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# A selective sampling approach to active feature selection

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#### Abstract

Feature selection, as a preprocessing step to machine learning, has been very effective in reducing dimensionality, removing irrelevant data, increasing learning accuracy, and improving result comprehensibility. Traditional feature selection methods resort to random sampling in dealing with data sets with a huge number of instances. In this paper, we introduce the concept of active feature selection, and investigate a selective sampling approach to active feature selection in a filter model setting. We present a formalism of selective sampling based on data variance, and apply it to a widely used feature selection algorithm Relief. Further, we show how it realizes active feature selection and reduces the required number of training instances to achieve time savings without performance deterioration. We design objective evaluation measures of performance, conduct extensive experiments using both synthetic and benchmark data sets, and observe consistent and significant improvement. We suggest some further work based on our study and experiments.

Keywords: Dimensionality reduction; Feature selection and ranking; Sampling; Learning

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# 1. Introduction

Inductive learning is one of the major approaches to automatic extraction of useful patterns (or knowledge) from data. Data becomes increasingly larger in both number of features and number of instances in many applications such as genome projects, text mining, customer relationship management, and market basket analysis [2,35,43,44,55,57]. This trend poses a severe challenge to inductive learning systems in terms of efficiency and effectiveness. Feature selection has proven to be an effective means when dealing with large dimensionality with many irrelevant features [17,42,57]. In particular, feature selection removes irrelevant features, increases efficiency of learning tasks, improves learning performance (e.g., predictive accuracy), and enhances comprehensibility of learned results [34,37]. Although there exist numerous feature selection algorithms [6,12,23], new challenging research issues arise for feature selection: from handling a huge number of instances, large dimensionality (e.g., thousands of features), to dealing with data without class labels. This work is concerned with the number of instances in the context of feature selection.

When the number of instances is large, how can one use a portion of data to achieve the original objective without performance deterioration? Sampling is a common approach to this problem and many sampling methods are available [9,22]. Random sampling is a method of selecting a sample of *n* out of *N* ( $n \le N$ ) units such that every one of the  $\binom{N}{n}$  distinct samples has an equal chance of being drawn. It has proven to be an effective approach to dealing with large data sets for many machine learning tasks including classification, clustering, and association rule mining [7,30,52]. However, random sampling is blind because it does not exploit any data characteristic. In this work, we explore if sampling can use data characteristics and achieve better performance than random sampling in the following sense: either maintaining the performance of feature selection with much fewer instances, or improving the performance of feature selection with the same amount of instances.

This work is about feature selection on labeled data, i.e., class information is available. For feature selection on unlabeled data, various work can be found in [13,15,17,18,27,53]. In Section 2, we briefly review the development of feature selection, its models, and active learning. In Section 3, we describe active feature selection and a formalism of selective sampling that exploits data variance. In Section 4, we demonstrate active feature selection using Relief and discuss implementation details. In Section 5, we design objective measures for performance evaluation including time savings. Section 6 is an empirical study in which we evaluate the performance improvement obtained with active feature selection and discuss the implications of the findings. Section 7 presents a conclusion and some work to be completed in the near future.

# 2. Related work

Feature selection refers to the study of algorithms selecting an optimal subset of the input feature set. Optimality is normally dependent on the evaluation criteria or the application's needs [37]. Major aspects of feature selection [34] include feature subset generation,

search strategies, goodness evaluation, etc. Feature subset generation studies how a subset is generated following search directions. Search strategies cover exhaustive and complete search, random search, and heuristic search. A search can start from an empty feature set and add new features, or begin with a full set and remove irrelevant features. The goodness of a feature subset can be evaluated using various measures: consistency, distance, information, dependency, accuracy, etc. Feature selection algorithms fall into two broad categories, the filter model or the wrapper model [11,31]. The filter model relies on the general characteristics of the training data to select some features independently of any learning algorithm, therefore it does not inherit any bias of a learning algorithm. The wrapper model requires one predetermined learning algorithm and uses the performance of the learning algorithm to evaluate and determine which features are selected. The wrapper model needs to learn a new hypothesis (or a classifier) [40] for each new feature subset. It tends to find features better suited to the predetermined learning algorithm resulting in good learning performance, but it also tends to be more computationally expensive than the filter model [34]. When the number of instances becomes large, the filter model is usually chosen due to its computational efficiency. In the context of this work, therefore, we focus on the *filter model* for feature selection.

The concept of active feature selection is inspired by the successful use of selected instances (or data points) in active learning [36,49]. Active learning [49,50] is different from traditional supervised learning: an active learner has the freedom to select which instances are added to the training set. An active learner may begin with a very small number of labeled instances, carefully select a few additional instances for which it requests labels, learn from the result of that request, and then using its newly-gained knowledge, carefully choose another few instances to request next. Several methods have been developed for active learning such as uncertainty sampling, adaptive sampling, and query-by-committee [10, 19,36]. The advantage of active learning is that the data requirements for some problems decrease drastically when the instances to be labeled are properly selected. In [50], they reported that when training the support vector machine (SVM) [8,26] on a small subset of the available data chosen by their heuristic, its performance is frequently better than that of an SVM trained on all available data. Thus, an active learner provides better generalization and requires less data than a passive learner trained on the entire data set. Similar results were observed in [36] with their probabilistic classifiers.

Before we delve into the details of active feature selection, let us briefly describe the difference and commonality between active learning and active feature selection. The essence of active learning lies in its control over the choice of instances used in the *iterative* learning process [49,54]. *Active feature selection* shares this essential characteristic with active learning in that it can influence the instances used for feature selection by exploiting some characteristics of the data. The selection process to form a representative sample data set is not iterative. As discussed earlier, we work with a filter model of feature selection and thus we do not employ a learning algorithm to actively choose instances. Therefore, the problem of active feature selection boils down to how we can employ *selective sampling* to choose representative instances for feature selection.

#### 3. Active feature selection via selective sampling

Traditional feature selection methods perform dimensionality reduction using whatever training data is given to them. When the training data set is very large, random sampling is commonly used to deal with memory and performance issues. Active feature selection avoids pure random sampling and is realized by selective sampling. The idea of selective sampling stems from the fact that instances are not uniformly distributed and some instances are more representative than others [3]. If one can identify and select representative instances, fewer instances are needed to achieve similar performance. Therefore, the objective of selective sampling for feature selection is to select only those instances with a high probability to be informative in determining feature relevance. By adopting the filter model for feature selection, we have ruled out the possibility to use a learning algorithm to determine which instances are most relevant [38,49]. In order to select representative instances for feature selection, we need to explore data characteristics: we first try to partition data according to data dissimilarity and then select representative instances from the resulting partitions.

There are many data partitioning techniques [21] in the literature on multi-dimensional indexing. We choose *kd*-tree [20] in this work because of its simplicity and popularity. A *kd*-tree is an index structure often used for fast nearest neighbor search [41]. It is a generalization of the simple binary tree which uses *k* dimensions (features) instead of a single dimension (feature) to split data points (instances) in a multi-dimensional space. In a *kd*-tree, the root presents all the instances. Each interior node has an associated splitting feature  $A_i$  and a splitting value  $V_i$  ( $1 \le i \le k$ ) that divide the instances into two partitions: those with  $A_i$ -values less than  $V_i$  and those with  $A_i$ -values equal to or greater than  $V_i$ . Splitting features at different levels of the tree are different, with levels rotating among the features of all dimensions. The splitting is done recursively in each of the successor nodes until the node contains no more than a predefined number of instances (called bucket size) or cannot be split further. The order in which features are chosen to split can result in different *kd*-trees.

Fig. 1 provides a typical example of *kd*-tree with four instances (2, 5), (3, 7), (5, 4), (8, 9) in a 2-dimension space: (a) shows how the instances are partitioned in the *X*, *Y* plane, and (b) gives a tree representation of the four instances. The root node, with point (2, 5), splits the plane along the *Y*-axis into two subspaces. The point (5, 4) lies in the lower subspace (i.e., (x, y) | y < 5), and thus is in the left subtree. The points (3, 7) and (8, 9) lie in the upper subspace (i.e.,  $(x, y) | y \ge 5$ ), and thus are in the right subtree. The point (3, 7) further splits the upper subspace into two parts along the *X*-axis.

