting can be seen as a generalization of it, but it is also useful to better understand a problem’s domain or to guide an inductor in its learning process. Relief family of algorithms are proven to be very effective in this task. Some other feature weighting methods are reviewed in order to give some context and then the different existing extensions to the original algorithm are explained.

One of Relief’s known issues is the performance degradation of its estimates when redundant features are present. A novel theoretical definition of redundancy level is given in order to guide the work towards an extension of the algorithm that is more robust against redundancy. A new extension is presented that aims for improving the algorithms performance. Some experiments were driven to test this new extension against the existing ones with a set of artificial and real datasets and denoted that in certain cases it improves the weight’s estimation accuracy.

1 Overview

Feature selection is undoubtedly one of the most important problems in machine learning, pattern recognition and information retrieval, among others. A feature selection algorithm is a computational solution that is motivated by a certain definition of relevance. However, the relevance of a feature may have several definitions depending on the objective that is looked after.

The generic purpose pursued is the improvement of the inductive learner, either in terms of learning speed, generalization capacity or simplicity of the
representation. It is then possible to understand better the obtained results, diminish the volume of storage, reduce noise generated by irrelevant or redundant features and eliminate useless knowledge.

On the other hand, feature weighting algorithms try to estimate relevance (in the form of weights to the features) rather than binarily deciding whether a feature is either relevant or not. This is a much harder problem, but also a more flexible framework from an inductive learning perspective. This kind of algorithms are confronted with the down-weighting of irrelevant features, the up-weighting of relevant ones and the problem of relevance assignment when redundancy is an issue.

In this work we review Relief, one of the most popular feature weighting algorithms. After a state-of-the-art in section 2 focused on feature weighting methods in general, in section we describe the algorithm and its more important extensions. We are primarily interested in coping with redundancy, and studying to what extent can the Relief algorithm be modified in order to better its treatment of redundancy, which is one of its known weaknesses. In this vein, section 3 points out a novel and general (though computationally infeasible) definition of redundancy level and try to relate it to the actual Relief performance. Next, we develop a "double" or feedback extension of the algorithm that takes its own estimations into account in order to improve general performance. We also complement this matter with a set of experiments in section 4. The work concludes with some open questions and clear avenues of continuation of the material herein presented.

2 State of the art

2.1 Introduction

In the last few years feature selection has become a more and more common topic of research. This popularity increase is probably due to the growth of the problem domains’ number of features. No more than ten years ago few problems treated domains with more than 50 features. Nowadays most papers deal with domains with hundreds and even tens of thousands of features. New techniques have to be developed to address this kind of problems with many irrelevant and redundant features and comparatively few instances to learn from. One example of these new domains is web page categorization, a domain currently of much interest for internet search engines where thousands of terms can be found in a document. Another example can be appearance-based image classification methods which may use every pixel in the image. Classification problems with thousands of features are very common in medicine and biology; e.g. molecule classification, gene selection or medical diagnostics. In medical problems we typically have less than a hundred patients and for each patient we can have thousands of features evaluated.

Feature selection can help us solving a classification problem with these characteristics for many reasons. Firstly it may make the task of data visualization
and understanding easier by eliminating irrelevant features which can mislead the interpretation of the data. It can also reduce the cost of the measurements as we can avoid measuring irrelevant features; this is especially important in domains where some features are very expensive to obtain, e.g., require a special medical test. In addition, a big benefit of feature selection is defying the curse of dimensionality to help the induction of good classifiers from the data. When many \textit{unuseful}, i.e., irrelevant or redundant, features are present in training data, classifiers may find false regularities in the input features and learn from that instead of learning from the features that really determine the instance class (also valid when predicting the instance target value in the case of regression).

There are two main approaches to feature selection: filter methods and wrapper methods. Both methods can be included in the framework shown on Fig. 1. The main difference between them is the use of a classifier for the estimation of a feature \textit{usefulness}. The two families of methods only differ in

![Feature selection framework](image)

Figure 1: Feature selection framework

the way they evaluate the candidate sets of features. While the former methods use a problem independent criterion, the latter use the performance of the final classifier to evaluate the quality of a feature subset. The basic idea of the filter methods is to select the features according to some prior knowledge of the data. For example, to select the features based on the conditional probability that a given instance is a member of a certain class given the value of its features. Another criterion commonly used by filter methods is the correlation of a feature with the class, i.e. selecting features with high correlation. More detailed criteria is given in section 2.2 where also more criteria are described. In contrast, wrapper methods suggest a set of features that are given to a classifier which uses them to classify some training data and returns the performance of the classification which is the acceptance criterion of the feature set.

Now we have explained two approaches of feature subset evaluation, but is clear to see that if we had to test all possible subsets, using either of the methods, of features we would have a combinatorial explosion. If our initial set of features is $\mathcal{F}$ and $|\mathcal{F}| = n$, the number of evaluations we would have to
do would be equal to the cardinality of the power set of $\mathcal{F}$: $|\mathcal{P}(\mathcal{F})| = 2^n$. For this reason diverse techniques have been developed to reduce the computational complexity of this problem.

A different technique of determining feature usefulness apart from feature selection is a technique called feature weighting (or feature ranking). It consists of assigning a numeric value to each feature so as to indicate the feature’s usefulness. Feature weighting can help solving the problem of feature selection. One possible approach to feature selection using feature weighting could be to first assign weights to features and then choose features according to their weights. This can be done either by having a rule to binarize the weights, e.g. select all the features with weight greater than zero, or by means of a weight guided feature subset evaluation, e.g. evaluating the subsets containing the features with greatest weight values. In fact, feature weighting could be seen as a generalization of feature selection, i.e. feature selection would be a specific kind of feature weighting where the weights assigned to features are binary.

In following sections we will explore various methods of existing feature weighting algorithms than and will discuss their properties to later have some starting point to describe and analyze the algorithm in the focus of this paper: Relief.

