Stability of Feature Selection Algorithms: a study on high dimensional spaces

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Abstract

With the proliferation of extremely high-dimensional data, feature selection algorithms have become indispensable components of the learning process. Strangely, despite extensive work on the stability of learning algorithms, the stability of feature selection algorithms has been relatively neglected. This study is an attempt to fill that gap by quantifying the sensitivity of feature selection algorithms to variations in the training set. We assess the stability of feature selection algorithms based on the stability of the feature preferences that they express in the form of weights-scores, ranks, or a selected feature subset. We examine a number of measures to quantify the stability of feature preferences and propose an empirical way to estimate them. We perform a series of experiments with several feature selection algorithms on a set of proteomics datasets. The experiments allow us to explore the merits of each stability measure and create stability profiles of the feature selection algorithms. Finally we show how stability profiles can support the choice of a feature selection algorithm.

1 Introduction

High dimensional datasets are becoming more and more abundant in classification problems. A variety of feature selection methods have been developed to tackle the issue of high dimensionality. The major challenge in these applications is to extract a set of features, as small as possible, that accurately classifies the learning examples.

A relatively neglected issue in the work on high dimensional problems, and in general in problems requiring feature selection, is the stability of the feature selection methods used. Stability, defined as the sensitivity of a method to variations in the training set, has been extensively studied with respect to the learning algorithm itself. We propose to investigate how different subsamples of a training set affect a method's assessment of a feature's importance and consequently the final set of selected features.

The stability of classification algorithms was examined by Turney [16] who proposed a measure based on the agreement of classification models produced by an algorithm when trained on different training sets. He defined the agreement of two classification models as the probability that they will produce the same predictions over all possible instances drawn from a probability distribution $P(X)$. Note that instances are drawn from $P(X)$ and not from $P(X, C)$, the joint probability distribution of class and training instances; the underlying reason is that the agreement of two concepts—classification models—should be examined in all possible input worlds. In order to estimate stability he suggested using $m \times 2$-fold cross-validation. In each of the m repetitions of cross-validation a classification model is produced from each one of the two folds. The two models are then tested on artificial instances drawn by sampling from $P(X)$ and their agreement is computed. The final estimation of stability is the average agreement over all m runs.

Related to the notion of stability is the bias-variance decomposition of the error of classification algorithms, [6, 2, 3]. The variance term quantifies instability of the classification algorithm in terms of classification predictions. Variance measures the percentage of times that the predictions of different classification models, learned from different training sets, for a given instance are different from the typical (average) prediction. Bias-variance decomposition is usually done via bootstrapping, where part of the data is kept as a hold-out test set and the remainder is used to create different training sets by using sampling with replacement. The final estimation of variance is also the average over the different bootstrap samples.

In both approaches described above, the predictions of the classification models are crucial in quantifying the sensitivity of classification algorithms to changes in the training sets (note that both approaches can also be used for error estimation which is then tightly coupled with the stability analysis). However when one wants to examine only feature selection algorithms without involving a classification algorithm, the above methods do not apply. Typical feature selection algorithms do not construct classification models and thus cannot provide classification predictions. They usually output what we call a feature preference statement (for conciseness, *feature preference*); this can take the form of a subset of selected features, or alternatively of a weighting-scoring or a ranking of the features, based on which a small set of features can be selected (either by specifying a threshold or asking for a specific number of features). A classification algorithm should then be applied on the selected feature set to produce a classification model. If we used the stability estimation methods described above to the combined feature selection and classification algorithms, we would be measuring their joint sensitivity to training set variations and we would have no way to delimit the (in)stability the feature selection algorithm from that of the classification algorithm.

To address this difficulty we introduce the notion of preferential stability, i.e., the stability of the feature preferences produced by a feature selection algorithm, to quantify its sensitivity to differences in training sets drawn from the same distribution. The same approach can in fact be used to measure the preferential stability of any classification algorithm that produces models from which weightings or rankings of the features can be extracted, e.g. linear discrimination algorithms.

Stability, as introduced in [16], and the bias-variance decomposition frameworks are not able to accurately quantify preferential stability. It is possible that different training samples lead to really different feature sets which however yield the same prediction patterns. This can be especially true when the initial features have a high level of redundancy which is not handled in a principled way by the algorithms used.

The motivation for investigating the stability of feature selection algorithms came from the need to provide application domain experts with quantified evidence that the selected features are relatively robust to variations in the training data. This need is particularly crucial in biological applications, e.g. genomics, DNA-micorarrays, and proteomics, mass spectrometry. These applications are typically characterized by high dimensionality, the goal is to output a small set of highly discriminatory features on which biomedical experts will subsequently invest considerable time and research effort. Domain experts tend to have less confidence in feature sets that change radically with slight variations in the training data. Data miners have to convince them not only of the predictive potential but also of the relative stability of the proposed features.

The rest of the paper is organized as follows: in Section 2 we introduce measures of stability that can be applied to any feature selection algorithm that outputs a feature preference as defined above; we also show how we can empirically estimate these measures. In Section 3 we describe the experimental setup, the datasets used, and the feature selection algorithms included in the study; in Section 4 we present the results of the experiments, investigate the behavior of the different stability measures and establish the stability profiles of the chosen feature selection algorithms; in Section 5 we examine together classification performance and stability of feature preferences, and suggest how we can exploit the latter to support the choice of the appropriate feature selection algorithm; finally we conclude in Section 6.

2 Stability

The generic model of classification comprises: a generator of random vectors x, drawn according to an unknown but fixed probability distribution $P(X)$; a supervisor that assigns class labels c, to the x random vectors, according to an unknown but fixed conditional probability distribution $P(C|X)$; a learning space populated by pairs (x, c) drawn from the joint probability distribution $P(X, C) = P(C|X)P(X)$.

We define the *stability* of a feature selection algorithm as the robustness of the feature preferences it produces to differences in training sets drawn from the same generating distribution $P(X, C)$. Stability quantifies how different training sets affect the feature preferences.

Measuring stability requires a similarity measure for feature preferences. This obviously depends on the representation language used by a given feature selection algorithm to describe its feature preferences; different representation languages call for different similarity measures. We can distinguish three types of representation languages for feature preferences. In the first type a weight or score is assigned to each feature indicating its importance. The second type of representation is a simplification of the first where instead of weights ranks are assigned to features. The third type consists of sets of selected features in which no weighting or ranking is considered. Obviously any weighting schema can be cast as a ranking schema, which in turn can be cast as a set of features by setting a threshold on the ranks or asking for a given number of features.

More formally, let training examples be described by a vector of features $f = (f_1, f_2, ..., f_m)$, then a feature selection algorithm produces either:

- a weighting-scoring: $w = (w_1, w_2, .., w_m), w \in W \subseteq R^m$,
- a ranking: $r = (r_1, r_2, .., r_m), 1 \leq r_i \leq m$,
- or a subset of features: $s = (s_1, s_2, .., s_m), s_i \in \{0, 1\}$, with 0 indicating absence of a feature and 1 presence.

