An efficient randomised sphere cover classifier

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Abstract: This paper describes an efficient randomised sphere cover classifier (αRSC) , that reduces the training dataset size without loss of accuracy when compared to nearest neighbour classifiers. The motivation for developing this algorithm is the desire to have a non-deterministic, fast, instance-based classifier that performs well in isolation but is also ideal for use with ensembles. Essentially we trade off decreased testing time for increased training time whilst retaining the simple and intuitive nature of instance-based classifiers. We use 24 benchmark datasets from UCI repository and six gene expression datasets for evaluation. The first set of experiments demonstrate the basic benefits of sphere covering. We show that there is no significant difference in accuracy between the basic αRSC algorithm and a nearest neighbour classifier, even though αRSC compresses the data by up to 75%. We then describe a pruning algorithm that removes spheres that contain α or fewer training instances and compare the results to three data reduction algorithms. The experiments show better average data reduction (89.5%) and improved overall accuracy. The second set of experiments demonstrate that when we set the α parameter through cross validation, the resulting αRSC algorithm outperforms several well known classifiers when compared using the Friedman rank sum test. Thirdly, we test the usefulness of αRSC when used with three attribute filtering methods on six gene expression datasets. Finally, we highlight the benefits of pruning with a bias/variance decomposition. In conclusion, we discuss why the randomisation inherent in αRSC makes them an ideal ensemble component and outline our future direction.

Keywords: classification; sphere cover; machine learning; gene expression classification; bias and variance decomposition; data reduction.

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1 Introduction

Instance-based learning techniques (Kibler et al., 1991) operate by keeping a typical sample of the training data then classifying new instances based on their similarity to the retained sample. Instance-based learning algorithms are defined by three characteristics: a similarity function that specifies the closeness of two instances, a selection function that selects the samples to be kept by the algorithm, and a classification function that decides on the class of unseen instances. The simplest and most popular IBL algorithm is the nearest neighbour (NN) algorithm which retains the entire training set. Although surprisingly effective, one well documented problem with NN classifiers is that classifying a new instance requires a distance calculation for each instance in the training set. Data reduction algorithms have been studied in great depth (Wilson and Martinez, 2000; Bezdek and Kuncheva, 2000; Kim and Oommen, 2003). In general, these algorithms search the training data for a subset of cases and/or attributes with which to classify new instances with the objective of achieving the maximum compression with the minimum reduction in accuracy. Recently, development in compression scheme rejuvenated research in compression algorithms (Shah, 2008). Compression scheme (Floyd and Warmuth, 1995) is put forward to explain the generalisation performance of sparse algorithms. In general, various algorithms are called sparse because they keep a subset from the training set as part of their learning process (Laviolette et al., 2005). In Younsi and Bagnall (2010), we proposed a new fast and efficient sparse algorithm based on the class cover method which we call randomised sphere cover classifier (αRSC). In this paper, we explore the generalisation and compression performance of αRSC using several experiments. In addition, we test the usefulness of αRSC on six gene expression datasets. Lastly, we explore the reason behind the good performance of this simple classifier using Domingo's bias/variance decomposition of the error (Domingos, 2000). The rest of this paper is structured as follows: Section 2 provides some further background into data reduction and class cover problem (CCP); Section 3 describes the αRSC algorithm and the α pruning scheme used in the experimentation; The results are reported in Section 5 and finally, we conclude in Section 6 and discuss future direction.

2 Background

The sphere covering mechanism we use stems from the class covering approach to classification (Cannon and Cowen, 2000). The CCP involves finding the smallest number of sets covering (i.e., containing) points from one class without covering any points from a second class. The solution to the CCP proposed in Priebe et al. (2003) involves constructing a class cover catch digraph (CCCD), a directed graph based on the proximity of training cases. However, finding the optimal covering via the CCCD is NP-hard (Cannon et al., 2002). Hence (Marchette and Priebe, 2003; Marchette, 2004) proposed a number of greedy algorithms to find an approximately optimal set covering. Whilst covering techniques have shown to be good classifiers that effectively compress the data (Priebe et al., 2003), these algorithms have the drawback that they are still time consuming and that they only find pure coverings, i.e., sets that only contain cases of a single class. An algorithm that relaxes the requirement of class purity was proposed by Priebe et al. (2003). This algorithm introduces two parameters to alleviate this constraint on a pure proper cover. Whilst effective, the parameters are non-intuitive and hard to set. The greedy algorithms proposed all have a run time complexity of $O(n^2)$, and hence (to the best of our knowledge) there has been very limited experimental evaluation of the algorithms proposed in Marchette and Priebe (2003) and Priebe et al. (2003) since most of them are impractical for large and complex datasets. The sphere covering algorithm we propose follow the same principles proposed in Marchette et al. (2003). The algorithm is computationally efficient, randomises the process of finding a set covering and allows for pruning through the setting of a single parameter α which directly penalise complex covers.