### 2.2 Feature weighting

This section will review some of the most used feature weighting algorithms. Although the section is focused on feature weighting, most of the methods described below can also be used for feature selection.

On following subsections $I$ and $\mathcal{F}$ represent the sets of instances and features respectively. $I$, $I_1$ or $I_i$ represent instances from $I$. $X$, $X_i$ or $Y$ are sets of possible feature values from a feature in $\mathcal{F}$. $C$ represents the set of possible class values. And their lower case versions represent single value in its correspondent upper case set, e.g. we will use $c \in C$ and $x \in X$. We also will use a short notation to express probabilities, e.g. will write $p(x)$ to represent the probability for feature $X$ to have value $x$ or $p(c|x)$ to express the conditional probability of the class to have value $c$ knowing that the feature $X$ has value $x$.

#### Conditional Probabilities based methods

The first group of methods we will look at are the ones based on conditional probabilities of class given a feature value. Two simple methods using this idea were introduced in [Creecy et al., 1992]: per-category feature importance and cross-category feature importance (or, in short, PCF and CCF). One important limitation is that they can only deal with binary features, so numerical features must be discretized and symbolic features converted to a group of binary features. The weights assigned to features in the case of PCF depends on the class of the feature as seen in Eq. 2.1

$$w_{PCF}(X, c) = P(c|x), \text{ where } x \text{ would be the positive feature value} \quad (2.1)$$
so we have a weight for each feature and class. CCF relies on the same idea but instead of having one weight for each feature and class it have only a weight per feature. It does so by averaging the weights across classes. In fact, as it shows Eq. 2.2 it uses the summation of squares of conditional probabilities.

\[ w_{CCF}(X) = \sum_{c \in C} P(c|x)^2, \text{ where } x \text{ would be the positive feature value} \] (2.2)

Later on [Mohri and Tanaka, 1994] showed that PCF is too sensitive to class proportions and tends to answer the most frequent class when using it for classifying.

A more sophisticated approach that also makes use of conditional probabilities is the one used by the value difference method (VDM) introduced by [Stanfill and Waltz, 1986]. This time no binarization of features is required, although numeric features still have to be discretized in order to calculate conditional probabilities as shown in Eq. 2.3. In addition this method does not assign weights to each feature but to each value of each feature.

\[ w_{VDM}(X, x) = \sqrt{\sum_{c \in C} \left( \frac{P(x|c)}{p(x)} \right)^2} \] (2.3)

This weighting scheme was originally used to calculate distances between features.

Finally we have Gini-index gain [Breiman et al., 1984] in Eq. 2.4 which can be interpreted as the expected error rate

\[ GG(X) = \sum_{x \in X} P(x) \sum_{c \in C} P(c|x)^2 - \sum_{c \in C} P(c)^2 \] (2.4)

and is proven to be biased towards multiple valued features. In further sections we will see that this particular measure has some relation with the Relief algorithm.

**Information theory based methods**

Not all the feature weighting methods are based on conditional probabilities, though. Now we will describe some methods based on information theory [Shannon, 1948, Shannon and Weaver, 1949].

The first one is just using Shannon’s mutual information (MI) between two features \(X\) and \(Y\) in Eq. 2.5

\[ MI(X, Y) = H(X) - H(X|Y) = \sum_{x \in X, y \in Y} p(x, y) \log_2 \frac{p(x, y)}{p(x)p(y)} \] (2.5)
which is defined using entropies and conditional entropies (see Eq. 2.7),

\begin{align*}
\text{Entropy:} & \quad H(X) = - \sum_{x \in X} P(x) \log_2 P(x) \\
\text{Conditional entropy:} & \quad H(X|Y) = H(X,Y) - H(Y) \\
\text{Joint entropy:} & \quad H(X,Y) = - \sum_{x \in X, y \in Y} P(x,y) \log_2 P(x,y)
\end{align*}

(2.6) (2.7) (2.8)

to weight features. A more informal but maybe more intuitive definition of mutual information is that MI measures the information of $X$ that is also in $Y$. If the features are independent no information is shared so mutual information is zero. In the other end we have that one feature is an exact copy of the other, all the information it contains is also shared by the other so the mutual information is the same as the information conveyed by one of them, namely its entropy. A very popular feature weighting method uses the idea of mutual information. It was proposed by [Hunt et al., 1966] and it is used in [Quinlan, 1986] when splitting nodes in top down induction of decision trees (TDIDT) known as ID3. The term information gain (IG) in Eq. 2.9 is used there. Its intuitive interpretation would be: The more an feature reduces class entropy when knowing its value, the more its weight. This is just another way to say: The more information is shared between an feature and the class, the more its weight. So if we have a set of classes $C$ we can define IG for the class knowing the value of a feature $X$ as shown in Eq. 2.9

\[
IG(C|X) = MI(C, X).
\] 

(2.9)

Later on, similar methods were introduced to reduce the bias of IG towards features with large number of values. The extreme case is using an feature with an ID code. It is clear to see that knowing the ID code we can precisely know the class of any instance in our training set. The problem is that we can say nothing about a new instance which will have another unknown ID code. One of these methods is gain ratio (GR) in Eq. 2.10 used by C4.5 decision tree induction algorithm [Quinlan, 1993] which normalizes IG by the amount of information needed to predict an features value (the entropy of the feature). But there are also various other proposals, among them there are entropy distance [MacKay, 2003] in Eq. 2.11 and the Mántaras distance between the class and the feature in Eq. 2.12 which was proved to be unbiased towards multiple-valued features.

\begin{align*}
GR(C|X) & = \frac{IG(C|X)}{H(X)} \\
D_H(C, X) & = H(C, X) - MI(C, X) \\
D_M(C, X) & = \frac{H(X|C) + H(C|X)}{H(C, X)} = 2 - \frac{H(X) + H(C)}{H(C, X)}
\end{align*}

(2.10) (2.11) (2.12)
Distribution distance based methods

Another way to find dependencies between a feature and the class is to measure differences between their distributions. Perhaps the simplest way to do so is to compute the difference between the joint and the product distributions as shown in Eq. 2.13

\[
\text{Diff}(C, X) = \sum_{c \in C, x \in X} |P(c, x) - P(x)P(c)| \quad (2.13)
\]

and this distance can be directly used as the features weight. Large differences between the joint and the product distributions indicate large dependency of the class on the feature, so the feature should be given a large weight. This can easily be applied to continuous features changing the sum for an integration. It can also easily be rescaled to the [0,1] interval as it has an upper bound of \(1 - \sum_{x \in X} P(x)^2\).