In order to measure stability we need a measure of similarity for each of the above representations. To measure similarity between two weightings w, w', produced by a given feature selection algorithm we use Pearson's correlation coefficient

$$S_W(w, w') = \frac{\sum_i (w_i - \mu_w)(w'_i - \mu_{w'})}{\sqrt{\sum_i (w_i - \mu_w)^2 \sum_i (w'_i - \mu_{w'})^2}},$$

where S_W takes values in [-1,1]; a value of 1 means that the weightings are perfectly correlated, a value of 0 that there is no correlation while a value of -1 that they are anticorrelated.

To measure similarity between two rankings r, r', we use Spearman's rank correlation coefficient

$$S_R(r, r') = 1 - 6 \sum_i \frac{(r_i - r'_i)^2}{m(m^2 - 1)},$$

where r_i and r'_i are the ranks of feature i in rankings r and r' respectively. Here too the possible range of values is in [-1,1]. A value of 1 means that the two rankings are identical, a value of 0 that there is no correlation between the two ranks, and a value of -1 that they have exactly inverse orders.

Finally we measure similarity between two subsets of features using a straightforward adaptation of the Tanimoto distance between two sets, [4]:

$$S_S(s, s') = 1 - \frac{|s| + |s'| - 2|s \cap s'|}{|s| + |s'| - |s \cap s'|}.$$

The Tanimoto distance metric measures the amount of overlap between two sets of arbitrary cardinality. S_S takes values in [0,1] with 0 meaning that there is no overlap between the two sets, and 1 that the two sets are identical.

To empirically estimate the stability of a feature selection algorithm for a given dataset, we can simulate the distribution $P(X, C)$ from which the training sets are drawn by using a resampling technique like bootstrapping or cross-validation. We opted for N-fold stratified cross-validation (N=10). In ten-fold cross-validation the overlap of training instances among the different training folds is roughly 78%. The feature selection algorithm outputs a feature preference for each of the training folds. The similarity of each pair of feature preferences, i.e. $N(N - 1)/2$ pairs, is computed using the appropriate similarity measure and the final stability score is simply the average similarity over all pairs.

We want to couple stability estimates with classification error estimates in view of identifying feature selection algorithms which maximize both stability and classification performance. To this end we embed the procedure described above within an error estimation procedure, itself conducted using stratified 10-fold cross-validation. In other words, at each iteration of the cross-validated error estimation loop, there is a full internal cross-validation loop aimed at measuring the stability of feature precedences returned by the feature selection algorithm. The outer loop provides a classification error estimate in the usual manner, while the inner loop provides an estimate of the stability of the feature selection algorithm.

3 Stability Experiments

3.1 Datasets

We have chosen to experiment with high dimensional data from three different application domains, namely proteomics, genomics and text mining. A short description of these datasets is given in table 1.

The proteomics datasets come all from the domain of mass-spectrometry. The goal is to construct classification models that discriminate between healthy and diseased individuals, i.e we have two class problems. We worked with three different datasets: ovarian cancer [11], (version 8-07-02), prostate cancer [12] and an extended version of the early stroke diagnosis dataset used in [14]. All features correspond to intensities of mass values and are continuous.

The genomics datasets are all datasets of DNA-microarray experiments. We worked with three different datasets: leukemia [7] where the goal is to distinguish between acute myeloid leukemia (AML) and acute lymphoblastic leukemia (ALL); classification of embryonal tumors of the central nervous system [13] where the goal is to predict whether a given treatment

dataset	class 1	# class 1	class 2	# class 2	# features
ovarian	normal	91	diseased	162	824
prostate	normal	253	diseased	69	2200
stroke	normal	101	diseased	107	4928
leukemia	ALL	47	AML	25	7131
nervous	survival	21	failure	39	7131
colon	normal	22	tumor	40	2000
alt	relevant	1425	not	2732	2112
disease	relevant	631	not	2606	2376
function	relevant	818	not	3089	2708
structure	relevant	927	not	2621	2368
subcell	relevant	1502	not	6475	4031

Table 1. Description of datasets.

will be effective or not (i.e., patient will or will not survive); and colon cancer [1] where the goal is to distinguish between healthy and tumor colon tissue. Features correspond to levels of expression of different genes and are continuous.

In text mining we worked with five datasets aimed at determining whether a sentence is relevant or not to a given topic: protein-disease relations (disease), protein-function and structure (function and structure respectively), protein subcellular location (subcell), and related protein sequences produced by alternative splicing of a gene or by the use of alternative initiation codons (alt) [10]. Sentence features are stemmed words, each described by a continuous value representing it standard *tf-idf* score.

Dimensionality reduction and stability of selected features are very important especially in the first two types of applications. The selected features provide the basis to distinguish between different types of pathologies, a first path to hypothesis construction, an initial understanding of the mechanisms involved in various diseases etc. In other words they provide a starting point which is followed by substantial laboratory research. As such the quality and the robustness of the selected features is of paramount importance.

3.2 Feature Selection Algorithms

For feature selection we considered the following methods: Information Gain (IG), Chi-Square (CHI) [4], Symmetrical Uncertainty (SYM), [9], ReliefF (RELIEF), [15], and SVMRFE [8]. Information gain, Chi-Square and Symmetrical Uncertainty are all univariate feature scoring methods for nominal attributes or continuous attributes which are discretized using the method of [5]. ReliefF delivers a weighting of the features while taking their interactions into account; it uses all features to compute distances among training instances and the K nearest neighbors of each of the M probe instances to update feature weights. We set K to 10 and M to the size of the training set, so that all instances were used as probes. SVMRFE is based on repetitive applications of a linear support vector machine algorithm where the P% lowest ranked features are eliminated at each iteration of the linear SVM. The ranks of the features are based on the absolute values of the coefficients assigned to them by the linear SVM. In our experiments, P was set to 10% and the complexity parameter C of the linear SVM to 0.5.

We also include a simple linear support vector machine to show that the same type of stability analysis can be applied to any linear classifier; here too the complexity parameter was set to 0.5. Provided that all features are normalized to a common scale, the absolute values or the squares of the coefficients of the linear hyperplane can be taken to reflect the importance of the corresponding features, in effect providing a feature weighting. This is actually the assumption under which SVMRFE works; alternatively the support vector machine is equivalent to SVMRFE with a single iteration, where the ranking of the features is simply based on the absolute values or the squares of the coefficients of the support vector machine. We consider this version of support vector machines as yet another feature selection algorithm and identify it as SVMONE. The implementations of all the algorithms are those found in the WEKA machine learning environment [17].

