

# Feature Selection Via Coalitional Game Theory

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## Abstract

We present and study the Contribution-Selection algorithm (CSA), a novel algorithm for feature selection. The algorithm is based on the Multi-perturbation Shapley Analysis (MSA), a framework which relies on game theory to estimate usefulness. The algorithm iteratively estimates the usefulness of features and selects them accordingly, using either forward selection or backward elimination. It can optimize various performance measures over unseen data such as accuracy, balanced error rate and area under receiver-operator-characteristic curve. Empirical comparison with several other existing feature selection methods shows that the backward elimination variant of CSA leads to the most accurate classification results on an array of datasets.

## 1 Introduction

Feature selection refers to the problem of selecting input variables, otherwise called features, that are relevant to predicting a target value for each instance in a dataset. Feature selection can either be used to rank all potentially relevant input variables or to build a good classifier, and each task may lead to a different methodological approach (Blum & Langley, 1997; Kohavi & John, 1997). Feature selection has several potential benefits: defying the curse of dimensionality to enhance the prediction performance, reducing measurement and storage requirements, reducing training and prediction times, providing

better understanding of the process that generated the data and allowing data visualization. This paper focuses on the first issue, namely selecting input variables in an attempt to maximize the performance of a classifier on previously unseen data. Clearly, this would not necessarily produce the most compact set of features.

Feature selection is a search problem, where each state in the search space corresponds to a subset of features. Exhaustive search is usually intractable, and methods to explore the search space efficiently must be employed. These methods are often divided into two main categories: filter methods and subset selection methods. The algorithms in the first category rank each feature according to some measure of association with the target, such as mutual information, Pearson correlation or  $\chi^2$  statistic, and features with high ranking values are selected. A major disadvantage of filter methods is that they are performed independently of the classifier, and it is not guaranteed that the same set of features is optimal for all classifiers. In addition, most filter methods disregard the dependencies between features, as each feature is considered in isolation.

The second category, the subset selection methods, includes two types of algorithms: a) embedded algorithms that select the features through the process of generating the classifier, e.g. regularization methods such as Grafting (Perkins, Lacker, & Theiler, 2003), Gram-Schmidt methods such as Stop-piglia, Dreyfus, Dubois, and Oussar (2003); Rivals and Personnaz (2003) or methods specific for Support Vector Machines such as Weston et al. (2000);

Guyon, Weston, Barnhill, and Vapnik (2002); b) wrapper algorithms which treat the induction algorithm as a black box, and interact with it in order to perform a search for an appropriate features set using search algorithms such as genetic algorithms or hill climbing (Kohavi & John, 1997). Although wrapper methods are successful in feature selection, they may be computationally expensive, because they require the retraining of a classifier on data with a large number of features. For a survey of the current methods in feature selection see Guyon and Elisseeff (2003).

In this paper we recast the problem of feature selection in the context of coalitional games, a notion from game theory. This perspective yields an iterative algorithm for feature selection, the Contribution-Selection algorithm (CSA), intent on optimizing the performance of the classifier on unseen data. The algorithm combines both the filter and wrapper approaches, where the features are reranked on each step by using the classifier as a black box. The ranking is based on the Shapley value (Shapley, 1953), a well known concept from game theory, to estimate the importance of each feature for the task at hand, specifically taking into account interactions between features. Due to combinatorial constraints the Shapley value cannot be calculated precisely and is estimated by the Multi-perturbation Shapley Analysis (MSA) (Keinan, Sandbank, Hilgetag, Meilijson, and Ruppin (2004, 2005)). Furthermore, since the classifier is trained and tested extensively, the classifier used by CSA must be fast both in training and in testing phases. This requirement can be moderated by parallel processing.

Throughout the paper we use the following notations. Three disjoint sets containing i.i.d. sampled instances of the form  $(\mathbf{x}_k, y_k)$  are denoted by  $T$ ,  $V$  and  $S$  representing the training set, validation set and test set respectively, where  $\mathbf{x}_k \in \mathbf{R}^n$  denotes the  $k$ 'th instance, and  $y_k$  is the target class value associated with it. Given an induction algorithm and a set of features  $S \subseteq \{1, \dots, n\}$ ,  $f_S(x)$  stands for a classifier constructed from the training set using the induction algorithm, after its input variables were narrowed down to the ones in  $S$ . Namely,  $f_S(x)$  labels each instance of the form  $(x_{i_1}, \dots, x_{i_{|S|}})$ ,  $i_j \in S$ ,  $1 \leq j \leq |S|$  with an appropriate class value. The task of feature selection is to choose a subset  $S$  of the input variables that maximizes the performance of the classifier on the test set. In what follows we shall focus on optimizing classifier accuracy, although we could as easily optimize other performance measures such as the area under the receiver operator characteristic, balanced error rate etc.

The rest of this paper is organized as follows: Section 2 introduces the necessary background from game theory and justifies the usage of game theory concepts for the task of feature selection. It also provides a detailed description of the CSA algorithm; Section 3 provides an empirical comparison of CSA with several other feature selection methods on artificial and real world datasets, accompanied by an analysis of the results, showing that the backward elimination version of CSA is significantly superior to other feature selection methods considered; Section 4 discusses the empirical results and provides further insights to the success and failure of the backward

elimination version of the CSA algorithm. Section 5 summarizes the results obtained.

## 2 Classification as a Coalitional Game

Cooperative game theory introduces the concept of “coalitional games”, in which a set of players is associated with a real function, that denotes the payoff achieved by different sub-coalitions in a game. Formally, a *coalitional game* is defined by a pair  $(N, v)$  where  $N = \{1, \dots, n\}$  is the set of all *players* and  $v(S)$ , for every  $S \subseteq N$ , is a real number associating a worth with the *coalition*  $S$ . Game theory further pursues the question of representing the contribution of each player to the game by constructing a value function, which assigns a real-value to each player. The values correspond to the contribution of the players in achieving a high payoff.

The contribution value calculation is based on the Shapley value (Shapley, 1953). An intuitive example of the potential use of the Shapley value is a scenario of a production machine in a factory which is composed of numerous components. During its yearly operation, the machine undergoes various malfunctions from time to time. In each such malfunction, the normal activity of a subset of its components may be shut down, resulting in a certain reduction in the machine’s productivity and output. Based on this annual data of these multi-component failures and their associated production drops, the Shapley Value provides a fair and efficient way to distribute the responsibility for

the machine’s failure among its individual components, identifying the ones needed the most attention and maintenance, while considering their possible intricate functional interactions. In reference to feature selection, the machine is analogous to the predictor and its components to the classification features. The task of feature selection then involves the identification of the features contributing most to the classification in hand.

