

Booster in high dimensional data classification

HyunJi Kim, Byong Su Choi and Moon Yul Huh

Abstract—Classification problems in high dimensional data with small number of observations are becoming more common especially in microarray data. During the last two decades, lots of efficient classification models and feature selection (FS) algorithms have been proposed for higher prediction accuracies. However, the result of an FS algorithm based on the prediction accuracy will be unstable over the variations in the training set, especially in high dimensional data. This paper proposes a new evaluation measure Q -statistic that incorporates the stability of the selected feature subset in addition to the prediction accuracy. Then we propose the Booster of an FS algorithm that boosts the value of the Q -statistic of the algorithm applied. Empirical studies based on synthetic data and 14 microarray data sets show that Booster boosts not only the value of the Q -statistic but also the prediction accuracy of the algorithm applied unless the data set is intrinsically difficult to predict with the given algorithm.

Index Terms—high dimensional data classification, feature selection, stability, Q -statistic, Booster

1 INTRODUCTION

THE presence of high dimensional data is becoming more common in many practical applications such as data mining, machine learning and microarray gene expression data analysis. Typical publicly available microarray data has tens of thousands of features with small sample size and the size of the features considered in microarray data analysis is growing. The statistical classification of the data with huge number of features and small sample size (under-sampled problem) presents an intrinsic challenge [29]. A striking result has been found that the simple and popular Fisher linear discriminant analysis can be as poor as random guessing as the number of features gets larger [7], [16].

As was reported in [14], [59], most of the features of high dimensional microarray data are irrelevant to the target feature and the proportion of relevant features or the percentage of up-regulated or down-regulated genes compared with appropriate normal tissues is only 2% ~ 5%. Finding relevant features simplifies learning process and increases prediction accuracy. The finding, however, should be relatively robust to the variations in training data, especially in biomedical study, since domain experts will invest considerable time and efforts on this small set of selected features. Hence, the proposed selection should

provide them not only of the high predictive potential but also with the high stability in the selection [40].

1.1 Previous studies

There have been lots of researches on the FS during the last two decades, and the research continues to be still one of the hot topics in machine learning area [1], [19], [26], [31], [33], [53], [58], [62], [67]. One often used approach is to first discretize the continuous features in the preprocessing step and use mutual information (MI) to select relevant features [13], [41], [49], [69]. This is because finding relevant features based on the discretized MI is relatively simple while finding relevant features directly from a huge number of the features with continuous values using the definition of relevancy is quite a formidable task.

Methods used in the problems of statistical variable selection such as forward selection, backward elimination and their combination can be used for FS problems. Most of the successful FS algorithms in high dimensional problems have utilized forward selection method but not considered backward elimination method since it is impractical to implement backward elimination process with huge number of features.

A serious intrinsic problem with forward selection is, however, a flip in the decision of the initial feature may lead to a completely different feature subset and hence the stability of the selected feature set will be very low although the selection may yield very high accuracy [10], [43], [77]. This is known as the stability problem in FS [40]. The research in this area is relatively a new field [3], [15], [24], [28], [30], [40], [47], and devising an efficient method to obtain a more stable feature subset with high accuracy is a challenging area of research.

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1.2 A new proposal for feature selection

This paper proposes Q -statistic to evaluate the performance of an FS algorithm with a classifier. This is a hybrid measure of the prediction accuracy of the classifier and the stability of the selected features. Then the paper proposes Booster on the selection of feature subset from a given FS algorithm.

The basic idea of Booster is to obtain several data sets from original data set by resampling on sample space. Then FS algorithm is applied to these resampled data sets to obtain different feature subsets. The union of these selected subsets will be the feature subset obtained by the Booster of FS algorithm. Empirical studies show that the Booster of an algorithm boosts not only the value of Q -statistic but also the prediction accuracy of the classifier applied.

Several studies based on resampling technique have been done to generate different data sets for classification problem [6], [34], [56], [65], [68], [73], and some of the studies utilize resampling on the feature space [6], [34], [65], [73]. The purposes of all these studies are on the prediction accuracy of classification without consideration on the selection of feature subset.

The paper is organized as follows. Section 2 describes the pre-processing steps to find weakly relevant features based on t-test and to remove irrelevant features based on MI. Section 3 introduces a new evaluation criterion Q -statistic and investigates its properties. Section 4 gives Booster algorithm and some theoretical backgrounds are provided. Then, section 5 presents the results of the experimentation based on synthetic data and 14 microarray data sets. Conclusion is given in Section 6.

2 PREPROCESSING STEP

FS in high dimensional data needs preprocessing process to select only relevant features or to filter out irrelevant features. Relevancy of a feature is defined as follows.

Let $\mathbf{X} = (X_1, X_2, \dots, X_p)$ be a set of p features and let Y be the target feature taking one of g possible classes. Then a feature X_i is defined to be *strongly relevant* iff the following is satisfied [37], [40], [77]:

$$P[Y|X_i, \mathbf{X}_{-i}] \neq P[Y|\mathbf{X}_{-i}], \quad (1)$$

where $\mathbf{X}_{-i} = \mathbf{X} - \{X_i\}$ for $i = 1, \dots, p$.

A feature X_i is defined to be *weakly relevant* iff there exists a feature subset $\mathbf{X}'_{-i} \subset \mathbf{X}_{-i}$ such that the following is satisfied:

$$P[Y|X_i, \mathbf{X}_{-i}] = P[Y|\mathbf{X}_{-i}] \quad (2)$$

and

$$P[Y|X_i, \mathbf{X}'_{-i}] \neq P[Y|\mathbf{X}'_{-i}]. \quad (3)$$

A feature X_i is defined to be *irrelevant* iff the following is satisfied:

$$P[Y = j|X_i, \mathbf{X}'_{-i}] = P[Y = j|\mathbf{X}'_{-i}], \forall \mathbf{X}'_{-i} \subseteq \mathbf{X}_{-i}. \quad (4)$$

An efficient FS algorithm should not include *redundant* features in the selection. A feature X_i is defined to be *redundant* if it is weakly relevant and has a Markov blanket \mathbf{M}_i within the current set $\mathbf{G} \subset \mathbf{X}$. \mathbf{M}_i is a Markov blanket of $X_i \notin \mathbf{M}_i$ if the following is satisfied [42]:

$$P[\mathbf{X} - \mathbf{M}_i - \{X_i\}, Y|X_i, \mathbf{M}_i] \quad (5)$$

$$= P[\mathbf{X} - \mathbf{M}_i - \{X_i\}, Y|\mathbf{M}_i]. \quad (6)$$

Hence, X_i is removed from $\mathbf{G} \subset \mathbf{X}$ when there exists \mathbf{M}_i of X_i within the current set \mathbf{G} . That is, the redundant features are removed from \mathbf{G} .

