A Numeric Comparison of Variable Selection Algorithms for Supervised Learning

G. Palombo[*]
University of Milan - Bicocca
E-mail: palombo@caltech.edu

I. Narsky
California Institute of Technology
E-mail: narsky@hep.caltech.edu

Datasets in modern High Energy Physics (HEP) experiments are often described by dozens or even hundreds of input variables. Reducing a full variable set to a subset that most completely represents information about data is therefore an important task in analysis of HEP data. We compare various variable selection algorithms for supervised learning using several datasets such as, for instance, imaging gamma-ray Cherenkov telescope (MAGIC) data found at the UCI repository. We use classifiers and variable selection methods implemented in the statistical package StatPatternRecognition (SPR), a free open-source C++ package developed in the HEP community (http://sourceforge.net/projects/statpatrec/). For each dataset, we select a powerful classifier and estimate its learning accuracy on variable subsets obtained by various variable selection algorithms. When possible, we also estimate the CPU time needed for the variable subset selection. The results of this analysis are compared with those published previously for these datasets using other statistical packages such as R and Weka. We show that the most accurate, yet slowest, method is a wrapper algorithm known as generalized sequential forward selection ("Add N Remove R") implemented in SPR.

XII Advanced Computing and Analysis Techniques in Physics Research
November 3-7 2008
Erice, Italy

[*]Speaker.

1. Introduction

A crucial task in analysis of High Energy Physics (HEP) data is separation of signal and background events [1]. In modern HEP analysis, Supervised Machine Learning (SML) techniques are often used to classify observed events as signal or background. SML is an inductive process of learning a function from a given set of events typically collected in a training set. Each event is described by a vector of input variable values (such as momenta, energy, etc.) and a class label (typically signal and background). The task is to derive a classifier that is able to predict accurately class labels for unseen events [2–5]. The measure of the classifier performance is called Figure-Of-Merit (FOM).

The number of input variables can be very high and the analysis can involve a huge number of events. Variable Selection (VS) in classification addresses the problem of reducing the variable set to a subset that most completely represents information about the SML problem [2]. VS is usually based on filter, wrapper, or embedded approaches. In the filter approach, the selection is performed using only information present in the data, without considering information from the underlying learning algorithm [6]. It can be seen as a pre-processing step which involves only intrinsic characteristics of the data. In the wrapper approach, VS optimizes directly the induction algorithm performance to select the best subset of variables [7]. To do that, many different possible subsets of variables are generated and, then, evaluated on an independent test set which is not used during the search. Embedded algorithms are specific to a given algorithm too, but, in contrast to wrapper algorithms, they incorporate VS directly into the learning process [6]. They typically select the most important variables according to a variable ranking strategy, where the variable rank depends on the relevance of this variable in the learning process. Embedded methods are not new: CART decision trees introduced by Breiman et al. [3] in 1984 already have a built-in mechanism to estimate variable importance. Since they evaluate the variable importance during the learning process, they are faster than wrappers. Filter algorithms are usually the fastest, however they are typically outperformed by methods which take into account the induction algorithm [6, 7].

Removing variables irrelevant for the classification problem can considerably reduce the time needed by the learning process and gives the chance to interpret and analyze the results more easily and quickly. Also, some algorithms are not robust with respect to irrelevant or noisy variables and their performance degrades when the variable pool is polluted with poor predictors.

In this paper we compare the performance of various VS methods applied to the same sets of data. Section II of the paper describes briefly statistical tools used in our study. Section III shows the performance of various VS algorithms on several datasets. Section IV draws conclusions from this analysis.

2. Statistical Analysis Tools

For the data analysis we use the statistical packages SPR (release 08-00-00) [8], R (release 2.6.2) [9], and Weka (release 3.5.7) [10]. We describe briefly the SPR package. For details on SPR, R, and Weka see the references above.

SPR is a C++ package for SML. It implements linear and quadratic discriminant analysis [11], logistic regression [2], a binary decision split, a bump hunter [12], two flavors of decision trees

[3, 4, 13] (one for fast machine optimization and the other for easy interpretation by humans), a feedforward backpropagation neural net with a logistic activation function [14] , several flavors of boosting [15] including the arc-x4 algorithm [16] , bagging [17] and random forest [18], and an algorithm for combining classifiers trained on subsets of input variables [19]. The algorithms listed above can only be used for separation of two classes, signal and background. The package also includes two multiclass methods [19], one of which is described later in this paper; these algorithms reduce a problem with an arbitrary number of classes to a set of two-class problems and then convert the solutions to these binary problems into an overall multi-category classification label.

In this study, we mainly use tree-based classifiers. Therefore, we briefly review Decision Trees (DT), Boosted Decision Trees (BDT) and Random Forest (RF). The structure of a single DT is rather simple. At every step, the algorithm considers all possible binary splits on each variable and splits on the variable which improves the FOM most. It continues to split the two daughter nodes into smaller nodes recursively until a stopping criterion is satisfied. A node which is not split into daughter nodes is a leaf. A leaf is labeled as signal if there are more signal events in this node than background events. Various measures are used to search for optimal decision splits; for details look elsewhere [13].

DT usually offer a weak predictive power. However, ensemble methods can significantly improve the accuracy of weak classifiers such as DT by combining and averaging many weak classifiers. One ensemble method is called boosting. Boosting grows decision trees sequentially increasing weights of misclassified events after every tree and growing a new tree on the reweighted training data. Classification labels for test data are then computed by taking a weighted average of all trees grown by the algorithm.

Another ensemble method is RF applied in conjunction with bagging. Many decision trees are grown on bootstrap replicas of training data, where each bootstrap replica is obtained by sampling N out of N with replacement. In addition, RF selects input variables for each decision split and thus introduces even more randomness in the algorithm. Classification labels for test data are then obtained by taking a majority vote of the grown trees.