3 An αRSC

The reason for designing the αRSC algorithm was to develop an instance-based classifier to use in ensembles. Hence our design criteria were that it should be randomised (to allow for diversity), fast (to mitigate against the inevitable overhead of ensembles) and comprehensible (to help produce meaningful interpretations from the models produced). The αRSC algorithm has a single integer parameter, α , that specifies the minimum size for any sphere. Informally, for any given α , αRSC works as follows.

- 1 Repeat until all data are covered.
 - a randomly select a data point and add it to the set of covered cases
 - b create a new sphere centred at this point
 - c find the closest case in the training set of a different class to the one selected as a centre
 - d set the radius of the sphere to be the distance to this case
 - e find all cases in the training set within the radius of this sphere
 - f if the number of cases in the sphere is greater than α , add all cases in the sphere to the set of covered cases and save the sphere details (centre, class and radius).

A more formal algorithmic description is given in Algorithm 1. For all our experiments we use the Euclidean distance metric, although the algorithm can work with any distance function.

Algorithm 1 A *aRSC*

1: Input: Cases $D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, distance function $d(\mathbf{x}_i, \mathbf{x}_j)$ parameter α . 2: Output: Set of spheres B3: Let covered cases set $C = \oslash$ 4: while $D \neq C$ do Select a random element $(\mathbf{x_i}, y_i) \in D - C$ 5: 6: Copy $(\mathbf{x_i}, y_i)$ to C Find $\min_{(\mathbf{x}_j, y_j) \in D} d(\mathbf{x}_i, \mathbf{x}_j)$ such that $y_i \neq y_j$ 7: Let $r_i = d(\mathbf{x_i}, \mathbf{x_j})$ 8: Create a B_i with a centre $\mathbf{c_i} = \mathbf{x_i}$, radius r_i 9: and target class y_i 10: Find all the cases in B_i and store in temporary set T11: if $|T| \ge \alpha$ then 12: $C = C \bigcup T$ Store the sphere B_i in B13: 14: end if 15: end while

The parameter α allows us to smooth the decision boundary, which has been shown to provide better generalisation by mitigating against noise and outliers, (see for instance Liu and Motoda, 2002). Figure 1 provides an example of the smoothing effect of removing small spheres on the decision boundary.





The αRSC algorithm classifies a new case by the following rules:

- Rule 1 a test example that is covered by a sphere, takes the target class of the sphere. If there is more than one sphere of different target class covering the test example, the classifier takes the target class of the sphere with the closest centre.
- Rule 2 in the case where a test example is not covered by a sphere, the classifier selects the closest spherical edge.

A case covered by Rule 2 will generally be an outlier or at the boundary of the class distribution. Therefore, it may be preferable not to have spheres over-covering areas where such cases may occur. These areas are either close to the decision boundary specifically when the high overlap between classes exist [an illustration is given in Figure 1(a)], and areas where noisy cases are within dense areas of examples of different target class. The αRSC method of compressing through sphere covering and smoothing via boundary setting provides a robust simple classifier that is competitive with other commonly used classifiers.

4 Bias and variance decomposition

In general, the bias/variance theory is used successfully to analyse the generalisation error of any classifier (Valentini and Dietterich, 2004). The main characteristic of the bias and variance decomposition is simplicity of use. The bias/variance decomposition essentially consists in decomposing the generalisation error into two components: bias and variance. In this section, we discuss briefly the bias/variance decomposition for the 0/1 loss function using Domingos framework (Domingos, 2000).

The bias is attributed to the systematic part of the error, while variance to the stochastic part of the error (Domingos, 2000). It is commonly recognised that.

- 1 bias arises when the classifier cannot represent the true function. That is, the classifier underfits the data
- 2 variance arises when the classifier overfits the data
- 3 there is often a trade-off between bias and variance.