The Shapley value is defined as follows. Let the *marginal importance* of player  $i$  to a coalition  $S$ , with  $i \notin S$ , be

$$\Delta_i(S) = v(S \cup \{i\}) - v(S). \quad (1)$$

Then, the Shapley value is defined by the payoff

$$\Phi_i(v) = \frac{1}{n!} \sum_{\pi \in \Pi} \Delta_i(S_i(\pi)) \quad (2)$$

where  $\Pi$  is the set of permutations over  $N$ , and  $S_i(\pi)$  is the set of players appearing before the  $i$ th player in permutation  $\pi$ . The Shapley value of a player is a weighted mean of its marginal value, averaged over all possible subsets of players.

Transforming these game theory concepts into the arena of feature selection, in which one attempts to estimate the contribution of each feature in generating a classifier, the players are mapped to the features of a dataset and the payoff is represented by a real-valued function  $v(S)$ , which measures the performance of a classifier generated using the set of features  $S$ .

The usage of Shapley value for feature selection may be justified by its axiomatic qualities:

**Axiom 1** (*Normalization or Pareto optimality*) For any game  $(N, v)$  it holds that  $\sum_{i \in N} \Phi_i(v) = v(N)$

In the context of feature selection, this axiom implies that the performance on the dataset is divided fully between the different features.

**Axiom 2** (*Permutation invariance or symmetry*) For any  $(N, v)$  and permutation  $\pi$  on  $N$  it holds that  $\Phi_i(v) = \Phi_{\pi(i)}(\pi v)$

This axiom implies that the value is not altered by arbitrarily renaming or reordering the features.

**Axiom 3** (*Preservation of carrier or dummy-property*) For any game  $(N, v)$  such that  $v(S \cup \{i\}) = v(S)$  for every  $S \subseteq N$  it holds that  $\Phi_i(v) = 0$

This axiom implies that a dummy feature that does not influence the classifier's performance indeed receives a contribution value 0.

**Axiom 4** (*Additivity or aggregation*) For any two games  $(N, v)$  and  $(N, w)$  it holds that  $\Phi_i(v + w) = \Phi_i(v) + \Phi_i(w)$  where  $(v + w)(S) = v(S) + w(S)$

This axiom applies to a combination of two different payoffs based on the same set of features. For a classification task these may be, for example, accuracy and area under the receiver operator characteristic curve or false positive rate and false negative rate. In such case, the Shapley value of a feature which measures its contribution to the combined performance measure is just the sum of the corresponding Shapley values. The linearity of

the Shapley value is a consequence of this property. Namely, if the payoff function  $v$  is multiplied by a real number  $\alpha$  then all Shapley values are scaled by  $\alpha$  namely  $\Phi_i(\alpha v) = \alpha \Phi_i(v)$ . In other words, multiplying the performance measure by a constant does not change the ranking of the features, a vital property for any scheme that ranks features by their 'importance'.

Since it was introduced, the Shapley value has been successfully applied to many fields. One of the most important applications is with cost allocation, where the cost of providing a service should be shared among the different receivers of that service (Shubik, 1962; Roth, 1979; Billera, Heath, & Raanan, 1978). This use of the Shapley value has received recent attention in the context of sharing the cost of multicast routing (Feigenbaum, Papadimitriou, & Shenker, 2001). In epidemiology, the Shapley value has been utilized as a means to quantify the population impact of exposure factors on a disease load (Gefeller, Land, & Eide, 1998). Other fields where the Shapley value has been used include, among others, politics (starting from the *strategic voting* framework introduced by Shapley and Shubik (1954)), international environmental problems and economic theory (see Shubik (1985) for discussion and additional references).

## 2.1 Estimating Features Contribution Using MSA

The calculation of the Shapley value requires summing over all possible subsets of players, which is impractical in typical feature selection problems. Keinan et al. (2005) have presented an unbiased estimator for the Shapley

value <sup>1</sup> by uniformly sampling permutations from  $\Pi$ . Still, the estimator considers both large and small features sets to calculate the contribution values. In our feature selection algorithm, we use the Shapley value heuristically to estimate the contribution value of a feature for the task of feature selection. Since in most realistic cases we assume that the size  $d$  of significant interactions between features is much smaller than the number of features,  $n$ , we will limit ourselves to calculating the contribution value from permutations sampled from the whole set of players, with  $d$  being a bound on the permutation size:

$$\varphi_i(v) = \frac{1}{|\Pi_d|} \sum_{\pi \in \Pi_d} \Delta_i(S_i(\pi)) \quad (3)$$

where  $\Pi_d$  is the set of sampled permutations on subsets of size  $d$ .

Limiting the extent of interactions taken into account is not uncommon in feature selection methods: Most filter methods are equivalent to using  $d = 1$  where no feature interactions are taken into account. Explicit restriction on the level of interactions characterizes also several ensemble methods, e.g. Random Forests (Breiman, 2001), where  $d \simeq \sqrt{n}$  is usually suggested.

The usage of bounded sets coupled with the method for the Shapley value estimation, yields an efficient and robust way to estimate the contribution of a feature to the task of classification. For a detailed discussion of the MSA framework and its theoretical background see Keinan et al. (2004, 2005).

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<sup>1</sup>The estimation in Keinan et al. (2005) is used in a different context - to analyze the functional contribution in artificial and biological networks; however, the method to estimate the Shapley value is valid for our purpose as well.

The MSA toolbox can be downloaded from <http://www.cns.tau.ac.il/msa/>.

## 2.2 The Contribution-Selection Algorithm

The Contribution-Selection algorithm (CSA) is iterative in nature, and can either adopt a forward selection or backward elimination approach. Its backward elimination version, which overall yields better prediction accuracy (see Section 3.2) is described in detail in Figure 1. In the backward elimination version, using the subroutine *contribution*, the CSA ranks each feature according to its contribution value, and then eliminates  $e$  features with the lowest contribution values (using the subroutine *elimination*). It repeats the phases of calculating the contribution values of the currently remaining features and eliminating new features, until the contribution values of all candidate features exceed a contribution threshold  $\Delta$ . Forward selection CSA works in a similar manner, selecting on each iteration  $s$  features with highest contribution values, as long as their contribution values exceed a some threshold.