As already mentioned the stability estimates are calculated within each training fold by a nested cross-validation loop and the final results reported are the averages, $\overline{S_W}, \overline{S_R}, \overline{S_S}$, over the ten external folds.

dataset	IG			CHI			SYM		
	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$
ovarian	0.9553	0.9105	0.4948	0.9560	0.9089	0.5614	0.9512	0.9068	0.5038
prostate	0.8247	0.4070	0.4080	0.8249	0.4011	0.4212	0.8196	0.4039	0.4125
stroke	0.8387	0.2042	0.1847	0.8434	0.2032	0.2152	0.8250	0.2023	0.2187
avg	0.8729	0.5072	0.3625	0.8747	0.5044	0.3992	0.8652	0.5043	0.3783
leukemia	0.8507	0.2492	0.7392	0.8467	0.2477	0.7557	0.8397	0.2479	0.7897
nervous	0.4652	0.0177	0.2320	0.4693	0.0166	0.2385	0.4652	0.0182	0.2436
colon	0.7606	0.1138	0.4865	0.7587	0.1157	0.5024	0.7504	0.1159	0.5069
average	0.6921	0.1269	0.4859	0.6915	0.1266	0.4988	0.6851	0.1273	0.5134
alt	0.9983	0.1254	0.9632	0.9985	0.1267	0.9640	0.9966	0.1268	0.9037
disease	0.9231	0.0900	0.7589	0.9267	0.0853	0.7470	0.9002	0.0853	0.7405
function	0.9151	0.1045	0.8055	0.9255	0.1058	0.7974	0.8972	0.1041	0.7491
structure	0.9771	0.1636	0.8855	0.9807	0.1641	0.8853	0.9643	0.1629	0.8485
subcell	0.9854	0.1136	0.8990	0.9873	0.1139	0.8599	0.9795	0.1135	0.8487
average	0.9594	0.1194	0.8624	0.9637	0.1191	0.8507	0.9476	0.1185	0.8181
average									
	RELIEF			SVMONE			SMVRFE		
	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$	$\overline{S_W}$	$\overline{S_R}$	$\overline{S_S}$
ovarian	0.9697	0.9537	0.7296	0.9379	0.8476	0.5965	NA	0.8386	0.4680
prostate	0.9572	0.9399	0.5529	0.8685	0.7389	0.5243	NA	0.7323	0.4484
stroke	0.8806	0.8230	0.3410	0.8174	0.7032	0.2721	NA	0.6971	0.1678
avg	0.9358	0.9055	0.5411	0.8746	0.7633	0.4175	NA	0.7560	0.3614
leukemia	0.9157	0.8675	0.5793	0.8757	0.7655	0.4878	NA	0.7632	0.2678
nervous	0.8078	0.7839	0.2873	0.8099	0.6751	0.4568	NA	0.6728	0.1065
colon	0.9063	0.8363	0.6931	0.7782	0.6818	0.3512	NA	0.6799	0.2392
average	0.8766	0.8292	0.5199	0.8213	0.7074	0.4319	NA	0.7053	0.2045
alt	0.8278	0.6945	0.6908	0.9889	0.7468	0.6676	NA	0.7307	0.6517
disease	0.8270	0.6892	0.5277	0.8366	0.7033	0.5269	-	-	-
function	0.6764	0.6417	0.5444	0.7826	0.7169	0.3255	-	-	-
structure	0.7636	0.6678	0.5072	0.8543	0.7156	0.5325	-	-	-
subcell	0.8016	0.6881	0.6794	0.9328	0.7345	0.7663	-	-	-
average	0.7793	0.6763	0.5899	0.8790	0.7234	0.5638			

Table 2. Stability results for the different stability measures. $\overline{S_S}$ is computed on feature sets comprising the top ten features proposed by each method.

4 Stability Results

In this section we will examine the stability results along two dimensions:

- the behavior of the stability measures per se,
- and the stability performance of the feature selection algorithms

Table 2 gives the stability results for $\overline{S_W}$, $\overline{S_R}$, and $\overline{S_S}$, i.e., for weightings-scorings, rankings and selected feature sets, for the six different methods considered. The imposed cardinality of the final feature set influences the values of $\overline{S_S}$ but not of $\overline{S_W}$ and $\overline{S_R}$. $\overline{S_S}$ was computed on the feature sets of the best ten features selected by each method. SVMRFE does not produce a weighting-scoring of features so the computation of $\overline{S_W}$ does not make sense in that case; moreover in the case of the text mining datasets SVMRFE produced results only for the alt dataset, in the remaining text mining datasets its execution did not terminate within a reasonable amount of time. For SVMONE the stability results are computed on the square values of the coefficients of the linear hyperplane found by the support vector machine.

4.1 Discussion on stability measures

$\overline{S_W}$ and $\overline{S_R}$ take into account the complete feature preferences produced by a method, while $\overline{S_S}$ focuses on a given number of top ranked or selected features. Thus the former two provide a global view of stability of feature preferences while the latter focuses on a more precise picture of greater utility since feature preferences are used to select a feature set. $\overline{S_W}$ provides a finer grain picture of stability in comparison to $\overline{S_R}$ since it is based on the actual feature coefficients produced by a given method while the $\overline{S_R}$ uses the ranking of these coefficients. However this does not mean that the information provided by $\overline{S_W}$ is of greater value than that provided by $\overline{S_R}$, on the contrary. First, in practice ranks are of more direct utility in selecting the final set of features. A second disadvantage of $\overline{S_W}$ is that since it directly operates on the actual weights-scores produced by each method, its results are not directly comparable among different methods due to possible differences in scales and intervals of the weights-scores, a problem that does not appear in the case of ranks.

The results that the three measures of stability deliver can be contradictory, each one indicating a considerably different level of stability, eg the stability measurements of IG on the colon dataset (table 2), where $\overline{S_W}$ has a value of 0.7606, $\overline{S_R}$ a value of 0.1138 and $\overline{S_S}$ a value of 0.4865. These differences are a result of the way the three different measures are computed. $\overline{S_W}$ operates directly on the weightings-scorings produced by the feature selection method, if it happens that a method assigns exactly the same score to a large set of features the resulting $\overline{S_W}$ value can be quite high. In fact this was often the case with all the univariate feature selection that we examine here, all of them assign a score of zero to a large number of features. That was a side effect of the discretization process, used in conjunction with the univariate feature selection methods, which resulted in a large number of features with a single value thus the corresponding score of the feature was zero. In the case of the multivariate feature selection methods this happens much less often. $\overline{S_R}$ addresses this issue by breaking ties randomly, i.e. when two features have exactly the same score which would mean assigning to both of them the same rank k then we randomly assign to one of them a rank of k and to the other a rank of $k+1$. The reasoning behind the random breaking of ties is that when we ask a feature selection algorithm to select exactly k features, usually we have no way to prefer one feature over another when both have the same rank k. This explains why there can be such large discrepancies between the values of $\overline{S_W}$ and $\overline{S_R}$. Table 3 shows how many zero weights-scorings each feature selection method produces; when the number of zero weights is low then the values of $\overline{S_W}$ and $\overline{S_R}$ will be similar. The discrepancy between $\overline{S_R}$ and $\overline{S_S}$ is explained by the fact that the latter is focusing on the top k ranked features which can be extremely stable, especially when the value of k is low as it was in the case of the results given in table 2 ($k = 10$). This observation points to possible improved versions of S_R where similarities or differences on the top ranks are more heavily accounted for while differences and similarities in the lowest ranks are less accounted.