The SPR classifiers are implemented in a flexible framework utilizing the full power of object-oriented programming. Because all classifiers inherit from the same abstract interface, one can easily substitute one classifier for another. This modular approach makes the package scalable for highly complex applications. For example, SPR is capable of boosting or bagging an arbitrary sequence of classifiers included in the package.

Besides multivariate classifiers, SPR implements tools for computation of data moments including correlations between variables, bootstrap analysis of data and others. SPR is distributed under General Public License (GPL) off Sourceforge [20]. Support is provided for two versions of the package: a standalone version that uses ASCII text for input and output of data, and a ROOT-dependent version [21]. The user can choose between the two versions during installation by setting an appropriate parameter of the configuration script. No graphical tools are offered for the ASCII version of the package; however, one can go through the full analysis chain using ASCII output from SPR executables, as long as one can tolerate digesting information in the form of text tables instead of plots. The ROOT version of the package allows the user to call SPR routines from an interactive ROOT session and plot output of various SPR methods using supplied ROOT scripts for graphical data analysis. Algorithms for variable selection implemented in SPR are discussed below.

One of the several VS algorithms for classification implemented in SPR is a quick filter algorithm which ranks variables by their correlation with the class label (we will call it "Correlations" in this work). The larger the correlation, the more important is this variable for classification.

Another method for estimation of variable importance is the "Permutations" algorithm implemented in SPR. The idea behind this method is similar to that proposed by Breiman [18] for out-of-bag estimates. A trained classifier is applied to events not included in the data used for training and a performance measure such as, e.g., quadratic loss

$$\Delta = \frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i))^2 , \tag{2.1}$$

is recorded, where y_i is the true class of event i, $f(x_i)$ is the predicted class of event i, and N is the number of events. Then, this classifier is applied to these events with class labels randomly permuted across each variable in turn and the change in the performance measure due to this permutation for each variable is estimated. The SPR implementation lets the user specify the number of permutations across each variable, producing more accurate estimates as this number increases. Unlike Breiman's method for the out-of-bag estimate, the classifier is applied to independent test data; furthermore, an ensemble of weak learners such as, e.g., RF is applied to the test events as a whole, without evaluating the out-of-bag performance for each tree. The "Permutations" method is versatile as it can be used with any classifier, not just ensemble members trained on bootstrap replicas.

For DT and their ensembles, one can estimate variable importance by adding up changes in the optimized FOM such as, e.g., the Gini index due to splits imposed on each variable [3]. We refer to this popular embedded algorithm as "FOM Importance".

Another algorithm for VS implemented in SPR sorts input variables by their interaction with the rest of the variables ("Interactions"). Interaction between two variable subsets S_1 and S_2 is defined as:

$$\rho = \frac{\Sigma_i(f(S_{1i}) - \overline{f}(S_1))(f(S_{2i}) - \overline{f}(S_2))}{\sqrt{\Sigma_i(f(S_{1i}) - \overline{f}(S_1))^2}\sqrt{\Sigma_i(f(S_{2i}) - \overline{f}(S_2))^2}}, \tag{2.2}$$

where $f(S_1)$ and $f(S_2)$ are classifier responses at a given point integrated over all the variables not included in subsets S_1 and S_2, respectively. $\overline{f}(S_1)$ and $\overline{f}(S_2)$ are the means of $f(S_1)$ and $f(S_2)$. The algorithm sorts variables by their interaction in the descendant order. In a stepwise manner it chooses the variable interacting most with all other variables except those included in the optimal subset at earlier steps. The order in which the variables are selected gives the variable importance rank. This algorithm needs to compute K*(K-1)/2 interactions, where K is the dimensionality of the dataset. For datasets with many variables and a huge number of events, this could be very time consuming. To reduce the CPU time needed by the algorithm, the SPR implementation allows the user to choose the number of points, picked randomly from the dataset, used to calculate the interactions.

A well-known wrapper VS method is Forward Stepwise Addition (FSA)[22] . This method, once defined a FOM, adds one variable at a time, trains the classifier, computes the FOM, and chooses the variable with the greatest improvement in the FOM. This addition continues as long as it is possible to improve the FOM. A disadvantage of FSA, as implemented in Weka and R, is that an added variable cannot be removed. For instance, if a variable is part of the best subset with x variables but is not part of the best subset with x+1 variables, FSA is not able to find the optimal subset with x+1 variables.

SPR overcomes the disadvantage of FSA by implementing a more flexible generalization of the forward stepwise addition method, “Add n Rem r”. At each step the subset with the smallest loss on the test set is selected by adding n and removing r variables, where the values of “n” and “r” are chosen by the user.

3. Tests of Variable Selection Methods

We evaluate several methods implemented in the statistical packages SPR, R, and Weka. The datasets used in this analysis are taken from the machine learning repository of the University of California at Irvine (UCI) [23]. We include one astrophysics dataset and 4 datasets related to medical research. We could have as well performed this study using HEP data. However, HEP data are proprietary and rarely shared among different HEP experiments. Moreover, well documented applications of SML algorithms to HEP data are hard to find. In contrast, datasets at the UCI repository are publicly available and were thoroughly studied from the SML perspective. The methodology described in this study can be applied to HEP data in exactly the same way.

If a dataset has more than 1000 events, it is split into a training set (2/3 of the events) and a test set (1/3 of the events). The classifier is optimized using the training set and the performance is evaluated using Receiver Operating Characteristic (ROC) curve for the independent test set, where ROC is a graphical plot of true signal rate (y-axis) vs. false signal rate (x-axis). The larger is the area under the ROC, the better is the classifier performance. For datasets with less than 1000 events, 10-fold cross-validation is used to train the classifier and estimate its accuracy. That is, if we take k as the number of cross-validation folds, the dataset is split into k folds. Then k-1 subsets are used for training and the remaining one is used for testing. This is done k times, with each of the k subsets used exactly once as the test set. At the end, the FOM is obtained by averaging the FOMs from all the folds.