The algorithm, without further specification of the *contribution* subroutine, is a known generalization of filter methods. However, the main idea of the algorithm is that the *contribution* subroutine, unlike common filter methods, returns a contribution value for each feature according to its role in improving the classifier's performance, which is generated using a specific induction algorithm, and in conjunction with other features. Using the notation in Section 2 and assuming that one maximizes the accuracy level of

Contribution-Selection-Algorithm-Backward-Elimination( $F ; t, d, \Delta, e$ )

1.  $c := F$
2. for each  $f \in F \setminus c$ 
  - 2.1. Sample permutations set  $\{\pi_1, \dots, \pi_t\}$  over  $F \setminus c$
  - 2.2.  $C_f := \text{contribution}(f, c ; d) = \frac{1}{t} \sum_{j=1}^t \Delta_f(S_f(\pi_j))$
3. if  $\max_f C_f < \Delta$ 
  - 3.1.  $c := c \setminus \text{elimination}(\{C_f\} ; e, \Delta)$
  - 3.2. goto 2
- else
- 3.3. return  $c$

Figure 1: *The Contribution-Selection algorithm in its backward elimination version.*  $F$  is the input set of features.  $t$ ,  $d$ ,  $\Delta$  and  $e$  are hyperparameters:  $t = |\Pi_d|$  is the number of permutations sampled (see Equation 3),  $d$  is the maximal permutation size for calculating the contribution values,  $\Delta$  is a contribution value threshold and  $e$  is the number of features eliminated in each phase. The variable  $c$  represents the set of candidate features for selection. The *contribution* subroutine calculates the contribution value of feature  $f$  according to Equation 3 where  $f$  corresponds to the  $i$ 'th player. The *elimination* subroutine eliminates at most  $e$  features with lowest contribution values that do not exceed  $\Delta$ . In the forward selection version, the *elimination* subroutine is replaced with an *selection* subroutine which selects  $s$  features in each phase and the halting criterion is changed accordingly.

the classifier, the *contribution* subroutine for backward selection calculates the contribution values  $\varphi_i$  by Eq. 1 and 3 where the payoff function  $v(S)$  is simply the validation accuracy of the base classifier  $f_S(x)$  trained on the training set  $T$ ,

$$v(S) = \frac{|\{x|f_S(x) = y, (x, y) \in V\}|}{|V|} .$$

The case  $S = \phi$  is handled by returning the fraction of majority class instances. The maximal permutation size  $d$  has an important role in deciding the contribution values of the different features, and should be selected in a way that ensures that different combinations of features that interact together are inspected. Its impact is demonstrated in Section 3.

The number of eliminated features  $e$  for the *elimination* subroutine controls the redundancies of the eliminated features; the higher  $e$  is, the more likely that correlated features with redundant contribution will be eliminated. Although  $e = 1$  minimizes the redundancy dependencies of the features, increasing  $e$  accelerates the algorithm’s convergence, and further provides some regularization as has been verified experimentally. The algorithm’s halting criterion depends on  $\Delta$ , which designates a trade-off between the number of selected features, and the performance of the classifier on the validation set. With the backward elimination version, choosing  $\Delta = 0$  means that CSA eliminates features as long as there exist features that are unlikely to improve the classifier’s performance. Increasing  $\Delta$  has the opposite effect on the size of the final set of features. The naive halting criterion that ter-

minates feature elimination when no further performance gain is expected, namely when the exclusion of no feature enhances the performance, is entirely different. For example, during CSA backward elimination there are occasionally features with negative contribution values that once eliminated, there is no performance improvement. Still the removal of such features tends to increase the generalization of the classifier by the mere reduction of its complexity. Indeed, testing this naive halting criterion has verified that it leads to considerably inferior performance levels.

## 3 Results

### 3.1 Experiments with Artificial Data

In order to demonstrate the algorithm’s behavior, we generated a dataset which consists of 9 features. The first three features are binary. The target labels are taken as the parity function of these three features. The other six features are correlated with the target by setting them to the target values and adding a random value taken from the normal distribution with expectancy 0 and standard deviation  $\sigma = 1$ . A simple calculation shows that the correlation between each of these six features and the target is  $\sqrt{(1 + \sigma^2)^{-1}} \simeq 0.71$ , and the correlation between the sum of these features and the target is  $\sqrt{(1 + \sigma^2/6)^{-1}} \simeq 0.92$ . The mean accuracy of a classifier that outputs the sign of the sum of these six features is 0.84, which will be considered a baseline accuracy (the accuracy of C4.5 classifier that uses all

nine features is 0.82). The dataset consists of 200 training examples and 100 test examples.

Using this dataset, we inspected the features selected and the performance of several feature selection methods. We used Random Forests (Breiman, 2001), mutual information, Pearson correlation, regular backward wrapper method (eliminating one feature at a time), regular forward wrapper method (selecting one feature at a time) and CSA in both backward elimination and forward selection using C4.5 as base learner. CSA was run with  $s = 1$ ,  $e = 1$ ,  $d = 3$  and  $t = 20$ .<sup>2</sup> No optimization was performed on these hyperparameters. In all ranking methods (Random Forests, mutual information and Pearson correlation) the first three features were ranked as least informative features. As expected, the accuracy obtained by using these methods did not exceed the baseline accuracy 0.84. Forward selection CSA together with backward wrapper and forward wrapper did not select any of the first three most relevant features. Yet, backward elimination CSA chose the three features for classification, and achieved 100% accuracy. The reason for this behavior is that the other six features were too confusing for the classifier with most algorithms. With decision trees, the first three features will always be used in deep nodes of the tree, due to the greedy criterion used by decision tree algorithm to select a feature for node splitting. Therefore, the inclusion or removal of any one of these features will have less influence on

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<sup>2</sup>While CSA evaluated 540 permutations, this toy example can be solved by an exhaustive search requiring only  $2^9 - 1 = 511$  evaluations.

