Scalability Analysis of mRMR for Microarray Data

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Keywords: Feature Selection, Microarray, Machine Learning, Scalability.

Abstract: Lately, derived from the Big Data problem, researchers in Machine Learning became also interested not only in accuracy, but also in scalability. Although scalability of learning methods is a trending issue, scalability of feature selection methods has not received the same amount of attention. In this research, an attempt to study scalability of both Feature Selection and Machine Learning on microarray datasets will be done. For this sake, the minimum redundancy maximum relevance (mRMR) filter method has been chosen, since it claims to be very adequate for this type of datasets. Three synthetic databases which reflect the problematics of microarray will be evaluated with new measures, based not only in an accurate selection but also in execution time. The results obtained are presented and discussed.

1 INTRODUCTION

The advent of DNA microarray technology has brought the possibility of simultaneously measuring the expressions of thousands of genes. However, due to the high cost of experiments, sample sizes of gene expression measurements remain in hundreds, a very small number compared to tens of thousands of genes involved (Mundra and Rajapakse, 2010). Theoretically, having more genes should give more discriminating power. But actually, this fact can cause several problems, such as increasing computational complexity and cost, too many redundant or irrelevant genes and estimation degradation in the classification error. Having much higher number of attributes than instances causes difficulties for most machine learning methods, since they cannot generalize adequately and therefore, they obtain very poor test performances. To deal with this problem, and according to Occams razor (Blumer et al., 1987), the need to reduce dimensionality was soon recognized and several works have used methods of feature (gene) selection (Saeys et al., 2007).

Feature selection consists of detecting the relevant features and discarding the irrelevant ones to reduce the input dimensionality, and most of the time, to achieve an improvement in performance (Guyon, 2006). Moreover, several studies show that most genes measured in a DNA microarray experiment are not relevant for an accurate distinction among different classes of the problem (Golub et al., 1999). To avoid this curse of dimensionality (Jain and Zongker, 1997), feature selection plays a crucial role in DNA microarray analysis. Although the efficiency of feature selection in this domain (and in other areas with high dimensional datasets), is out of doubt, it is often forgotten in discussions of scaling, which is an important issue when dealing with high dimensional datasets, as it is the case in this research.

Among the different feature selection methods (Guyon, 2006), filters only rely on general characteristics of the data, and not on the learning machines; therefore, they are faster, and more suitable for large data sets. A common practice in this approach is to simply select the top-ranked genes where the ranks are determined by some dependence criteria, and the number of genes to retain is usually set by human intuition with trial-and-error. A deficiency of this ranking approach is that the selected features could be dependent among themselves. Therefore, a minimum Redundancy Maximum Relevance (mRMR) approach is preferred in practice (Peng et al., 2005), that also minimizes the dependence among selected features. This filter method has been widely used to deal with microarray data (Mundra and Rajapakse, 2010; Zhang et al., 2008; El Akadi et al., 2011). However, it is a computationally expensive method and its scalability should be evaluated. Therefore, this preliminary research will be focused on the scalability of the mRMR method over an artificial controlled experimental scenario, paving the way to its application to real microarray datasets.

The rest of the paper is organized as follows: section 2 describes the mRMR feature selection method,

Rego-Fernández D., Bolón-Canedo V. and Alonso-Betanzos A..
Scalability Analysis of mRMR for Microarray Data.
DOI: 10.5220/0004807703800386
In *Proceedings of the 6th International Conference on Agents and Artificial Intelligence* (ICAART-2014), pages 380-386
ISBN: 978-989-758-015-4

section 3 introduces the experimental settings, section 4 presents the experimental results and, finally, section 5 reveals the conclusions and future lines of research.

2 THE FILTER: mRMR

As mentioned in the Introduction, filters are more suitable for large datasets, as it is the case in this research. Within filters, one can distinguish between univariate and multivariate methods (Bolón-Canedo et al., 2013). Univariate methods (such as filters which just evaluate the information gain between a feature and the class label) are fast and scalable, but ignore feature dependencies so the features could be correlated among themselves. On the other hand, multivariate filters (such as mRMR) model feature dependencies and detect redundancy, but at the cost of being slower and less scalable than univariate techniques.