In practice, the bias and variance are computed by running the algorithm several times on different training sets. To this end, we need to sample repeatedly from a set U in order to make s training datasets $\{D_i\}_{i=1}^s$. Each bootstrap D_i is made of t training examples $D_i = \{\mathbf{x}_j, y_j\}_{i=1}^t$, where each point is a pair $(\mathbf{x}_j, y_j), y_j \in C, \mathbf{x} \in \mathbb{R}^n, n \in \mathbb{N}$, and C is the set of class labels. D_i can be seen as a random variable. A learning algorithm \mathcal{A} produces a hypothesis f_{D_i} using a training set D_i such as $f_{D_i} = \mathcal{A}(D_i)$. For each point $\mathbf{x} \in \mathbb{R}^n$ the hypothesis produces a prediction $f_{D_i}(\mathbf{x}) = p$, and L(y, p)represents the 0/1 loss, if p = y then L(y, p) = 0, else L(y, p) = 1. The goal of our learning algorithm \mathcal{A} consists in minimising the expected loss EL. Thus, the expected loss at point \mathbf{x} can be written as: $EL(\mathcal{A}, \mathbf{x}) = E_{D_i}[E_y[L(y, f_{D_i}(\mathbf{x})]], E_{D_i}[.]$ indicate the expected value with respect to the distribution of D_i . $E_y[.]$ is the expectation with respect to y since the randomness in y due to the choice of a particular test point (\mathbf{x}, y) .

The two important variables are the optimal prediction p_* and the main prediction (also known as central tendency) p_c . Both p_* and p_c are evaluated using 0/1 loss

function and without considering noise (Noise is only considered for theoretical analysis as it is impossible to calculate in practice) (Domingos, 2000).

Definition 4.1 [Optimal prediction p_* (Domingos, 2000)]: An optimal prediction p_* is the prediction that the optimal classification algorithm does (which is the prediction obtained by the Bayes classifier).

In practice we cannot compute this optimal prediction p_* so instead we replace it with y the target value.

Definition 4.2 [Main prediction p_c (Domingos, 2000)]: The main prediction p_c for the example (\mathbf{x}, y) is the class most often predicted.

To compute p_c for an example (\mathbf{x}, y) of the test set, we need to get all the $f_{D_i}(\mathbf{x})$ predictions for that example from different hypotheses, and then find the prediction that appears most often, this will be p_c .

The bias B(x) is the loss of the main prediction relative to the optimal prediction p_* .

Bias measures how far are the predictions that a learning algorithm does for an example (\mathbf{x}, y) from the optimal prediction, p_* . For the 0/1 loss, the bias is always 0 or 1. Thus, it is said that the learning algorithm \mathcal{A} is biased at point \mathbf{x} , if $B(\mathbf{x}) = 1$. The **bias** $B(\mathbf{x})$ is:

$$B(\mathbf{x}) = L(p_*, p_c) \tag{1}$$

Definition 4.2 [Net variance $V(\mathbf{x})$ (Domingos, 2000)]: The net variance $V(\mathbf{x})$ is the average loss of the predictions relative to the main prediction.

Net variance measures how the choice of the training set affects the predictions of the learning algorithm. In our case, it measures how the predictions of a learning algorithm for a specific example, derived from the D_i different training sets, fluctuate around the most often prediction p_c associated with that example. The variance is:

The *net*-variance $V(\mathbf{x})$ is:

$$V(\mathbf{x}) = E_{D_i}[L(p_c, f_{D_i}(\mathbf{x}))]$$
⁽²⁾

The biased variance V_b and the unbiased variance V_u constitute the two components of the net variance. The unbiased variance corresponds to the variance of incorrect predictions for the case where the main prediction is correct $(p_c = p_*)$. Thus, unbiased variance captures the extents to which the learner deviates from the correct prediction p_c . In this case, the unbiased variance is added to the error. On the other hand, the biased variance corresponds to the variance of correct predictions for the case where the main prediction is incorrect $(p_c \neq p_*)$. Thus, biased variance captures the extents to which the learner deviates from the incorrect prediction p_c . As a consequence, the net variance is the difference of the two: $V = V_u - V_b$. This means that variance hurts on unbiased examples while it helps on biased examples.

Domingos decomposition is:

$$EL(\mathcal{A}, \mathbf{x}) = c_1 N(\mathbf{x}) + B(\mathbf{x}) + c_2 V(\mathbf{x})$$

Noise part $c_1 N(\mathbf{x})$ is disregarded simplifying the decomposition to

$$EL(\mathcal{A}, \mathbf{x}) = B(x) + c_2 V(\mathbf{x})$$

 c_2 is +1 if $B(\mathbf{x}) = 0$ and -1 if $B(\mathbf{x}) = 1$.