For the purpose of selective sampling, we want to select features that can split instances into different groups based on their dissimilarity measures as early as possible. Hence, in our building a *kd*-tree, a splitting feature is chosen if the data variance is maximized along the dimension associated with the feature. The variance of a feature  $A_i$  is calculated according to the formula  $Var(A_i) = \frac{1}{N} \sum_{j=1}^{N} (V_j - V_i)^2$ , where  $V_i$  is the median value of feature  $A_i$ , and j is the index of each instance in a data set with N instances. Once feature  $A_i$  is determined, value  $V_i$  is then used to split the instances into two partitions. Fig. 2 shows a modified *kd*-tree of the example shown in Fig. 1. At the root level, since Var(X) = 5.5 (with median value 4) and Var(Y) = 3.75 (with median value 6), the space



Fig. 1. A typical kd-tree example. (a) The splitting of the X, Y plane; (b) A 2d-tree representation.



Fig. 2. A modified use of kd-tree. (a) The splitting of the X, Y plane; (b) A 2d-tree representation.

is split along the X-axis (x = 4) into two subspaces. The points (2, 5) and (3, 7) lie in the left subspace (i.e., (x, y) | x < 4), and thus are in the left subtree. The points (5, 4) and (8, 9) lie in the right subspace (i.e.,  $(x, y) | x \ge 4$ ), and thus are in the right subtree. Each of the two subspaces are further split along the y-axis (y = 6, y = 6.5, respectively) into two parts, producing four leaf nodes in the tree. Since the median value (instead of mean) of feature  $A_i$  is used in the calculation of variance, the resulting kd-tree is theoretically a balanced tree. The time complexity of building such an optimized kd-tree is  $O(kN\log N)$ . However, in some cases, a feature selected to split the tree may contain duplicate values, which may result in an unbalanced tree. The kd-tree can be built once if necessary, or dynamically when required.

In building a modified kd-tree (as shown in Fig. 2), the leaf nodes (buckets) represent mutually exclusive small subsets of instances which collectively form a partition of the whole data set.<sup>1</sup> The size of a bucket can be an input parameter and determined *a pri*-

<sup>&</sup>lt;sup>1</sup> Every node at each level of the tree only records indexes of the instances this node contains.

*ori*. Since instances in each bucket are relatively close to each other, we can randomly select one instance from each bucket to represent the effect of all the instances in its corresponding bucket. Therefore, a subset of the instances chosen by selective sampling is used to approximate the full sample space. Selective sampling can be summarized by a 3-step procedure:

- 1. Determine the size *t* of a bucket;
- 2. Build a variance-based kd-tree with m buckets;
- 3. Randomly select an instance from each bucket.

We provide next details of selective sampling for feature selection.

# 4. Applying selective sampling to feature selection

Efficiency is critical for feature selection algorithms in the context of large data sets. To demonstrate selective sampling, we use a well-known and efficient algorithm Relief that can select statistically relevant features in linear time of the numbers of features and instances [28,47]. After introducing Relief in Section 4.1, we illustrate how selective sampling can be applied to Relief and present a new algorithm of active feature selection in Section 4.2. In Section 4.3, we discuss other related work on Relief.

# 4.1. Relief algorithm

The key idea of Relief (given in Fig. 3) is to estimate the quality of features according to how well their values distinguish between instances that are near to each other. For this purpose, given a randomly selected instance X from a data set S with k features, Relief searches the data set for its two nearest neighbors: one from the same class, called nearest hit H, and the other from a different class, called nearest miss M. It updates the quality estimation  $W[A_i]$  for all the features  $A_i$  based on the values of difference function diff() about X, H, and M. The process is repeated m times, where m is a user-defined parameter [28,32]. For instances  $X_1, X_2, diff(A_i, X_1, X_2)$  calculates the difference between the values<sup>2</sup> ( $x_{1i}$  and  $x_{2i}$ ) of feature  $A_i$ :

$$diff(A_i, x_{1i}, x_{2i}) = \begin{cases} |x_{1i} - x_{2i}| & \text{if } A_i \text{ is numeric,} \\ 0 & \text{if } A_i \text{ is nominal } \& x_{1i} = x_{2i}, \\ 1 & \text{if } A_i \text{ is nominal } \& x_{1i} \neq x_{2i}. \end{cases}$$

Normalization with *m* in calculation of  $W[A_i]$  (line 6 in Fig. 3) guarantees that all weights are in the interval of [-1, 1].

The time complexity of Relief for a data set with N instances is O(mkN). Efficiency is one of the major advantages of the Relief family over other algorithms [12]. With m being a constant, the time complexity becomes O(kN). However, since m is the number of in-

 $<sup>^{2}</sup>$  Numeric values should be normalized into the range between 0 and 1.

Given *m*—desired number of sampled instances, and *k*—number of features,

set all weights W[A<sub>i</sub>] := 0.0;
for j := 1 to m do begin
randomly select an instance X;
find nearest hit H and nearest miss M;
for i := 1 to k do begin
W[A<sub>i</sub>] := W[A<sub>i</sub>] - diff(A<sub>i</sub>, X, H)/m + diff(A<sub>i</sub>, X, M)/m;
end;

Fig. 3. Original Relief algorithm.

stances used to approximate probabilities, a larger *m* implies more reliable approximations. When *N* is very large, it is often required that  $m \ll N$ .

## 4.2. Relief with selective sampling

Although random sampling of *m* instances for Relief reduces the time complexity from  $O(kN^2)$  to O(kN), the optimal results of Relief are not guaranteed. When applying selective sampling to Relief, we aim to obtain results that are better than using random sampling and similar to the results using all the instances.

In our attempt to selectively sample *m* instances based on the modified *kd*-tree introduced in Section 3, we can use either sample size *m* or bucket size *t* to control the *kd*-tree splitting process. Since only one instance is selected from each bucket, one can easily establish that t = N/m, where *N* is the total number of instances. Therefore, if *m* is predetermined, the splitting process stops when it reaches the level where each bucket contains N/m or fewer instances. For example, in Fig. 2(b), if m = 2, the splitting process stops after the first split when each bucket contains two instances. On the other hand, given a *t*, we can estimate *m* based on *t*. In Fig. 2(b), if we choose *t* to be 1 (i.e., each bucket contains only one instance), all the four instances will be selected. For a bucket size t = N, the root node is not split at all, and only one instance will be selected. As we mentioned earlier, in practical, the resulting *kd*-tree may not be a balanced tree due to duplicate feature values. Therefore, for 1 < t < N, the number of selected instances *m* will be within  $(\frac{1}{t}N, N)$ .

In this work, we use bucket size t to control the number of selected instances m which is equal to the number of buckets. The algorithm of Relief with selective sampling is detailed in Fig. 4. One important point in buildKDTree(t) is that each feature should be normalized [56] before the variance calculation in order to choose to split on the feature with largest variance.

In the empirical study, we use ReliefF [32,56] which is an extension to the original Relief. It handles multiple classes and searches for several nearest neighbors to be robust to noise. We compare ReliefF with its counterpart ReliefS which applies selective sampling for instance selection in the same way as described in Fig. 4. The difference between the two is illustrated in Fig. 5. The top flow shows ReliefF with random sampling of 4 instances from the data. The bottom flow shows ReliefS with random sampling of one instance from each of the four buckets of the kd-tree.

Given t-bucket size,

1. set all weights  $W[A_i] := 0.0$ ; buildKDTree(t); 3. m := number of buckets; 4. for j := 1 to *m* do begin randomly select an instance *X* from *Bucket*[*j*]; 5. find nearest hit H and nearest miss M; 6. 7. for i := 1 to k do begin 8.  $W[A_i] := W[A_i] - diff(A_i, X, H)/m + diff(A_i, X, M)/m;$ 9. end; 10. end;



Fig. 5. The difference between ReliefF and ReliefS: the top and bottom flows show how ReliefF and ReliefS work, respectively.