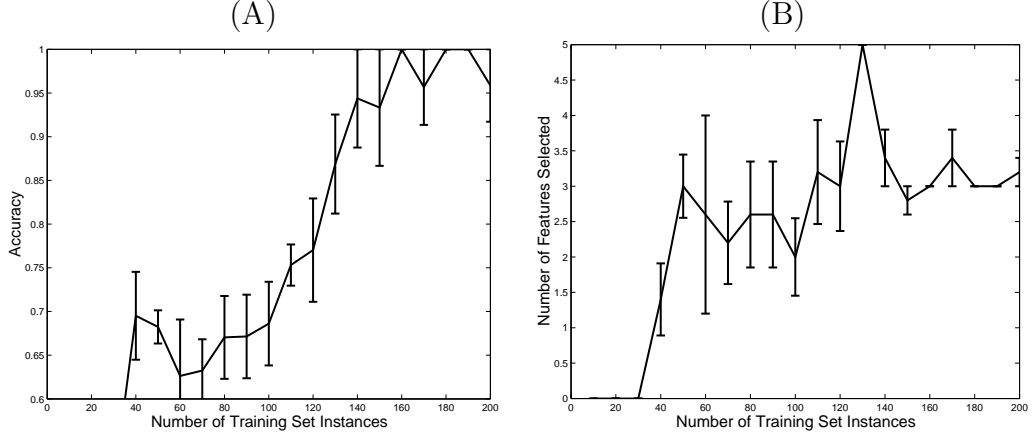


Figure 2: *Behavior of backward selection CSA on the artificial dataset.* (A) The accuracy of the backward selection CSA changes with respect to  $n$ , the number of training set instances. (B) The average number of features selected as a function of  $n$ .

the classifier’s accuracy than any of the six features linearly correlated with the target.

We further tested the behavior of CSA with respect to the number of training instances,  $n$ . To this end, we produced training sets of different values of  $n$  and ran the algorithm on each sample. For each value of  $n$  five different training sets were sampled and scored, and the average accuracy and average number of features selected were computed. The results for the backward selection CSA with are described in Figure 2. As can be seen, for  $n \gtrsim 140$  many instances of the backward elimination CSA identify the 3 salient features and achieve perfect categorization of the test examples.

## 3.2 Experiments with Real-world Data

To test CSA empirically we ran a number of experiments on seven real-world datasets with number of features ranging from 278 to 20,000 (Table 1):

- Following Koller and Sahami (1996) we constructed the Reuters1 dataset from the Reuters-21578 document collection (Reuters, 1997). The dataset consists of articles from the categories *coffee* (99 documents), *iron-steel* (137 documents) and *livestock* (54 documents). These topics do not have many overlapping words, making the task of classification easier. As a preprocessing step, we removed all words that appeared less than 3 times. Each article was then encoded into a binary vector, where each element designates whether the word appeared in the document or not.
- The Reuters2 dataset was constructed, similarly to the Reuters1 dataset, only from the categories *gold* (68 documents), *gross national product* (124 documents) and *reserves* (136 documents). These topics are more similar, and contain many overlapping words, making the task of classification harder. For both of the Reuters datasets, our splits are not identical to the one in Koller and Sahami (1996), and contain fewer documents, because we could not obtain the exact same dataset.
- The Arrhythmia database from the UCI repository (Blake & Merz, 1998). The task for this database is to distinguish between normal and abnormal heartbeat. We used a version of the data which was

slightly modified by Perkins et al. (2003): features that were missing in most of the instances were removed. The dataset contains 237 positive instances and 183 negative instances. It can be found in <http://www.lanl.gov/~simes/data/jmlr03>.

- The Internet Advertisements database from the UCI repository (Blake & Merz, 1998). It was collected for research on identifying advertisements in web pages (Kushmerick, 1999). The features in the database describe different attributes in a web page, such as the domain which it was downloaded from, the domain which referred to it and its size. There are two classes: each instance is either an advertisement or not an advertisement. The dataset contains 2581 positive instances, and 419 negative instances.
- The Dexter dataset from the NIPS 2003 workshop on feature selection (Guyon, 2003). The Dexter dataset is a two-class text categorization dataset constructed from a subset of the Reuters dataset, using documents from the category in *corporate acquisitions*. The dataset is abundant with irrelevant features; for the exact details of how the dataset was constructed see Guyon (2003). The dataset contains 300 positive instances, and 300 negative instances. As a preprocessing step, we binarized each of the instances, which originally contained the word frequency in each document, and removed words that appeared less than 3 times. The validation set of the data served in the following

experiments as T, the test set.

- The Arcene dataset from the NIPS 2003 workshop on feature selection (Guyon, 2003). The Arcene dataset is a two-class categorization dataset, describing mass spectrometry analysis of blood serum of patients with a certain kind of cancer and without it. It is affluent with features and poor with data instances. For the exact details of how the dataset was constructed see Guyon (2003). The dataset contains 88 positive instances, and 112 negative instances. The validation set of the data served in the following experiments as T, the test set.
- I2000, a microarray colon cancer dataset by Alon et al. (1999). The dataset is a two-class categorization dataset for discriminating between healthy and ill tissues in colon cancer. The data contains the expression of 2000 genes with highest minimal intensity across 62 tissues. The dataset contains 31 positive instances, and 31 negative instances. It has a very high features to instances ratio, making the task of feature selection harder.

In principle, CSA can work with any induction algorithm  $L$ . However, due to computational constraints we focused on fast induction algorithms or algorithms that may be efficiently combined into CSA. We experimented with Naive Bayes, C4.5 and 1NN. For each of the datasets, we measured the training set accuracy of each classifier using ten-fold cross validation on the whole set features. For each dataset, all subsequent work used the induction

| Name         | # Classes | # Features | Training Set Size | Testing Set Size |
|--------------|-----------|------------|-------------------|------------------|
| Reuters1     | 3         | 1579       | 145               | 145              |
| Reuters2     | 3         | 1587       | 164               | 164              |
| Arrhythmia   | 2         | 278        | 280               | 140              |
| Internet Ads | 2         | 1558       | 2200              | 800              |
| Dexter       | 2         | 20000      | 300               | 300              |
| Arcene       | 2         | 10000      | 100               | 100              |
| I2000        | 2         | 2000       | 40                | 22               |

Table 1: Description of datasets used.

algorithm  $L$  that gave the highest cross validation accuracy, as detailed in Table 2.