Thus, the average loss $E_{\mathbf{x}}[EL(\mathcal{A}, \mathbf{x})]$ for a learning algorithm \mathcal{A} on all the examples is calculated using the average bias, variance (unbiased, biased and net variance), averaged over the entire set of the examples of the test set is:

$$E_{\mathbf{x}}[EL(\mathcal{A}, \mathbf{x})] = E_{\mathbf{x}}[B(\mathbf{x})] + E_{\mathbf{x}}[V_u(\mathbf{x})] - E_{\mathbf{x}}[V_b(\mathbf{x})]$$

= $E_{\mathbf{x}}[B(\mathbf{x})] + E_{\mathbf{x}}[(1 - 2B(\mathbf{x}))V(\mathbf{x})]$ (3)

To give a simple interpretation, we use a similar illustration presented in Webb (2000). Let (\mathbf{x}, y) , be an example where $y \in \mathcal{C} = \{a, b, c\}$ is the target value of an example \mathbf{x} .

Let say that an algorithm is run ten times on different training set. For each case (example (\mathbf{x}, y)), we get a prediction, for a total of ten predictions as shown in Table 1. The main prediction for an example (\mathbf{x}, y) is the class most often predicted. For the 0/1 loss, the bias is always 0 or 1. The contribution of bias to error depends on the loss of the main prediction relative to the optimal prediction. The contribution of variance to error depends on the average loss of the predictions relative to the main prediction. Thus, the error in Domingos bias/variance decomposition is:

Case 1
$$E_{\mathbf{x}}[B(\mathbf{x})] + E_{\mathbf{x}}[(1 - 2B(\mathbf{x}))V(\mathbf{x})] = 0 + ((1 - 0) * 0.6) = 0.6$$

Case 2
$$E_{\mathbf{x}}[B(\mathbf{x})] + E_{\mathbf{x}}[(1 - 2B(\mathbf{x}))V(\mathbf{x})] = 1 + ((1 - 2) * 0.4) = 0.6$$

Case 3
$$E_{\mathbf{x}}[B(\mathbf{x})] + E_{\mathbf{x}}[(1-2B(\mathbf{x}))V(\mathbf{x})] = 0 + ((1-0)*0.2) = 0.2$$

Correct class	Case 1	Case2	Case3
Correct cluss	a	b	С
Prediction 1	а	а	а
Prediction 2	а	а	b
Prediction 3	а	а	с
Prediction 4	а	а	с
Prediction 5	b	а	с
Prediction 6	b	а	с
Prediction 7	b	b	с
Prediction 8	с	b	с
Prediction 9	с	b	с
Prediction 10	с	b	с
Main prediction	а	а	с
Bias	0	1	0
Variance	0.6	0.4	0.2
Error	0.6	0.6	0.2

 Table 1
 Table showing an example of BV calculation

In the second case, the error comes from both bias and variance, whereas in the two other cases, the error comes from variance only. As stated above, the interesting point about Domingos decomposition is that reducing unbiased variance in Case 1 will help reduce variance. Hence, the overall error is reduced. In the other hand, reducing the biased variance of Case 3 will increase the overall error. It becomes clear that in order to reduce the overall error, it is required that both bias $(B(\mathbf{x}))$ and unbiased variance $(V_u(\mathbf{x}))$ are reduced.

5 Results

In this section, we perform four sets of experiments. The first set is meant to demonstrate the general principle that we can intelligently compress the dataset using αRSC without significantly increasing classification error. The second set of experiments shows that the αRSC classifier performs as well as or better than other classifiers based on similar principles. The third set of experiments investigates the usefulness of αRSC in real domains on gene expression datasets. Finally, we show the reason pruning (α parameter) is the main reason for the good performance of αRSC using the bias/variance decomposition of the generalisation error.

5.1 Experimental setup

To evaluate the performance of αRSC , we used twenty four datasets from both UCI data repository (Asuncion and Newman, 2007), and boosting repository (http://ida.first.gmd.de/raetsch/data/benchmarks.htm). These datasets are summarised in Table 2. They were selected because they vary in the numbers of training examples, classes and attributes and thus provide a diverse testbed. In addition, they all have only continuous attributes.