# 4.3. Related work on Relief

There has been substantial research on the Relief family of algorithms (Relief, ReliefF, and RReliefF) [25,28,32,33,45–48]. Relief (introduced in Section 4.1) was designed for feature subset selection [28,29] and it is considered one of the best algorithms for this purpose [16]. Relief only deals with binary classes. This limitation was overcome by ReliefF [32] which handles multiple classes and incomplete and noisy data. ReliefF was further extended to RReliefF [45] in order to handle continuous classes in regression. The Relief family of algorithms are general and successful feature estimators and are especially good in detecting conditional dependencies between features [48]. In inductive learning, ReliefF was successfully employed in building decision trees for classification. The resulting decision trees achieved superior predictive accuracy over Naive Bayesian classifiers

and k-NN classifiers across various artificial and real-world data sets [33]. It was also shown in [45] that RReliefF is effective in selecting features in learning regression trees for regression problems.

Albeit a broad spectrum of successful uses of the Relief family of algorithms, little work has shown how to determine an optimal sample size.<sup>3</sup> Therefore, work regarding Relief usually circumvents the issue of optimal m by simply choosing m to be the full size of the data set [32] as the larger m leads to better performance.<sup>4</sup> Robnik-Sikonja and Kononenko showed in [48] that although feature selection results become stable after a number of iterations for simple data sets, the quality of results keeps improving as the sample size increases for more complicated data sets. The goal of this work is to show that for a given sample size m, instances obtained by selective sampling are more effective for feature selection than those selected by random sampling. Hence, in our work, we observe how selective sampling differs from random sampling by varying m from 10% to 100% of N using ReliefF with all N instances as the performance reference.

Recall that Relief relies on the search of a predefined number of nearest neighbors [32], and the *kd*-tree data structure is often used for fast nearest neighbor search [41]. In [51], *kd*-trees are applied to speed up Relief and its extensions by providing a fast way to locate nearest neighbors for each class, thus reducing the overall time complexity of the algorithms to  $O(kN\log N)$ . Additional time savings can be achieved by building the *kd*-tree once and using it for both bucket generation and the nearest neighbor search. However, the focus of this work is not to speed up current algorithms in the Relief family, but to investigate the effectiveness of selective sampling in partitioning data points for feature selection.

# 5. Issues of performance evaluation

Before we proceed to define performance measures for selective sampling, let us first discuss some criteria for a suitable performance measure:

- 1. It is a function of the features of the data.
- 2. Its value improves as *m* increases.
- 3. Its value reaches the best when m = N.

In ReliefF, since *m* is the number of instances used to approximate probabilities, a larger *m* implies more reliable approximations. Therefore, it is reasonable to assume that the optimal result ReliefF can achieve is the features ranked according to their weights when m = N. This ranked list of features is named  $S_N$ . Given various sizes of *m*, the results of ReliefF and ReliefS can be compared in two aspects: (1) subset selection—we compare which resulting subset is more similar to the optimal subset obtained from  $S_N$ ; and (2) feature order—we compare the order of features determined by ReliefF or ReliefS to the order

<sup>&</sup>lt;sup>3</sup> One heuristic suggested in [25] is to choose  $m = \log N$  in an algorithm similar to Relief.

<sup>&</sup>lt;sup>4</sup> Doing so increases the complexity of the algorithm to  $O(kN^2)$ .

of features in  $S_N$ . In Section 5.1, we discuss the reason why it is important to consider the order of features. In Section 5.2, we present three different measures with different emphasis on feature order and check if they satisfy the above three criteria. In Sections 5.3 and 5.4, we discuss time savings and accuracy improvement when using active feature selection.

#### 5.1. Importance of feature order

Based on the output type, feature selection algorithms can be grouped into two categories, minimum subset algorithms and feature ranking algorithms [37]. Minimum subset algorithms return a minimum feature subset but do not rank features in the subset [14,24, 53]. Features in the subset are relevant, others are irrelevant. Feature ranking algorithms assign a weight to each feature of the data set and rank the relevance of features according to their weights [15,32,58]. Order information is important for these algorithms because it indicates relative relevance. Order information is also important if one aims to select a feature subset from the resulting ranked list. Below, we illustrate how order information can affect the selection of relevant features for ReliefF and other feature ranking algorithms.

We first define some terms. For an optimal list of features  $S_N$ , a target subset of features T is defined as an optimal subset of features which contains the top n weighted features in  $S_N$ . For a data set with an unknown number of relevant features (n), T contains the top n features whose weights  $\ge \gamma$ , where  $\gamma$  is a threshold equal to W[i] (the *i*th largest weight in  $S_N$ ) and the gap defined by W[i] and W[i + 1] is sufficiently large (e.g., greater than the average gap among the k - 1 gaps). Let  $S_{ReliefF}$  and  $S_{ReliefS}$  be the two resulting lists obtained by ReliefF and ReliefS, respectively. To compare the performance of both ReliefF and ReliefS with different sizes of m, we can define a performance measure  $\mathcal{P}(S_N, R)$  where R can be either  $S_{ReliefF}$  or  $S_{ReliefS}$  with varying m. Fig. 6(a) illustrates the relationships among  $S_N$ , T, R, and  $R_n$  (the subset of the top n features in R). Fig. 6(b) shows five cases for a set of five features. Column I shows the optimal ranking of the five features ( $S_N$ ), and each of the remaining four columns (II–V) represents a ranking from either ReliefF or ReliefS with m instances, assuming m < N.



Fig. 6. An example for the importance of feature order. (a) Relationships among terms; (b) Results with different feature orders.

For a given *n* (either known *a priori* or determined by threshold  $\gamma$ ), the order of features in *R* directly affects the selection of a feature subset  $R_n$ . For example, in Fig. 6(b), the threshold  $\gamma$  is chosen to include the top three features from each resulting list. All the three relevant features ( $A_1$ ,  $A_2$ ,  $A_3$ ) are selected into  $R_n$  in cases II and III, while only two of them are selected in cases IV and V. However, given the same ordered lists II–V, if  $\gamma$  is chosen to include the top two features, the selected subset  $R_n$  in case III will fail to include both of the two relevant features  $A_1$  and  $A_2$ , while  $R_n$  in case IV will become an optimal subset. Therefore, it is important to develop performance measures that take order information into consideration. Below we examine sensible candidates for  $\mathcal{P}()$ .

#### 5.2. Performance measures

#### 5.2.1. Precision

Precision (P) is computed as the number of features that are in both T and  $R_n$ , divided by the number of features in T:

$$\mathbf{P} = \frac{|T \cap R_n|}{|T|}.$$

P ranges from 0 to 1, where P is 1 when subsets T and  $R_n$  are equal and 0 when none of the features in T appears in  $R_n$ . In Fig. 6(b), P is 1 for cases II and III and 2/3 for cases IV and V.

#### 5.2.2. Distance

Precision treats all features in *T* and  $R_n$  equally without considering the orders of the features. In order to account for the order of features in both  $S_N$  and R, Distance (D) is defined based on the sum of distances between common features in *T* and *R*. The distance of a feature between two sets is the difference between its positions in the two ranked lists. Let  $S'_N$  be  $S_N$  in reverse order. The maximum possible ranking distance between two sets that share the same features is:

$$D_{\max} = \sum_{\forall A_i \in S_N} \left| position(A_i \in S_N) - position(A_i \in S'_N) \right|.$$

D is then defined as the follows:

$$D = \frac{\sum_{\forall A_i \in T} |position(A_i \in T) - position(A_i \in R)|}{D_{max}}$$

Since the subset  $R_n$  may not contain all the features in T, we use the full set R in the definition of D.  $D_{max}$  is used to normalize D so that D ranges from 0 to 1, where D is 0 when the two sets T and  $R_n$  have identical ranking (as shown in case II), otherwise, D is larger than 0. In Fig. 6(b), with  $D_{max} = 12$ , the D values for cases II, III, IV, and V are 0, 4/12, 3/12, and 5/12, respectively.