The pattern of agreement or disagreement between the three different measurements is as follows: usually the highest stability value will be given by $\overline{S_W}$; depending on whether there are fewer or more features with zero weighting, the value of $\overline{S_R}$ can be as high as that of $\overline{S_W}$ or considerably lower. The value of $\overline{S_S}$ does not correlate with that of the other two measurements, i.e. a low value of S_R does not necessarily translate to a low value of $\overline{S_S}$. Overall the most important information is delivered by $\overline{S_S}$, when we are examining the stability of the methods for sets of selected features of given cardinality, followed by $\overline{S_R}$ which provides an indication of stability of the complete feature preference. In the following sections we will focus on these two measures of stability.

	IG	CHI	SYM	RELIEF	SVMONE
ovarian	35.07	35.07	35.07	0	01.08
prostate	85.63	85.63	85.63	0	00.99
stroke	91.25	91.25	91.25	0	02.33
leukemia	87.68	87.68	87.68	0	16.21
nervous	98.48	98.48	98.48	0	09.91
colon	93.98	93.98	93.98	0	02.51
alt	94.33	94.33	94.33	05.56	09.72
disease	96.15	96.15	96.15	06.06	05.03
function	95.17	95.17	95.17	07.35	05.64
structure	92.82	92.82	92.82	06.88	05.69
subcell	95.19	95.19	95.19	06.13	07.91

Table 3. Percentage of features with zero score for each method.

4.2 Discussion on stability of feature selection algorithms

First of all there is no feature selection method that is consistently more stable than all the others for all the different problems that we examined. However it seems that there are types of problems for which a given method is more stable than the others.

In the case of the proteomics problems the most stable method seems to be RELIEF which achieved the highest stability scores in all three problems both in terms of $\overline{S_R}$ and $\overline{S_S}$. The feature preferences that RELIEF produces for the given type of problem are stable both globally, i.e. the ranking of the features does not change considerably with different training sets, and at the top, i.e. the ten top ranked features do not change considerably with changes in the training set. The global stability of RELIEF's feature preferences as measured by $\overline{S_R}$ is on average 0.9055 for the three proteomics datasets, considerably higher than all the other feature selection methods. For $\overline{S_S}$ RELIEF scores 0.7295, 0.5529 and 0.3410 for the ovarian, prostate and stroke datasets respectively. These scores correspond to an average overlap of 8.43, 7.12 and 5.08 features, out of the ten contained in the final set of selected features, among the different subsets of the training folds[1]. The rest of the methods have a considerably lower score.

In the case of the genomics datasets the picture is mixed. In terms of the global stability of the feature preferences measured by $\overline{S_R}$ the clear winner is again RELIEF, with an average score of 0.8292. The results of all the univariate methods are catastrophic, on average around 0.126, a fact that is due to the very large number of features to which these methods assigned a score of zero resulting in random rankings for these features. SVMONE and SVMRFE have relatively stable feature preferences, around 0.7. However when we turn to $\overline{S_S}$ the picture changes. For the leukemia dataset the univariate methods achieve the highest stability compared to all the other methods, the best being SYM with a score of 0.7897 (8.82 common features out of ten on average); for the nervous dataset the most stable algorithm is by far SVMONE and for colon RELIEF.

For the text mining problems in terms of the global stability the clear winner is SVMONE, with an $\overline{S_R}$ that is consistently higher than 0.7 for all datasets, followed by RELIEF. All univariate methods have a very low $\overline{S_R}$ score, in the best case around 0.16, again this is due to the large number of features to which these methods assign a score of zero. The picture changes radically when we examine the stability behavior with respect to $\overline{S_S}$. This time the most stable methods are the univariate methods with an average $\overline{S_S}$ score always above 0.8 (8.88 common features).

Overall RELIEF produces very stable feature preferences as these are evaluated by $\overline{S_R}$, being the most stable in all the proteomics and genomics datasets and the second most stable in the text mining datasets. When we evaluate the stability of the top ten selected features RELIEF is the clear winner in the proteomics datasets and on average the best for the genomics datasets. The univariate feature selection methods perform badly in terms of their global stability but better when we evaluate the stability of the top ten features, in fact for the text mining applications they are by far more stable than the other methods. The SVM based algorithms are somewhere in the middle getting the second place in terms of global stability in two out of the three application domains (proteomics, genomics). In what concerns the stability of the top ten selected features they do not have an application domain in which they excel.

[1] It is easy to compute the actual number of common features when we know the S_S score and the cardinality of the final feature set simply by the definition of S_S.

Examining the stability profiles of the different feature selection algorithms three groups of algorithms arise naturally, where the algorithms that belong to a given group share a very similar stability behavior. The first group consists of all the univariate feature selection algorithms, the second contains SVMONE and SVMRFE, while RELIEF is a group on each own since it does not have a stability behavior similar to any of the other methods.

IG, SYM and CHI have almost identical stability scores for all three measures of stability and all application domains considered. This is not a surprise since all of them are based in a similar principle, i.e. they select individual features on the basis of how well they discriminate among the different classes.

SVMONE and SVMRFE are quite similar in terms of $\overline{S_R}$—a fact that can be easily explained since the ranking of features provided by SVMONE can be considered as a less refined version of the ranking provided by SVMRFE, the former being the result of a single execution of the SVM algorithm and the latter the result of an iterative execution where each time 10% of the lower ranked features are removed. However in terms of $\overline{S_S}$ SVMONE appears to be more stable; for the proteomics datasets SVMONE has an average overlap of 7.47, 6.87, 4.27 features out of ten against 6.37, 6.19, 2.87 for SVMRFE for ovarian, prostate and stroke respectively. In the case of genomics datasets the difference is even greater, SVMONE has an average feature overlap of 6.55, 6.27, 5.19 against 4.22, 1.92, 3.86 for SVMRFE for leukemia, nervous and colon respectively; finally in alt the only text dataset in which SVMRFE terminated, the difference is small: 8 and 7.9. Here too the fact that SVMRFE is based on multiple iterations explains its higher instability on the top ten ranked features. When the differences of the coefficients of two features are rather small and a choice is about to be made on which of the two to eliminate, different training sets could result in opposite rankings for these two features thus eliminating a different feature each time.

The results of the estimation process of $\overline{S_S}$ can be very eloquently visualized, not only providing insight on the stability of each method, but also clearly indicating which features are considered important by each method. An example of such a visualization for one dataset from each application domain is given in figure 1, where the cardinality of the final feature set is set to ten. In each of the graphs the x-axis corresponds to the individual features. The y-axis is separated into 10 rows, each one corresponding to one of the outer cross-validation folds. Within each row we find 10 rows (not visibly separated) corresponding to each of the inner cross-validation folds of the outer fold. A perfectly stable method, i.e. one that always chooses the same features, would have in its graph as many vertical lines as the cardinality of the final feature set. Each line would correspond to one selected feature.