Table 2 Benchmark datasets used for the empirical evaluations

Dataset	Examples	Attributes	Classes	Dataset	Examples	Attributes	Classes
Sonar	208	60	2	Vehicle	846	18	4
Glass6	214	9	6	Vowel	990	10	11
Glass2	214	9	2	German	1,000	20	2
Thyroid	215	5	2	Concentric	2,000	2	2
Heart	270	13	2	Image segment	2,310	18	2
Haberman	306	3	2	Abalone	4,177	8	3
Cancer	315	13	2	Clouds	5,000	2	2
Ecoli	336	7	8	Waveforme	5,000	40	3
Ionosphere	351	34	2	Ringnorm	7,400	20	2
wdbc	569	30	2	Twonorm	7,400	20	2
Winsconsin	699	9	2	Pendigitis	10,991	14	10
Pima diabetes	768	8	2	Magic	19,020	2	10

For the experiments in Section 5.2 we used a stratified ten-fold cross validation (CV). In the first experiments, we compare the proposed classifier with several state of the art data reduction algorithms. We used Wilson's programme written in C for Drop3, IB3, and Explore (Wilson and Martinez, 2000). For the later experiments we performed model selection on the parameter values, in that for each fold of the overall cross-validation we first took a test sample, then cross validated on the remainder to set the parameter. For comparison purposes we compare to K-nearest neighbour (K-NN), the non-nested generalised exemplar (NNge) (Martin, 1995), C4.5, Naive Bayes (NB) and Naive Bayes tree (NBTree. K-NN and NNge are the most relevant for comparison purposes, the other three are included for completeness. Weka implementations are used for the standard classifiers, bespoke implementations for αRSC and NNge.

Dataset	1-NN	uRSC	(%)	Dataset	1-NN	uRSC	(%)
Vehicle	69.61 ± 4.62	68.13 ± 4.75	50	Glass6	70.30 ± 8.96	$69.00~\pm~9.49$	52
Segment	97.14 ± 1.07	96.10 ± 1.21	89	Cancer	67.65 ± 7.80	68.08 ± 7.76	52
Abalone	50.13 ± 2.25	49.46 ± 2.02	32	Breastw	95.67 ± 2.48	95.36 ± 2.42	90
Waveform	85.88 ± 1.57	85.41 ± 1.55	73	Concentric	98.54 ± 0.79	$98.21~\pm~0.82$	97
Ringnorm	72.59 ± 0.53	95.16 ± 0.49	63	Clouds	84.64 ± 1.68	84.75 ± 1.48	76
Magic	80.16 ± 0.32	79.95 ± 0.35	68	wdbc	94.01 ± 2.95	95.38 ± 2.65	88
Pendigits	98.95 ± 0.10	97.72 ± 0.25	93	Thyroid	$96.80~\pm~3.33$	95.40 ± 4.44	88
Vowel	$98.90~\pm~1.05$	95.70 ± 2.34	77	German	70.70 ± 4.34	70.30 ± 3.86	52
Twonorm	94.51 ± 0.29	93.78 ± 0.34	83	Diabetes	70.62 ± 4.67	68.87 ± 5.02	51
Glass2	94.25 ± 4.72	93.86 ± 5.67	87	Ionosphere	87.10 ± 5.12	92.80 ± 3.75	69
Ecoli	80.66 ± 6.16	81.75 ± 6.26	66	Heart	75.78 ± 7.34	$75.26~\pm~8.98$	60
Haberman	$65.77\ \pm\ 6.92$	$68.58~\pm~7.38$	53	Sonar	$86.23\ \pm\ 7.41$	$82.80~\pm~8.48$	61

Table 3 10-fold CV classification accuracy (in %) and standard deviation over the folds

Note: The final column gives the average compression rate for unpruned RSC (uRSC).

Table 4 10-fold CV classification accuracy (in %)