More distance functions can be used here. An interesting one is the Kullback-Leibler divergence which is not a distance in fact as it is not symmetric (i.e., \(D_{KL}(X||Y) \neq D_{KL}(Y||X)\)). The application on feature weighting is to have the weight be equal to the distance between the joint and the product distributions, see Eq. 2.14

\[
D_{KL}(P(X, C)||P(X)P(C)) = \sum_{c \in C, x \in X} P(c, x) \log \frac{P(c, x)}{P(x)P(c)} \quad (2.14)
\]

Note that this is exactly the same as the mutual information between the feature and the class (see Eq. 2.5) so we have \(D_{KL}(P(X, C)||P(X)P(C)) = MI(X, C)\).

Correlation based methods

Even though this approach to feature weighting is treated last, maybe is one of the simplest as it does not care about continuous feature discretization or probability density estimations. It is usual in statistics to construct contingency tables for pairs of discrete variables to analyze their correlation. In our case (see Table 1) we will define a contingency table between the set of classes \(c_i \in C\) and the values of a feature \(x_j \in X\). The inner cells in row \(i\) and column \(j\) of the table contain the number of instances of class \(c_i\) that have feature \(X = x_j\). The row marginal totals will tell the number of instances for the corresponding class and the column marginal totals the number of instances with the corresponding value on feature \(X\). Finally the sum of either marginal totals should be the total number of instances \(m\). Looking at this table we can define chi-squared weight for feature \(X\) as shown on Eq. 2.15

\[
X^2(X) = \sum_{x \in X, c \in C} \frac{(N_{cx} - E_{cx})^2}{E_{cx}} \quad (2.15)
\]

where \(E_{cx}\) is the expected number of instances of class \(c\) with value \(x\) on feature \(X\) calculated as \(N_c N_x/m\). \(X^2\) is distributed approximately as a \(\chi^2\) with \((v -
2.3 Relief

One common characteristic of the previously cited methods is that they treat features individually assuming conditional independence of features upon the class. In the other hand, Relief takes all other features in care when evaluating a specific feature. Another interesting characteristic of Relief is that it is aware of contextual information being able to detect local correlations of feature values and their ability to discriminate from an instance of a different class.

The main idea behind Relief is to assign large weights to features that contribute in separating near instances of different class and joining near instances belonging to the same class. The word "near" in the previous sentence is of crucial importance since we mentioned that one of the main differences between Relief and the other cited methods is the ability to take local context into account. Relief does not reward features that separate (join) instances of different (same) classes in general but features that do so for near instances.

In Fig. 2 we can see the original algorithm presented by Kira and Rendell in [Kira and Rendell, 1992]. We maintained the original notation that slightly differs from the used above as now features (attributes) are labeled A. There we can see that in the aim of detecting whether the feature is useful to discriminate near instances it selects two nearest neighbors of the current instance $R_i$. One from the same class $H$ called the nearest hit and one from the different class $W$.
Input: for each training instance a vector of feature values and the class value
Output: the vector $W$ of estimations of the qualities of features

1. set all weights $W[A] := 0$;
2. for $i := 1$ to $m$ do begin
   3. randomly select an instance $R_i$;
   4. find nearest hit $H$ and nearest miss $M$;
   5. for $A := 1$ to $a$ do
      6. $W[A] := W[A] − \text{diff}(A, R_i, H)/m + \text{diff}(A, R_i, M)/m$
   7. end;

Figure 2: Pseudo code of the original Relief algorithm

$M$ (the original Relief algorithm only dealt with two class problems) called the nearest miss. With these two nearest neighbors it increases the weight of the feature if it has the same value for both $R_i$ and $H$ and decreases it otherwise. The opposite occurs with the nearest miss, Relief increases the weight of a feature if it has opposite values for $R_i$ and $M$ and decreases it otherwise.

One of the central parts of Relief is the difference function $\text{diff}$ which is also used to compute the distance between instances as shown in Eq. 2.16.

$$\delta(I_1, I_2) = \sum_i \text{diff}(A_i, I_1, I_2)$$  \hspace{1cm} (2.16)

The original definition of $\text{diff}$ was an heterogeneous distance metric composed of the overlap metric in Eq. 2.17 for nominal features and the normalized Euclidean distance in Eq. 2.18 for linear features, which [Wilson and Martinez, 1997] called HEOM.

$$\text{diff}(A, I_1, I_2) = \begin{cases} 0 & \text{if } \text{value}(A, I_1) = \text{value}(A, I_2) \\ 1 & \text{otherwise} \end{cases}$$  \hspace{1cm} (2.17)

$$\text{diff}(A, I_1, I_2) = \frac{|\text{value}(A, I_1) - \text{value}(A, I_2)|}{\max(A) - \min(A)}$$  \hspace{1cm} (2.18)

The difference normalization with $m$ guarantees that the weight range is $[-1,1]$. In fact the algorithm tries to approximate a probability difference in Eq. 2.20.

$$W[A] \approx P(\text{different value of } A|\text{nearest instance from different class}) − P(\text{different value of } A|\text{nearest instance from same class})$$  \hspace{1cm} (2.19)

$$W[A] \approx P(\text{different value of } A|\text{nearest instance from different class}) − P(\text{different value of } A|\text{nearest instance from same class})$$  \hspace{1cm} (2.20)

We can see that for a set of instances $I$ having a set of features $F$ this algorithm has cost $O(m \times |I| \times |F|)$ as it has to loop over $m$ instances. For each instance in
the main loop it has to compute its distance from all other instances so we have \(O(m \times |I|)\) times the complexity of calculating \(D_{\text{Relief}}\) and we can easily see from Eq. 2.10 that its complexity is \(O(|\mathcal{F}|)\), so we have our complexity: \(O(m \times |I| \times |\mathcal{F}|)\). As \(m\) is a user defined parameter we can in some measure control the cost of Relief algorithm having a tradeoff between accuracy of estimation (for large \(m\)) and low complexity of the algorithm (for small \(m\)). However \(m\) can never be greater than \(|I|\).