To check how sensitive are results obtained by the same algorithm to the number of cross-validation folds, we also run 3-fold cross-validation. For any dataset, results from 3-fold and 10-fold cross-validation are consistent within statistical errors. This is why we show only results obtained by 10-fold cross-validation. The error on the classification accuracy estimate obtained by cross-validation is computed using:

$$\varepsilon = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(a_i - \overline{a})^2} \tag{3.1}$$

where a_i is the classification accuracy for the test subset i, $\overline{a}$ is the average accuracy and N is the number of folds. This estimate is biased [24], because it does not account for correlations between the splits.

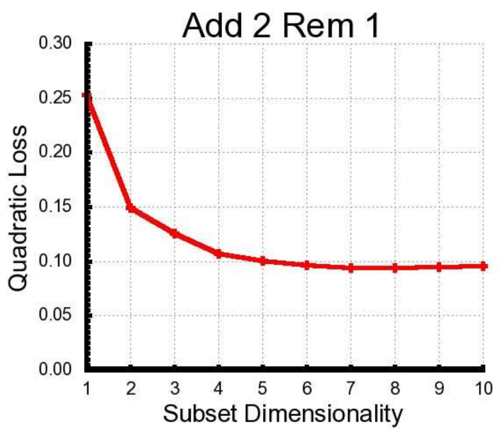


Figure 1: Magic telescope dataset: quadratic classification loss as a function of the best subset dimensionality. The best 6 variables selected are: Alpha, Length, Size, Width, Dist, and Conc.

For the "Interactions" method, we choose 500 points for integration for datasets with more than 500 events and all points for datasets with less than 500 events.

For each dataset, we find the best classifier among those available in SPR by comparing their predictive power. If several classifiers show comparable performance, we choose the fastest.

3.1 Magic Gamma-ray Telescope

This simulated dataset involves a binary classification task with 10 variables and 19020 events (12332 signal events and 6688 background events). Performance of several classifiers on these data has been studied in Ref. [25].

We use a RF classifier with 200 trees, at least 1 event per leaf, and with each split chosen among 3 variables randomly selected at each node.To find important variables, we run "Add 2 Rem 1", adding 2 and removing 1 variable each time. The best subset with 3 variables is found adding variables "Size" and "Width" and removing "Length", a variable that was added at an earlier step of the forward selection. At all the other steps, the removed variable is one of two added at the same step. Quadratic classification loss versus added variables is plotted in Fig. 1.

We conclude that the optimal predictive power can be achieved using only 4 variables and use 6 to be conservative. The two ROC curves, for 6 and 10 variables, are in statistical agreement.

Figure 2 shows the ROC curves corresponding to the configurations with six and all the ten variables.

We then test five other VS methods implemented in SPR: "Add 1 Rem 0", Interactions, Permutations, FOM Importance, and Correlations. We take the best six variables from each method. In this case "Add 1 Rem 0" selects the same six variables as "Add 2 Rem 1", while all the other methods select a different subset with 6 variables. The ROC curves for the best 6 variable obtained by "Add 2 Rem 1", by the Interactions method, and by the FOM Importance method (the two methods with the worst results) are shown in Fig. 3. In this analysis, all methods except FOM Importance give good results.

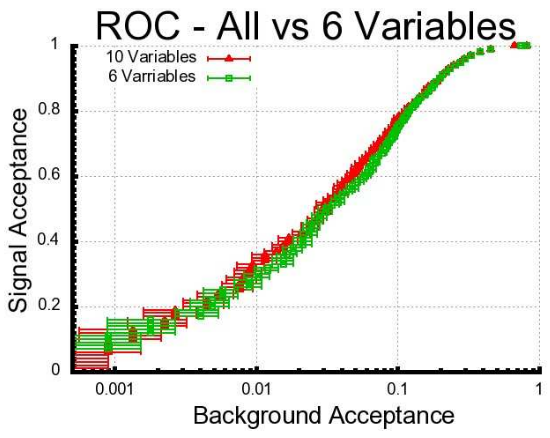


Figure 2: Magic telescope dataset: ROC distributions for the random forest classifier with 10 and 6 variables. A logarithmic axis is used to magnify the low-acceptance region.

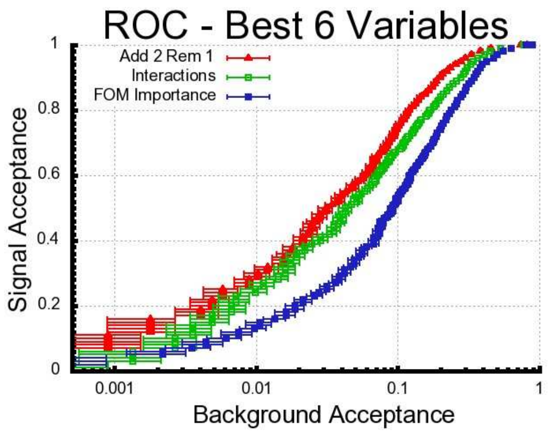


Figure 3: Magic telescope dataset: ROC curves for best 6 out of 10 variables for “Add 2 Rem 1”, Interactions, and FOM Importance. The ROC curves for all other methods lie between the curves for Interactions and “Add 2 Rem 1”. A logarithmic axis is used to show the low-acceptance region in more detail.

R.K. Bock et al. [25] define LOACC as average S_A for B_A=0.01, 0.02, and 0.05, HIACC as the average S_A for B_A=0.1 and 0.2, and Q=$\frac{S_A}{\sqrt{B_A}}$ at S_A=0.5; where S_A is the signal acceptance and B_A is the background acceptance. In Table 1, the results obtained by an SPR implementation of RF for this study are compared with those from Ref. [25] obtained by a FORTRAN program RF [26].

3.2 Cardiac Arrhythmia

The task of this analysis is to classify a patient into one of the 16 classes of cardiac arrhythmia. A slightly modified version of the dataset is used as described in Ref. [27]. After removing the 17 variables whose values are always zero for each event and removing the 14th variable which has a high incidence of missing values, the final data set has 261 variables, 12 classes (4 classes have no events in the original dataset), and 420 events. We consider the accuracy of 10-fold cross-validation as a measure of predictive power of the learning algorithm.