To rank the importance of the features of the datasets included in this research, the mRMR method, that was first developed by Peng, Long and Ding (Peng et al., 2005) was used for the analysis of microarray data. The mRMR method can rank features based on their relevance to the target, and at the same time, the redundancy of features is also considered. Features that have the best trade-off between maximum relevance to target and minimum redundancy are considered as “good” features. The feature selection purpose is to find *maximum dependency*, a feature set S with m features $\{x_i\}$, which have the largest dependency on the target class c, described by the authors (Peng et al., 2005) as:

$$max\ D(S,c),\ D = I(\{x_i, i = 1, ..., m\}; c)$$

Implementing the maximum dependency criterion is not an easy-to-solve task because of the characteristics of high-dimensional spaces. Specifically, the number of samples is often insufficient and, moreover, estimating the multivariate density usually implies expensive computations. An alternative is to determine the *maximum relevance* criterion. The maximum relevance consists of searching features which satisfy the following equation:

$$maxD(S,c), D = \frac{1}{|S|}\sum_{x_i \in S} I(x_i;c) \qquad (1)$$

Selecting the features according to the maximum relevance criterion can bring a large amount of redundancy. Therefore, the following criterion of minimum redundancy must be added, as suggested by (Peng et al., 2005) :

$$min\ R(S),\ R = \frac{1}{|S|^2}\sum_{x_i, x_j \in S} I(x_i, x_j)$$

Combining the above two criteria and trying to optimize D and R at the same time, the criterion called minimum redundancy maximum relevance (mRMR) arises.

$$max\ \Phi(D,R),\ \Phi = D - R$$

In practice, the next incremental algorithm can be employed:

$$max_{x_j \in X - S_{m-1}} [I(x_j;c) - \frac{1}{m-1}\sum_{x_i \in S_{m-1}} I(x_j;x_i)]$$

As mentioned above, mRMR is a multivariate method so it is expected to be slow and its scalability might be compromised. For these reason it is very interesting to perform a scalability study, which will be presented in next sections.

3 EXPERIMENTAL SECTION

3.1 Materials

Three synthetic datasets were chosen to evaluate the scalability of mRMR. Several authors choose to use artificial data since the desired output is known, therefore a feature selection algorithm can be evaluated with independence of the classifier used. Although the final goal of a feature selection method is to test its effectiveness over a real dataset, the first step should be on synthetic data. The reason for this is twofold (Belanche and González, 2011):

1. Controlled experiments can be developed by systematically varying chosen experimental conditions, like adding more irrelevant features. This fact facilitates to draw more useful conclusions and to test the strengths and weaknesses of the existing algorithms.
2. The main advantage of artificial scenarios is the knowledge of the set of optimal features that must be selected; thus, the degree of closeness to any of these solutions can be assessed in a confident way.

The three synthetic datasets selected (SD1, SD2 and SD3) (Zhu et al., 2010) reflect the problematic of microarray data. They are challenging problems because of their high number of features (around 4,000) and the small number of samples (75), besides of a high number of irrelevant attributes. In this context, Zhu et al. (Zhu et al., 2010) introduced two new definitions of multiclass relevancy features: full class relevant (FCR) and partial class relevant (PCR) features. On the one hand, FCR features are useful for distinguishing any type of cancer. On the other hand, PCR features only help to identify subsets of cancer types.

SD1, SD2 and SD3 are three-class synthetic datasets with 75 samples (each class containing 25 samples) and 4000 irrelevant features, generated following the directions given in (Díaz-Uriarte and De Andres, 2006). The number of relevant features is 20, 40 and 60, respectively, which are divided in groups of 10. Within each group of 10 features, only one of them must be selected, since they are redundant with each other.

To sum up, the characteristics of these three datasets are depicted in Table 1, where one can see the number of features, the number of features and samples and the relevant attributes which should be selected by the feature selection method, as well as the number of full class relevant (FCR) and partial class relevant (PCR) features. Notice that G_i means that the feature selection method must select only one feature within the *i*-th group of features.