2.4 Extensions of Relief

The first modification proposed to the algorithm is to make it deterministic by changing the outer loop through \(m\) randomly chosen instances for a loop over all instances. This obviously increases the algorithm’s computation cost which becomes \(O(|I|^2 \times |\mathcal{F}|)\) but makes experiments with small datasets more reproducible. Kononenko uses this simplified version of the algorithm in its paper [Kononenko, 1994] to test his new extensions to the original Relief. This version is also used by other authors [Kohavi and John, 1997] and it’s given the name Releaved with the final \(d\) for "deterministic".

We can find some extensions to the original Relief algorithm proposed in [Kononenko, 1994] in order to overcome some of its limitations: It couldn’t deal with incomplete datasets, it was very sensible to noisy data and it could only deal with multi-class problems by splitting the problem into series of 2-class problems.

To able Relief to deal with incomplete datasets, i.e. that contained missing values, a modification of the diff function is needed. The new function must be capable of calculating the difference between a value of a feature and a missing value and between two missing values in addition to the calculation of difference between two known values. Kononenko proposed various modifications of this function in its paper and found one that performed better than the others it was the one in a version of Relief he called RELIEF-D (not to be confused with Releaved mentioned above). The difference function used by RELIEF-D can be seen in Eq. 2.21.

\[
\text{diff}(A, I_1, I_2) = \begin{cases} 
1 - P(\text{value}(A, I_2)|\text{class}(I_1)) & \text{if } I_1 \text{ is missing} \\
1 - \sum_{a \in A} [P(a|\text{class}(I_1)) \times P(a|\text{class}(I_2))] & \text{if both missing}
\end{cases}
\]

(2.21)

Now we will focus on giving Relief greater robustness against noise. This robustness can be achieved by increasing the number of nearest hits and misses to look at. This mitigates the effect of choosing a neighbor that would not have been the nearest without the effect of noise. The new algorithm has a new user defined parameter \(k\) that controls the number of nearest neighbors to use. In choosing \(k\) there is a tradeoff between locality and noise robustness. [Kononenko, 1994] states that 10 is a good choice for most purposes.

The last limitation was that the algorithm was only designed for 2-class problems. The straightforward extension to multi-class problems would be to
take as the near miss the nearest neighbor belonging to a different class. This variant of Relief is the so-called Relief-E by Kononenko. But later on he proposes another variant which gave better results: This was to take the nearest neighbor (or the \( k \) nearest) from each class and average their contribution so as to keep the contributions of hits and misses symmetric and between the interval \([0,1]\). That gives the Relief-F (ReliefF from now on) algorithm seen in Fig. 3.

Input: for each training instance a vector of feature values and the class value
Output: the vector \( W \) of estimations of the qualities of features

1. set all weights \( W[A] := 0; \)
2. \textbf{for} \( i := 1 \) \textbf{to} \( m \) \textbf{do begin}
3. randomly select an instance \( R_i; \)
4. find \( k \) nearest hits \( H_j; \)
5. \textbf{for} each class \( C \neq \text{class} (R_i) \) \textbf{do}
6. find \( k \) nearest misses \( M_j(C); \)
7. \textbf{for} \( A := 1 \) \textbf{to} \( a \) \textbf{do}
8. \( W[A] := W[A] - \sum_{j=1}^{k} \text{diff}(A, R_i, H_j)/(m \cdot k) + \)
9. \( \sum_{C \neq \text{class}(R_i)} \left[ \frac{P(C)}{1 - P(\text{class}(R_i))} \sum_{j=1}^{k} \text{diff}(A, R_i, M_j(C)) \right] / (m \cdot k); \)
10. \textbf{end};

Figure 3: Pseudo code of the ReliefF algorithm

The above mentioned relation to impurity functions, in specific with Gini-index gain in Eq. 2.3 can be seen in Robnik-Sikonja and Kononenko, 2003 when developing the probability difference in Eq. 2.20 in the case that the algorithm uses a large number of nearest neighbors (i.e., when the selected instance could be anyone from the set of instances). This version of the algorithm is called myopic ReliefF as it loses its context of locality property. Rewriting Eq. 2.20 by removing the neighboring condition and by applying Bayes’ rule, we obtain Eq. 2.22

\[
W'[A] = \frac{P_{\text{samecl|equal}}P_{\text{equal}}}{P_{\text{samecl}}} - \frac{(1 - P_{\text{samecl|equal}})P_{\text{equal}}}{1 - P_{\text{samecl}}} \quad (2.22)
\]
For sampling with replacement we obtain we have:

\[ P_{\text{eqval}} = \sum_{c \in C} P(c)^2 \]

\[ P_{\text{samecl}\mid \text{eqval}} = \sum_{x \in X} \left( \frac{P(x)^2}{\sum_{x \in X} P(x)^2} \times \sum_{c \in C} P(c|x)^2 \right) \]

Now we can rewrite Eq. 2.22 to obtain the myopic Relief weight estimation:

\[ W'[A] = \frac{P_{\text{eqval}} \times GG'(X)}{P_{\text{samecl}} 1 - P_{\text{samecl}}} \quad (2.23) \]