2.1 Finding weakly relevant features by t-test

When preprocessing is performed on the original numeric data, t-test or F-test has been conventionally applied to reduce feature space in the preprocessing step [16], [25], [35], [44], [74]. We will show that the t-test will remove irrelevant features.

Assume $g = 2$, or there are two classes and let $\mu_j = E[X|Y = j]$, $j = 1, 2$. Then the two sample t-test is to test the equality of the two means, or $H_0 : \mu_1 = \mu_2$. Under normality, this is equivalent to the test of the equality of two distributions $f(x|Y = 1)$ and $f(x|Y = 2)$. Hence, under the null hypothesis, X and Y are independent of each other, or $f(x|y) = f(x)$. From Bayes rule, we have the following:

$$f(x|y) = \frac{f(x, y)}{f(y)} = \frac{f(y|x)f(x)}{f(y)}. \quad (7)$$

Since $f(x|y) = f(x)$ under the null hypothesis, we have $f(y|x) = f(y)$ under the null hypothesis. Hence, when the null hypothesis is rejected, we have $f(x|y) \neq f(x)$ with the size of type I error α , where $\alpha = P[\text{reject } H_0 | H_0 \text{ is true}]$. This shows that the feature X is relevant with probability $1 - \alpha$ by setting $\mathbf{X}'_{-i} = \emptyset$ in the definition of (3).

For the problems with more than two classes, F-test can be used instead. The null hypothesis in this case is $H_0 : \mu_1 = \dots = \mu_g$, $g > 2$. Under the null hypothesis, Y and X are independent. Hence, the features selected by the F-test are also weakly relevant with the size of type I error α .

2.2 Removing irrelevant features by discretization

It has been observed that MI is an equivalent concept to feature relevance [9], [20], [39], [49]. The MI between two continuous random variables X and Y having marginal and joint densities $f(x)$, $f(y)$ and $f(x, y)$, respectively, is defined as follows:

$$I(Y; X) = \int \int f(x, y) \log \frac{f(x, y)}{f(x)f(y)} dx dy. \quad (8)$$

Similarly, the MI between the two discrete random variables X and Y with marginal and joint probability

mass functions $f(x)$, $f(y)$ and $f(x, y)$, respectively, is defined as follows:

$$I(Y; X) = \sum \sum f(x, y) \log \frac{f(x, y)}{f(x)f(y)}. \quad (9)$$

The basic concept and properties of MI can be found in [13].

The MI estimation with numerical data involves density estimation of high dimensional data. Although much researches have been done on multivariate density estimation [8], [45], [55], [57], high dimensional density estimation with small sample size is still a formidable task.

The MI estimation based on discretized data is straightforward. In this respect, lots of researches on FS algorithms work on discretized data and huge number of researches have been done in the area of discretization. Most of the recent successful FS algorithms based on discretized data [27], [46], [50], [62], [77] utilized the well known minimum description length principle (MDLP) method [18] for discretization. Hence, this paper also uses the MDLP method for discretization.

When a feature has only one distinct value after discretization, it has MI=0 with the target feature and it does not contribute any information to the target feature. Hence, this feature is considered as an irrelevant feature and is filtered out.

Some authors suggested to filter out the feature X_i if $I(Y; X_i) < \delta$ where δ corresponds to the value of the w^{th} largest $I(Y; X_i)$, $w = \sqrt{p} \log(p)$ [32], [62], [77].

3 A NEW EVALUATION CRITERION Q -STATISTIC

Several studies have been done on the measure of the stability of the selected feature subset [40], [43], [61], [75]. A simple and straightforward measure for the similarity of a set of sequences of features V_1, V_2, \dots, V_h , for a given set size h , is given as follows [40]:

$$K(V_1, \dots, V_h) = \frac{2}{h(h-1)} \sum_{i=1}^{h-1} \sum_{j=i+1}^h T_{ij}, \quad (10)$$

where T_{ij} is the Tanimoto distance between two sets V_i and V_j which are defined as follows:

$$T_{ij} = \frac{|V_i \cap V_j|}{|V_i \cup V_j|}, \quad (11)$$

where $|A|$ is the cardinality of a set A .

Another measure is suggested by [43] and it considers the correction for chance in selecting the feature set in addition to the cardinality of the intersection of two feature sets. It is given as follows:

$$U(V_1, \dots, V_h) = \frac{2}{h(h-1)} \sum_{i=1}^{h-1} \sum_{j=i+1}^h U_{ij}, \quad (12)$$

where $U_{ij} = \frac{rp-u^2}{u(p-u)}$, $r = |V_i \cap V_j|$, $u = |V_i| = |V_j|$ and p is the total number of features in the original full feature set.

The measure U , however, is targeted to the evaluation of different feature selectors based on the wrapper method with equal prefixed size of selected features. For this measure, an FS algorithm is applied to each data set to find the set of first u features giving the highest accuracies.

This paper considers only filter approach for FS. For filter approach, the selection of features is performed independently of a classifier and the evaluation of the selection is obtained by applying a classifier to the selected features. The evaluation of FS in this paper is based on both the accuracy of the classifier and the stability of the selection. For this, we propose Q -statistic as follows by modifying the Tanimoto measure of (10) and (11):

$$Q(V_1, \dots, V_h, a_1, \dots, a_h) = \frac{2}{h(h-1)} \sum_{i=1}^{h-1} \sum_{j=i+1}^h Q_{ij}. \quad (13)$$

Q_{ij} is defined as follows:

$$Q_{ij} = \frac{\sqrt{a_i a_j} |V_i \cap V_j|}{|V_i \cup V_j|}, \quad (14)$$

where a_i and a_j are the accuracies of a classifier based on the feature sets V_i and V_j , respectively.

From the definition, $K \geq Q$. When a classifier gives perfect prediction accuracies ($a_i = 1$ for all i), $K = Q$. We can consider two special cases. First case is $V_i = V_j = V$ for all i, j . This gives $Q = a$ where a is the accuracy of a classifier with the same V . Second case is $V_i \cap V_j = \emptyset$ for all i, j . In this case, $Q = 0$.

If an FS algorithm provides a feature subset whose accuracy is almost perfect but gives very small Q -statistic, the algorithm is not preferable based on the Q -statistic criterion.

4 BOOSTER

Booster is simply a union of feature subsets obtained by a resampling technique. The resampling is done on the sample space. Assume we have training sets and test sets. For Booster, training set \mathcal{D} is divided into b -partitions $\mathcal{D}_i, i = 1, \dots, b$ such that $\mathcal{D} = \cup_{i=1}^b \mathcal{D}_i$. From these b \mathcal{D}_i 's, we obtain b training subsets \mathcal{D}_{-i} such that $\mathcal{D}_{-i} = \mathcal{D} - \mathcal{D}_i, i = 1, \dots, b$. To each of these b generated training subsets, an FS algorithm s is applied to obtain the corresponding feature subsets $V_i, i = 1, \dots, b$. The subset selected by the Booster of s is $V^* = \cup_{i=1}^b V_i$.