Table 1: Characteristics of SD1, SD2 and SD3 datasets.

Dataset	No. of features	No. of samples	Relevant features	No. of FCR	No. of PCR
SD1	4020	75	G_1, G_2	20	–
SD2	4040	75	$G_1 - G_4$	30	10
SD3	4060	75	$G_1 - G_6$	–	60

It has to be noted that the easiest dataset in order to detect relevant features is SD1, since it contains only FCR features and the hardest one is SD3, due to the fact that it contains only PCR genes, which are more difficult to detect.

For assessing the scalability of the mRMR method, different configurations of these datasets were used. In particular, the number of features ranges from 2^6 to 2^{12} whilst the number of samples ranges from 3^2 to 3^5 (all pairwise combinations). Notice that the number of relevant features is fixed (2 for SD1, 4 for SD2 and 6 for SD3) and it is the number of irrelevant features the one that varies. When the number of samples increases, the new instances are randomly generated.

3.2 Evaluation Metrics

At this point, it is necessary to remind that mRMR does not return a subset of selected features, but a ranking of the features where the most relevant one should be ranked first. The goal of this research is to assess the scalability of mRMR feature selection method. For this purpose, some evaluation measures need to be defined, motivated by the measures proposed in (Zhang et al., 2009). One_error, coverage, ranking_loss, average_precision and training time were considered. In all measures, $feat\_sel$ is the ranking of features returned by the mRMR method, $feat\_rel$ is the subset of relevant features and $feat\_irr$ stands for the subset of irrelevant features. Notice that all measures mentioned below except training time are bounded between 0 and 1.

- The *one_error* measure evaluates if the top-ranked (the first selected in the ranking) feature is not in the set of relevant features.

$$\mathit{one\_error} = \begin{cases} 1; feat\_sel(1) \notin (feat\_rel) \\ 0; otherwise \end{cases}$$

- The *coverage* evaluates how many steps are needed, on average, to move down the ranking in order to cover all the relevant features. At worst, last ranking feature would be relevant so coverage would be 1 (since this measure is bounded between 0 and 1).

$$\mathit{coverage} = \frac{\max(feat\_sel(feat\_rel(i)))}{\#feat\_sel}$$

- The *ranking_loss* evaluates the number of irrelevant features that are better ranked than the relevant ones. The fewer irrelevant features are on the top of the ranking, the best classified are the relevant ones.

$$\mathit{ranking\_loss} = \frac{(coverage * \#feat\_sel) - \#feat\_rel}{\#feat\_rel * \#feat\_irr}$$

- The *average_precision:* evaluates the mean of average fraction of relevant features ranked above a particular feature of the ranking.

$$\mathit{average\_precision} = \frac{1}{\#feat\_rel} * \frac{\sum j; feat\_sel(j) \in feat\_rel \cap j<i}{i; feat\_rel(i)}$$

- The *training time* is reported in seconds.

For example, suppose we have 4 relevant features, $x_1, \ldots, x_4$, 4 irrelevant features, $x_5, \ldots, x_8$ and the following ranking returned by mRMR: $x_5, x_3, x_8, x_1, x_4, x_2, x_7, x_6$. In this case, the *one_error* is 1, because the first feature in the ranking is not a relevant one. For calculating the *coverage*, it is necessary to move down 6 steps in the ranking to cover all the relevant features. Regarding the *ranking_loss*, there are 2 irrelevant features better ranked than the relevant ones. As for the *average_precision*, the number of relevant features ranked above each feature of the ranking are the following: $0, 0, 1, 1, 2, 3, 4, 4$.

Motivated by the methodology proposed in (Sonnenburg et al., 2008), we define 5 figures from which 13 scalar measures are extracted. Note that the evaluation of mRMR algorithm relies on the bidimensional features-samples space (X-Y -axes). So, these evaluation measures shape a surface (Z-axis) in a three-dimensional space.

- One_error surface: *Feature size* vs *Sample size* vs *One_error*. It is obtained by displaying the evolution of the One_error measure across the feature-sample space. The following scalar measures are computed:

1. *OeMin*: the minimum amount of data (features x samples) for which the One_error measure achieves its minimum value.
2. *VuOe*: volume under the One_error surface.