Where \( GG'(A) \) is a modified Gini-index gain of attribute \( A \) as seen in Eq. 2.24

\[ GG'(X) = \sum_{x \in X} \left( \frac{P(x)^2}{\sum_{x \in X} P(x)^2} \times \sum_{c \in C} P(c|x)^2 \right) - \sum_{c \in C} P(c)^2 \quad (2.24) \]

As we can see the difference in this modified version from its original Gini-index gain described above in Eq. 2.4 is that Gini-index gain used a factor:

\[ \frac{P(x)}{\sum_{x \in X} P(x)} = P(x) \]

while myopic ReliefF uses:

\[ \frac{P(x)^2}{\sum_{x \in X} P(x)^2} \]

So we can see how this myopic ReliefF in Eq. 2.23 holds some kind of normalization for multi-valued attributes when using the factor \( P_{\text{eqval}} \). This solves the bias of impurity functions towards attributes with multiple values. Another improvement compared with Gini-index is that Gini-index gain values decrease when the number of classes increase. The denominator of Eq. 2.23 avoids this strange behavior.

## 3 New apporations

### 3.1 Redundancy analysis

To begin with the redundancy analysis of Relief, we first of all have to define exactly the meaning of redundancy. In general the definitions of redundancy we find in the literature are based on feature correlation, i.e. two features are redundant if their values are correlated. One interesting particular case is when one feature is an exact copy of another so their values are completely correlated, one feature is obviously redundant. But in reality a feature may not be completely correlated with another feature but may be (partially) correlated with a set of features. In such case it’s not straightforward to determine redundancy. We can take as an example the features shown in Table 2. The feature
Table 2: Two relevant and one redundant features: $C = f_1 \land f_2$ and $f_r = f_1 \land f_2$

$f_r$ is intuitively redundant with the set $\{f_1, f_2\}$ but is not correlated with any of them, so it would not be redundant according to the correlation based definition of redundancy. So we have to find a better definition for feature redundancy that enables us to identify not only pairs of redundant features but features redundant with any set of other features. Before giving the formal definition of redundancy let’s introduce some previous definitions:

**Definition 3.1** Let $U = \{\alpha, \beta, \ldots\}$ be a set of discrete variables in a problem domain. Each variable is associated with a set of possible values. A configuration or a tuple $u'$ of $U'$ is an assignment of values to every variable in $U$.

**Definition 3.2** A probabilistic domain model (PDM) $P$ over $U$ determines the probability $P(u')$ of every tuple $u'$ of $U'$ for each $U' \subseteq U$.

**Definition 3.3** For three disjoint subsets $X$, $Y$ and $Z \subseteq U$, $X$ and $Y$ are said to be conditionally independent given $Z$ under $P$, noted $I(X, Z, Y)$ or simply $I(X, Z, Y)$ from now on, if (see [Pearl, 1988, pp 83–97])

$$I(X, Z, Y) \equiv P(x|y, z) = P(x|z) \text{ whenever } P(y, z) > 0 \quad (3.1)$$

Using this notation we can express unconditional independence as $I(X, \emptyset, Y)$, i.e.,

$$I(X, \emptyset, Y) \equiv P(x|y) = P(x) \text{ whenever } P(y) > 0$$

Note that $I(X, Z, Y)$ implies the conditional independence of all pairs of variables $\alpha \in X$ and $\beta \in Y$, but the converse is not necessarily true.

**Definition 3.4** A Markov Blanket $BL_I(\alpha)$ of an element $\alpha \in U$ is any subset $S \subseteq U$ for which (see [Pearl, 1988])

$$I(\alpha, S, U - S - \alpha) \text{ and } \alpha \notin S. \quad (3.2)$$

An intuitive interpretation of Def. 3.3 would be: Once $Z$ is given, the probability of $X$ will not be affected by the discovery of $Y$. Or $Y$ is irrelevant to $X$ once we know $Z$. Note that the Markov blanket condition in Def. 3.4 is stronger than conditional independence. It is saying that not only that knowing $\alpha$ is irrelevant to the class, but also to the rest of the features, so $S$ has all the information that $\alpha$ has about $C$ and all the information $\alpha$ has about $U - S - \alpha$. This takes us to our definition of redundancy:
Definition 3.5 Given a set of features $F$ and a class feature $C$, a redundant feature $\alpha \in F$ is a feature for which exists a Markov blanket $S = BL_I(\alpha)$ within $\{F, C\}$ such that $S \subset F$.

An interesting property of Markov blankets is that if we removed a feature $\alpha$ such that existed $BL_I(\alpha) \subset U$ and now we are eliminating another feature $\beta$ such that exists $BL_I(\beta) \subset U - \alpha$ then we can prove that also exists $BL_I(\alpha) \subset U - \beta$, we can see the proof in [Koller and Sahami, 1996]. That is, a redundant feature remains redundant when other redundant features are removed. So if we proceed to remove features using this criterion, we will never have to reconsider our decisions.

Unfortunately, there we rarely find a fully redundant feature, but rather one that its information is nearly subsumed by other features. So we would like to know not only whether a feature is redundant or not but its redundancy grade. We would like a function $R'$ which given an feature $\alpha \in U$ and a set of features $U \in U$ gives us a degree of redundancy of this feature to the set. Ideally we would like a function $R'$:

$$R'(\alpha, U) = 1 - \max_{S \subset U - \alpha} \left( \frac{\sum_{u \in U} |P(\alpha_u|s_u) - P(\alpha_u|s_u^{-1}, s_u)|}{|U|} \right)$$

Note that the calculation of this redundancy level is exponential in the number of features in our set, as it compares the conditional probabilities of all possible subsets of $U$, so the max function will have to compare $|P(U)| = 2^{|U|}$ terms. And for each subset we also have an exponential cost in the number of values of the features because the sum is over each configuration $u$ of $U$.