Table 1: Magic telescope dataset: summary of results in this analysis and in ref. [25].

FOM	FORTRAN	SPR
LOACC	0.452	0.456 ± 0.006
HIACC	0.852	0.837 ± 0.010
Q	2.8	2.91 ± 0.18

We use the Allwein-Schapire-Singer algorithm [28], which reduces a multi-class problem to a series of binary problems. The chosen classifier is a DT with at least 15 events per node. To reduce the multi-class problem to a series of binary problems, the Allwein-Schapire-Singer algorithm uses an indicator matrix of size C*L (C rows and L columns), where C is the number of classes and L is the number of binary classifiers. The elements of the indicator matrix can take only three values: 1, -1 and 0. In each column, 1 represents signal, -1 represents background, and 0 means that the corresponding class is not considered in that particular binary classification problem. There are many ways in which the indicator matrix can be built. In one approach, for instance, each class is compared to all others (One-vs-All). This means that the indicator matrix has C binary classifiers. For each binary classifier, one element is equal to 1 and all others are equal to -1. In another approach, every binary classifier uses a pair of classes and the indicator matrix has C*(C-1)/2 columns. Each column has one 1, one -1 and all other elements are zeros. Both, All-vs-One and One-vs-One approaches, are implemented in SPR. SPR also lets the user specify an arbitrary indicator matrix.

Table 2: Indicator matrix used for the arrhythmia dataset. Rows are classes and columns are binary classifiers. Matrix elements can take only three values: -1, 0 and 1, where 1 means that the corresponding class is treated as signal, -1 as background and 0 means that this class does not participate in this binary problem. The last row represents weights given to binary classifiers.

row/col	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1	0	-1	1	-1	-1	-1	-1	-1	-1	-1	-1	-1	0
2	-1	1	1	0	-1	-1	-1	-1	-1	-1	-1	-1	0	0
3	0	0	0	0	1	-1	-1	-1	-1	-1	-1	-1	-1	0
4	-1	0	0	0	-1	1	-1	-1	-1	-1	-1	-1	-1	1
5	-1	0	0	0	-1	-1	1	-1	-1	-1	-1	-1	-1	0
6	0	0	0	0	-1	-1	-1	1	-1	-1	-1	-1	-1	0
7	0	0	0	0	-1	-1	-1	-1	1	-1	-1	-1	-1	-1
8	0	0	0	0	-1	-1	-1	-1	1	-1	-1	-1	-1	0
9	0	0	0	0	-1	-1	-1	-1	-1	1	-1	-1	-1	0
10	0	0	0	-1	-1	-1	-1	-1	-1	-1	1	-1	-1	0
14	-1	0	0	0	-1	-1	-1	-1	-1	-1	-1	1	0	0
16	-1	-1	0	0	-1	-1	-1	-1	-1	-1	-1	-1	1	0
W	1	7	2	5	1	1	1	1	1	1	1	1	1	5

To classify a test event, we compute quadratic loss for each row of the indicator matrix with weighted contributions from the constructed binary classifiers:

$$\Delta_c = \frac{\sum_{l=1}^{L} \mathbf{I}(I_{cl} \neq 0) w_l (I_{cl} - f(x_l))^2}{\sum_{l=1}^{L} w_l}. \tag{3.2}$$

Each of the L classifiers is used to compute response $f(x_l)$ for a given event, with l=1,2,...,L where w_l is the relative weight for each classifier. I_{cl} is an element of the indicator matrix (c-th row and l-th column). $\mathbf{I}(I_{cl} \neq 0)$ is an indicator function equal to 1 if the indicator expression is true and 0 otherwise. The loss is evaluated for each row of the indicator matrix and an event is classified as class c if Δ_c is the least of loss values computed for all rows.

In this analysis we test all three different approaches: One-vs-All, One-vs-One and user-configured matrix. We obtain the best accuracy by building our own matrix. With the One-vs-All approach, the results are 2-3 % worse than those obtained with the user-configured matrix. With the One-vs-One approach, the results are about 10% worse. The user-configured matrix shown in Table 2 first separates class “Normal” (the most numerous class) from the classes that are most likely to be misclassified as “Normal” and then separates the remaining classes among themselves.

The 10-fold cross-validation accuracy for the model with all 261 variables is 75.95%. We then run the “Add 2 Rem 1” method to search for the optimal subset of variables.

The results of this analysis are shown in Fig. 4. The output of “Add 2 Rem 1” is shown in Fig. 5.

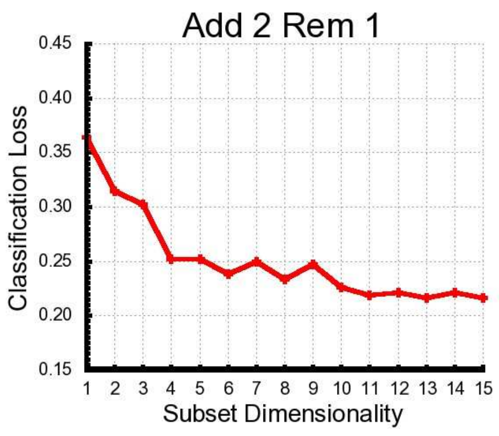
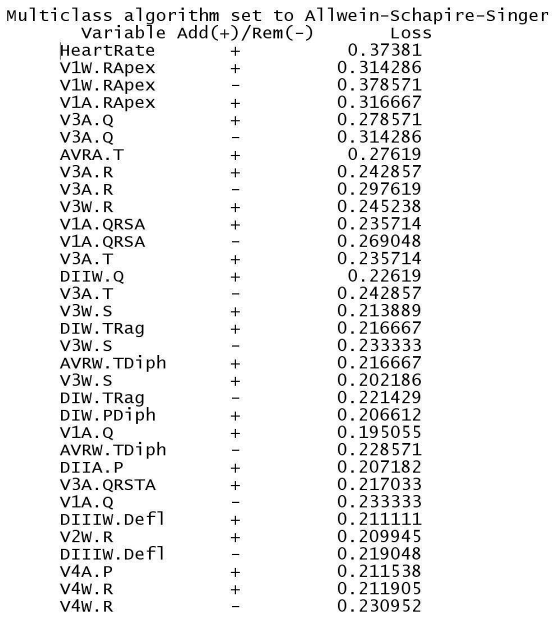