Examining figure 1 it is obvious that the most stable behavior for all algorithms is attained for the alt dataset while the less stable in the case of the nervous dataset, with prostate being somewhere in the middle. In the case of the alt dataset it is clear that the univariate methods are more stable than RELIEF, SVMONE and SVMRFE. The visual inspection of the graphs allows for a clear understanding of which features are considered most important by each method. We can see that the three univariate methods select roughly the same features on each dataset. The feature patterns established by SVMONE and SVMRFE are also similar between them, albeit to a lesser extent, while RELIEF has a distinctively different pattern from all the other methods. Moreover it is clear that the actual value of stability is affected by the dataset examined with some datasets resulting in systematically higher levels of stability for all algorithms.

4.3 Stability profiles with $\overline{S_S}$

The more interesting stability estimation is provided by $\overline{S_S}$ since it focuses on a subset of features, the ones selected by each method, which is actually what interests us when we are performing feature selection. Nevertheless this estimation is specific to a given number of selected features. To get a more global picture of the stability profile of the different methods with respect to $\overline{S_S}$ we computed its values for different sizes of selected feature sets, ranging from 10 up to the cardinality of the full feature set in increments of five, the results are given in figure 2. However as the cardinality of the selected feature set increases so does the estimated value of stability simply because with a larger number of selected features there is also a higher probability that there will be more features in common only due to chance. To quantify the increase in stability attributed to the increasing cardinality of the selected feature set we included as a stability baseline a random feature selector that outputs random feature sets of a given cardinality. We should note here that the computation of the curves does not require any extra application of the feature selection algorithms other than that described in the previous section for estimating the different stability measures, the reason is that each algorithm simply outputs a complete feature preference which can be readily used to compute the values of $\overline{S_S}$ for different feature set cardinalities.

The univariate feature selection methods have an acceptable stability performance only for low cardinalities of feature sets for almost all datasets, with the exception of ovarian. After a point their behavior converges to that of the random selector and they are dominated by the remaining three algorithms, a fact that as already mentioned is due to the discretization method used with them. For low feature set cardinalities they dominate all other algorithms in all the text mining problems and they

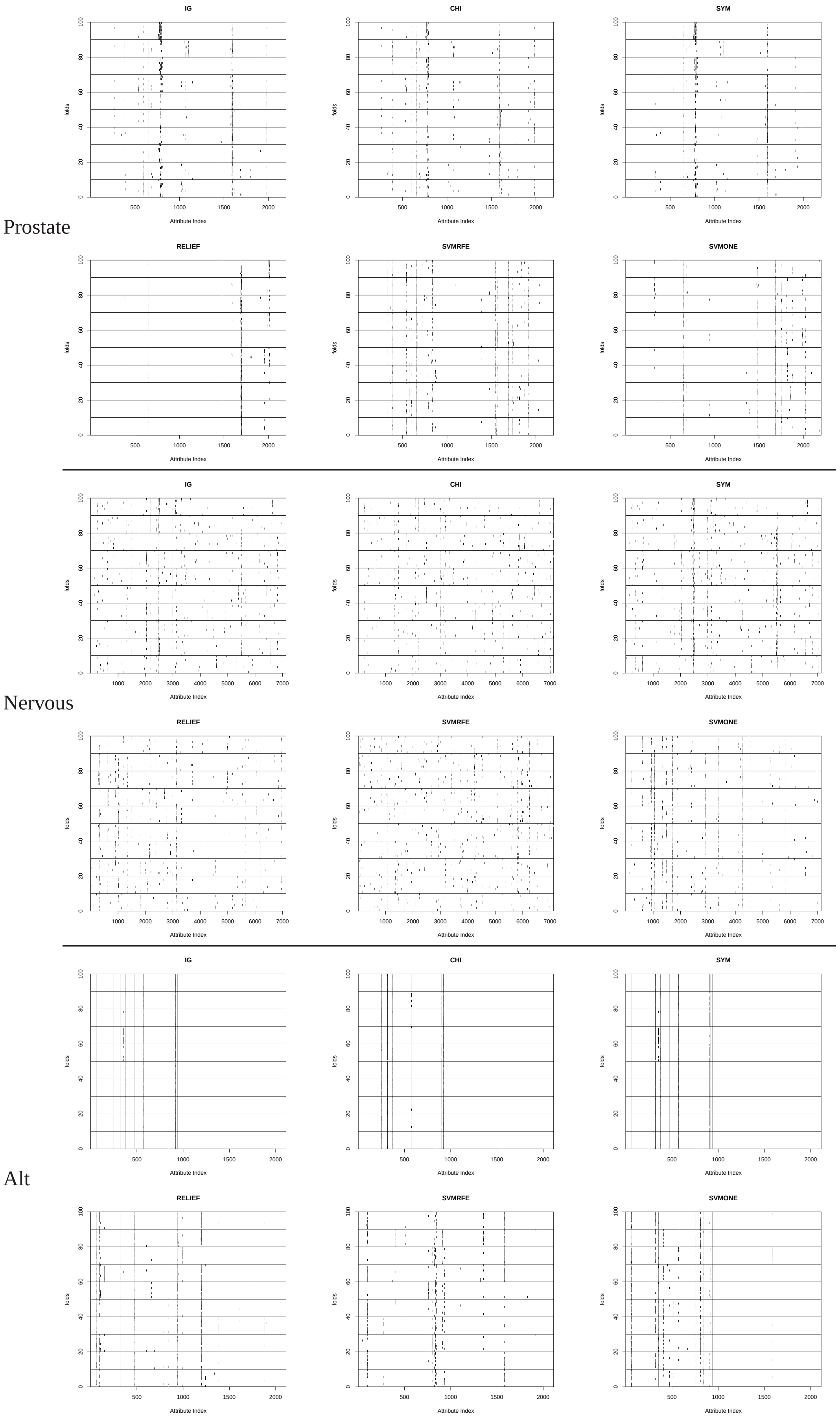


Figure 1. Stability results for three selected datasets, one from each type of application (selected feature sets of cardinality 10).

have a slight advantage in the proteomics and in two of the three genomics datasets (leukemia and colon) over the SVM based algorithms. RELIEF has an almost systematic advantage over the other methods for two out of the three proteomics datasets (prostate, stroke). For all types of problems it appears to have a better (proteomics, genomics problems) or similar (text mining problems) stability profile with the SVM based algorithms.

The global relation of the stability profiles of the different algorithms is nicely summarized by the $\overline{S_R}$ measure. For example in the case of the leukemia dataset RELIEF which has the best stability profile overall the other algorithms has also the highest $\overline{S_R}$ value (0.8675). The SVM based algorithms have the next better stability profile with an $\overline{S_R}$ value around 0.754, while the univariate methods are the worst with an $\overline{S_R}$ value around 0.247. While $\overline{S_R}$ captures the global picture it is not able to capture the finer details, for example in the same dataset there is a range of feature set cardinalities in which the univariate methods clearly dominate the SVM based algorithms, and they are very similar to RELIEF.