# 5.2.3. Raw Distance

Both Precision and Distance require choosing a threshold  $\gamma$  to decide the target set T. In some cases, it is difficult to determine an optimal threshold. If  $\gamma$  is wrongly estimated, meaning that the target set T is not an optimal subset, evaluation using these measures will be incorrect. For example, in Fig. 6(b), if  $\gamma$  is chosen between features  $A_2$  and  $A_3$ in  $S_N$ , the target set will be  $\{A_1, A_2\}$  instead of  $\{A_1, A_2, A_3\}$ . Thus, Precision for case III will become 1/2 instead of 1, and Precision for case IV will become 1 instead of 2/3. A straightforward performance measure is to directly calculate the sum of the differences of weights for each of the feature pairs (same features) in the optimal list  $S_N$  and the resulting list R. We name it Raw Distance (RD):

$$\mathrm{RD} = \sum_{i=1}^{k} |W_{S}[A_{i}] - W_{R}[A_{i}]|,$$

where  $W_S[A_i]$  and  $W_R[A_i]$  are associated with  $S_N$  and R, respectively. RD considers all k features in the two results. Thus, this measure does not rely on threshold  $\gamma$ . It is designed to compare the results of ReliefF and ReliefS, but it cannot be used for measuring the performance of subset selection as it uses all the features.

# 5.2.4. Comparison of measures

Each measure serves a unique purpose in the evaluation of feature selection results. Table 1 provides a summary of these four measures. The setting of  $\gamma$  is required in ReliefF for feature subset selection. Precision is a simple measure of subset selection, but it is not sufficient due to its insensitivity to the order of features. Both Distance and Raw Distance are order-sensitive, but Raw Distance does not require the threshold setting.

# 5.3. Measuring time savings

It is sensible to question whether the use of selective sampling in feature selection would result in any time savings overall because the initial building of *kd*-tree incurs certain costs. This question is best answered by measuring computation time during experiments. ReliefS and ReliefF require different numbers of instances to achieve the same level of performance. We can compare the running times required to achieve a given level of performance. Let  $T_{kd-tree}$ ,  $T_{ReliefS}$ , and  $T_{ReliefF}$  be the times for *kd*-tree building, running ReliefS, and running ReliefF, respectively, with a given performance. A straightforward approach is to report  $T_{kd-tree}$ ,  $T_{ReliefS}$ , and  $T_{ReliefF}$  and compare  $T_{kd-tree} + T_{ReliefS}$  with  $T_{ReliefF}$ . Their difference can be either the saving or the loss of computation time.

Table 1 Summary of performance measures

	Precision	Distance	Raw distance
Complexity	$O(n^2)$	O(nk)	$O(k^2)$
Upper bound	1	1	None
Lower bound	0	0	0
Ordering	No	Yes	Yes
$\gamma$ setting	Yes	Yes	No

#### 5.4. Measuring accuracy improvement

One can indirectly measure the results of feature selection using a learning algorithm to check its effect on accuracy. Likewise, the effectiveness of selective sampling for feature selection can be further verified by comparing the learning accuracy on the subsets of features chosen by ReliefF and ReliefS. For the two resulting lists produced by RelieF and ReliefS with the same number of sampled instances of a data set, two different feature subsets of the same cardinality can be chosen from the top of the two lists and then used to obtain the learning accuracy for a certain leaning algorithm. We expect an accuracy gain from the subset chosen by ReliefS over the subset chosen by ReliefF.

# 6. Empirical study

The objective of this section is to empirically evaluate if selective sampling can do better in selecting m instances than random sampling in the context of ReliefF. We examine if the results of feature selection are consistently better when using instances sampled from kd-tree buckets than when using the same number of instances selected by random sampling. In Section 6.1, we present two groups of data sets (synthetic and benchmark) and the experimental procedures. In Sections 6.2 and 6.3 we present and discuss results for synthetic data sets and benchmark data sets. In Section 6.4, we further examine the effectiveness of selective sampling in terms of learning accuracy.

# 6.1. Data and experimental procedures

We choose synthetic data sets in our experiments because the relevant features of these data sets are known beforehand. The use of synthetic data in our experiments serves three purposes: (1) to verify the effectiveness of ReliefF, (2) to avoid choosing the optimal threshold  $\gamma$  for subset selection, and (3) to evaluate the effectiveness of active feature selection. Since we rarely know the relevant features beforehand in practice, we also conduct experiments on benchmark data sets to evaluate selective sampling. We describe the two groups of data sets below.

#### 6.1.1. Synthetic data

We use functions described in [1] to generate synthetic data sets so that we know exactly which features are relevant. The nine features are described in Table 2. Ten classification functions of Agrawal et al. [1] were used to generate classification problems with different complexities. Efforts were made to generate data sets as described in the original functions. Each data set consists of 5000 instances. The values of the features of each instance were generated randomly according to the distributions given in the table. For each instance, a class label was determined according to the rules that define the functions.

As an example, we give Function 2 that uses two features and classifies an instance into Group A if

Feature	Description	Value
salary	salary	uniformly distributed from 20,000 to 150,000
commission	commission	if salary $\ge 75000 \rightarrow \text{commission} = 0$
		else uniformly distributed from 10000 to 75000.
age	age	uniformly distributed from 20 to 80.
elevel	education level	uniformly distributed from $[0, 1, \ldots, 4]$ .
car	make of the car	uniformly distributed from $[1, 2, \ldots, 20]$ .
zipcode	zip code of the town	uniformly chosen from 9 available zipcodes.
hvalue	value of the house	uniformly distributed from 0.5k10000 to 1.5k1000000
		where $k \in \{09\}$ depends on zipcode.
hyears	years house owned	uniformly distributed from $[1, 2,, 30]$ .
loan	total amount of loan	uniformly distributed from 1 to 500000.

Table 2 Features of the test data adapted from Agrawal et al. [1]

 $((\mathbf{age} < 40) \land (50000 \leq \mathbf{salary} \leq 100000)) \lor$ 

$$\left((40 \leqslant \mathbf{age} < 60) \land (75000 \leqslant \mathbf{salary} \leqslant 125000)\right) \lor$$

 $((age \ge 60) \land (25000 \le salary \le 75000)).$ 

Otherwise, the instance is classified into Group B.

# 6.1.2. Benchmark data

All together 23 data sets are selected from the UCI Machine Learning Data Repository [5] and the UCI KDD Archive [4]. They all have nominal classes with varied numbers of instances (from 150 to 145000), numbers of features (from 4 to 85), and numbers of classes (from 2 to 22). A summary of these data sets is presented in Table 3 which is divided into three groups: Group 1 contains only numeric data, Group 2 only nominal data, and Group 3 mixed data.

# 6.1.3. Experimental procedures

The experiments are conducted using Weka's implementation of ReliefF, and ReliefS is also implemented in the Weka environment [56]. We use different percentages of data (varying *m*). The performance of ReliefF with m = N is set as the performance reference point. The departure from the reference point is a measure of performance deterioration. In particular, we choose six increasing bucket sizes  $t_i$  ( $1 \le i \le 6$ ) from 1 to 6 corresponding to six percentage values  $P_i$ . For example,  $t_2$  corresponds to  $P_2 \approx 50\%$ . For each data set, the experiment is conducted as follows:

- 1. Run ReliefF with bucket size  $t_1$  ( $P_1 = 100\%$ ), and obtain the optimal ranked list of features ( $S_N$ ) according to their weights. The parameter for k in the k-nearest neighbor search is set to 5 (neighbors). This parameter remains the same for all experiments.
- 2. Run ReliefS with bucket sizes  $t_i$  ( $2 \le i \le 6$ ). At each  $t_i$ , run ReliefS 30 times with different seeds and calculate values of Precision, Distance, and Raw Distance for each iteration to obtain average values of these performance measures to eliminate any idio-syncrasy in a single run. A curve is plotted for each measure for comparison. Some of the curves are shown in Figs. 7 and 8.