Figure 4: Arrhythmia dataset: classification error as a function of the best subset dimensionality. The best 11 variables selected are: AVFA.Q, AVRW.PDiph, DIIIA.JJ, DIIIW.Defl, HeartRate, V1A.Rapex, V3A.Q, V3A.QRSA, V3A.T, V6A.T, and V6W.R.



```
Multiclass algorithm set to Allwein-Schapire-Singer
       Variable Add(+)/Rem(-)        Loss
     HeartRate       +          0.37381
     V1W.RApex       +         0.314286
     V1W.RApex       -         0.378571
     V1A.RApex       +         0.316667
     V3A.Q           +         0.278571
     V3A.Q           -         0.314286
     AVRA.T          +          0.27619
     V3A.R           +         0.242857
     V3A.R           -         0.297619
     V3W.R           +         0.245238
     V1A.QRSA        +         0.235714
     V1A.QRSA        -         0.269048
     V3A.T           +         0.235714
     DIIW.Q          +          0.22619
     V3A.T           -         0.242857
     V3W.S           +         0.213889
     DIW.TRag        +         0.216667
     V3W.S           -         0.233333
     AVRW.TDiph      +         0.216667
     V3W.S           +         0.202186
     DIW.TRag        -         0.221429
     DIW.PDiph       +         0.206612
     V1A.Q           +         0.195055
     AVRW.TDiph      -         0.228571
     DIIA.P          +         0.207182
     V3A.QRSTA       +         0.217033
     V1A.Q           -         0.233333
     DIIIW.Defl      +         0.211111
     V2W.R           +         0.209945
     DIIIW.Defl      -         0.219048
     V4A.P           +         0.211538
     V4W.R           +         0.211905
     V4W.R           -         0.230952
```

Figure 5: Arrhythmia dataset: part of the output of “Add 2 Rem 1” showing which variables are added and removed at every step.

It displays the order in which the variables are added and removed and the corresponding classification loss at each step. Often, at a given step, two new variables are added and one variable, which was part of the best subset with lower dimensionality, is removed. That is, for a dataset with many variables the advantage of a generalized forward addiction selection, which takes into account the combined effect of several variables, is more evident.

We use the estimates of the classification error obtained by the Add 2 Rem 1 algorithm and shown in Fig.. 5 to choose the best variable subset. Therefore we cannot use these numbers as unbiased estimates of the classification error. To obtain unbiased estimates, we retrain the classifier on the 3-, 4- and 11-variable subsets using new random seeds for the 10-fold cross-validation. The best accuracy is obtained using 11 variables. The accuracy obtained with 4 variables is not statistically different at 0.05 level from the model with all 261 variables.

We also analyze the performance of VS algorithms FCBF (Fast Correlation-Based Filter) [29], ReliefF [30], and CFS-SF [29]. As a classifier, we use a C4.5 decision tree [31] with at least 15 events per node; same as in our previous analysis with SPR. All these algorithms are used in the Weka environment [10].

In the top sector of Table 3, the accuracy obtained by using the best 11 variables from “Add 2 Rem 1” is compared with the accuracy obtained by using the best 11 variables from “Add 1 Rem 0” and the best 3 and 4 variables from “Add 2 Rem 1”; as well as with the accuracy of the full model. In the 2^{nd} section from the top, results of the S methods implemented in Weka are compared with the result of the 11-variable subset from “Add 2 Rem 1”. In the 3^{rd} section from the top, we give published results [29] obtained with the same dataset, in a similar analysis configuration, and using the package Weka. Our results using ReliefF, CFS-SF and FCBF are in good agreement with the published results. In the bottom section of the table, we compare our results with those obtained by the FOS-MOD method with the k-nearest-neighbor (k-NN) algorithm [32].

We use a 10-fold cross-validation paired t test [33] to compare the accuracies obtained by various methods. This test is widely used in machine learning applications and has the advantage of giving results independent of the specific splitting used to separate training and test sets. To perform this test, it is necessary to know not only the average accuracy of 10-fold cross-validation, but also the accuracy of each of ten splits. Since the published results report only the average accuracy, we can calculate the p-values only for the results obtained by SPR and Weka.

Results of these tests are shown in table 3. “Add 2 Rem 1” and the multi-class algorithm implemented in SPR give the best accuracy.

3.3 WDBC

Wisconsin Diagnostic Breast Cancer (WDBC) dataset has 569 events, 30 variables, and involves a binary classification task. The goal is to predict whether a tumor is benign or malignant. We use a random forest classifier with 50 trees, at least 2 events per leaf and 23 variables randomly chosen for each DT. The accuracy is evaluated using a 10-fold cross-validation.

VS is carried out using “Add 2 Rem 1“, “Add 1 Rem 0”, Correlations, Interactions, and FOM Importance methods implemented in SPR; as well as with the RuleFit method [34] implemented in R [9].

Table 3: Arrhythmia dataset: accuracy and p-value obtained using different VS methods. 1st two sectors from the top: best 11 variables selected by “Add 2 Rem 1” compared with different models (see text for details). (-) indicates that the best 11 variables model is better than the model it is compared with. P-value smaller or equal to 0.05 indicates that the model with 11 variables is statistically, at 0.05 level, better. These results $*$ from Ref.[29]. These results † from Ref.[32].