It is clear to see that, although Eq. 3.6 gives an intuitively consistent definition of redundancy level, its computational cost might be too large for $R'$ to be directly applied in a feature weighting (or feature selection) algorithm. We should use an estimation of $R'$ that maximized the tradeoff between accuracy and complexity. But in fact the aim of the definition of $R'$ was not to have an
efficient algorithm to calculate the redundancy level of a feature. The definition
had three basic (related) objectives: first of all to provide a suitable formal def-
nition of redundancy in order to study the effect of feature redundancy in the
different existing algorithms, for instance ReliefF. And second to serve as some
starting point for new extensions to methods which performance decreases in
the presence of redundant features, again Relief is an example. And finally, to
direct the developing of new algorithms that effectively and efficiently estimate
redundancy.

3.2 Double Relief

When more and more irrelevant features are added to a dataset the distance
calculation of Relief degrades its performance as instances may be considered
neighbors when in fact they are far from each other if we compute its distance
only with the relevant features. In such cases the algorithm may lose its context
of locality and in the end it may fail to recognize relevant features.

The \( \text{diff}(A_i, I_1, I_2) \) function calculates the difference between the values of
the feature \( A_i \) for two instances \( I_1 \) and \( I_2 \). Sum of differences over all features
is used to determine the distance between two instances in the nearest hit and
miss calculation (see equation (2.16)).

As seen in the k-nearest neighbors classification algorithm (kNN) many
weighting schemes which assign different weights to the features in the cal-
culation of the distance between instances (see equation (3.3)).

\[
\delta'(I_1, I_2) = \sum_{i=1}^{a} w(A_i) \text{diff}(A_i, I_1, I_2) \tag{3.3}
\]

In the same way that in [Wettschereck et al., 1997] Relief’s estimates of fea-
tures’ quality have been used successfully as weights for the distance calculation
of kNN we could use their estimation in the previous iteration to compute the
distance between instances while searching the nearest hits and misses. We
will refer to this version of ReliefF as double ReliefF or in short dReliefF. The
problem using the weights estimates could be that in early iterations these es-
timations could be too biased to the first instances and could be far from the
optimal weights. So, for small \( t \), \( W[A_i] \) is very different from \( W[A_i]^t \).

What we want is to begin the distance calculation without using the weight
estimates and then, as Relief’s weight estimates become more accurate (because
more instances have been taken into account), increase the importance of these
weights in the distance calculation. Let’s have a distance calculation like the one
in equation (3.4)

\[
\delta(I_1, I_2) = \sum_{i=1}^{a} f(W(A_i), t) \text{diff}(A_i, I_1, I_2) \tag{3.4}
\]

We would like a function \( f : \mathbb{R} \times (0, \infty) \rightarrow \mathbb{R} \) such that:

- \( f(w, t) \) is increasing with respect to \( t \)
• is continuous
• \( f(w, 0) = 1 \)
• \( f(w, \infty) = w \)

One such function could be the one in equation 3.5. And we will refer to the version of ReliefF using this distance equation as progressively weighted double relief or in short pdReliefF.

\[
f(w, t) = -\frac{w + 1}{t^T} + w
\]  

(3.5)

Where \( T \) is a control parameter that determines the steepness of the curve described by \( f \) (see figure 4). Another desirable property for our function would be that it always gives the same results regardless of the number of iterations. In other words, if \( m \) is the total number of iterations, we would like \( f(w, m) \) to be the same value whatever the value of \( m \). To achieve that we must vary the value of \( T \) according to the total number of iterations so as to decrement the steepness of the function as the number of total iterations increases. The value of \( T \) for \( f(w, m) \) to be the same is \( T = \frac{2}{\log(m)} \). In figure 5 we can see how \( f \) varies the influence of different weights (even a non realistic one that is greater than 1) as iterations go on. We can see that with this value for \( T \) the function converges in the first few iterations and then it stabilizes its value near \( w \). For problems with many iterations a softer function may be tried if values converge prematurely.

Figure 4: Plot of function \( f \) for 10 instances with \( w = 0.5 \)
4 Empirical results

To begin with the empirical results we have to define a measure of success for the weights estimations. First of all we need to have a success criterion. For problems where we know which of the features are important (e.g., artificial datasets) some we can use this knowledge to evaluate estimates. In [Kononenko, 1994] separability and usability, two more indicators may be useful in case of negative separability - minimality and completeness - which can help in determining the quality of the given solution. See more precise definitions below.

**separability** Shows the ability of the weight estimates to distinguish between important and unimportant features. Positive separability ($s > 0$) means that important features are correctly separated from unimportant ones.

\[ s = W_{I_{worst}} - W_{R_{best}} \in [-2, 2] \]

**usability** Shows the ability of the weight estimates to distinguish one of the important feature from the unimportant ones. Positive usability ($u > 0$) means that almost one of the important features is correctly separated from unimportant ones.

\[ u = W_{I_{best}} - W_{R_{best}} \in [-2, 2] \]

**minimality** Shows the ratio of important features in the minimum set of features that contains all the important features if we select features in decreasing weight order. Note that $s > 0 \Rightarrow m = 1$.

\[ m = |Z|/|\mathcal{M}| \in (0, 1] \text{ where } \mathcal{M} = \{ F | W_F \geq W_{I_{worst}} \} \]
completeness Shows the ratio of important features that we would take if selecting features in decreasing weight order we stopped before selecting the first unimportant feature. Note that again $s > 0 \Rightarrow m = 1$.

$$c = \frac{|C|}{|I|} \in (0, 1] \text{ where } C = \{F | W_F > W_{R_{best}}\}.$$  

The first set of artificial problems to use is the so-called Modulo-$p$-$I$. In these datasets we will find $I$ important features and $R$ random ones. All of them integers in the range $[0,p)$. The class value $C$ is also an integer in the same range and can be calculated for an instance $X$ having values $X_1, X_2, \ldots, X_I$ in its important features as seen on Eq. (4.1). We will test our criteria for various parameters of ReliefF on two different problems (Modulo-2-2 and Modulo-4-3) incrementally adding random features.

$$C(X) = \left(\sum_{i=1}^{I} X_i\right) \mod p \quad (4.1)$$

In Fig. 6 and 7 we can see the different behaviors of the three algorithms when more and more random features are added. While ReliefF seems to gradually degrade its performance, dReliefF is more erratic and pdReliefF obtains the best results. This supports our theory that although it seems a good idea to use ReliefF’s own estimates as weights for its distance function, a bad start can make dReliefF’s estimates even poor than ReliefF’s.