Title	Ν	Num	Nom	#C
Iris	150	4	0	3
Glass	214	9	0	7
WDBC	569	30	0	2
Balance	625	4	0	3
Pima-Indian	768	8	0	2
Vehicle	846	18	0	4
German	1000	24	0	2
Segment	2310	19	0	7
Abalone	4177	8	0	3
Satimage	4435	36	0	6
Waveform	5000	40	0	3
Page-blocks	5473	10	0	5
CoIL2000	5822	85	0	2
Shuttle	14500	8	0	7
Breast-cancer	286	0	9	2
Primary-tumor	339	0	17	22
KRKPA7	3196	0	36	2
Mushroom	8124	0	22	2
Zoo	101	1	16	7
Autos	205	15	10	7
Colic	368	7	15	2
Vowel	990	10	3	11
Hypothyroid	3772	7	22	4

Table 3 Summary of benchmark data sets: N—number of instances, Num—numeric features, Nom nominal features, #C—number of classes

3. Run ReliefF with each  $P_i$  ( $2 \le i \le 6$ ) determined by corresponding  $t_i$  in step 2. For each  $P_i$ , run ReliefF 30 times and calculate Precision, Distance, and Raw Distance each time, and obtain their average values after 30 runs. A curve is plotted for each measure for comparison. Some of the curves are shown in Figs. 7 and 8.

# 6.2. Results on synthetic data

Table 4 reports the set of relevant features used to determine the class labels in the definition of each function and the optimal ranking list obtained from running ReliefF on the whole data set of 5000 instances generated by each function. From Table 4, we observe that given the cardinality of a relevant feature set (n), for each of these 10 functions except Function 4 and Function 10,<sup>5</sup> the set of the top n features in each ranking list matches exactly with the known relevant feature set. This verifies that ReliefF can indeed find the relevant features of a data set in most cases. Thus we can use the results obtained from the first step of the experimental procedures as a reference to evaluate the performance of ReliefF and ReliefS with varying size m.

<sup>&</sup>lt;sup>5</sup> For these two functions, one relevant feature is just outside the selected set. This could be due to the inability of ReliefF to differentiate redundant features with strong correlation.



Fig. 7. Three illustrative numeric data sets: Average results of 30 runs in three performance measures (P, D, RD).

Table 5 presents a summary of the three performance measures for each synthetic data set. For a given measure, let  $\mathcal{P}_i$  be the averaged value (over 30 runs) obtained at percentage  $P_i$  ( $2 \le i \le 6$ ). Each value in Table 5 is averaged over five percentage values, i.e.,

$$val_{Avg} = \left(\sum_{i=2}^{6} \mathcal{P}_i\right) / 5.$$

Recall that Precision varies from 0 (worst) to 1 (best); Distance varies from 0 (best) to 1 (worst); and Raw Distance starts at 0 (best) and increases. The last row (W/L/T) in Table 5 summarizes Win/Loss/Tie in comparing ReliefS with ReliefF for each measure. It is clear that for the ten synthetic data sets, taking all the three measures into account, ReliefS is as



Fig. 8. Three illustrative **non-numeric** data sets: Average results of 30 runs in three performance measures (P, D, RD).

good as or better than ReliefF. This suggests that m instances selected using kd-trees are more effective than m instances selected at random.

# 6.3. Results on benchmark data

We present and discuss separately the results on numeric data and non-numeric data below.

# 6.3.1. Results on numeric data

Two sets of results on numeric data sets are reported in Table 6 and Fig. 7, respectively. Like Table 5, Table 6 shows that ReliefS is better than or as good as ReliefF in determining

	Relevant feature set	Result from ReliefF $(m = N)$
Function 1	{A3}	A3,  A5, A6, A8, A4, A7, A9, A2, A1
Function 2	{ <i>A</i> 1, <i>A</i> 3}	A1, A3,  A2, A9, A7, A4, A8, A6, A5
Function 3	$\{A3, A4\}$	A4, A3,  A7, A1, A9, A2, A6, A8, A5
Function 4	$\{A1, A3, A4\}$	A1, A4, A2,  A3, A7, A6, A5, A9, A8
Function 5	$\{A1, A3, A9\}$	A9, A3, A1,  A2, A7, A4, A8, A6, A5
Function 6	$\{A1, A2, A3\}$	A1, A3, A2,  A8, A4, A5, A7, A9, A6
Function 7	$\{A1, A2, A9\}$	A9, A1, A2,  A8, A5, A7, A6, A3, A4
Function 8	$\{A1, A2, A4\}$	A1, A4, A2,  A5, A7, A9, A6, A3, A8
Function 9	$\{A1, A2, A4, A9\}$	A9, A1, A4, A2,  A5, A3, A7, A6, A8
Function 10	$\{A1, A2, A4, A7, A8, A9\}$	A4, A1, A2, A8, A3, A9,  A7, A6, A5

Effectiveness of ReliefF on synthetic data. The order of features in a relevant feature set has no significance based on function definitions

Table 5

Average values of three different measures using ReliefF and ReliefS on synthetic data

	Precision		Distance		Raw distance	
	ReliefF	ReliefS	ReliefF	ReliefS	ReliefF	ReliefS
Function 1	1.0	1.0	0.0	0.0	0.049	0.041
Function 2	0.997	1.0	0.017	0.0	0.047	0.044
Function 3	1.0	1.0	0.0	0.0	0.046	0.044
Function 4	0.930	0.932	0.075	0.061	0.049	0.043
Function 5	0.860	0.886	0.182	0.169	0.045	0.044
Function 6	0.891	0.927	0.280	0.225	0.047	0.026
Function 7	0.852	0.881	0.157	0.137	0.047	0.041
Function 8	1.0	1.0	0.039	0.007	0.053	0.042
Function 9	0.915	0.935	0.135	0.109	0.050	0.040
Function 10	0.900	0.910	0.079	0.072	0.061	0.046
W/L/T	7/	0/3	8/	0/2	10/	/0/0

relevant instances for feature selection. Now let us look at the trends of the three performance measures when the number of instances increases for both ReliefF and ReliefS. Fig. 7 shows the results of three illustrative data sets for Precision, Distance, and Raw Distance. For the Segment data, we notice that both ReliefF and ReliefS perform equally well in Precision but differently in Distance and Raw Distance. Precision being 1 indicates that all feature subsets selected are the same as if we use all N instances (recall that the order of selected features is not considered by Precision). Distance and Raw Distance have values greater than 0, which suggests that the selected results are not in the same order as those obtained using all N instances. It can be observed that the more instances used for both ReliefF and ReliefS, the better the performance of feature selection. A similar trend can be observed for the Vehicle data and Satimage data as well.

Fig. 7 and Table 6 indicate that active feature selection can significantly improve performance on numeric data over feature selection with random sampling with the same amount of instances. In other words, the use of kd-trees to partition the data makes the difference. However, as mentioned earlier, the building of kd-trees incurs certain costs. To

Table 4

	Precision		Distance	Distance		Raw distance	
	ReliefF	ReliefS	ReliefF	ReliefS	ReliefF	ReliefS	
Iris	1.0	1.0	0.020	0.013	0.054	0.019	
Glass	0.988	0.992	0.141	0.090	0.069	0.046	
WDBC	0.991	0.994	0.139	0.103	0.111	0.068	
Balance	0.864	0.940	0.468	0.247	0.037	0.018	
Pima-Indian	0.906	0.930	0.248	0.209	0.019	0.016	
Vehicle	0.996	1.0	0.206	0.105	0.052	0.026	
German	0.898	0.920	0.360	0.309	0.154	0.125	
Segment	1.0	1.0	0.074	0.029	0.054	0.020	
Abalone	0.947	0.971	0.257	0.176	0.003	0.001	
Satimage	0.998	1.0	0.088	0.047	0.065	0.022	
Waveform	1.0	1.0	0.080	0.056	0.047	0.036	
Page-blocks	1.0	1.0	0.202	0.043	0.006	0.003	
CoIL2000	1.0	1.0	0.060	0.041	0.110	0.074	
Shuttle	1.0	1.0	0.0	0.0	0.003	0.001	
W/L/T	8/	/0/6	13	/0/1	14	/0/0	

Table 6 Average values of three different measures using ReliefF and ReliefS on **numeric** data

#### Table 7

Time savings by ReliefS w.r.t. ReliefF for **numeric** data.  $m_{ReliefS}$  and  $m_{ReliefF}$  are numbers of instances used by ReliefS and ReliefF to achieve the same performance in raw distance

	ReliefS			ReliefF	
	<i>T<sub>kd-tree</sub></i> (ms)	T <sub>ReliefS</sub> (ms)	m <sub>Relief</sub> S	T <sub>ReliefF</sub> (ms)	m <sub>Relief</sub> F
Iris	20	14	18	60	87
Glass	61	140	62	259	126
WDBC	455	1414	125	3282	313
Balance	136	223	88	743	313
Pima	246	484	77	2684	476
Vehicle	530	2874	195	6790	499
German	697	6274	420	8310	590
Segment	1520	10870	277	53300	1317
Abalone	1359	23879	961	58228	2423
Satimage	4630	63901	577	255716	2572
Waveform	7170	359840	1900	529860	2950
Page	1858	43774	1095	125709	3284
CoIL	14117	612203	1979	983601	3377
Shuttle	6058	187156	1885	802001	8700

actually compare the running time of ReliefS with that of ReliefF, we consider the case of bucket size 2 for ReliefF (i.e.,  $m_{ReliefF}$  is around 50% of the whole data set) and use the performance measured by Raw Distance to find corresponding  $m_{ReliefS}$  for ReliefS.