Booster needs an FS algorithm s and the number of partitions b . When s and b are needed to be specified, we will use notation s -Booster $_b$. Hence, s -Booster $_1$ is equal to s since no partitioning is done in this case and the whole data is used. When s selects relevant features while removing redundancies, s -Booster $_b$ will

also select relevant features while removing redundancies.

We now give a proof that V^* will cover more relevant features in probability than the relevant features obtained from the whole data set \mathcal{D} . Since $V^* \supseteq V_i$ for any i , we have $P[v \in V^*] \geq P[v \in V_i]$ for any relevant feature $v \in V$. Since the data set \mathcal{D}_{-i} is a random sample from the data \mathcal{D} , V_i obtained from \mathcal{D}_{-i} will have the same distributional property as $V_{\mathcal{D}}$ from the whole data \mathcal{D} . Hence, $P[v \in V^*] \geq P[v \in V_i] = P[v \in V_{\mathcal{D}}]$.

From the above result, we can observe that if the selected subsets V_1, \dots, V_b obtained by s consist only of the relevant features where redundancies are removed, V^* will include more relevant features where redundancies are removed. Hence, V^* will induce smaller error of selecting irrelevant features. However, if s does not completely remove redundancies, V^* may result in the accumulation of larger size of redundant features.

The number of partitions b plays the key factor for Booster. Larger b will find more relevant features but may include more irrelevant features, and also may induce more redundant features. This is because no FS algorithm can select all relevant features while removing all irrelevant features and redundant features. Another problem with larger b is more computing burden. In contrast, too small b may fail to include valuable (strong) relevant features for classification. We will investigate this problem in more detail in the next section and will suggest appropriate choice of b .

Algorithm 1. s -Booster _{b}

Input: Data set \mathcal{D} , FS algorithm s , number of partitions b

Output: selected feature subset V^*

- 1: Split \mathcal{D} into b -partitions $\mathcal{D}_i, i = 1, \dots, b$.
 - 2: $V^* = \emptyset$
 - 3: **for** $i = 1$ to b **do**
 - 4: $\mathcal{D}_{-i} = \mathcal{D} - \mathcal{D}_i$ # remove \mathcal{D}_i from \mathcal{D}
 - 5: $V_i \leftarrow s(\mathcal{D}_{-i})$ # obtain V_i by applying s on \mathcal{D}_{-i}
 - 6: $V^* = V^* \cup V_i$
 - 7: **end for**
 - 8: return V^*
-

5 EXPERIMENTATION

Our experimentation first filters out irrelevant features or selects weakly relevant features by the preprocessing methods described in section 2. Three preprocessing methods explained in section 2 are applied here, and the size of the subset of features left out after preprocessing is equal to $N = \min(p_t, p_D, p_L)$ where p_t is the number of features having p-value < 0.05 by t-test or F-test, p_D is the number of features with more than two distinct values after discretization, p_L is the number of preprocessed features left out by the δ criterion explained in the subsection 2.2. When N is

decided, the features having the first N largest MI's with the target will be used for the evaluation of FS algorithms and their corresponding Boosters.

Three FS algorithms considered in this paper are minimal-redundancy-maximal-relevance (mRMR) [50], Fast Correlation-Based Filter (FCBF) [77], and Fast clustering-based feature Selection algorithm (FAST) [62]. All three methods work on discretized data. For mRMR, the size of the selection m is fixed to 50 after extensive experimentations. Smaller size (30 or smaller) gives lower accuracies and lower values of Q -statistic while the larger selection size, say 100, gives not much improvement over 50.

The background of our choice of the three methods is that FAST is the most recent one we found in the literature and the other two methods are well known for their efficiencies. FCBF and mRMR explicitly include the codes to remove redundant features. Although FAST does not explicitly include the codes for removing redundant features, they should be eliminated implicitly since the algorithm is based on minimum spanning tree. Our extensive experiments supports that the above three FS algorithms are at least as efficient as other algorithms including CFS [27] and Relief [46].

For convenience, we will use the notation FAST-Booster, FCBF-Booster, and mRMR-Booster for the Booster of the corresponding FS algorithm.

To obtain the value of Q -statistic, we need a classifier. This paper considers 3 classifiers: Support Vector Machine (SVM) [12], k-Nearest Neighbors algorithm (KNN) [2], and Naive Bayes classifier (NB) [38]. We will first consider choosing the appropriate number of partitions b for Booster. Then we will evaluate the relative performance efficiency of s -Booster over the original FS algorithm s based on prediction accuracy and Q -statistic.

To evaluate the efficiencies of the three FS algorithms - FAST, FCBF, and mRMR - and their corresponding Boosters, we apply k -fold cross validation. For this, k training sets and their corresponding k test sets are generated. For each training set, Booster is applied to obtain V^* . Classification is performed based on the training set with the selection V^* , and the test set is used for prediction accuracy. This process is repeated for the k pairs of training-test sets, and the value of the Q -statistic is computed. In this paper, $k = 5$ is used. The flow of the evaluation process is given in algorithm 2.

5.1 Synthetic data

In this section, Monte Carlo experimentation is performed to evaluate the usefulness of Q -statistic and to show the efficiency of the Booster in FS process. For the generation of synthetic data, we follow the approach of the works on generating microarray data [14], [59] and the method used here is following the works by [16], [17].

Algorithm 2. Evaluation process of FS

Input: FS algorithm s ,
 number of folds k , original data set \mathcal{D} and k -folded data subsets $\mathcal{D}_i, i = 1, \dots, k$.

- 1: **for** $i = 1$ to k **do**
- 2: $\mathcal{D}_{-i} = \mathcal{D} - \mathcal{D}_i$ # apply \mathcal{D}_{-i} to s -Booster $_b$
- 3: $V_i^* \leftarrow f$ -Booster $_5(\mathcal{D}_{-i})$
- 4: $a_i \leftarrow \text{Classifier}(\mathcal{D}_i)$
- 5: **end for**
- 6: $Q \leftarrow$ compute Q using k -pairs of (V_i^*, a_i)

Synthetic data consists of 1,200 features with two classes and 30 samples from each class. Each feature X is generated from the following statistical model.

$$X = \begin{cases} \mu + \epsilon & \text{from class 1} \\ \epsilon & \text{from class 2} \end{cases}$$

μ is from the following distribution:

$$\mu \sim (1 - c)\delta_0 + \frac{1}{2}ce^{-2|x|}, \quad (15)$$

where $c \in (0, 1)$ is a constant, $-\infty < x < \infty$ and ϵ is from a mixture of random noise of distributions as defined in [16]. c is the percentage of significant (relevant) features among the 1,200 features. For our data, we set $c = 0.02$. Hence, among the 1,200 features, 2% or 24 genes are relevant. This process is repeated 1,000 times to obtain the results.