Another good test is CorrAl dataset introduced in [Kohavi and John, 1997]. This dataset is composed of 6 features ($A_0, A_1, B_0, B_1, C, I$). $C$ is 75%
correlated with the class and four other features that can fully determine the class of the instance when used together. The class can be expressed as: ($A_0 \land A_1) \lor (B_0 \land B_1)$. And the last one, $I$, is completely random. Results are shown in table 3. So for CorrAl dataset the three algorithms correctly identify the

| Feature | ReliefF | dReliefF | pdReliefF |
|---------|---------|----------|-----------|
| $B_0$   | 0.259   | 0.272    | 0.272     |
| $B_1$   | 0.197   | 0.273    | 0.273     |
| $A_0$   | 0.194   | 0.277    | 0.278     |
| $A_1$   | 0.128   | 0.277    | 0.278     |
| $C$     | 0.281   | 0.042    | 0.044     |
| $I$     | -0.141  | -0.222   | -0.222    |

|        | separability | usability   |
|--------|--------------|-------------|
|        | -0.153       | 0.422       |
|        | 0.230        | 0.047       |
|        | 0.228        | 0.050       |

Table 3: Weights and separability for CorrAl dataset. (With 5 nearest neighbors).

irrelevant feature and rank it last, but the normal version of ReliefF give a larger weight to the correlated feature than it should be given. The double versions of the algorithm in the other hand correctly identify the four features that completely determine the class and give them larger weights, followed by the correlated one and leaving the random one last. We can see that the behavior of the two double versions is very similar, although the progressive weighted
estimation is a little more usable, it’s a little less separable.

The next dataset (led24) is one of the LED display domain datasets from [S. Hettich and Merz, 1998]. In fact it is an extension of the led7 dataset. The led7 dataset consists of 7 boolean valued features \((I_1, \ldots, I_7)\) each of them representing one of the light-emitting diodes contained on a LED display. They indicate whether the corresponding segment is on or off (see Fig. 8). And the class feature has range \([0,9]\) and coincides with the digit represented by the display. This dataset has another added difficulty as it has a 10% of noise in its features, i.e., each instance’s feature has a 10% chance of having its value negated. This is a quite difficult problem for classifiers and the version with 17 unimportant features is especially difficult, e.g. a nearest neighbor classification algorithm falls from a 71% of classification success with the 7 feature version to a poor 41% with the other one. So it would be desirable for ReliefF to separate the important features from the rest. Table 4 shows separability and usability

![Figure 8: A LED display indicating the meaning of the features](image)

| Algorithm | \(s\)  | \(u\)  |
|-----------|-------|-------|
| ReliefF   | 0.131 | 0.340 |
| dReliefF  | 0.084 | 0.234 |
| pdReliefF | 0.104 | 0.278 |

Table 4: Separability and usability for led24 dataset.

for this dataset. There it can be seen that the behavior for the three algorithms is extremely similar for this domain. All of them are able to separate the seven important features from the rest and even the values for \(s\) and \(u\) are almost the same for the three algorithms.

Finally, the last artificial datasets to be tested are Monks datasets. They are interesting because even though they do not consist of lots of features, they are well known datasets, have interesting feature interactions and can serve us to compare the algorithms order of each feature with its intended ordering. There are three Monks datasets but we will only use Monk-1 and Monk-3 because Monk-2 does not contain unimportant features. They consist of six numerical features \(A_1, \ldots, A_6\) with ranges varying from \([1,2]\) to \([1,4]\) and a boolean class
value. For Monk-1 the class \( C_{M1} \) can be calculated as 
\[ C_{M1} = (A_1 = A_2) \lor (A_5 = 1) \]
and the class \( C_{M3} \) for Monk-3 as 
\[ C_{M3} = (A_5 = 3 \land A_4 = 1) \lor (A_5 \neq 4 \land A_2 \neq 3) \].
So for the first problem, \( A_3, A_4, \) and \( A_6 \) are unimportant and among the other three, \( A_1 \) and \( A_2 \) would help us better determine the class value than \( A_5 \) as only one of the four possible values of \( A_5 \) is important. For Monk-3 the important features will only be \( A_5, A_4, \) and \( A_2 \) and the rest do not influence the instance’s class. Among these three features, \( A_5 \) and \( A_2 \) should be preferred over \( A_4 \) as using only the second term of the disjunct we can achieve a 97% performance. It is important to say that Monk-3 has a 5% of additional noise (misclassifications).

Table 5 shows the results for the three variants of ReliefF when applied to

| Algorithm  | s u Feature ordering |
|------------|----------------------|
| ReliefF    | 0.26 0.38 A_1,A_2,A_5,A_3,A_6,A_4 |
| dReliefF   | 0.42 0.44 A_5,A_1,A_2,A_3,A_6,A_4 |
| pdReliefF  | 0.41 0.43 A_1,A_5,A_2,A_3,A_6,A_4 |

Table 5: Separability, usability and feature ordering for Monk-1 dataset.

| Algorithm  | s u Feature ordering |
|------------|----------------------|
| ReliefF    | 0.05 0.43 A_5,A_2,A_4,A_3,A_1,A_6 |
| dReliefF   | 0.08 0.29 A_2,A_5,A_4,A_3,A_1,A_6 |
| pdReliefF  | 0.05 0.31 A_2,A_5,A_4,A_3,A_1,A_6 |

Table 6: Separability, usability and feature ordering for Monk-3 dataset.