Table 7 records the running times  $T_{kd-tree}$ ,  $T_{ReliefS}$  and  $T_{ReliefF}$  as well as  $m_{ReliefS}$  and  $m_{ReliefF}$ . We can observe that:

	Precision		Distance		Raw distance	
	ReliefF	ReliefS	ReliefF	ReliefS	ReliefF	ReliefS
Breast-cancer	0.765	0.821	0.695	0.601	0.203	0.162
Primary-tumor	0.957	0.965	0.259	0.207	0.296	0.246
KRKPA7	0.970	0.977	0.103	0.070	0.152	0.101
Mushroom	1.0	1.0	0.065	0.032	0.141	0.063
Zoo	0.986	0.994	0.136	0.119	0.633	0.539
Autos	0.9	0.928	0.308	0.259	0.380	0.298
Colic	0.854	0.867	0.351	0.316	0.382	0.334
Vowel	1.0	1.0	0.056	0.023	0.043	0.021
Hypothyroid	0.965	0.981	0.110	0.085	0.065	0.050
W/L/T	7/0	0/2	9/	0/0	9/	0/0

Table 8		
Average values of three different	ent measures using ReliefF ar	nd ReliefS on non-numeric data

- 1. The time savings are consistent with the time complexity analysis of ReliefF: it is usually O(mkN), or linear in N if m and k are fixed. Now, k and N are fixed, its time complexity is O(m). That is, the reduction of m results in direct time savings.
- 2. The larger the data set, the more savings in time.
- 3. The ratio of  $T_{kd-tree}/T_{ReliefS}$  decreases when data size increases. In other words, the time spent on kd-tree building becomes immaterial when  $T_{ReliefS}$  increases. This is consistent with earlier theoretical analysis.

### 6.3.2. Results on non-numeric data

Based on previous results, it is clear that ReliefS works well on numeric data. We then experiment if ReliefS can be directly extended to non-numeric data (Groups 2 and 3 in Table 3). Since variance is calculated on numeric data when building the *kd*-tree, in our experiments we apply ReliefS to non-numeric data by associating a distinct number to a nominal value, e.g., assigning 1, 2 and 3 to nominal values A, B, and C, respectively.

Results for the three performance measures are reported in Table 8 and Fig. 8. From Table 8, we still notice that for each data set, ReliefS is better than or as good as ReliefF. This suggests that active feature selection works for non-numeric data as well. However, by comparing the results in Table 8 with Table 6, we observe that both ReliefF and ReliefS generally work better on numeric data than on non-numeric data. In addition, the performance gains obtained by ReliefS on non-numeric data are not as significant as those on numeric data, especially for small data sets (this can also be observed in Fig. 8). Through three illustrative data sets from Groups 2 and 3, Fig. 8 demonstrates similar trends of performance measures as those in Fig. 7 when the number of instances increases for both ReliefF and ReliefF, but as we can see that the two curves for each measure are very close to each other, which suggests that the performance gains obtained by selecting m instances using kd-trees are not significant.

Table 9 records the running times  $T_{kd-tree}$ ,  $T_{ReliefS}$  and  $T_{ReliefF}$  as well as  $m_{ReliefS}$  and  $m_{ReliefF}$  for data sets in Groups 2 and 3. From this table, we observe similar results: (1) the larger the data set, the more savings in time; and (2) the ratio of  $T_{kd-tree}/T_{ReliefS}$  decreases

	ReliefS			ReliefF	
	T <sub>kd-tree</sub> (ms)	T <sub>ReliefS</sub> (ms)	m <sub>ReliefS</sub>	T <sub>ReliefF</sub> (ms)	m <sub>Relief</sub> F
Breast-cancer	90	234	123	300	166
Primary-tumor	175	546	112	836	176
KRKPA7	4559	84880	1055	145520	1950
Mushroom	7668	248336	1950	491665	4062
Zoo	50	73	40	105	65
Autos	161	417	82	568	123
Colic	303	1047	151	1518	221
Vowel	484	2633	218	6570	574
Hypothyroid	4950	98094	1094	173950	2112

Time savings by ReliefS w.r.t. ReliefF for non-numeric	c data. $m_{ReliefS}$ and $m_{ReliefF}$ are numbers of instances
used by ReliefS and ReliefF to achieve the same performa	ance in raw distance

when data size increases. However, five small data sets out of the nine do not show significant time savings. This observation is consistent with what we saw in Table 8 and Fig. 8. For these data sets, selective sampling using ReliefS does not significantly reduce the number of instances required to achieve a given level of performance when compared to random sampling using ReliefF. Thus the extra time spent on building a *kd*-tree is not compensated by the modest time savings obtained from using fewer instances.

# 6.4. Examining learning accuracy

Table 9

In this section, we first show how ReliefF using all instances as suggested by [32] affects the learning accuracy, and then examine how the reduction of training instances affect the results of feature selection in terms of learning accuracy. The first set of comparisons is shown in Table 10 and the second set of comparisons is shown in Table 11.

In Section 6.2, we have demonstrated the effectiveness of ReliefF using all instances on a group of synthetic data sets for which we know the relevant features in advance. We now examine the effectiveness of ReliefF using all instances on benchmark data through a learning algorithm. Table 10 records the 10-fold cross validation results of the 5-NN (nearest neighbor) classifier on the full sets of features and the target sets of features chosen by ReliefF with all instances (defined in Section 5.1) for the 14 numeric data sets (shown in Table 3). In order to evaluate the statistical significance of the difference between the two averaged accuracy values for a given data set, a Student's paired two-tailed t-Test is conducted for the two underlying samples of individual accuracy values. The P value in each row of Table 10 reports the probability that the two underlying samples are different. The smaller the P value, the more significant the difference of the two average values is. The last row (W/L/T) summarizes Win/Loss/Tie in comparing the averaged accuracy values on the target sets with those on the full sets based on a significance threshold 0.1. It is clear that out of the 14 data sets, seven pairs of results are significantly different. ReliefF significantly improves the accuracy of the 5-NN classifier for 3 data sets and maintains the accuracy for 7 data sets with selected subsets of features.