Tables 1 and 2 give the summary of the Monte Carlo experiments for various choices of Booster size b : $b = 1, 2, 3, 5$, and 10. Table 1 gives the increase of the average size of the selected feature subsets as Booster size b increases, and Table 2 gives the accuracies and the Q -statistics of the three FS algorithms (FAST, FCBF, and mRMR) based on the three classifiers (SVM, KNN, and NB) for different values of b .

5.1.1 Choice of b for s -Booster $_b$

Table 1 shows that the average $|V^*|$ increases rapidly to 18 as b increases to 5 but does not increase much after $b = 5$. The plots in Figure 1 show that the Q -statistics of FAST-Booster and FCBF-Booster increase rapidly until $b = 5$ and remains stable after $b = 5$. The Q -statistic of mRMR-Booster, however, reaches its maximum at $b = 3$, and remains stable after $b = 3$. From these results, $b = 5$ is a safe choice for s -Booster $_b$.

5.1.2 Outperformance of mRMR-Booster

Also noted in Figure 1 is the outperformance of mRMR-Booster over the other two Boosters, FAST-Booster and FCBF-Booster. However, the choice of m is crucial for mRMR, where m denotes the initial number of features for the algorithm. One option is to set $m = c \times p$ where c is the proportion of the significant genes in p features. It has been noted that

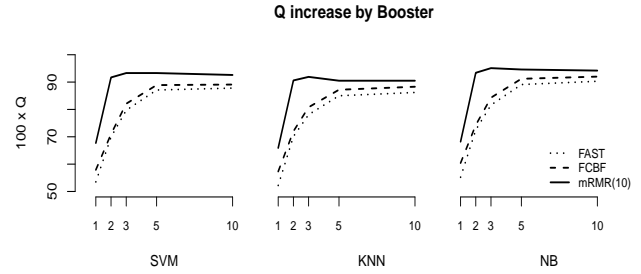


Fig. 1: Accuracy and Q -statistic from s -Booster $_b$ with $b=1, 2, 3, 5$, and 10. The values are the averages across 1000 repetitions.

generally 2 ~ 5% genes are significant in microarray data [14].

For the synthetic data, c was set to 0.02 and hence $m = 0.02 \times 1,200 = 24$ is suggested. When the size of the feature set is large, this rule will set m too large which results in the burden of computation and interpretation. With Booster, however, we may set smaller value to m because $V^* = \cup_{i=1}^b V_i$ has the effect of setting larger value to m . Monte-Carlo experiment supports this. $m = 10$ is set to obtain each V_i , and Table 1 shows that mRMR-Booster $_5$ gives average $|V^*| = 18.64$. The table also shows that the average of Q -statistic is 0.65 ~ 0.68 from mRMR with $m = 10$, and the average of Q -statistic is 0.9 ~ 0.95 from mRMR-Booster $_5$.

5.2 Real data

14 microarray data sets are considered for experiments. These are all high dimensional data sets with small sample sizes and large number of features. Among the 14 data sets, 5 data sets have the number of classes (g) larger than 2. They are summarized in Table 3. The number of features ranges from 457 to 24,482 and the sample sizes are in the range of 47 ~ 248.

5.2.1 Choice of b for Booster

Table 4 gives the average number of selected features ($|V^*|$) for the 14 data sets with $b = 1, 2, 3, 5, 10$, and 20. It shows the trend that the increase of $|V^*|$ is rapid up to $b = 5$ and $|V^*|$ remains relatively stable after $b = 5$.

Specifically, for mRMR-Booster, m for mRMR is initially set to 50. Hence $|V^*| = 50$ when $b = 1$. When mRMR is boosted 5 times, or when mRMR-Booster $_5$ is applied, average $|V^*|$ of the mRMR-Booster $_5$ is 93. When $b > 5$, average $|V^*|$ remains almost the same. Hence, $b = 5$ is a reasonable choice as was the case with the synthetic data.

Now, we consider the effect of b on the change of the accuracy and the Q -statistic for all the combinations of the 3 FS algorithms and the 3 classifiers. Table 5 summarizes the average accuracies and the Q -statistics of

TABLE 1: Results from the synthetic data. Average size of the feature subsets selected by the three Boosters with $b = 1, 2, 3, 5$, and 10 . m for mRMR is set to 10 .

| b | FAST | FCBF | mRMR |
|----|-------|-------|-------|
| 1 | 8.93 | 9.32 | 10 |
| 2 | 10.47 | 11.79 | 11.31 |
| 3 | 13.10 | 13.47 | 14.94 |
| 5 | 17.27 | 17.62 | 18.64 |
| 10 | 19.46 | 19.73 | 20.47 |

TABLE 2: Results from the synthetic data. Average accuracy, K-statistic and Q -statistic from s -Booster $_b$ with $b = 1, 2, 3, 5$, and 10 for the three FS algorithms and the three classifiers. Each value of the table is the average based on 1,000 repetitions. s -Booster $_1$ is the same as the original FS algorithm s . m for mRMR is set to 10 .

| | b | FAST | | | FCBF | | | mRMR | | |
|----------------|----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| accuracy(%) | 1 | 95.3 | 94.2 | 96.8 | 95.3 | 94.8 | 97.2 | 97.2 | 95.9 | 97.4 |
| | 2 | 94.3 | 94.5 | 96.0 | 94.1 | 94.8 | 96.3 | 95.9 | 95.4 | 96.8 |
| | 3 | 96.7 | 95.7 | 97.8 | 96.6 | 95.9 | 97.8 | 97.3 | 96.5 | 98.2 |
| | 5 | 97.7 | 96.6 | 98.8 | 97.6 | 96.7 | 99.0 | 98.3 | 96.8 | 99.0 |
| | 10 | 97.7 | 96.8 | 99.1 | 97.5 | 97.0 | 99.0 | 98.3 | 97.1 | 99.1 |
| $100 \times K$ | 1 | 58.5 | 58.5 | 58.5 | 63.6 | 63.6 | 63.6 | 71.5 | 71.5 | 71.5 |
| | 2 | 78.6 | 78.6 | 78.6 | 80.2 | 80.2 | 80.2 | 99.6 | 99.6 | 99.6 |
| | 3 | 85.2 | 85.2 | 85.2 | 87.9 | 87.9 | 87.9 | 98.6 | 98.6 | 98.6 |
| | 5 | 91.3 | 91.3 | 91.3 | 93.3 | 93.3 | 93.3 | 96.6 | 96.6 | 96.6 |
| | 10 | 92.0 | 92.0 | 92.0 | 93.8 | 93.8 | 93.8 | 95.9 | 95.9 | 95.9 |
| $100 \times Q$ | 1 | 53.5 | 52.2 | 55.2 | 57.9 | 57.3 | 60.4 | 67.7 | 65.9 | 68.2 |
| | 2 | 69.9 | 70.1 | 72.5 | 71.0 | 72.0 | 74.3 | 91.7 | 90.6 | 93.4 |
| | 3 | 79.7 | 78.1 | 81.6 | 82.1 | 80.8 | 84.3 | 93.3 | 91.9 | 95.1 |
| | 5 | 87.1 | 85.0 | 89.1 | 88.9 | 87.2 | 91.2 | 93.3 | 90.5 | 94.6 |
| | 10 | 87.8 | 86.2 | 90.3 | 89.1 | 88.3 | 92.0 | 92.6 | 90.5 | 94.2 |