Examining the graphs in figure 2 the separation of the feature selection algorithms in three groups is clearly visible. The three univariate feature selection methods have an indistinguishable stability profile for all the datasets to the point that the lines depicting their profile become one. SVMONE and SVMRFE have also a very similar profile with SVMONE being more stable on feature sets of lower cardinality, nevertheless as the cardinality increases their profiles converge and after a point, which depends on the dataset, they become indistinguishable. As we move to higher cardinalities, both methods add low ranked features; these should be more or less the same for both methods since for SVMRFE they are determined at the earliest iterations of the algorithm, thus resembling closely the behavior of SVMONE's single run. For lower cardinalities the instability of SVMRFE increases due to the already mentioned fact that small differences in the coefficients can inverse the rank and thus remove different features. The difference in instability between SVMONE and SVMRFE increases as we move to lower cardinalities where the final feature sets of SVMRFE are determined during the last iterations of the SVM algorithm.

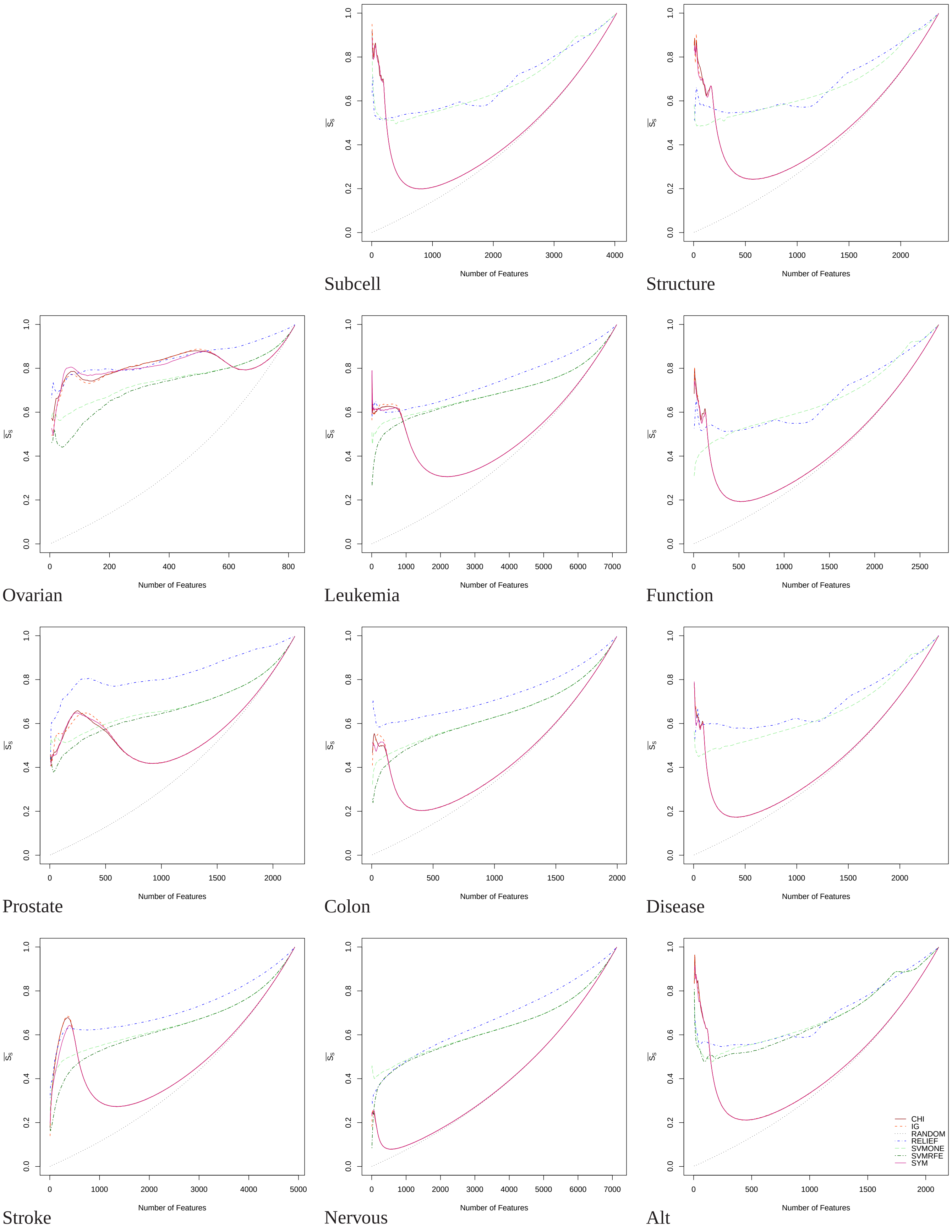
Looking more closely at the behavior of the univariate methods we see that they reach a peak after which their stability drops dramatically and their stability profile converges to that of the random feature selector. The peak before the dramatic drop in stability corresponds to the inclusion of all features whose score was different than zero. After this point features are actually included randomly. The three remaining algorithms, RELIEF, SVMONE and SVMRFE exhibit a different pattern of stability. In almost all the datasets their $\overline{S_S}$ value reaches a plateau, either starting from lower values and increasing creating an upwards looking ”knot” (this can be observed in all the proteomics datasets), or starting from higher values and decreasing creating a downwards looking ”knot” (this can be observed in all the text mining datasets). After reaching the plateau their stability values increase very slowly. In both cases reaching the plateau means that afterwards the stability value changes mainly due to the increase of the feature set cardinality, i.e. the algorithms do not select anymore features in an strongly informative manner. In some sense the stability of the algorithms converges at the stability value observed in the beginning of the plateau. A similar plateau is observed also for the univariate feature selection methods in the case of the ovarian dataset. Note that the beginning of the plateau does not necessarily correspond to the most stable feature set size. In the cases where it defines an upward looking knot this is true; in the cases where it defines a downwards looking knot it corresponds to the minimal stability feature set size, all feature sets with less features would have a higher stability.

The identification of the start of the plateau can provide a means of bounding the maximum cardinality, k, of the selected feature sets. In terms of information content it would not make sense to have feature sets of higher cardinality since the new features will not be incorporated in an strongly informative manner. This is an important observation that could guide the selection of the appropriate number of features. In almost all feature selection algorithms we have to set either a threshold or a number of selected features but usually there is no informed way this could be done and we most often rely on extensive cross validation using accuracy estimations to select the appropriate values. Reaching the plateau indicates that we should stop adding new features since selection is not done anymore in an informative manner.

5 Stability and Classification Performance

A feature selection algorithm alone can provide an indication of which features are informative for classification but it cannot provide an estimate of the discriminatory power of these features, since it does not construct classification models whose error could be estimated. In the same manner stability results cannot provide the sole basis on which to select an appropriate feature selection algorithm; nevertheless they can support the selection of a feature selector when the latter is coupled with a classification algorithm, and increase the confidence of the users in the analysis results (provided that the feature selection is found to be stable).