#### Table 10

Effectiveness of ReliefF on benchmark data: 10-fold cross validation accuracy (%) of 5-NN on original features (full sets without feature selection) and target sets of features chosen by ReliefF (with m = N). P reports the probability associated with a Student's paired two-tailed t-Test

	Full set	Target set	Р
		(m = N)	
Iris	96.67	97.33	0.32
Glass	65.80	71.95	0.07
WDBC	96.67	95.43	0.15
Balance	88.00	77.42	0.00
Pima-Indian	74.49	73.84	0.69
Vehicle	69.97	69.27	0.66
German	71.00	72.50	0.19
Segment	95.80	95.76	0.94
Abalone	53.72	52.79	0.17
Satimage	90.73	86.16	0.00
Waveform	79.20	83.74	0.00
Page-blocks	95.87	93.92	0.00
CoIL2000	93.63	93.89	0.07
Shuttle	99.71	99.60	0.01
W/L/T	3/4/7		

# Table 11

Comparison of ReliefF and ReliefS on benchmark data: 10-fold cross validation accuracy (%) of 5-NN on target sets of features chosen by ReliefF (with m = N), subsets of features chosen by ReliefF (with  $m \approx \frac{1}{10}N$ ), and subsets of features chosen by ReliefS (with  $m \approx \frac{1}{10}N$ ). P reports the probability associated with a Student's paired two-tailed t-Test

	$\frac{A}{\text{Target set}}$ $(m = N)$	$\frac{B}{\text{ReliefF}}$ $(m \approx \frac{1}{10}N)$	$\frac{C}{\text{ReliefS}}$ $(m \approx \frac{1}{10}N)$			
				Р		
				(A, B)	(A, C)	(B, C)
Iris	97.33	97.33	97.33	1	1	1
Glass	71.95	65.84	67.23	0.01	0.04	0.40
WDBC	95.43	95.43	96.71	0.99	0.09	0.08
Balance	77.42	76.97	77.42	0.79	1	0.79
Pima-Indian	73.84	65.61	72.27	0.02	0.21	0.04
Vehicle	69.27	66.01	69.16	0.04	0.92	0.09
German	72.50	70.60	72.60	0.06	0.94	0.06
Segment	95.76	95.84	96.19	0.44	0.25	0.35
Abalone	52.79	52.79	54.51	1	0.04	0.04
Satimage	86.16	85.75	86.11	0.18	0.84	0.27
Waveform	83.74	83.48	83.38	0.49	0.36	0.83
Page-blocks	93.92	91.17	89.73	0.00	0.00	0.00
CoIL2000	93.89	93.77	93.77	0.15	0.15	1
Shuttle	99.60	99.60	99.60	1	1	1
W/L/T				0/5/9	2/2/10	5/1/8

To examine the effect of reduction of training instances and verify the effectiveness of ReliefS, for each data set, two feature subsets of the same cardinality are selected from the top of the two resulting lists produced by ReliefF and ReliefS with the same number of sampled instances (we choose  $m \approx 10\% N$ , corresponding to the smallest bucket size, in our experiments). Table 11 records the 10-fold cross validation results of 5-NN on the subsets of features chosen by ReliefF (column B) or ReliefS (column C). We use the results on the target sets of features chosen by ReliefF with all instances (m = N) as the reference point (column A) in comparison of ReliefF and ReliefS. As discussed in Section 5.1, for feature ranking methods like ReliefF, the order of features in a resulting list is important for subset selection. However, learning accuracy on a selected subset may not be sensitive to the order of features; as long as two subsets contain the same features (having equal Precision values), they can result in the same learning accuracy for a given learning algorithm. Therefore, in order to show the effect of the different orders of features, we choose two subsets of different features of cardinality n from the top of the two resulting feature lists to obtain the accuracy for 5-NN.

Table 11 also contains P values resulting from pair-wised comparisons of columns A, B, and C. P (A, B) values for columns A and B suggest that there are 5 pairs of average accuracy rates that are significantly different and the subsets selected by ReliefF with  $m \approx \frac{1}{10}N$  cause accuracy decrease in all 5 cases. P (A, C) values for columns A and C show that there are 4 pairs of average accuracy rates that significantly different, and the subsets selected by ReliefS with  $m \approx \frac{1}{10}N$  result in accuracy increase for 2 data sets and decrease for 2 data sets among the 4 cases. We then further compare the 5-NN results using the feature subsets of ReliefS and ReliefF with  $m \approx \frac{1}{10}N$  directly. P (B, C) values for columns B and C indicate that there are 6 pairs of average accuracy rates that are significantly different. It is clear that the subsets selected by ReliefS with  $m \approx \frac{1}{10}N$  for 5 data sets and worse accuracy for only one data set among the 6 cases. According to the above results, we conclude that with the same number of sampled instances, ReliefS in general achieves better performance than ReliefF in terms of learning accuracy and hence selective sampling is an effective approach for active feature selection.

#### 7. Conclusions and further work

In this paper, we present a case for active feature selection using a formalism of selective sampling. We choose an efficient feature selection algorithm ReliefF in our case study to evaluate whether selective sampling has consistent advantages over random sampling. In particular, we use the kd-tree to partition data and select instances from the partitions. We conduct extensive experiments to evaluate the performance of active feature selection. Significant time savings are observed using the Raw Distance performance measure. Improvement of learning accuracy is reported for the nearest neighbor classifier on numeric data.

Although the experimental study demonstrates the effectiveness of active feature selection, we plan future work along the following lines: (1) to investigate why ReliefS still works in cases where data is not purely numeric and explore different methods of handling nominal features; (2) to automatically determine the cost-effective percentage of instances for selective sampling and investigate its performance on large data sets (e.g., Web data); (3) to investigate other means of exploiting data characteristics for selective sampling; and (4) to apply selective sampling to the vast body of feature selection and other data preprocessing algorithms [38].

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## References

- R. Agrawal, T. Imielinski, A. Swami, Database mining: a performance perspective, IEEE Trans. Knowledge Data Engrg. 5 (6) (1993) 914–925.
- [2] R. Agrawal, R. Srikant, Fast algorithms for mining association rules, in: Proc. Internat. Conf. Very Large Data Bases, Santiago, Chile, 1994, pp. 487–499.
- [3] D.W. Aha, D. Kibler, M.K. Albert, Instance-based learning algorithms, Machine Learning 6 (1991) 37-66.
- [4] S.D. Bay, The UCI KDD archive, 1999, http://kdd.ics.uci.edu.
- [5] C.L. Blake, C.J. Merz, UCI Repository of machine learning databases, 1998, http://www.ics.uci. edu/~mlearn/MLRepository.html.
- [6] A.L. Blum, P. Langley, Selection of relevant features and examples in machine learning, Artificial Intelligence 97 (1997) 245–271.
- [7] P.S. Bradley, U. Fayyad, C. Reina, Scaling clustering algorithms to large databases, in: Proceedings of the Fourth International Conference on Knowledge Discovery & Data Mining, New York, AAAI Press, Menlo Park, CA, 1998, pp. 9–15.
- [8] C.J.C. Burges, A tutorial on support vector machines for pattern recognition, Data Mining and Knowledge Discovery 2 (1998) 121–167.
- [9] W.G. Cochran, Sampling Techniques, Wiley, New York, 1977.
- [10] D. Cohn, L. Atlas, R. Ladner, Improving generalization with active learning, Machine Learning 15 (1994) 201–221.
- [11] S. Das, Filters, wrappers and a boosting-based hybrid for feature selection, in: Proceedings of the Eighteenth International Conference on Machine Learning, Williamstown, MA, 2001, pp. 74–81.
- [12] M. Dash, H. Liu, Feature selection for classification, Intelligent Data Analysis: An Internat. J. 1 (3) (1997) 131–156.
- [13] M. Dash, H. Liu, Feature selection for clustering, in: Proceedings of the Fourth Pacific Asia Conference on Knowledge Discovery and Data Mining, (PAKDD-2000), Kyoto, Japan, Springer, Berlin, 2000, pp. 110– 121.
- [14] M. Dash, H. Liu, H. Motoda, Consistency based feature selection, in: Proceedings of the Fourth Pacific Asia Conference on Knowledge Discovery and Data Mining, (PAKDD-2000), Kyoto, Japan, Springer, Berlin, 2000, pp. 98–109.