the 14 data sets for $b = 1, 2, 3, 5, 10$, and 20 . Figure 2 graphically summarizes Table 5. The figure has two plots. The left hand side plot gives the change of the accuracy and the right hand side plot gives the change of the Q -statistic depending on the values of b . From the Table 5 and the Figure 2, we can observe that the improvement of accuracy and Q -statistic is rapid from $b = 1$ to $b = 5$, and is slow or decreases after $b = 5$. Hence, $b = 5$ is suggested for the Booster $_b$.

We can also observe that classification methods do not have much effect on the prediction accuracy and the stability of the selected feature subset. The Q -statistic of mRMR-Booster is far better than the Q -statistic of the other two algorithms for all b considered in this paper.

5.2.2 Efficiency of Booster

Tables 6 and 7 give detailed results of the accuracies and the Q -statistics for all combinations of the three FS algorithms and three classifiers. Tables 8 and 9 give the rate of the increase of accuracy and Q -statistic by the Booster with $b = 5$. From now on, $b = 5$ is the default value assigned to a Booster if there is no ambiguity.

Figure 3 graphically presents the effect of s -Booster on accuracy and Q -statistic against the original s 's. Classifier used here is NB. Separate plots are drawn for the data sets with $g = 2$ and $g > 2$. Upper two plots are for the comparison of the accuracies and the lower two plots are for the comparison of the Q -statistics: y -axis is for s -Booster and x -axis is for s . Hence, if a

point lies above $y = x$ line, s -Booster is more efficient than s . Since three FS algorithms are considered for each of the 14 data sets, there are 42 cases in each plot.

5.2.3 Booster boosts accuracy

Tables 6 and 8 demonstrate that mRMR-Booster improves accuracy considerably: overall average accuracy increases from 0.91 to 0.96. One interesting point to note here is that mRMR-Booster is more efficient in boosting the accuracy of the original mRMR when it gives low accuracies. Table 6 shows that data sets giving three lowest accuracies with mRMR are D7, D9, and D11: 0.76, 0.71, and 0.62, respectively. Table 8, however, shows that these three data sets give highest increase rates of accuracies with mRMR-Booster: 1.23, 1.13, and 1.24, respectively.

From the two tables, we can observe that FAST-Booster also improves accuracy, but not as high as mRMR. For FCBF-Booster, overall average accuracy remains the same, but the average accuracy for the data sets with $g > 2$ decreases by 0.4%.

5.2.4 Booster boosts Q -statistic

Table 7 shows that mRMR is outstanding in its performance on Q -statistic as we have already noticed with the synthetic data. Overall average is 0.44: 0.38 for the data sets with $g = 2$ and 0.57 for the data sets with $g > 2$.

FCBF gives poor performance on Q -statistic in contrast to its high performance on accuracy. Overall average is 0.28: 0.20 for the data sets with $g = 2$ and 0.42 for the data sets with $g > 2$.

FAST gives quite poor performance on Q -statistic. The highest value for the data sets with $g = 2$ is 0.28 (D6), and most of the values are below 0.1.

Figure 3 graphically demonstrates that Booster improves the Q -statistic for all the cases considered except the case with the data set D6.

The improvement of Booster is generally more significant for the data sets with $g = 2$ than for the data sets with $g > 2$. This is because of the fact that the Q -statistic from original FS algorithm gives higher value for $g > 2$ than for $g = 2$.

Now, consider the improvement of the Q -statistic by mRMR-Booster. From Table 9, the rate of overall increase is 1.40: 1.53 for the data sets with $g = 2$ and 1.16 for the data sets with $g > 2$. Specifically, for mRMR-Booster, overall average Q -statistic is 0.62: 0.581 for the data sets with $g = 2$ and 0.661 for the data sets with $g > 2$.

An interesting observation is that the Q -statistic for D7 is extremely low by mRMR: 0.075, 0.077, and 0.075 for SVM, KNN, and NB, respectively (Table 7). Table 9, however, shows that mRMR-Booster gives extremely high improvement on the Q -statistic for all three cases. It shows that the increase rate for the three classifiers is 305%, 273%, and 285%, respectively.

All the codes in this paper are programmed in R [52]. Booster and FAST codes are programmed by the authors, mRMR is from [36], FCBF is implemented in Weka [72], SVM and NB are from [48] and KNN is from [71]. The computing burden of Booster depends upon the FS algorithm applied. The choice of $b = 5$ consumes 5 times more computing time of the original algorithm.

6 CONCLUSION

This paper proposed a measure Q -statistic that evaluates the performance of an FS algorithm. Q -statistic accounts both for the stability of selected feature subset and the prediction accuracy. The paper proposed Booster to boost the performance of an existing FS algorithm. Experimentation with synthetic data and 14 microarray data sets has shown that the suggested Booster improves the prediction accuracy and the Q -statistic of the three well-known FS algorithms: FAST, FCBF, and mRMR. Also we have noted that the classification methods applied to Booster do not have much impact on prediction accuracy and Q -statistic. Especially, the performance of mRMR-Booster was shown to be outstanding both in the improvements of prediction accuracy and Q -statistic.

It was observed that if an FS algorithm is efficient but could not obtain high performance in the accuracy or the Q -statistic for some specific data, Booster of the FS algorithm will boost the performance. However, if an FS algorithm itself is not efficient, Booster may not be able to obtain high performance. The performance of Booster depends on the performance of the FS algorithm applied.

If Booster does not provide high performance, it implies two possibilities: the data set is intrinsically difficult to predict or the FS algorithm applied is not efficient with the specific data set. Hence, Booster can also be used as a criterion to evaluate the performance of an FS algorithm or to evaluate the difficulty of a data set for classification.