Nine different classification algorithms were then compared on the datasets described above:

- Classification using the induction algorithm  $L$  without performing any feature selection.
- Classification using soft margin linear  $SVM$  with the  $SVM^{light}$  package (Joachims, 1999). Datasets that had more than two classes were decomposed to few one-versus-all binary classification problems.
- Classification using  $L$  after performing feature selection by estimation of the Pearson correlation coefficient. The number of features was selected by performing ten-fold cross validation on the training set and averaging the results, each time adding more features with the highest correlation value to the current features set. After this process, the set that obtained the best result was selected.

- Classification using  $L$  after performing feature selection by estimation of mutual information. For datasets with continuous domain (*Arrhythmia*, *Internet Ads*, *Arcene* and *I2000*), we used binning to estimate the mutual information. The number of features selected was optimized like with the Pearson correlation coefficient.
- Classification using  $L$  after performing feature selection with Random Forests (Breiman, 2001). We used the “randomForest” library implementation for the R environment (Bengtsson, 2003). The number of features selected was optimized like with the Pearson correlation coefficient.
- Classification using  $L$  after performing feature selection with backward elimination CSA with  $d = 1$ . The number of permutations selected was large enough so each feature is sampled with high probability. This is equivalent to regular wrapper technique, in which backward elimination is used to eliminate the features that most degrades the accuracy of the classifier. This algorithm is chosen to check whether it is sufficient to examine each feature separately for performing feature selection on the dataset.
- Classification using  $L$  after performing feature selection with forward selection CSA with  $d = 1$ . The number of permutations selected was large enough so each feature is sampled with high probability. This is equivalent to regular wrapper technique, in which forward selection

is used to select the features that most improve the accuracy of the classifier. This algorithm is similar to that of the backward wrapper.

- Classification using  $L$  after performing feature selection with backward elimination CSA and parameters as described in Table 2. The parameters  $d$  and  $t$  were chosen such that the expected number of times that each feature is sampled is higher than 5. This number was chosen according to error analysis considerations of MSA (Keinan et al., 2004) and following preliminary experimentation with an artificial datasets. When computation times allowed, the number of permutations sampled was much larger than the minimal value. The contribution value threshold for stopping elimination was  $\Delta = 0$ . No hyperparameter selection was performed on either  $d$ ,  $t$  or  $\Delta$ .
- Classification using  $L$  after performing feature selection with forward selection CSA and parameters as described in Table 2. The parameters  $d$  and  $t$  were chosen such that the expected number of times that each feature is sampled is higher than 5. The termination of feature selection was fixed by choosing a contribution value threshold  $\Delta = 0$ . No hyperparameter selection was performed on either  $d$ ,  $t$  or  $\Delta$ .

CSA is prone to overfitting on the validation set; when the classifier’s performance is always evaluated on a possibly small validation set, the curse of dimensionality appears, and irrelevant features are selected, even if the classifier itself is trained using techniques that avoid overfitting. It might

| Dataset      | Induction Alg. (L) | $s$ (Fwd.) | $e$ (Bwd.) | $d$ | $t$   |
|--------------|--------------------|------------|------------|-----|-------|
| Reuters1     | Naive Bayes        | 1          | 100        | 20  | 1500  |
| Reuters2     | Naive Bayes        | 1          | 100        | 20  | 1800  |
| Arrhythmia   | C4.5               | 1          | 50         | 20  | 500   |
| Internet Ads | 1NN                | 1          | 100        | 20  | 1500  |
| Dexter       | C4.5               | 50         | 50         | 12  | 3500  |
| Arcene       | C4.5               | 100        | 100        | 5   | 10000 |
| I2000        | C4.5               | 100        | 100        | 3   | 2000  |

Table 2: *The parameters and the classifier used with the CSA algorithm for each dataset.*  $s$  is the number of features selected in forward selection in each phase,  $e$  is the number of features eliminated in backward elimination in each phase,  $d$  is the permutation size and  $t$  is the number of permutations sampled to estimate the contribution values. For an explanation how hyperparameters are chosen, see the description of the backward CSA algorithm.

seem at first that evaluating the classifier each time on a different training set and validation set split can solve the problem. However, this leads to another problem: the classifier’s performance depends on the split so the marginal contributions of the different features do not reflect their real value. In order to avoid both of these problems, we used ten-fold cross validation; the training set was split into several parts, and the payoff function was evaluated by averaging a classifier’s performance on the whole training set.

### 3.3 Feature Selection and Classification Results

Table 3 summarizes the classifiers’ performance on the test set and the number of features selected in each of the experiments. The accuracy levels are the fraction of correctly classified test set instances:

- *The Reuters1 dataset.* Feature selection using CSA with backward elimination did best, yielding accuracy level of 98.6% with 51 features. Koller and Sahami (1996), for example, report that the Markov Blanket algorithm yields approximately 600 selected features with accuracy levels of 95% to 96% on this dataset.
- *The Reuters2 dataset.* Wrapper with backward elimination did best, yielding accuracy level of 95% with 53 features. For comparison, Koller and Sahami (1996) report that the Markov Blanket algorithm yields approximately 600 selected features with accuracy levels of 89% to 93% on this dataset. <sup>3</sup>
- *The Arrhythmia dataset.* This dataset is considered to be a difficult one. CSA with backward elimination did best, yielding an accuracy level of 84% with 21 features. Forward selection with higher depth value ( $d = 20$ ) did better than with  $d = 1$ , implying that one should consider many features concomitantly to perform good feature selection for this dataset. For comparison, the grafting algorithm (Perkins et al., 2003) yields an accuracy level of approximately 75% on this dataset.
- *The Internet Ads dataset.* All the algorithms did approximately the same, leading to accuracy levels between 94% and 96% with CSA slightly outperforming the others. Interestingly enough, with  $d = 1$

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<sup>3</sup>The datasets used in Koller and Sahami (1996) are not identical to the datasets we used. We were unable to obtain the same datasets, and had to reconstruct them from the original Reuters-21578 collection.

the algorithm did not select any feature; in the first phase, the 1NN algorithm had neighbors from both classes with the same distance for each feature checked, leading to arbitrary selection of one of the classes, and the classifier’s performance was constant through all the phase, yielding zero contribution values. However, when selecting the higher depth levels, the simple 1NN algorithm was boosted up to outperform classifiers such as *SVM*.