Dataset	K-NN	αRSC	Comp %	IB3	Comp %	Drop3	Comp %	Explore	Comp %
Sonar	87.02	81.22	80.28	76.57	83.07	80.38	79.49	77.45	98.88
Glass2	94.37	94.76	90.50	93.42	88.42	94.83	92.16	92.99	98.96
Glass6	72.42	70.44	75.65	64.03	67.97	67.34	76.12	67.81	96.57
Tyroid	95.76	94.26	95.32	91.65	91.27	93.94	89.20	92.90	98.50
Heart	83.33	82.81	99.09	58.89	93.21	81.85	80.16	83.33	99.18
Haberman	73.56	74.89	91.41	26.48	98.98	73.88	91.65	73.19	99.56
Cancer	74.11	74.40	93.09	39.48	95.92	74.50	90.69	68.36	99.48
Ecoli	84.84	85.09	81.29	81.86	70.08	84.24	81.25	83.03	98.08
Iono	85.75	93.40	78.74	85.49	86.17	86.03	92.97	79.77	99.02
wdbc	96.31	96.26	92.91	93.50	90.57	95.60	89.87	95.78	99.61
Wins	96.57	97.03	95.97	96.28	93.96	96.28	95.55	96.43	99.68
Diabetes	73.70	74.63	82.29	70.30	90.26	75.66	82.15	74.48	99.71
Vehicle	71.26	66.23	83.84	65.48	72.60	68.79	75.85	47.87	99.29
Vowel	99.09	93.16	79.01	93.94	79.28	94.65	70.38	71.01	93.29
German	75.30	73.87	89.30	70.50	90.19	73.60	83.60	69.40	99.78
Conc	98.68	98.64	98.33	97.00	93.00	98.28	91.11	63.16	99.96
Image	97.71	96.20	89.96	94.42	93.11	95.76	91.39	87.75	99.59
Abalone	53.77	54.44	92.16	53.05	80.37	54.78	82.86	53.00	99.92
Clouds	88.52	88.81	95.26	87.26	95.37	88.10	93.10	77.94	99.96
Waveform	88.80	89.56	99.44	86.26	96.83	89.28	87.20	85.36	99.96
Ringnorm	72.45	95.60	81.37	86.18	85.58	91.69	92.88	86.19	99.46
Twonorm	97.24	96.59	98.98	95.72	96.82	96.77	90.69	95.92	99.95
Pendigitis	99.07	97.83	94.24	97.39	94.80	97.85	94.13	95.27	98.89
Magic	83.53	83.12	89.48	80.10	95.44	83.70	89.06	76.50	79.88
Average	85.13	85.55	89.50	78.55	88.47	84.91	86.81	78.95	98.22

Note: The final column gives the average compression rate (comp) for αRSC .

5.2 Experiment 1: compression without loss of accuracy

The average compression rate for unpruned RSC was 75%. These experiments clearly show that by using the simplest form of αRSC we can discard a large proportion of the data whilst maintaining the same level of accuracy. In order to verify the compression rate and the accuracy of the pruned RSC (αRSC), we used Drop3, IB3 and Explore. Drop3 was shown to be the best reduction algorithm in terms of reduction and accuracy

in comparison to 14 other data reduction algorithms (Wilson and Martinez, 2000). IB3 is an algorithm which was proposed to rectify shortcomings of the famous IB1 and IB2 (Wilson and Martinez, 2000). Explore was shown to produce very good reduction without too much deterioration in accuracy (Wilson and Martinez, 2000). The results produced in Table 4 shows the best accuracy produced by K-NN and αRSC trained over a range of parameter values while the reduction algorithms use internal tuning to produce the best results.

The results shown in Table 4 demonstrate once more the good performance of αRSC in comparison of state of the art data reduction algorithms. In addition, the average accuracy is comparable to that of K-NN.