The second group of experiments is with some well known datasets from UCI [S. Hettich and Merz, 1998]. These are datasets of real data, so we don’t know which of the features may be important and which may be not. For this reason we will not be able to compute the above criteria for these datasets. So to evaluate the quality of the algorithms’ estimates we will use the performance obtained with a classifier. We will make various tests with the classifier. We will first of all try a classification with the feature with the greatest weight, then will use the two most weighted variables, end so on until all variables are used.
When all tests are completed we will compare the performance of the classifier when using all features with the performance when using the best subset found using Relief’s estimates. We will use the 1NN classifier because of its simplicity and sensibility to a bad choice of features.

The first chosen dataset is the E. coli promoter gene sequences. This dataset contains a set of 57 nominal variables representing a DNA sequence of nucleotides. A promoter is a DNA sequence that enables a gene to be transcribed. The promoter is recognized by RNA polymerase, which then initiates transcription. For the RNA polymerase to make contact, the DNA sequence must have a valid conformation so that the two pieces of the contact region spatially align. But shape of the DNA molecule is a very complex function of the nucleotide sequence due to the so complex interactions between them, so strong interactions among features are expected. In Fig. 9 we can see the results of applying feature selection in the way described above for the 1-NN classifier. As can be seen

Figure 9: Classification success % with for the promoter gene problem

the results for the classification task are in general not very good, but we can see that for all the three versions of the algorithm the maximum performance is achieved when the number of used features is 2, much less than the initial 57 features. The three versions of the algorithm agree in the first two features to be add (15 and 16), although the ordering in the case of normal Relief is inverted it selects 16 first and then 15.

Another problem that can serve us to determine whether the weighted distance calculation makes sense is the lung cancer dataset also from UCI. It consists of data from 32 patients suffering three different types of pathological lung cancers. The objective is to distinguish among the three types of cancer given
a set of 56 nominal features with ranges \([0,3]\). Authors of the dataset gave no information on the meaning of individual features. But probably data may be from different types of tests performed on patients and as there are many features one can venture the hypothesis that many of them may be standard tests that cannot help in determining the patient’s type of disease. So these unimportant features may affect the way that ReliefF chooses the nearest neighbors. Moreover, it is especially important to reduce the number of features in this problem because the number of instances is very low compared to it so classifiers may be fooled by unimportant features. We can see in Fig. 10 that

![Figure 10: Classification success % for the lung cancer problem](image)

| Algorithm  | Max. 1-NN Performance | # of features |
|------------|-----------------------|--------------|
| ReliefF    | 93.75                 | 28           |
| dReliefF   | 96.88                 | 37           |
| pdReliefF  | 96.88                 | 33           |

Table 7: Best results obtained with 1-NN classifier for the lung cancer problem.

...in this case performance of the 1-NN classifier is significantly improved when we apply feature selection for this problem. While a classification using all of the features gives us a correct classification percent of 43.75, the best results obtained with a subset of the features is above 90% with all of the versions of ReliefF. Although the same performance is achieved with the best subset given by dReliefF and the one given by pdReliefF, the results of the latter are better as the same performance is achieved with 4 less features.
5 Conclusions and future work

In our experiments we have seen how the double versions of the algorithm helped in the correct feature weighting of some problems while in other cases performance is not improved and even it is diminished. An interesting property of these new versions of the algorithm is that they seem to help in problems where many irrelevant features exist, which was the initial objective. The performance of the algorithm improved in the modulo-p-I problems as more and more random features were added. We saw in the experiments that although ReliefF’s performance with few attributes was better, as the number of random features increased it began to decrease and for a relatively small number of random features dReliefF and pdReliefF overperformed the original algorithm. Furthermore the performance of the latter methods did not vary with the addition of random features. In contrast, the results obtained with the LED dataset were not that encouraging. Although the dataset had more than twice random features than relevant ones the results for the three algorithms were very similar. This might be because the separability for this problem was so low (though positive) due to the difficulty of the problem (even without random features) for the presence of noise. The try with datasets having fewer irrelevant features, i.e. the Monks problems, gave very similar results for all the versions. This has a logical explanation: the behavior of the double version if all the attributes are relevant is not very different from the original one.

The experiments with real data from the UCI Machine Learning Repository [Hunt et al., 1966] that consisted in running a 1-NN classifier using successive subsets of features proposed by the three versions of ReliefF showed interesting results. The success evaluation criteria was the percentage of instances classified correctly using 5-fold crossvalidation. Two datasets were chosen for this experiments because of their large number of features and the intuition that they might contain large number of irrelevant features. In both of them the double versions of the algorithm chose a subset of features that helped the 1-NN best in classifying the instances. In the case of the DNA promotors dataset the performance increase was not significant but this may be due to the fact that 1-NN do not seem to be capable of solving this problem as it gave poor results in all cases. On the other hand, for the lung cancer dataset, we obtained significantly better classifying performance with the subset from the double versions and, in addition, the subset found by the pdReliefF had less variables than the one found by dReliefF.

We experienced almost no difference between the two double versions. This may be because of the progressive weighting function used. The function attenuates the weight estimates influence at first iterations but rapidly increases their influence and after the first few iterations the algorithm behaves exactly as dReliefF. So as a future work some other softer functions may be tested.

Another clear line of future work is the formal study of the influence that having redundant features has to ReliefF, dReliefF and pdReliefF. Robnik-Šikonja and Kononenko started this study in [Robnik-Šikonja and Kononenko, 2003] where they proved that the addition of successive copies of one feature divided
the initial weight ReliefF assigned to the feature among all the copies. And they received the same weight. But still some crucial questions have to be answered: Do equal weights for two features mean that features are redundant to each other? Does an equal sequence of weight actualizations for two features mean that they are redundant to each other? How can Relief be extended to diminish or eliminate the negative effect of redundant features? Does ReliefF compute some kind of approximation to $R'$?

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