- *The Dexter dataset.* For the Dexter dataset, we used algorithm *L* (*C4.5* decision trees) only for the process of feature selection, and Linear *SVM* to perform the actual prediction on the features selected. This was done because *C4.5* did not give satisfying accuracy levels for any of the feature selection algorithms, and it is impractical to use *SVM* with CSA for large datasets. To overcome the difference between the classifiers performing feature selection and the classifier used for the actual classification, we added an optimization phase for the forward selection algorithm after it stopped. In this phase, a ten-fold cross-validation is performed on the dataset in a similar way to the one used to optimize filter methods. The simple mutual information feature selection performed best, followed closely by the Contribution-Selection algorithm in its backward elimination version and by Random Forests. This implies that in Dexter the contribution of single features significantly outweigh the contribution of feature combinations for the task of classification. The forward selection algorithm did as well as *Linear*

*SVM* without feature selection, but with a significantly lower number of features.

- *The Arcene dataset.* Here, just as in the case of Dexter, we use *C4.5* for the process of feature selection, and Linear *SVM* to perform the actual prediction on the features selected. The CSA with backward elimination obtained better performance than the rest of the algorithms.
- *The I2000 dataset.* CSA with backward elimination together with feature selection using mutual information yielded the best results. The poor performance of CSA with forward selection can be explained by the poverty of data compared to the number of features; the algorithm selected in the first phases features which explain well the training data by coincidence, and avoided from selecting features that truly contribution to the task of classification. This phenomenon is explained in portrait in Section 3.5.2.

### 3.4 Significance of the Results

Using McNemmar test (Gillick & Cox, 1989) on the results summarized in Table 3 has shown no significant superiority of any feature selection method on any of the datasets. The accuracies are too close to each other compared to the size of the test sets.

However, in five out of the seven datasets, CSA with backward elimination achieved the highest accuracy. In the other case it achieved the second

best accuracy. So even though the results are not significant per dataset, the overall picture may suggest otherwise. To test whether the backward elimination version of CSA is indeed superior to the other feature selection algorithms, we performed a one-sided Wilcoxon Signed-Rank Test (Kanji, 1994). This test takes into account the ranking of feature selection methods across all datasets, and tests whether the set of rankings significantly deviates from the  $H_0$  distribution that assumes that all methods are equal. Table 4 lists the p-values of these tests. As can be seen, the backward elimination version of CSA has significantly higher performance than most of the other methods tried.

## 3.5 A Closer Inspection of the Results

### 3.5.1 Behavior of the Algorithm With Different Parameters

In order to examine the effect of different parameter values on the algorithm we ran the CSA on the Arrhythmia dataset with different values of  $d$  (size of subsets analyzed) and values of  $t$  (number of permutations examined in each phase of eliminating new features). The results were averaged over five experiments for each value of  $d$  and  $t$ .

Figure 3 describes the result. Figure 3A implies that there are optimal values of  $d$  for which the performance achieved is highest. For small values of  $d$ , not enough interactions between the different features are considered. As  $d$  increases, the performance on the dataset increases as well until it reaches a

| Dataset      | No FS | SVM   | Corr         | MI                  | RF          |
|--------------|-------|-------|--------------|---------------------|-------------|
| Reuters1     | 84.1% | 94.4% | 90.3% (20)   | 94.4% (20)          | 96.3% (6)   |
| Reuters2     | 81.1% | 91.4% | 88.4% (20)   | 90.2% (5)           | 87.2% (21)  |
| Arrhythmia   | 76.4% | 80%   | 71.4% (20)   | 70% (20)            | 80% (40)    |
| Internet Ads | 94.7% | 93.5% | 94.2% (15)   | 95.75% (70)         | 95.6% (10)  |
| Dexter       | 92.6% | 92.6% | 92.6% (1240) | <b>94%</b> (230)    | 93.3% (800) |
| Arcene       | 83%   | 83%   | 83% (6600)   | 81% (5600)          | 82% (6000)  |
| I2000        | 86.3% | 72.7% | 81.8% (260)  | <b>90.9%</b> (1060) | 86.3% (100) |

| Dataset      | Wrapper Bwd       | Wrapper Fwd | CSA Bwd             | CSA Fwd     |
|--------------|-------------------|-------------|---------------------|-------------|
| Reuters1     | 94.4% (35)        | 92.4% (7)   | <b>98.6%</b> (51)   | 96.5% (10)  |
| Reuters2     | <b>95.7%</b> (53) | 91.4% (5)   | 93.2% (109)         | 90.1% (14)  |
| Arrhythmia   | 77.8% (17)        | 70% (5)     | <b>84.2%</b> (21)   | 74.2% (28)  |
| Internet Ads | 95% (62)          | -           | <b>96.1%</b> (158)  | 95.6% (8)   |
| Dexter       | 92.6% (653)       | 80% (10)    | 93.3% (717)         | 92.6% (100) |
| Arcene       | 82% (6800)        | 58% (7)     | <b>86%</b> (7200)   | 81% (600)   |
| I2000        | 86.3% (1600)      | 86.3% (550) | <b>90.9%</b> (1100) | 86.3% (500) |

Table 3: *Accuracy levels and number of features selected in the different datasets.* Upper table: No FS (no feature selection), SVM (linear soft margin SVM without feature selection), Corr (feature selection using Pearson correlation), MI (feature selection using mutual information), RF (feature selection using Random Forests). Bottom table: Wrapper Bwd and Wrapper Fwd (Wrapper with backward and forward selection respectively), CSA Bwd and CSA Fwd (CSA with backward elimination and forward selection respectively with parameters from Table 2). Accuracy levels are calculated by counting the number of misclassified instances. The number of features selected is given in brackets. Notice that the accuracies obtained by our algorithms on the Dexter and Arcene datasets are inferior to those of the winners of NIPS 2003, feature selection competition.

|       | CFwd. | WBwd. | WFwd. | RF    | MI    | No FS | SVM   | Corr. |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| CBwd. | 0.015 | 0.078 | 0.031 | 0.093 | 0.015 | 0.015 | 0.015 | 0.015 |
| CFwd. | -     | 0.672 | 0.219 | 0.625 | 0.218 | 0.625 | 0.687 | 0.156 |
| WBwd. |       | -     | 0.016 | 0.031 | 0.094 | 0.016 | 0.016 | 0.016 |
| WFwd. |       |       | -     | 0.156 | 0.046 | 0.625 | 0.437 | 0.937 |
| RF    |       |       |       | -     | 0.562 | 0.156 | 0.156 | 0.156 |
| MI    |       |       |       |       | -     | 0.078 | 0.437 | 0.109 |
| No FS |       |       |       |       |       | -     | 0.812 | 0.812 |
| SVM   |       |       |       |       |       |       | -     | 0.109 |