- Coverage surface: *Feature size* vs *Sample size* vs *Coverage*. It is obtained by displaying the evolution of the Coverage across the feature-sample space.

3. *Coverage*: minimum coverage.
4. *Co5%*: the minimum amount of data (features x samples) for which the coverage drops below a threshold (5% of coverage).
5. *VuCo*: volume under the coverage surface.

- Ranking_loss surface: *Feature size* vs *Sample size* vs *Ranking_loss*. It is obtained by displaying the evolution of the ranking_loss across the feature-sample space.

6. *Ranking_loss*: minimum ranking_loss.
7. *Rl5%*: the minimum amount of data (features x samples) for which the ranking_loss drops below a threshold (5% of ranking_loss).
8. *VuRl*: volume under the ranking_loss surface.

- Average_precision surface: *Feature size* vs *Sample size* vs *Average_precision*. It is obtained by displaying the evolution of the average_precision across the feature-sample space.

9. *Average_precision*: maximum average_precision.
10. *Ap95%*: the minimum amount of data (features x samples) for which the average_precision rises above a threshold (95% of average_precision).
11. *VuAp*: volume under the Average_precision surface.

- Training time surface: *Feature size* vs *Sample size* vs *Traning time*. It is obtained by displaying the evolution of the average_precision across the feature-sample space.

12. *Training time*: training time in seconds for the maximum amount of data tested.
13. *VuTt*: volume under the training time surface.

Those measures related to One_error, Coverage, Ranking_loss and Training time (i.e. VuOe, Coverage, VuCo, Ranking_loss, VuRl, Training time and VuTt) are desirable to be minimized, whilst those related to Average_precison and amount of data (i.e. Average_precison, VuAp, Co5%, Rl5% and Ap95%) are desirable to be maximized.