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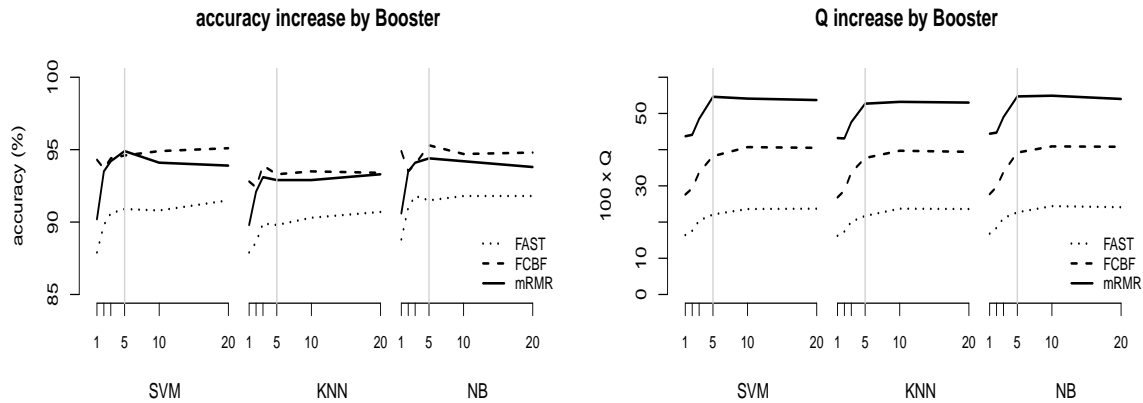


Fig. 2: Accuracy and Q -statistic of s -Booster $_b$ for $b = 1, 2, 3, 5, 10,$ and 20 (x -axis). Each value is the average over the 14 data sets. s -Booster $_1$ is s . The grey vertical line is for $b = 5$.

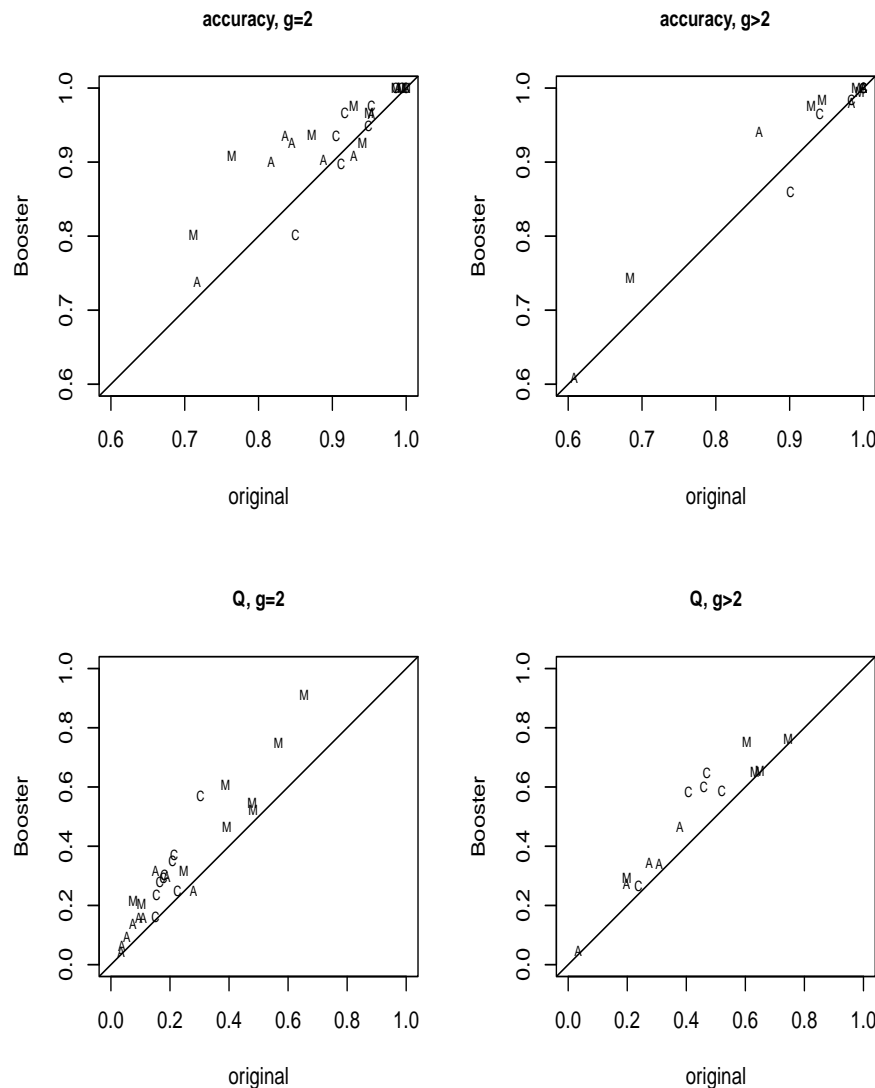


Fig. 3: Comparison of s -Booster $_5$ over s for prediction accuracy and Q -statistic. Plots are drawn separately for the data sets with $g = 2$ and $g > 2$. Classifier used is NB. "A" stands for FAST, "C" for FCBF, "M" for mRMR.

TABLE 3: 14 data sets used in this paper. n : the number of samples; p : the number of features including target feature; p_L : the number of features after filtering using the δ criterion explained in the subsection 2.2, p_t : the number of features after filtering based on t-test or F-test, $\alpha = 0.05$; p_D : the number of features with more than two distinct values after discretization; g : the number of class categories.

| ID | Dataset | n | p | g | p_L | p_t | p_D |
|-----|--|-----|-------|-----|-------|-------|-------|
| D1 | B-cell1 [4] | 47 | 4026 | 2 | 527 | 902 | 2264 |
| D2 | coloncancer [5] | 62 | 2000 | 2 | 340 | 478 | 135 |
| D3 | embryonal-tumours [51] | 60 | 7129 | 2 | 749 | 521 | 69 |
| D4 | leukemia [22] | 72 | 7129 | 2 | 749 | 2046 | 1012 |
| D5 | lungcancer [23] | 181 | 12533 | 2 | 1056 | 4857 | 4937 |
| D6 | prostate [60] | 136 | 12600 | 2 | 1060 | 5430 | 2185 |
| D7 | breastcancer [70] | 97 | 24481 | 2 | 1581 | 2264 | 756 |
| D8 | GLI-85 [21] | 85 | 22283 | 2 | 1494 | 7307 | 3545 |
| D9 | SMK-CAN-187 [64] | 187 | 19993 | 2 | 1400 | 4961 | 1815 |
| D10 | tissue-specific DNA (christensen) [11] | 217 | 1413 | 3 | 273 | 1328 | 1312 |
| D11 | TOX-171 [54] | 171 | 5748 | 4 | 656 | 3484 | 1537 |
| D12 | multiple tissues (su) [66] | 102 | 5565 | 4 | 643 | 4659 | 3446 |
| D13 | breastcancer (sorlie) [63] | 85 | 456 | 5 | 131 | 359 | 160 |
| D14 | leukemia (yeoh) [76] | 248 | 12625 | 6 | 1061 | 6360 | 2660 |