Lets suppose that we use some resampling technique to perform error estimation of a pair of feature selection and classification algorithms. If the feature selection algorithm selects consistently the same features then we can have more confidence



Subcell

Structure

Ovarian

Leukemia

Function

Prostate

Colon

Disease

Stroke

Nervous

Alt

Figure 2. $\overline{S_S}$ **plots for varying cardinalities of the final feature set.**

in the importance of the selected features and a higher confidence in the error estimates. The latter because the models produced in the different folds of the resampling will be similar (at least in terms of the features they contain) a fact that means that the averaged error estimation we get corresponds to a model that remains relatively constant among different folds. One of the problems of the resampling based error estimations is that they evaluate algorithms and not specific classification models, nevertheless in practice what is going to be used is a single classification model that is the result of the learning phase of the algorithms. If the models are similar among the different resamples then we move closer to an estimate of the performance of a given model. The simplest scenario of using the stability and error estimation to select the appropriate algorithms goes as follows: couple a given classification algorithm with a number of feature selection algorithms and estimate the classification performance and the stability of the feature selector using the process described in section 2. Then calculate the statistical significance of error differences. Among the feature selection algorithm-classification algorithm combinations that are found to be better than all the others, choose the combination that contains the most stable feature selector.

To demonstrate the above idea we selected as classification algorithm a linear SVM, setting its complexity parameter to 0.5. We performed a series of experiments in which we paired each feature selection algorithm and the linear SVM. In the following when we will refer to a feature selection algorithm we will actually mean the pair of the feature selection algorithm with the linear SVM. From the univariate feature selection methods we have chosen to report results only for Information Gain since the others had a very similar behavior. For every dataset we fixed the number of selected features to N, with N ranging from 10 to 50 in steps of 10. For a given N the four feature selection algorithms were compared with respect to their classification error and their stability. The statistical significance of error differences was computed using McNemar's test with a significance level of 0.05. To rank the feature selection algorithms on a given dataset and for a given number N of selected features we used the following approach: if two algorithms A and B had a classification performance that was not significantly different, then each was assigned 0.5 points; if A was significantly better than B then A was assigned one point and B zero. The rank of an algorithm is given by the sum of its points. The complete results are given in tables 4,5, 6 for the proteomics, genomics and text mining datasets respectively. Each entry in the above tables gives the rank, classification error, and the $\overline{S_S}$ stability estimate for a given feature selection algorithm, top ranked algorithms are noted in *italics*.

Applying the algorithm selection scenario mentioned above we see that there are many cases in which there is a number of algorithms ranked on the top position in terms of classification error but whose stability values differ considerably. In the case of the proteomics datasets this is observed often in the Stroke dataset and less often in the case of ovarian. In the Stroke dataset the algorithms do not have a significantly different classification performance for $N = 30, 40$ and 50. In these cases SVMRFE is by far the less stable algorithm with an $\overline{S_S}$ which is always less than 0.20, while RELIEF has a value of stability which is more than double. Similar observations can be done in the case of ovarian dataset. In the genomics datasets we can see that for leukemia the algorithms have an indistinguishable performance for any value of N but a great difference in their stability values. Again SVMRFE has systematically a very low stability which can be as low as 1/3 of the stability value of the most stable algorithm. For example for $N = 10$ IG has a stability value of 0.7392 while SVMRFE has a value of 0.2678. A similar picture appears also in the colon dataset, with SVM and SVMRFE being very far from the most stable algorithm, RELIEF ($N = 10, 20$ and 30). Similar observations are in order also in the case of the text mining datasets; the most stable feature selection algorithm, for the range of N values examined here, is IG, which also appears in the top position in terms of classification performance in all datasets and almost all values of N.

We should note here that high instability, as measured by $\overline{S_S}$, is not necessarily associated with a low classification performance. Among the cases examined there were many in which the best performing algorithm was the most unstable, e.g. SVMRFE in stroke, ovarian for $N = 10, 20$, and prostate for all values of N, or cases in which among the best performing there were also algorithms with high instability e.g. SVM and SVMRFE in the colon dataset, $N = 10, 20$ and 30. One possible explanation for that is redundancy. Among the initial full feature set there are possibly many different subsets on which classification models can be constructed that can accurately predict the target concept. Such cases of instability coupled with high classification performance, can be an indication of redundancy within the full feature set. Nevertheless this is a hypothesis that remains to be verified.

Stability provides an objective criterion on which we can base our choice of feature selection algorithm in the absence of any significant difference in classification performance. Selecting the most stable algorithm we have a higher confidence in the quality of the features that it selects but also a higher confidence in the corresponding classification performance. Moreover coupling the selection procedure with a visual representation of stability, as the one given in figure 1, we get a clear picture of the important features and how robust they are to perturbations of the training set.

6 Conclusions and Future Work

To the best of our knowledge this is the first proposal of a framework that measures the stability of feature selection algorithms. We defined the stability of feature selection algorithms as the robustness of the ”feature preferences” they produce to training set perturbations. We examined three different stability measures and proposed a resampling technique to empirically estimate them. The most interesting one was based on S_S, a measure of the overlap of two feature sets. We exploited the framework to investigate the stability of some well known feature selection algorithms on high dimensional datasets from different application domains. We showed how we can use stability to support the selection of a feature selection algorithm among a set of equally performing algorithms.

We believe that the notion of stability is central in real world applications where the goal is to determine the most important features. If these features are consistent among models created from different training data, the confidence of the users in the analysis results is strengthened. The results of the empirical estimation of stability can be elegantly visualized and provide a clear picture of the relevant features, their robustness to different training sets, and the stability of the feature selection algorithm.

Future work includes refining the S_R stability measure in order to reflect better large differences and similarities on top ranked features. Exploring the stability profile in order to perform feature selection. Exploiting the notion of similarities between feature preferences to quantify the similarities of different feature selection algorithms. Aggregating the different feature sets produced from subsamples of a given training set in what can be viewed as the analogue of ensemble learning and model combination for feature selection; to draw a parallel with bias-variance, where aggregating models of a learning algorithm with a high variance can reduce classification error, we could combine feature sets of an unstable feature selection algorithm to increase stability and possibly classification performance afterwards.