Table 4: *Wilcoxon Signed-Rank test p-values.* This table specifies the Wilcoxon Signed-Rank test p-values related to the results in Table 3. The entry on row  $i$  and column  $j$  specifies the p-value related to testing whether the method  $i$  is superior to method  $j$ . CBwd stands for CSA with backward elimination and WBwd stands for Wrapper with backward elimination. CFwd and WFwd follow similar naming. p-values were calculated using the exact distribution for  $n = 7$  tests, which can easily be calculated by enumeration. It can be seen that the backward elimination CSA is better than the other methods tried with significance level 0.05, except for Random Forests and Wrapper backward elimination where only a marginal significance is achieved. Notice that no other feature selection method was found to be significantly better than majority of the remaining methods.

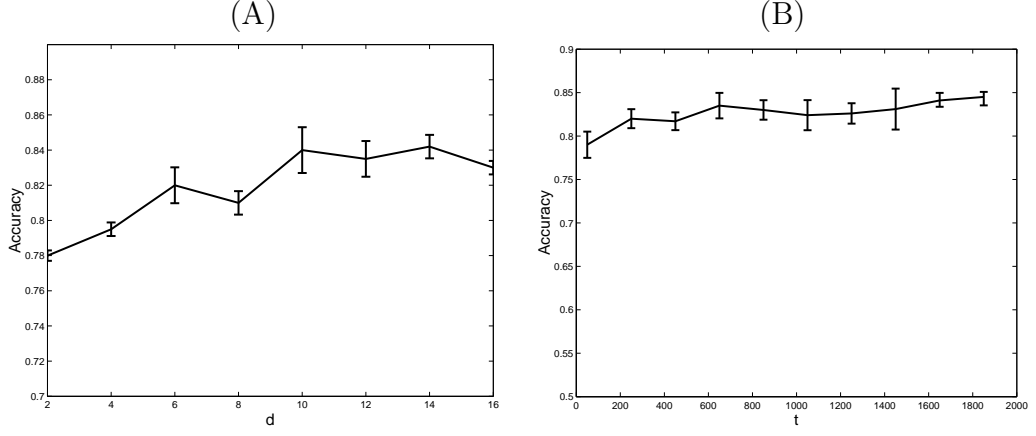


Figure 3: *Dependency of CSA performance on its hyperparameters:* (A) the accuracy of backward elimination version of CSA for various values of  $d$ , size of subsets. As expected, for small values of  $d$  there is a substantial improvement of performance as  $d$  is increased. But beyond a certain point (here around  $d = 10$ ), the accuracy stays stable around 83%. ;(B) the accuracy of backward elimination of CSA for various values of  $t$ , the number of permutations sampled. The overall picture is compatible with the fact that the estimate of the Contribution value becomes more robust as more samples taken.

critical value. For values of  $d$  larger than that critical value, the performance stays stable around the critical value's performance.

Figure 3B implies that the algorithm is rather robust to the number of permutations analyzed in each phase. For very small  $t$  values, the algorithm's performance is limited. But as  $t$  grows to values a little higher, the performance grows as well, until it stays rather stable.

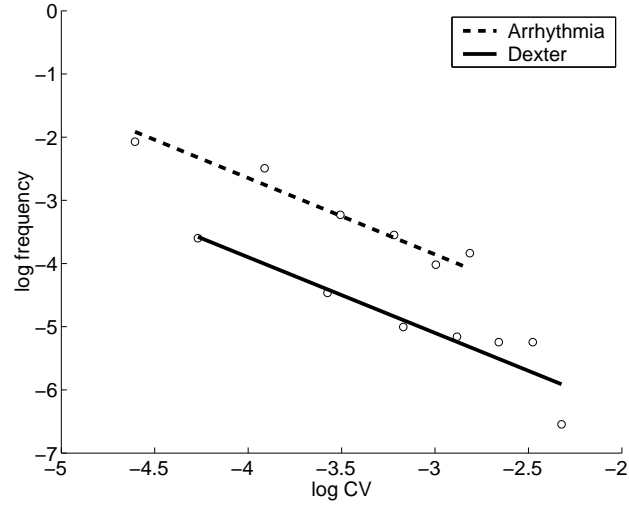


Figure 4: *Power-law distribution of contribution values.* This log-log plot of the distribution of the contribution values (absolute value) in the first phase for *Arrhythmia* and *Dexter*, prior to making any feature selection, demonstrates a power law behavior. For both axes natural logarithms are used. The p-values for the regression were 0.0047 (*Arrhythmia*) and 0.0032 (*Dexter*). The corresponding plots for the other datasets show power-law characteristics with different slopes and were eliminated for the sake of clarity.

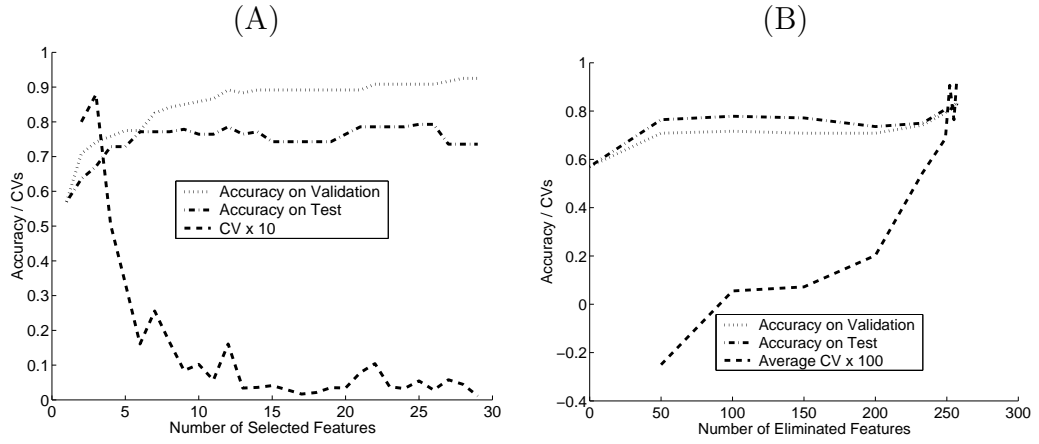


Figure 5: *Prediction accuracy and feature contribution during forward selection (A) and backward elimination (B) for the Arrhythmia dataset.* Both figures show how the performance of the C4.5 classifier improves on the validation set as the algorithm selects (eliminates) new features, while the contribution values of the selected features decrease (increase). The backward elimination generalizes better on the test set through the algorithm's progress. The behavior for the other datasets is similar.