TABLE 4: Average size of the feature subset from s -Booster $_b$ for the three FS algorithms with $b = 1, 2, 3, 5, 10$, and 20.

| b | FAST | FCBF | mRMR |
|-----|------|-------|------|
| 1 | 32.8 | 63.6 | 50.0 |
| 2 | 47.0 | 101.2 | 68.4 |
| 3 | 58.7 | 122.2 | 80.4 |
| 5 | 74.0 | 144.9 | 93.1 |
| 10 | 79.1 | 156.0 | 97.3 |
| 20 | 79.4 | 158.1 | 98.4 |

TABLE 5: Accuracy and Q -statistic from s -Booster $_b$ for the three FS algorithms and the three classifiers with $b = 1, 2, 3, 5, 10$, and 20. Each value is the averages over the 14 data sets.

| | b | FAST | | | FCBF | | | mRMR | | |
|----------------|-----|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| accuracy (%) | 1 | 87.9 | 87.9 | 88.8 | 94.3 | 92.8 | 94.9 | 90.2 | 89.8 | 90.6 |
| | 2 | 89.8 | 88.6 | 91.0 | 93.7 | 92.4 | 93.5 | 93.5 | 92.1 | 93.5 |
| | 3 | 90.6 | 89.9 | 91.8 | 94.4 | 93.9 | 94.0 | 94.2 | 93.1 | 94.1 |
| | 5 | 90.9 | 89.8 | 91.5 | 94.6 | 93.3 | 95.3 | 94.9 | 92.9 | 94.4 |
| | 10 | 90.8 | 90.3 | 91.8 | 94.9 | 93.5 | 94.7 | 94.1 | 92.9 | 94.2 |
| | 20 | 91.5 | 90.7 | 91.8 | 95.1 | 93.4 | 94.8 | 93.9 | 93.3 | 93.8 |
| $100 \times Q$ | 1 | 16.4 | 16.2 | 16.8 | 27.6 | 26.8 | 27.7 | 43.7 | 43.2 | 44.4 |
| | 2 | 17.6 | 17.4 | 18.4 | 29.3 | 28.7 | 29.7 | 44.1 | 43.1 | 44.7 |
| | 3 | 20.4 | 20.1 | 21.1 | 33.7 | 33.7 | 33.8 | 48.5 | 47.6 | 49.0 |
| | 5 | 22.1 | 21.7 | 22.7 | 38.2 | 37.7 | 39.2 | 54.6 | 52.7 | 54.7 |
| | 10 | 23.6 | 23.7 | 24.4 | 40.7 | 39.7 | 40.9 | 54.1 | 53.2 | 54.9 |
| | 20 | 23.7 | 23.6 | 24.1 | 40.5 | 39.4 | 40.8 | 53.7 | 53.0 | 54.0 |

TABLE 6: Accuracies obtained by the three classifiers based on the features selected by the three FS algorithms: FAST, FCBF, and mRMR.

| Dataset | FAST | | | FCBF | | | mRMR | | |
|-----------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| D1 | 0.77 | 0.86 | 0.84 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| D2 | 0.85 | 0.85 | 0.89 | 0.90 | 0.90 | 0.90 | 0.89 | 0.90 | 0.87 |
| D3 | 0.80 | 0.80 | 0.82 | 0.93 | 0.88 | 0.92 | 0.93 | 0.90 | 0.95 |
| D4 | 1.00 | 1.00 | 1.00 | 0.97 | 0.97 | 0.99 | 1.00 | 0.99 | 0.99 |
| D5 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 |
| D6 | 0.84 | 0.84 | 0.84 | 0.93 | 0.91 | 0.91 | 0.95 | 0.94 | 0.94 |
| D7 | 0.94 | 0.91 | 0.93 | 0.94 | 0.87 | 0.95 | 0.76 | 0.77 | 0.76 |
| D8 | 0.96 | 0.95 | 0.95 | 0.93 | 0.94 | 0.95 | 0.92 | 0.93 | 0.93 |
| D9 | 0.76 | 0.76 | 0.72 | 0.80 | 0.74 | 0.85 | 0.76 | 0.76 | 0.71 |
| D10 | 0.99 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 0.99 | 0.99 | 0.99 |
| D11 | 0.58 | 0.60 | 0.61 | 0.87 | 0.85 | 0.90 | 0.66 | 0.62 | 0.68 |
| D12 | 0.99 | 0.95 | 1.00 | 1.00 | 1.00 | 1.00 | 0.99 | 0.94 | 0.99 |
| D13 | 0.86 | 0.80 | 0.86 | 0.98 | 0.95 | 0.94 | 0.91 | 0.88 | 0.93 |
| D14 | 0.97 | 0.98 | 0.98 | 0.96 | 0.97 | 0.98 | 0.89 | 0.95 | 0.94 |
| average $g=2$ | 0.88 | 0.89 | 0.89 | 0.93 | 0.91 | 0.94 | 0.91 | 0.91 | 0.91 |
| average $g > 2$ | 0.88 | 0.87 | 0.89 | 0.96 | 0.95 | 0.97 | 0.89 | 0.88 | 0.91 |
| overall average | 0.88 | 0.88 | 0.89 | 0.94 | 0.93 | 0.95 | 0.90 | 0.90 | 0.91 |

TABLE 7: Q -statistics obtained by the three classifiers based on the features selected by the three FS algorithms: FAST, FCBF, and mRMR.

| Dataset | FAST | | | FCBF | | | mRMR | | |
|-----------------|------|------|------|------|------|-------------|-------------|-------------|-------------|
| | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| D1 | 0.05 | 0.06 | 0.05 | 0.18 | 0.18 | 0.18 | 0.39 | 0.39 | 0.39 |
| D2 | 0.10 | 0.10 | 0.11 | 0.21 | 0.21 | 0.21 | 0.40 | 0.42 | 0.39 |
| D3 | 0.14 | 0.14 | 0.15 | 0.32 | 0.28 | 0.30 | 0.63 | 0.59 | 0.66 |
| D4 | 0.10 | 0.10 | 0.10 | 0.17 | 0.17 | 0.18 | 0.49 | 0.48 | 0.48 |
| D5 | 0.19 | 0.19 | 0.19 | 0.21 | 0.21 | 0.21 | 0.57 | 0.57 | 0.57 |
| D6 | 0.28 | 0.28 | 0.28 | 0.23 | 0.23 | 0.23 | 0.49 | 0.48 | 0.48 |
| D7 | 0.08 | 0.07 | 0.07 | 0.16 | 0.14 | 0.17 | 0.08 | 0.08 | 0.08 |
| D8 | 0.04 | 0.04 | 0.04 | 0.15 | 0.15 | 0.15 | 0.24 | 0.25 | 0.25 |
| D9 | 0.04 | 0.04 | 0.04 | 0.13 | 0.12 | 0.15 | 0.12 | 0.12 | 0.10 |
| D10 | 0.37 | 0.38 | 0.38 | 0.47 | 0.47 | 0.47 | 0.74 | 0.74 | 0.75 |
| D11 | 0.03 | 0.03 | 0.03 | 0.22 | 0.21 | 0.24 | 0.18 | 0.16 | 0.20 |
| D12 | 0.30 | 0.28 | 0.31 | 0.46 | 0.46 | 0.46 | 0.65 | 0.59 | 0.65 |
| D13 | 0.20 | 0.17 | 0.20 | 0.44 | 0.42 | 0.41 | 0.58 | 0.55 | 0.61 |
| D14 | 0.27 | 0.27 | 0.27 | 0.50 | 0.51 | 0.52 | 0.56 | 0.64 | 0.63 |
| average $g=2$ | 0.11 | 0.11 | 0.11 | 0.20 | 0.19 | 0.20 | 0.38 | 0.37 | 0.38 |
| average $g > 2$ | 0.23 | 0.23 | 0.24 | 0.42 | 0.41 | 0.42 | 0.54 | 0.53 | 0.57 |
| overall average | 0.16 | 0.15 | 0.16 | 0.28 | 0.27 | 0.28 | 0.44 | 0.43 | 0.44 |