Datasets	αRSC	DT	K-NN	NB	NBT	NNge
Sonar	83.43 ± 5.37	$73.52~\pm~5.63$	85.57 ± 4.11	73.38 ± 4.91	74.14 ± 3.96	58.29 ± 4.48
Heart	$78.85\ \pm\ 3.62$	77.19 ± 5.52	$81.56\ \pm\ 2.75$	85.11 ± 3.12	80.48 ± 3.70	78.74 ± 3.66
Haberman	73.37 ± 0.72	70.98 ± 4.19	$74.44\ \pm\ 2.62$	$73.95\ \pm\ 2.32$	$72.61\ \pm\ 3.27$	67.25 ± 3.91
Cancer	$70.93\ \pm\ 1.89$	$69.82 \ \pm \ 6.76$	$74.77\ \pm\ 3.22$	$75.05\ \pm\ 3.25$	$74.52\ \pm\ 3.16$	68.03 ± 5.15
Ecoli	$71.13\ \pm\ 2.50$	81.28 ± 3.30	$85.80\ \pm\ 2.78$	$85.33\ \pm\ 2.91$	81.96 ± 2.76	83.78 ± 2.96
Liver	$60.90 \ \pm \ 4.44$	63.88 ± 4.37	$62.32\ \pm\ 3.83$	$64.41\ \pm\ 4.01$	$63.71\ \pm\ 4.14$	61.48 ± 5.01
Iono	93.19 ± 1.46	$75.05 \ \pm \ 2.45$	$86.87\ \pm\ 2.58$	91.99 ± 2.17	$89.52 \ \pm \ 1.72$	$91.23~\pm~2.98$
wdbc	$92.33 \ \pm \ 1.93$	93.49 ± 2.05	$95.11 \ \pm \ 1.74$	$89.33\ \pm\ 5.52$	93.79 ± 1.63	91.96 ± 2.91
Wins	96.65 ± 1.10	$94.03 \ \pm \ 1.22$	96.49 ± 0.57	$97.18\ \pm\ 0.77$	$96.14\ \pm\ 1.08$	96.01 ± 1.16
Diabetes	74.09 ± 2.40	$72.77\ \pm\ 2.55$	$74.66\ \pm\ 1.95$	$75.55\ \pm\ 1.88$	73.87 ± 2.29	$72.79\ \pm\ 2.28$
Vehicle	67.32 ± 1.93	70.91 ± 2.94	$68.44\ \pm\ 1.50$	58.96 ± 2.56	$68.00~\pm~2.06$	$61.81 \ \pm \ 4.86$
Vowel	76.32 ± 1.60	74.54 ± 2.06	$97.45\ \pm\ 1.09$	$66.37\ \pm\ 3.11$	75.63 ± 3.06	$83.40 \ \pm \ 2.68$
German	72.29 ± 1.70	70.68 ± 1.97	$74.72\ \pm\ 1.64$	71.16 ± 1.06	$72.48\ \pm\ 2.32$	63.29 ± 9.09
Yeast	$55.82 \ \pm \ 2.52$	$53.44 \ \pm \ 1.52$	$57.01\ \pm\ 1.78$	57.95 ± 2.16	$56.33 \ \pm \ 1.92$	$52.77 \ \pm \ 2.93$
Segment	95.48 ± 0.66	93.94 ± 0.86	96.99 ± 0.54	$78.40\ \pm\ 1.84$	93.37 ± 0.94	86.46 ± 2.65
Concentric	$98.01 \ \pm \ 0.57$	$98.42 \ \pm \ 0.31$	$98.51 \ \pm \ 0.32$	98.19 ± 0.27	98.51 ± 0.27	$89.72~\pm~7.90$
Abalone	53.86 ± 1.09	51.67 ± 1.39	54.20 ± 1.16	$52.13\ \pm\ 0.99$	$53.73 \ \pm \ 1.44$	50.51 ± 1.75
Clouds	88.50 ± 0.75	88.29 ± 0.56	$88.62 \ \pm \ 0.50$	$86.24\ \pm\ 0.51$	88.51 ± 0.59	$83.22 \ \pm \ 1.02$
Waveform	89.31 ± 0.62	84.93 ± 0.64	$89.64 \ \pm \ 0.54$	85.19 ± 0.65	$88.12 \ \pm \ 0.93$	78.44 ± 3.73
Banana	89.93 ± 0.43	88.78 ± 0.64	$89.83 \ \pm \ 0.66$	$72.51 \ \pm \ 0.95$	$88.82 \ \pm \ 0.76$	82.67 ± 5.53
Phono	87.35 ± 0.63	85.58 ± 0.80	$88.86\ \pm\ 0.45$	78.29 ± 0.74	$84.20 \ \pm \ 1.09$	$81.81 \ \pm \ 1.60$
Satimage	90.21 ± 0.52	85.60 ± 0.62	90.55 ± 0.40	82.00 ± 0.69	$82.43\ \pm\ 1.48$	$86.75 \ \pm \ 0.90$
Twonorm	96.67 ± 0.46	84.35 ± 0.74	$97.27\ \pm\ 0.31$	$97.53\ \pm\ 0.32$	$93.74 \ \pm \ 1.63$	79.04 ± 1.47
Ringnorm	95.41 ± 0.40	90.82 ± 0.51	$73.94 \ \pm \ 0.62$	$98.44\ \pm\ 0.19$	96.77 ± 0.66	91.62 ± 1.18
Pend	98.19 ± 0.20	95.71 ± 0.30	99.08 ± 0.16	$85.41\ \pm\ 0.46$	$94.34 \ \pm \ 0.58$	95.69 ± 0.65
Magic	83.63 ± 0.37	84.63 ± 0.38	83.56 ± 0.34	75.80 ± 0.42	85.09 ± 0.33	81.60 ± 0.59
F-Avg.	3.96	2.77	5.06	3.38	3.79	2.04
Ranks	2	5	1	4	3	6

Table 5Classification accuracy (in %) and standard deviation of five classifiers in comparison
with αRSC

Notes: αRSC is used for the baseline. F-Avg stands for Friedman averages and Ranks stands for Friendam ranks

5.3 Experiment 2: performance equivalent to other classifiers

The accuracy results in Table 5 are based on an independent test set drawn randomly from the dataset. We use 2/3 of the dataset for training and tested the classifiers on the same remaining test set. However, given the randomisation nature of αRSC , we choose to use the average of 30 runs on each algorithm in order to make a fair comparison. Tuning the parameters for both α and K is based on the average of 15 runs using ten CV

on the training set alone. NNge was trained based on the best parameters suggested by its authors. The decision tree is trained without pruning (J48) using the default parameters in WEKA. NB has no parameters.