Variable set	accuracy (%)	p-value
Best 11 Add2Rem1	80.95	
Best 11 Add1Rem0	76.19	0.49 (-)
Best 3 Add2Rem1	71.90	0.04 (-)
Best 4 Add2Rem1	75.24	0.22 (-)
All 261 SPR	75.95	0.10 (-)
Best 25 ReliefF	72.14	0.20 (-)
Best 25 CFS-SF	73.33	0.54 (-)
Best 5 FCBF	69.05	0.01 (-)
Full Dataset $*$	68.80	
Best 25 ReliefF $*$	68.80	
Best 25 CFS-SF $*$	69.02	
Best 5 FCBF $*$	71.47	
Full Dataset 95-NN †	56.92 ± 7.70	
Best 96 95-NN †	56.92 ± 7.70	
Full DataSet 7-NN †	65.38 ± 7.20	
Best 96 5-NN †	63.65 ± 4.39	

According to “Add 2 Rem 1”, a subset of three variables is enough for this classification problem (see Fig. 6). At each of the first 3 steps, the variable removed is one of the two added at the same step.

We take the best three variables from each method and compare the results. Table 4 shows the accuracy of each method as a function of the selected variables as well as the results of FOS-MOD published in [32]. For each method, the accuracy is compatible within statistical error with the accuracy obtained using all variables. “Add 1 Rem 0” chooses different variables from “Add 2 Rem 1”, obtaining a slightly worse accuracy.

“Add 2 Rem 1”, selecting just 3 variables, again outperforms the FOS-MOD method which selects 13 variables.

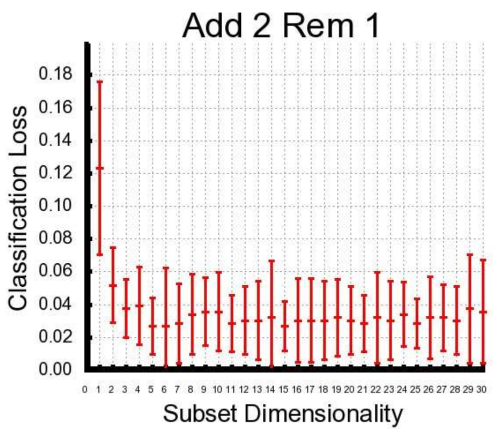


Figure 6: WDBC dataset: variation of the classification loss as a function of the best subset dimensionality. The best 3 variables selected are: WorstArea, WorstSmoothness, and WorstConcavity.

Table 4: WDBC dataset: accuracy with different variable sets. Rulefit method implemented in R doesn't show statistical errors. These results † from Ref. [32].

Variables set	accuracy (%)
Full Dataset Random Forest	96.25 ± 3.09
Full Dataset RuleFit	95.78
Best 3 Add2Rem1	96.07 ± 2.77
Best 3 Add1Rem0	94.89 ± 4.29
Best 3 Correlations	93.10 ± 2.65
Best 3 Permutations	96.21 ± 2.63
Best 3 Interactions	93.21 ± 3.65
Best 3 RuleFit	93.85
Best 3 FOM Importance	91.25 ± 3.20
Full Dataset†	97.94 ± 1.67 (5-NN)
13 Variables †	97.04 ± 1.65 (7-NN)

3.4 WBC

Wisconsin Breast Cancer (WBC) dataset is similar to WDBC dataset. It has 699 events (458 are benign samples and 241 are malignant) and 9 variables. We use an AdaBoost classifier with binary splits with 100 cycles. We compare VS methods "Add 2 Rem 1", "Add 1 Rem 0", Correlations, and Interactions in SPR , RuleFit in R, and FOS-MOD [32]. As shown in Fig. 7, "Add 2 Rem 1" selects three variables without loosing predictive power. At each of the first 3 steps, "Add 2 Rem 1" removes 1 of the 2 variables added at the same step. The FOS-MOD method selects a minimum of four variables in order to not loose predictive power.

We, then, take the best three variables subset from "Add 2 Rem 1", "Add 1 Rem 0" (same

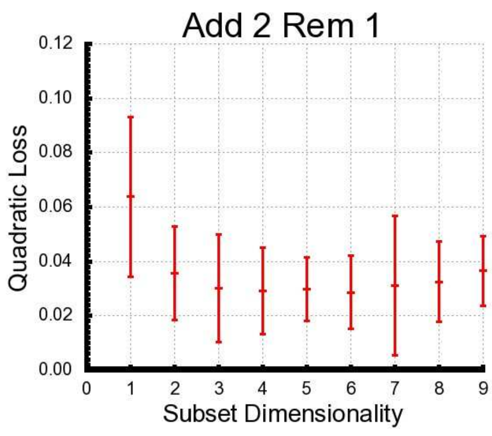


Figure 7: WBC dataset: variation of classification loss as a function of the best subset dimensionality. The best 3 variables selected are: Uniformity of Cell Shape, Normal Nucleoli, and Bland Chromatin

Table 5: WBC dataset: accuracy with different variable sets. Rulefit method implemented in R does not show statistical errors. These results † from Ref. [32].

Variables set	accuracy (%)
Full Dataset Boosted Decision Split	96.24 ± 2.59
Full Dataset RuleFit	95.82
Best 3 Add2Rem1	95.77 ± 1.71
Best 3 Add1Rem0	95.77 ± 1.71
Best 3 Correlations	95.28 ± 2.54
Best 3 Permutations	95.72 ± 2.98
Best 3 Interactions	94.85 ± 3.03
Best 3 RuleFit	95.61
Full Data Set †	98.16 ± 2.03 (5-NN)
4 Variables †	97.42 ± 2.16 (15-NN)

variables as “Add 2 Rem 1”), Correlations, Interactions, and RuleFit. For each method, the resultant accuracy is not statistically different from the one obtained using all 9 variables. In this dataset, which is particularly simple for a binary classification task, all methods give similar results, even when selecting different variables, as shown in Table 5.