TABLE 8: Ratio of the accuracy from s -Booster₅ to the accuracy from s .

| Dataset | FAST | | | FCBF | | | mRMR | | |
|-----------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| D1 | 1.18 | 1.09 | 1.12 | 1.00 | 1.00 | 1.00 | 1.00 | 0.98 | 1.00 |
| D2 | 1.06 | 1.02 | 1.02 | 1.05 | 1.07 | 1.03 | 1.05 | 1.00 | 1.07 |
| D3 | 1.15 | 1.04 | 1.10 | 1.00 | 1.00 | 1.05 | 1.04 | 1.00 | 1.02 |
| D4 | 1.00 | 1.00 | 1.00 | 1.03 | 1.03 | 1.01 | 1.00 | 1.00 | 1.01 |
| D5 | 1.01 | 1.01 | 1.01 | 1.00 | 1.00 | 1.01 | 1.00 | 1.01 | 1.01 |
| D6 | 1.07 | 1.05 | 1.10 | 0.98 | 1.03 | 0.98 | 0.99 | 1.00 | 0.98 |
| D7 | 0.97 | 1.01 | 0.98 | 1.01 | 1.02 | 1.00 | 1.23 | 1.16 | 1.19 |
| D8 | 1.01 | 1.00 | 1.01 | 1.05 | 1.01 | 1.02 | 1.05 | 1.04 | 1.05 |
| D9 | 1.06 | 0.97 | 1.03 | 1.05 | 1.02 | 0.94 | 1.10 | 1.06 | 1.13 |
| D10 | 1.00 | 1.00 | 1.00 | 0.99 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |
| D11 | 1.03 | 1.05 | 1.00 | 0.97 | 0.91 | 0.95 | 1.24 | 1.17 | 1.09 |
| D12 | 1.01 | 1.03 | 1.00 | 1.00 | 0.99 | 1.00 | 1.01 | 1.05 | 1.01 |
| D13 | 1.03 | 1.07 | 1.10 | 0.94 | 0.99 | 1.03 | 1.04 | 1.08 | 1.05 |
| D14 | 0.97 | 0.99 | 1.00 | 0.98 | 1.00 | 1.00 | 1.08 | 1.02 | 1.04 |
| average $g=2$ | 1.06 | 1.02 | 1.04 | 1.02 | 1.02 | 1.01 | 1.05 | 1.03 | 1.05 |
| average $g > 2$ | 1.008 | 1.029 | 1.018 | 0.975 | 0.978 | 0.996 | 1.074 | 1.066 | 1.038 |
| overall average | 1.04 | 1.02 | 1.03 | 1.00 | 1.01 | 1.00 | 1.06 | 1.04 | 1.05 |

TABLE 9: Ratio of the Q -statistic from s -Booster₅ to the Q -statistic from s .

| Dataset | FAST | | | FCBF | | | mRMR | | |
|-----------------|-------------|------|-------------|-------------|-------------|-------------|-------------|------|-------------|
| | SVM | KNN | NB | SVM | KNN | NB | SVM | KNN | NB |
| D1 | 1.92 | 1.63 | 1.77 | 1.66 | 1.66 | 1.66 | 1.19 | 1.14 | 1.19 |
| D2 | 1.51 | 1.47 | 1.43 | 1.79 | 1.86 | 1.74 | 1.50 | 1.35 | 1.56 |
| D3 | 2.32 | 1.90 | 2.10 | 1.67 | 1.69 | 1.87 | 1.44 | 1.34 | 1.39 |
| D4 | 1.66 | 1.66 | 1.66 | 1.69 | 1.69 | 1.65 | 1.11 | 1.11 | 1.14 |
| D5 | 1.56 | 1.56 | 1.58 | 1.66 | 1.66 | 1.67 | 1.31 | 1.32 | 1.32 |
| D6 | 0.86 | 0.85 | 0.89 | 1.10 | 1.20 | 1.11 | 1.11 | 1.12 | 1.09 |
| D7 | 1.85 | 2.05 | 1.88 | 1.71 | 1.76 | 1.68 | 3.05 | 2.73 | 2.85 |
| D8 | 1.76 | 1.72 | 1.73 | 1.59 | 1.48 | 1.51 | 1.29 | 1.25 | 1.28 |
| D9 | 1.35 | 1.12 | 1.24 | 1.32 | 1.23 | 1.06 | 1.85 | 1.71 | 1.96 |
| D10 | 1.23 | 1.23 | 1.23 | 1.35 | 1.38 | 1.38 | 1.02 | 1.03 | 1.02 |
| D11 | 1.52 | 1.62 | 1.41 | 1.14 | 1.02 | 1.11 | 1.93 | 1.72 | 1.48 |
| D12 | 1.13 | 1.17 | 1.10 | 1.31 | 1.28 | 1.31 | 1.01 | 1.09 | 1.01 |
| D13 | 1.21 | 1.32 | 1.37 | 1.20 | 1.32 | 1.43 | 1.22 | 1.32 | 1.24 |
| D14 | 1.19 | 1.24 | 1.26 | 1.08 | 1.14 | 1.13 | 1.11 | 0.99 | 1.03 |
| average $g=2$ | 1.64 | 1.55 | 1.59 | 1.58 | 1.58 | 1.55 | 1.54 | 1.45 | 1.53 |
| average $g > 2$ | 1.25 | 1.32 | 1.27 | 1.22 | 1.23 | 1.27 | 1.26 | 1.23 | 1.16 |
| overall average | 1.50 | 1.47 | 1.47 | 1.45 | 1.46 | 1.45 | 1.44 | 1.37 | 1.40 |

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