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Stroke				
N	IG	Relief	SVM	SVMRFE
10	1.5-32.22-0.1847	1.5-30.29-0.3410	1.0-37.02-0.2721	*2.0-26.45-0.1678*
20	1.0-31.73-0.2612	1.0-28.85-0.3670	1.0-35.10-0.3101	*3.0-21.64-0.1679*
30	*1.5-27.89-0.2944*	*1.5-27.41-0.3830*	*1.5-28.37-0.3390*	*1.5-23.56-0.1802*
40	*1.5-29.81-0.3261*	*1.5-25.97-0.3887*	*1.5-25.00-0.3583*	*1.5-25.49-0.1886*
50	*1.5-27.89-0.3576*	*1.5-28.37-0.4013*	*1.5-26.45-0.3801*	*1.5-25.49-0.1997*
Ovarian				
N	IG	Relief	SVM	SVMRFE
10	1.0-10.28-0.4948	1.0-10.28-0.7296	1.0-07.11-0.5965	*3.0-01.19-0.4680*
20	1.0-05.53-0.6111	1.0-05.93-0.6933	1.5-03.95-0.5897	*2.5-01.19-0.4749*
30	0.0-04.74-0.6567	*2.0-01.58-0.6966*	*2.0-01.19-0.5631*	*2.0-00.40-0.4498*
40	0.5-03.16-0.7011	1.5-01.58-0.7080	*2.0-00.40-0.5682*	*2.0-00.40-0.4401*
50	*1.5-02.77-0.7496*	*1.5-01.58-0.7368*	*1.5-00.40-0.5825*	*1.5-00.40-0.4473*
Prostate				
N	IG	Relief	SVM	SVMRFE
10	1.0-18.64-0.4073	1.0-18.95-0.5842	1.0-18.02-0.5308	*3.0-13.05-0.4417*
20	1.0-17.71-0.4299	1.0-17.09-0.6044	1.0-16.46-0.5131	*3.0-11.50-0.4006*
30	1.0-16.46-0.4639	1.0-15.84-0.6170	1.0-14.91-0.5193	*3.0-10.87-0.3786*
40	1.0-16.15-0.5044	1.0-14.91-0.6214	1.0-13.36-0.5280	*3.0-09.01-0.3848*
50	1.0-14.60-0.5374	1.0-13.36-0.6304	1.0-13.05-0.5343	*3.0-09.32-0.3890*

Table 4. Results on the proteomics datasets, each triplet of the form $x-y-z$ gives the ranking, x, of the feature selection algorithm for the specific number of selected features, the classification error, y, and the $\overline{S_S}$ value, z. In *italics* the feature selection algorithms that are ranked at the top.

leukemia				
N	IG	Relief	SVM	SVMRFE
10	*1.5-05.55-0.7392*	*1.5-06.94-0.5793*	*1.5-05.55-0.4878*	*1.5-05.55-0.2678*
20	*1.5-05.55-0.6570*	*1.5-04.16-0.6553*	*1.5-04.16-0.4544*	*1.5-01.38-0.2979*
30	*1.5-05.55-0.6294*	*1.5-02.77-0.6338*	*1.5-02.77-0.4681*	*1.5-01.38-0.3108*
40	*1.5-05.55-0.5958*	*1.5-02.77-0.6360*	*1.5-02.77-0.4852*	*1.5-01.38-0.3336*
50	*1.5-04.16-0.5938*	*1.5-02.77-0.6255*	*1.5-02.77-0.4921*	*1.5-01.38-0.3526*
nervous				
N	IG	Relief	SVM	SVMRFE
10	*1.5-40.00-0.2320*	*1.5-30.00-0.2873*	*1.5-35.00-0.4568*	*1.5-36.66-0.1065*
20	*1.5-38.33-0.2491*	*1.5-30.00-0.2973*	*1.5-30.00-0.4469*	*1.5-40.00-0.1498*
30	*1.5-35.00-0.2506*	*1.5-36.66-0.3124*	*1.5-36.66-0.4288*	*1.5-28.33-0.1909*
40	1.5-35.00-0.2488	1.0-40.00-0.3158	1.0-36.66-0.4174	*2.5-23.33-0.2129*
50	1.5-31.66-0.2501	1.0-41.66-0.3283	1.0-38.33-0.4127	*2.5-23.33-0.2349*
colon				
N	IG	Relief	SVM	SVMRFE
10	*1.5-17.74-0.4856*	*1.5-16.12-0.6931*	*1.5-25.80-0.3512*	*1.5-16.12-0.2392*
20	*1.5-17.74-0.5143*	*1.5-14.51-0.6530*	*1.5-22.58-0.3950*	*1.5-19.35-0.2810*
30	*1.5-14.51-0.5224*	*1.5-14.51-0.6174*	*1.5-16.12-0.4121*	*1.5-19.35-0.3115*
40	1.5-14.51-0.5459	*2-12.90-0.5937*	1.5-16.12-0.4229	1.0-22.58-0.3261
50	1.5-14.51-0.5519	*2-12.90-0.5837*	1.5-14.51-0.4311	1.0-22.58-0.3470

Table 5. Results on the genomics datasets.

		alt			disease	
N	IG	Relief	SVM	IG	Relief	SVM
10	*1.0-10.77-0.9623*	*1.0-10.87-0.6908*	*1.0-10.89-0.6676*	*1.0-19.67-0.7589*	*1.0-19.46-0.5277*	*1.0-19.64-0.5269*
20	*1.5-10.56-0.8631*	1.0-10.84-0.6187	0.5-11.01-0.6191	*1.0-19.74-0.6778*	*1.0-19.36-0.5766*	*1.0-19.43-0.4790*
30	*1.0-10.68-0.8209*	*1.0-10.80-0.6103*	*1.0-10.58-0.5832*	*1.0-19.83-0.6282*	*1.0-19.24-0.6282*	*1.0-19.80-0.4691*
40	*1.0-10.58-0.7996*	*1.0-10.65-0.5719*	*1.0-10.65-0.5549*	0.5-19.98-0.6124	*2.0-19.09-0.6670*	0.5-19.92-0.4536
50	*1.0-10.46-0.7733*	*1.0-10.58-0.5545*	*1.0-10.51-0.5311*	*1.0-19.52-0.6133*	*1.0-19.02-0.6250*	*1.0-19.77-0.4489*
		function			structure	
N	IG	Relief	SVM	IG	Relief	SVM
10	*1.5-20.24-0.8055*	0.5-20.93-0.5444	1.0-20.37-0.3255	*2.0-21.02-0.8855*	0.5-22.66-0.5072	0.5-21.84-0.5325
20	*1.0-20.29-0.7129*	*1.0-20.93-0.6304*	*1.0-20.45-0.3694*	*2.0-19.78-0.8141*	0.0-22.26-0.6296	1.0-20.77-0.4977
30	*1.0-20.27-0.6824*	*1.0-20.93-0.6566*	*1.0-20.47-0.3789*	*2.0-19.39-0.8481*	0.0-21.95-0.6486	1.0-20.40-0.4853
40	*2.0-20.06-0.6824*	0.5-20.93-0.6032	0.5-20.68-0.3916	*2.0-19.05-0.7718*	0.5-20.54-0.6288	0.5-19.80-0.4889
50	*2.0-19.98-0.6649*	0.5-20.93-0.5732	0.5-20.68-0.3996	*1.5-19.08-0.7331*	0.0-20.71-0.6062	*1.5-19.50-0.4866*

		subcell	
N	IG	Relief	SVM
10	*1.5-15.97-0.8980*	0.0-16.72-0.6794	*1.5-15.80-0.7663*
20	*1.5-15.84-0.8646*	0.0-16.47-0.7110	*1.5-15.43-0.6749*
30	*1.5-15.48-0.8039*	0.0-16.49-0.5878	*1.5-15.19-0.6349*
40	*1.5-14.86-0.8117*	0.0-16.48-0.5438	*1.5-15.03-0.6044*
50	*1.5-14.64-0.8460*	0.0-16.44-0.5339	*1.5-14.93-0.5773*

Table 6. Results on the text mining datasets.

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