### 3.5.2 The Distribution of the Contribution Values

The MSA, intent on capturing correctly the contribution of elements to a task, enables us to examine the distribution of the contribution values of the features. Figure 4 depicts a log-log plot of the distribution of the contribution values in the first phase for *Arrhythmia* and *Dexter*, prior to making any feature selection. This distribution follows a scale-free power law, implying that large contribution values (in absolute value) are very rare, while small ones are quite common, justifying quantitatively the need of feature selection. The other datasets were also observed to possess a similar power law characteristic.

The behavior of the algorithm through the process of feature selection and feature elimination is displayed in Figure 5; after the forward selection algorithm identifies the significant features in the first few phases, there is a sharp decrease in the contribution values of the features selected in the following phases, while with backward elimination, there is a gradual and rather stable increase in the contribution values of the non-eliminated features. The peaks in the graph of the contribution values in Figure 5A demonstrate that the contribution values do change as the CSA iterates. In this case, the selection of a single feature considerably increased the contribution value of another feature, pointing at intricate dependencies between features.

Figures 4 and 5 also assist in explaining why backward elimination usually outperforms several feature selection methods, including forward selection; due to the high dimensionality of the datasets, a feature that assists

in prediction merely by coincidence may be selected on the account of other truly informative features. Forward selection is penalized severely in such case: among the few significant features, some will not be chosen. However, backward elimination always maintains the significant features in the non eliminated set; a feature that truly enhances the classifier’s generalization will do so for the validation set as well, and will not be eliminated. This leads to a more stable generalization behavior for backward elimination on the test set through the algorithm’s progress (Figure 5).

## 4 Discussion

CSA evaluates on each phase  $t$  feature sets for each coalition size in the range 1 to  $d$ , leading to  $O(\frac{td}{\epsilon}n)$  sets being evaluated. However, in order to obtain reliable estimates of the contribution values,  $td$  should scale linearly with  $n$ . Therefore, in practice CSA requires  $O(n^2)$  evaluations, just like standard forward selection or backward elimination (Wrappers). The filter methods, ranking features by their Pearson correlation (Corr) or by their mutual information (MI) with the targets, have both linear time complexity. The time complexity of Random Forest (RF) is difficult to assess, since in order to get a reliable estimate of feature importance one should increase the number of trees, the resulting trees are usually deeper and with each node  $O(\sqrt{n})$  features are being considered.

The  $O(n^2)$  behavior of CSA poses a real challenge when using it with

non-trivial problems. To cope with it, fast induction algorithms such as naive bayes, KNN, or decision trees must be used. Running times can be further reduced by parallelizing, an advantage not shared by wrapper algorithms which use search methods such as hill climbing; At each phase the permutations can be computed in parallel and upon completion combined to obtain an estimate of contribution values. Furthermore, as the algorithm progresses, the number of candidate features for either selection (forward selection) or elimination (backward elimination) decreases. Consequently, the number of permutations sampled may be reduced, speeding up the algorithm significantly. The restriction in selecting the learning algorithm for CSA does not apply to the prediction once the features are selected. After a set of features is found by the CSA, it may be used by any induction algorithm as demonstrated in section 3.3 with the *Dexter* and *Arcene* datasets.

Several learning algorithms, such as *KNN with Euclidean metric*, *Naive Bayes Classifier* and *Fisher's Linear Discriminant*, allow an optimization which dramatically reduces the time spent in the *contribution* subroutine. Without such optimizations running times can be considerable: For example, using C4.5 as a base learning algorithm, the total running time for the Arrhythmia dataset was on average 41 minutes on a 1.73 Ghz Pentium 4 for backward elimination, and 34 minutes for forward selection. The standard deviations of running times were approximately 8 minutes and 6 minutes respectively. For comparison, the running times for the filter algorithms (Mutual Information and Pearson Correlation) were less than 4 minutes. Forward

selection and backward elimination wrapper methods took 28 minutes and 33 minutes respectively and the running time of Random Forests on the same dataset was 12 minutes.

Since the contribution value is based on extensive sampling of feature sets, the CSA algorithm is capable of identifying intricate dependencies between features and the target. We therefore expect that CSA will be effective for datasets where feature independence is strongly violated, as demonstrated in section 3.1. However, CSA may fail in certain circumstances, for example when a large coalition should be formed to aid in prediction. In such a case, it may well be that this coalition will not be sampled - and hence the contribution value of the corresponding features will not be increased. Obviously, forward selection CSA is more prone to this pitfall. Furthermore, when the data is scarce overfitting could pose a real problem for CSA – the significance of contribution estimates can be rather low, and the resulting noise can play a substantial role in driving the algorithm. Further incorporation of regularization into CSA may help to deal with such a situation.

## 5 Conclusion

The Contribution-Selection algorithm presented in this paper views the task of feature selection in the context of coalitional games. It uses a wrapper-like technique combined with a novel ranking method that is based on the Shapley contribution values of the features to the classification accuracy.

The CSA works in an iterative manner, each time selecting new features (or eliminating them) while taking into account the features that were selected (or eliminated) so far.

We verified that the feature sets selected by CSA are significantly different than those selected by other filter methods. It turns out that the first “strong” features are selected by most methods. But within few iterations, CSA selects entirely different features than other methods due to the fact that the contribution values of the candidate features are modified along the run of the algorithm, sometimes drastically, according to the features already selected.

The CSA was tested on number of datasets, and the results show that the algorithm can improve the performance of the classifier, and successfully compete with an existing array of filter and feature selection methods, especially in cases where the features interact with each other. In such cases performing feature selection with a permutation size higher than one, namely not using the common greedy wrapper approach, can enhance the classifier’s performance significantly.

The results successfully demonstrate the value of applying game theory concepts to feature selection. While the forward selection version of the algorithm is competitive with other feature selection methods, our experiments show that overall, the backward elimination version is significantly superior to them, and produces features sets which can be used to generate a highly performing classifier.

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