3.5 Colic Horse Data

Colic Horse dataset has 368 events, 22 variables and involves a binary classification task. The task is to predict whether the lesion is surgical. This dataset has a high number of missing values which are replaced using the median value of the variable. We used a SPR tree classifier with 15 as minimum number of events per leaf.

The output of “Add 2 Rem 1” (Fig. 8) shows that 2 variables are enough to achieve an accuracy comparable to the one obtained with all the 22 variables. “Add 2 Rem 1”, at each of the first 2 steps, removes one of the two variables added at the same step.

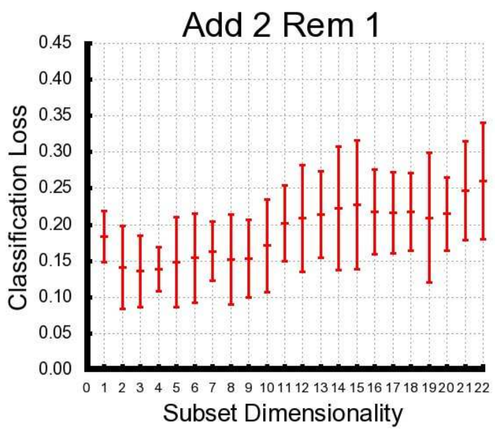


Figure 8: Colic dataset: variation of classification loss as a function of the best subset dimensionality. The 2 variables selected are: Surgery and Abdomal Distension.

We then evaluate the performance of VS methods implemented in SPR taking the 2 most important variable from each method. In this comparison, the minimum number of events per leaf of the SPR tree is taken equal to 1. In Table 6 we show the results of this study (top section of the table) together with published results obtained using, over the same dataset, different VS methods and as classifiers ID3 [7] (2^{nd} sector of the table from the top), and C4.5 [35, 36] (3^{rd} and bottom sector of the table). In this analysis we also see a better performance of “Add 2 Rem 1” compared to the other VS methods, since it selects fewer variables than any other published result while achieving similar accuracy. The variables selected by “Correlations” give a good result too, whilst “FOM Importance” obtains the worst result among the methods implemented in SPR.

3.6 CPU Time

In Table 7 is shown the CPU time required by each method used to select the variables of the best subset. When we run the wrapper algorithms, we use the option implemented in SPR which allows to monitor step by step which variables are added (and also removed in case of “Add 2 Rem 1”) and the corresponding classification loss at each step. That allows to select the best subset without waiting that the algorithms find the best subset for each dimensionality. This is particularly useful in the case of datasets with hundreds of variables, like arrhythmia dataset. “Add n Rem r” and Interactions in the magic gamma telescope analysis take longer than in any other analysis, this is why we use a very time consuming classifier, i.e. RF with 200 cycles and 1 minimum event per leaf, in conjunction with the largest data set (19020 events). All these experiments are conducted on a Intel Dual-Core Xeon 2.8 GHz with 1 GB RAM.

Table 6: Colic dataset: method, accuracy(%), and number of selected variables. Results on the accuracy of VS methods implemented in SPR compared with published results using different VS methods. "Add 2 Rem 1" and "Add 1 Rem 0" select the same variables.

Method	accuracy (%)	No of sel. feat.
All	85.85 ± 5.25	
Add2Rem1	85.85 ± 5.25	2
Add1Rem0	85.85 ± 5.25	2
Correlations	82.05 ± 5.44	2
Permutations	78.59 ± 7.33	2
Interactions	77.43 ± 4.87	2
FOM Importance	61.36 ± 4.21	2
ID3	81.52 ± 2.0	17.4
ID3 HC-FSS	83.15 ± 1.1	2.8
ID3 BFS-FSS Forward	82.07 ± 1.5	3.4
ID3 BFS-FSS Backward	82.61 ± 1.7	7.2
C4.5 GA-Wrapper	82.4	13
C4.5 ReliefF-GA-Wrapper	83.8	10
C4.5 ReliefF	85.3	20
C4.5 All	85.3	22
C4.5-RelFss	85.9	4
C4.5-RelFss'	84.5	12

4. Summary

We have evaluated the performance of five VS methods implemented in the statistical package StatPatternRecognition using datasets hosted at the UCI repository. We have compared their performance with that of other methods present in the literature. From these tests, we found that "Add 2 Rem 1" has the best performance. The difference in terms of results between "Add 2 Rem 1" and the other VS methods considered increases in significance with the complexity of the dataset. On the other hand, filter and embedded methods are faster. Noticeably faster if the dataset set is huge and the wrapper algorithm has to interact with a time consuming classifier. In general, filter and embedded methods are often able to achieve good results; however their reliability does not seem to be guaranteed for every kind of analysis.

Table 7: CPU elapsed real time in minutes (m) and seconds (s) to select the best variables from each dataset for all the methods used.

Dataset	Events	Classes	Sel. variables/ Tot. variable	Program	Method	Time
Magic	19020	2	6/10	SPR	Add 2 Rem 1	238*m*
					Add 1 Rem 0	97*m* 20*s*
					Correlations	2.53*s*
					Permutations	2*m* 58*s*
					Interactions	360*m*
					FOM Importance	2*m* 05*s*
Arrhythmia	420	12	11/261	SPR	Add 2 Rem 1	44*m* 30*s*
					Add 1 Rem 0	19*m*10*s*
			5/261	Weka	FCBF	2.11*s*
			25/261		ReliefF	9.01*s*
			25/261		CFS-SF	2.65*s*
WDBC	569	2	3/30	SPR	Add 2 Rem 1	7*m* 52*s*
					Add 1 Rem 0	4*m* 29*s*
					Correlations	0.250*s*
					Permutations	0.637*s*
					Interactions	7*m* 20*s*
					FOM Importance	1.02*s*
				R	Rulefit	2.81*s*
WBC	699	2	3/9	SPR	Add 2 Rem 1	12.7*s*
					Add 1 Rem 0	4.90*s*
					Correlations	0.078*s*
					Permutations	2.04*s*
					Interactions	23*m* 20*s*
				R	Rulefit	2.24*s*
Colic	368	2	2/22	SPR	Add 2 Rem 1	2.78*s*
					Add 1 Rem 0	1.89*s*
					Correlations	0.142*s*
					Permutations	0.171*s*
					Interactions	30.86*s*
					FOM Importance	0.071*s*

References

[1] K. Cranmer, Statistics for the LHC: Progress, Challenges, and Future, Proceed. of PhyStat-LHC Workshop, 47-60, Geneva, 27-29 June 2007 (http://phystat-lhc.web.cern.ch/phystat-lhc/2008-001.pdf). B. P. Roe et al., Boosted Decision Tree, an Alternative to Artificial Neural Networks, Nucl. Instr. and Meth. A543, 577-584 (2005).