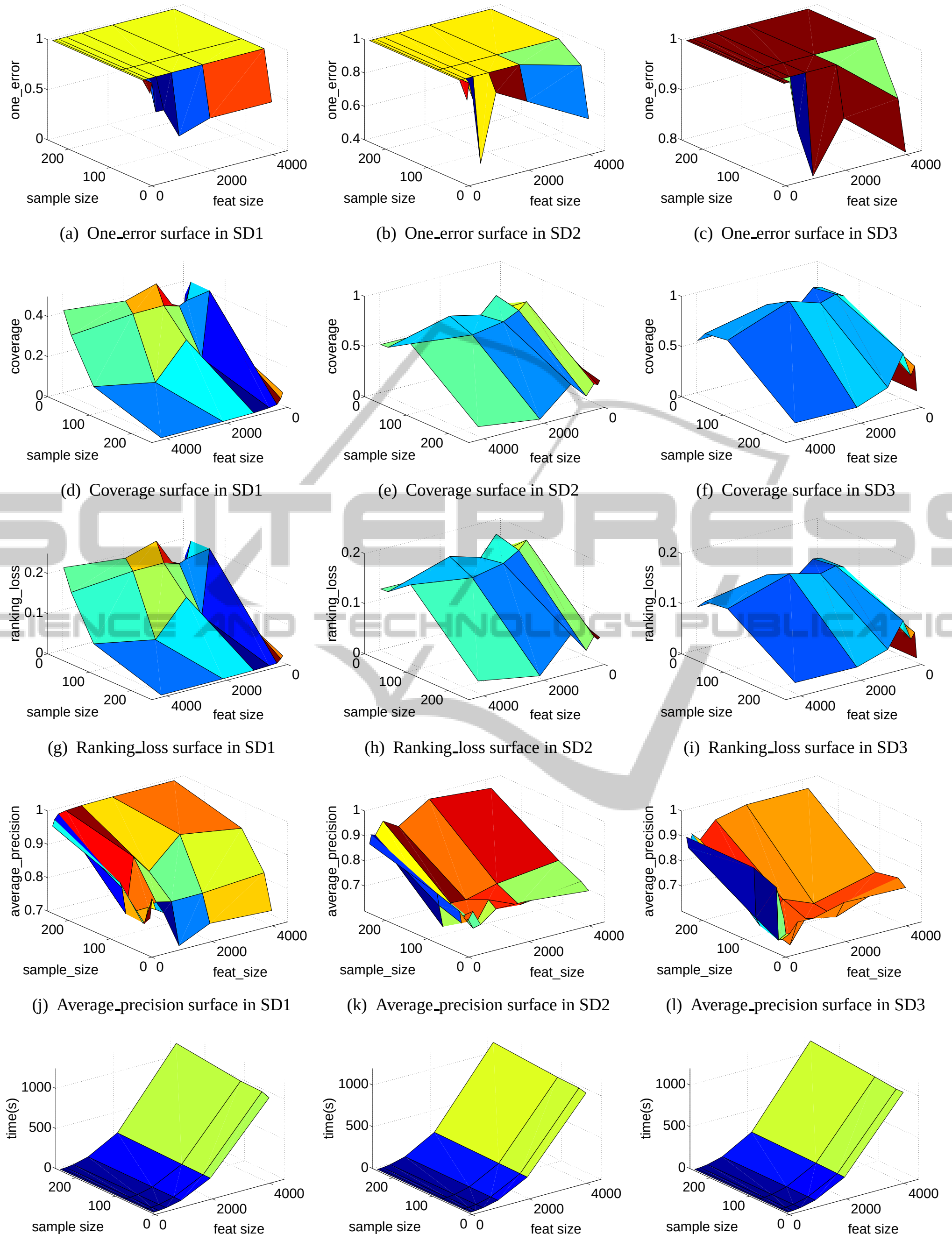
4 RESULTS

This section shows the scalability results for mRMR according to the measures explained above. Figure 1 plots these measures of scalability after applying a 10-fold cross validation. Remind that all the metrics but Average_precision are desirable to be minimized. In general terms, One_error, Coverage and Ranking_loss are more influenced by sample size whilst the training time is more affected by feature size. In the case of Average_precision, which should be maximized, this measure seems to be affected by feature size, since having more features would make harder the task of ranking the relevant features on top. Notice that in the figures related with Coverage and Ranking_loss the X-Y axes are shifted for visualization purposes.

As expected, the best results on the measures that assess the adequacy for selecting the most relevant features in the highest positions of the ranking (Coverage, Ranking_loss and Average_precision) are obtained on SD1 (the easiest dataset) whilst the performance deteriorates on SD2 and SD3. It has to be noticed that the coverage depends on the dataset, since the number of relevant features has influence on the calculation of this measure. Regarding One_error, it can be seen for all the three datasets that, in most of the cases, the top ranked feature is not in the subset of relevant features, which gives an idea of the hard challenge of the microarray problem.

Regarding the training time (see Figures 1(m), 1(n) and 1(o)), mRMR is sharply affected by the feature size (as expected for a multivariate filter technique), remaining almost constant with respect to the sample size.

Table 2 depicts the thirteen scalar measures related with Figure 1. These results confirm the trends seen in Figure 1, reflecting the adequacy of these measures which are reliable and confident and can give us a global picture of the scalability properties of the mRMR filter method. In terms of Coverage and Ranking_loss, it can be seen that mRMR achieves good results, especially on SD1 dataset. In fact, for this



(a) One_error surface in SD1 (b) One_error surface in SD2 (c) One_error surface in SD3

(d) Coverage surface in SD1 (e) Coverage surface in SD2 (f) Coverage surface in SD3

(g) Ranking_loss surface in SD1 (h) Ranking_loss surface in SD2 (i) Ranking_loss surface in SD3

(j) Average_precision surface in SD1 (k) Average_precision surface in SD2 (l) Average_precision surface in SD3

(m) Training time surface in SD1 (n) Training time surface in SD2 (o) Training time surface in SD3

Figure 1: Measures of scalability of mRMR filter in the SD1 (Figures a, d, g, j and m), SD2 (Figures b, e, h, k and n) and SD3 datasets (Figures c, f, i, l and o).

dataset, the minimum value of these metrics is really close to zero. As for the Average_precision, it is remarkable the result obtained on SD1, which obtains a maximum value very close to one, and an acceptable value (95 % of the maximum) is achieved with a small number of data (15552).