- [15] M. Dash, H. Liu, J. Yao, Dimensionality reduction of unsupervised data, in: Proceedings of the Ninth IEEE International Conference on Tools with AI (ICTAI'97), Newport Beach, CA, IEEE Computer Society, 1997, pp. 532–539.
- [16] T.G. Dietterich, Machine learning research: four current directions, AI Magazine 18 (4) (1997) 97–136.
- [17] J.G. Dy, C.E. Brodley, Feature subset selection and order identification for unsupervised learning, in: Proceedings of the Seventeenth International Conference on Machine Learning, Stanford, CA, 2000, pp. 247–254.
- [18] J.G. Dy, C.E. Brodley, Visualization and interactive feature selection for unsupervised data, in: Proceedings of the Sixth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Boston, MA, 2000, pp. 360–364.
- [19] Y. Freund, H. Seung, E. Shamir, N. Tishby, Selective sampling using the query by committee algorithm, Machine Learning 28 (1997) 133–168.
- [20] J.H. Friedman, J.L. Bentley, R.A. Finkel, An algorithm for finding best matches in logarithmic expected time, ACM Trans. Math. Software 3 (1977) 209–226.
- [21] V. Gaede, O. Günther, Multidimensional access methods, ACM Comput. Surv. 30 (2) (1998) 170-231.
- [22] B. Gu, F. Hu, H. Liu, Sampling: knowing whole from its part, in: H. Liu, H. Motoda (Eds.), Instance Selection and Construction for Data Mining, Kluwer Academic, Boston, MA, 2001, pp. 21–38.
- [23] M.A. Hall, Correlation based feature selection for machine learning, PhD Thesis, University of Waikato, Dept. of Computer Science, 1999.
- [24] M.A. Hall, Correlation-based feature selection for discrete and numeric class machine learning, in: Proceedings of the Seventeenth International Conference on Machine Learning (ICML-00), Stanford, CA, Morgan Kaufmann, San Francisco, CA, 2000.
- [25] Se June Hong, Use of contextual information for feature ranking and discretization, IEEE Trans. Knowledge Data Engrg. 9 (5) (1997) 718–730.
- [26] T. Joachims, Text categorization with support vector machines: learning with many relevant features, in: C. Nedellec, C. Rouveirol (Eds.), Proceedings of 10th European Conference on Machine Learning, Chemnitz, Germany, Springer, Berlin, 1998, pp. 137–142.
- [27] Y. Kim, W. Street, F. Menczer, Feature selection for unsupervised learning via evolutionary search, in: Proceedings of the Sixth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Boston, MA, 2000, pp. 365–369.
- [28] K. Kira, L.A. Rendell, The feature selection problem: traditional methods and a new algorithm, in: Proceedings of the Tenth National Conference on Artificial Intelligence, San Jose, CA, AAAI Press/The MIT Press, Menlo Park, CA, 1992, pp. 129–134.
- [29] K. Kira, L.A. Rendell, A practical approach to feature selection, in: Sleeman, P. Edwards (Eds.), Proceedings of the Ninth International Conference on Machine Learning (ICML-92), Aberdeen, Scotland, Morgan Kaufmann, San Francisco, CA, 1992, pp. 249–256.
- [30] J. Kivinen, H. Mannila, The power of sampling in knowledge discovery, in: SIGMOD/PODS'94, ACM, 1994, pp. 77–85.
- [31] R. Kohavi, G.H. John, Wrappers for feature subset selection, Artificial Intelligence 97 (1-2) (1997) 273-324.
- [32] I. Kononenko, Estimating attributes: Analysis and extension of RELIEF, in: F. Bergadano, L. De Raedt (Eds.), Proceedings of the European Conference on Machine Learning, Catania, Italy, Springer, Berlin, 1994, pp. 171–182.
- [33] I. Kononenko, E. Simec, M. Robnik-Sikonja, Overcoming the myopia of inductive learning algorithms with RELIEFF, Appl. Intelligence 7 (1997) 39–55.
- [34] P. Langley, Selection of relevant features in machine learning, in: Proceedings of the AAAI Fall Symposium on Relevance, AAAI Press, 1994, pp. 140–144.
- [35] E. Leopold, J. Kindermann, Text categorization with support vector machines. How to represent texts in input space?, Machine Learning 46 (2002) 423–444.
- [36] D. Lewis, W. Gale, A sequential algorithm for training text classifiers, in: Proceedings of the Seventeenth Annual ACM-SIGR Conference on Research and Development in Information Retrieval, 1994, pp. 3–12.
- [37] H. Liu, H. Motoda, Feature Selection for Knowledge Discovery and Data Mining, Kluwer Academic, Boston, MA, 1998.
- [38] H. Liu, H. Motoda (Eds.), Instance Selection and Construction for Data Mining, Kluwer Academic, Boston, MA, 2001.

- [39] H. Liu, H. Motoda, L. Yu, Feature selection with selective sampling, in: Proceedings of the Nineteenth International Conference on Machine Learning, Sidney, Australia, 2002, pp. 395–402.
- [40] T.M. Mitchell, Machine Learning, McGraw-Hill, New York, 1997.
- [41] A.W. Moore, An introductory tutorial on kd-trees, Extract from PhD Thesis Tech Report No. 209, Computer Laboratory, University of Cambridge, Robotics Institute, Carnegie Mellon University, Pittsburgh, PA, 1991.
- [42] A.Y. Ng, On feature selection: learning with exponentially many irrelevant features as training examples, in: Proceedings of the Fifteenth International Conference on Machine Learning, Madison, WI, 1998, pp. 404– 412.
- [43] K.S. Ng, H. Liu, Customer retention via data mining, AI Rev. 14 (6) (2000) 569-590.
- [44] K. Nigam, A.K. Mccallum, S. Thrun, T. Mitchell, Text classification from labeled and unlabeled documents using EM, Machine Learning 39 (2000) 103–134.
- [45] M. Robnik-Sikonja, I. Kononenko, An adaptation of relief for attribute estimation in regression, in: Proceedings of Fourteenth International Conference on Machine Learning, Nashville, TN, 1997, pp. 296–304.
- [46] M. Robnik-Sikonja, I. Kononenko, Attribute dependencies, understandability and split selection in tree based models, in: Proceedings of Sixteenth International Conference on Machine Learning, Bled, Slovenia, 1999, pp. 344–353.
- [47] M. Robnik-Sikonja, I. Kononenko, Comprehensible interpretation of relief's estimates, in: Proceedings of Eighteenth International Conference on Machine Learning, Williamstown, MA, 2001, pp. 433–440.
- [48] M. Robnik-Sikonja, I. Kononenko, Theoretical and empirical analysis of Relief and ReliefF, Machine Learning 53 (2003) 23–69.
- [49] N. Roy, A. McCallum, Toward optimal active learning through sampling estimation of error reduction, in: Proceedings of the Eighteenth International Conference on Machine Learning, Williamstown, MA, 2001, pp. 441–448.
- [50] G. Schohn, D. Cohn, Less is more: active learning with support vector machines, in: Proceedings of the Seventeenth International Conference on Machine Learning, Stanford, CA, 2000, pp. 839–846.
- [51] M.R. Sikonja, Speeding up Relief algorithms with k-d trees, in: Proceedings of the Electrotechnical and Computer Science Conference, ERK'98, 1998.
- [52] N.A. Syed, H. Liu, K.K. Sung, A study of support vectors on model independent example selection, in: S. Chaudhuri, D. Madigan (Eds.), Proceedings of ACM SIGKDD, International Conference on Knowledge Discovery and Data Mining, ACM, New York, 1999, pp. 272–276.
- [53] L. Talavera, Feature selection as a preprocessing step for hierarchical clustering, in: Proceedings of International Conference on Machine Learning (ICML'99), Bled, Slovenia, 1999, pp. 389–397.
- [54] C.A. Thompson, M.E. Califf, R.J. Mooney, Active learning for natural language parsing and information extraction, in: Proceedings of the Sixteenth International Conference on Machine Learning, Bled, Slovenia, Morgan Kaufmann, San Francisco, CA, 1999, pp. 406–414.
- [55] S. Tong, D. Koller, Support vector machine active learning with applications to text classification, Machine Learning Res. 2 (2001) 45–66.
- [56] I.H. Witten, E. Frank, Data Mining—Practical Machine Learning Tools and Techniques with JAVA Implementations, Morgan Kaufmann, San Francisco, CA, 2000.
- [57] E. Xing, M. Jordan, R. Karp, Feature selection for high-dimensional genomic microarray data, in: Proceedings of the Eighteenth International Conference on Machine Learning, Williamstown, MA, 2001.
- [58] L. Yu, H. Liu, Feature selection for high-dimensional data: a fast correlation-based filter solution, in: Proceedings of the Twentieth International Conference on Machine Learning, Washington, DC, 2003, pp. 856–863.