[2] T. Hastie, R. Tibshirani and J. Friedman, The elements of Statistical Learning, Springer Series in Statistics, 2001; A. Webb, Statistical Pattern Recognition, John Wiley & Sons Ltd, 2002.

[3] L. Breiman, J. H. Friedman, R. Olshen, and C. Stone, Classification and Regression Trees, Wadsworth and Brooks, 1984.

[4] J.R. Quinlan, Induction of decision trees, Machine Learning 1, 81-106 (1986).

[5] J. H. Friedman, Recent advances in (machine) learning, J. of Classification 23, 175-197 (2006).

[6] I. Guyon et al., An introduction to variable and feature selection, J. of Machine Learning Research 3, 1157-1182 (2003).

[7] R. Kohavi and G. H. John, Wrappers for feature subset selection, Artificial Intelligence J., Special Issue on Relevance 97, 273-324 (1997).

[8] `https://sourceforge.net/projects/statpatrec`

[9] `http://www.r-project.org`

[10] `http://www.cs.waikato.ac.nz/ml/weka`

[11] R.A. Fisher, The use of multiple measurements in taxonomic problems, Annals of Eugenics 7, 179-188 (1936).

[12] J. Friedman and N. Fisher, Bump hunting in high dimensional data, Statistics and Computing 9, 123-143 (1999).

[13] I. Narsky, StatPatternRecognition: A C++ Package for Statistical Analysis of High Energy Physics Data, axXiv:physics/0507143v1, 20 Jul 2005.

[14] S. Haykin, Neural Networks: A comprehensive Foundation, Prentice Hall, 1999.

[15] Y. Freund and R.E. Schapire, A decision theoretic generalization of on-line learning and an application to boosting, Jour. of Computer and System Sciences 55, 119-139 (1997); J. Friedman, t. Hastie and R. Tibshirani, Additive Logistic Regression: A statistical view of boosting, Annals of Statistics 28(2), 337-407 (2000).

[16] L.Breiman, Arcing Classifiers, The Annals of Statistics 26, 801-849 (1998).

[17] L. Breiman, Bagging Predictors, Machine Learning 26, 123-140 (1996); L. Lam and C.Y. Suen, Application of majority vote to pattern recognition: An analysis of its behaviour and performance, IEEE Transactions on Systems, Man, and Cybernetics 27, 533-568 (1997).

[18] L. Breiman, Random Forests, Machine Learning 45, 5-32 (2001).

[19] See README in the package distribution [8].

[20] `http://sf.net`

[21] `http://root.cern.ch`

[22] R.B. Bendel and A.A. Afifi , Comparison of Stopping Rules in Forward "Stepwise" Regression, J. of the American Statistical Association 72, 46-53 (1977).

[23] `http://www.ics.uci.edu/~mlearn/MLRepository.html`
Asuncion, A. & Newman, D.J. (2007). UCI Machine Learning Repository, Irvine, CA: University of California, School of Information and Computer Science.

[24] Y. Bengio, Y. Grandvalet, No unbiased estimator of the variance of k-fold cross-validation, J. of Machine Learning Research 5, 1089-1105 (2004).

[25] R. K. Bock et al., Methods for multidimensional event classification: a case study using images from Cherenkov gamma-ray telescope, A516, 511-528 (2004).

[26] L.Breiman, FORTRAN program Random Forests, Version 3.1, available at http://oz.berkeley.edu/users/breiman.

[27] S.Perkins et al., Grafting: Fast, incremental feature selection by gradient descent in function space, J. of Machine Learning Research 3, 1333-1356 (2003).

[28] E. Allwein, R. E. Schapire and Y. Singer, Reducing Multiclass to binary: a unifying approach for margin classifiers, J. of Machine Learning Research 1, 113-141 (2000).

[29] L. Yu and H. Liu, Efficient feature selection via analysis of relevance and redundancy, Jour. of Machime Learning Research 5, 1205-1224 (2004).

[30] M. Robnik-Sikonja and I. Kononenko, Theoretical and empirical analysis of ReliefF and RReliefF, Machine Learning 53, 23-69 (2003).

[31] J. R. Quinlan, C4.5:Programs for Machine Learnings, Morgan Kaufmann, 1993.

[32] H-L. Wei and S. A. Billings, Feature subset selection and ranking for data dimensionality reduction, IEEE Trans. Pattern Analysis and Machine Intelligence 29 (1), 162-166 (2007).

[33] T. G. Dietterich, Approximate statistical tests for comparing supervised classification learning algorithms, Neural Computation 10, 1895-1923 (1998).

[34] J. H. Friedman and B. E. Popescu,

`http://www-stat.stanford.edu/~jhf/ftp/RuleFit.pdf`

[35] L-X. Zhang et al., A novel hybrid feature selection algorithm: using ReliefF estimation for GA-Wrapper search, Proceed. of the Second International Conference on Machine Learning and Cybernetics, Xi'an, (2003).

[36] D. A. Bell and H. Wang, A formalism for relevance and its application in feature subset selection, Machine Learning 41, 175-195 (2000).