Table 3 shows an overview of the behavior of mRMR according to the different evaluation metrics over the different datasets studied, where the larger the number of dots, the better the behavior. To evaluate the goodness of the method it was computed a trade-off between the scalability in terms of number

Table 2: Evaluation metrics of mRMR filter in the SD1, SD2 and SD3 datasets.

Measure	SD1	SD2	SD3
One_error	0.4	0.5	0.8
Oe5%	9216	4608	9216
VuOe	17.00	17.38	17.70
Coverage	0.0017	0.0293	0.1474
Co5%	995328	497664	497664
VuCo	4.49	9.70	11.79
Ranking_loss	0.0006	0.0068	0.0115
Rl5%	995328	497664	15552
VuRl	2.19	2.39	1.93
Average_precision	0.9990	0.9893	0.9676
Av95%	15552	124416	248832
VuAp	15.61	13.85	13.25
Training time	1179	1144	1162
VuTt	2577	2577	2589

Table 3: Overview of the behavior regarding scalability of mRMR on the SD1, SD2 and SD3 datasets.

Measure	SD1	SD2	SD3
One_error	●	●	●
Coverage	●●●	●●	●●
Ranking_loss	●●●●	●●●	●
Average_precision	●●●●	●●●	●●
Training time	●●●	●●●	●●●

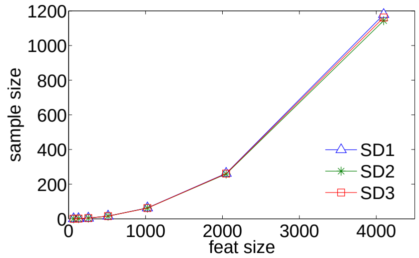


Figure 2: Training time vs. number of features for mRMR on SD1, SD2 and SD3 datasets.

of samples and number of features. In this manner, it is easy to see at a glance that mRMR does not achieve good results in terms of One_error, whilst shows strength in terms of Coverage and Ranking_loss, especially with SD1. With regard to the training time, the difficulty of the dataset has little impact on the time required to apply the filter, since it is almost constant for the three datasets tested. As can be seen in Figure 2, the training time is not linear for the number of features employed. In fact, when using 2000 features, the training time takes around 300 seconds, while when using double of features (4000), the training time increases by a factor of four.

5 CONCLUSIONS

With the advent of high dimensional scenarios in machine learning, scalability is becoming a very important trending issue. An algorithm is said to be scalable if it is suitable, efficient and practical when applied to large datasets. However, the current state is that the issue of scalability is far from being solved although is present in a diverse set of problems such as learning, clustering or feature selection.

In this research, our attention was focused on the scalability of feature selection, that has not received yet as much consideration in the literature as in the case of learning. In particular, this work is devoted to analyze the scalability of the well-known mRMR filter method, which is said to be suitable for microarray datasets. The method was evaluated over three synthetic datasets which reflect the problematic of microarray data. For analyzing scalability, these measures needed to be based not only in the accuracy of the selection, but also taking into account the execution time. Finally, the adequacy of the proposed measures to give a global picture on the mRMR method on the issue of scalability was shown.

In terms of accuracy of the selection, the mRMR method was demonstrated to be suitable and scalable for microarray datasets, since for most of the evaluation measures an increase in the amount of data does not produce a significantly degradation in performance. As for the training time, this filter is multivariate, and so the time raises exponentially when the number of features increases.

For future work, we plan to extend this research to other datasets and feature selection methods (filters, wrappers and embedded) in order to draw reliable conclusions. A methodology for fusing the proposed evaluation measures seems to be also necessary when comparing different methods so as to be able to obtain a ranking of the results, to establish final conclusions.

ACKNOWLEDGEMENTS

This research has been partially funded by the Secretaría de Estado de Investigación of the Spanish Government and FEDER funds of the European Union through the research project TIN 2012-37954. Verónica Bolón-Canedo acknowledges the support of Xunta de Galicia under *Plan I2C* Grant Program.

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