We are primarily interested in the relative performance of the classifiers over the range of datasets. In order to compare the algorithms on the overall datasets, we use Friedman ranks sum test (Janez, 2006). This test ranks the classifiers over each dataset (with the best performing algorithm getting the Rank of 1, the second best Rank 2, etc.). Let r_{ij} be the rank of the *j*th of *k* algorithms on the *i*th of *N* datasets. The average rank of classifier, $R_j = \frac{1}{N} \sum_i r_{ij}$ gives a non-parametric summary of the relative performance over all the datasets, and it has been shown that the ranking themselves provide a fair comparison of the algorithms (Janez, 2006). αRSC has the second highest average rank of the five classifiers tested. K-NN has the highest number of top ranks but on some datasets it performed relatively badly. These results suggest that αRSC can perform well on a variety of datasets in comparison to other classifiers, and that the smoothing process reduces the tendency of αRSC to perform very badly on some datasets.

5.4 Experiment 3: gene expression datasets

In this section we use six benchmark gene expression datasets in order to evaluate the usefulness on the proposed algorithm in real world application. We know that gene expression datasets contains a very large number of attributes most of which are irrelevant for the classification task (Zhang et al., 2004). For this reason, it was suggested that preprocessing would help to remove unnecessary attributes (Zhang et al., 2004). The two popular preprocessing methods used for the experiments rank best attributes according to the χ^2 statistics and information gain (IG) (Molina et al., 2002; Guyon and Elisseeff, 2003). In addition, we use the attribute filtering algorithm called relief (RL) (Molina et al., 2002). The three methods are implemented in WEKA. We evaluate the five classifiers on the first 5, 10, 20 30, 40 and 50 best ranked attributes. For these experiments we divide the datasets into a training set and a testing set. We use a stratified 10-fold CV (10CV) on the training set only to select the best values for α and K based on the average accuracy results of 15 experiments (model selection). The average classification accuracy of 30 experiments is calculated on each test set. For the comparison purpose, we continue with a single Decision tree (J48), NB, K-NN, NBTree and non-nested hyper-rectangle generalisation algorithm (NNge).

The experiments produced 648 accuracy results over the six gene expression datasets using the six classifiers each on three attribute filtering methods (χ^2 , information gain and RL). In order to collate the results into a single table we calculated the Friedman ranking. Tables 6 shows the best performing classifier for each attribute filtering method. It is interesting to note that αRSC has ranked first on each attribute filtering method and, in most cases, has not ranked below third place. NNge and the decision tree classifiers performed very badly in comparison to other classifier. These results suggest that αRSC performed very well over the six gene expression datasets on all the three attribute filtering methods.

Algorithms	αRSC	DT	K-NN	NB	NBTree	NNge
Ranked all dataset χ^2						
Top 5	3	5	6	4	1	2
Top 10	1	6	2	5	3	4
Top 20	3	6	4	1	2	5
Top 30	3	6	2	1	5	4
Top 40	3	6	1	2	4	5
Top 50	2	6	1	4	3	5
Avg.	2.5	5.83	2.67	2.83	3	4.17
Total ranks	1	6	2	3	4	5
Ranked all dataset IG						
Top 5	2	6	5	4	1	3
Top 10	2	6	1	4	3	5
Top 20	3	6	1	4	2	5
Top 30	5	6	1	2	3	4
Top 40	4	6	1	5	3	2
Top 50	1	6	2	5	3	4
Avg.	2.83	6	1.83	4	2.5	3.83
Total ranks	3.5	6	1	5	2	3.5
Ranked all dataset relief						
Top 5	2	6	4	5	5	3
Top 10	1	6	3	2	5	4
Top 20	1	6	3	2	5	4
Top 30	1	6	3	2	4	5
Top 40	2	6	3	1	5	4
Top 50	3	6	1.50	1.50	4	5
Avg.	1.67	6	2.92	2.25	4.67	4.17
Total ranks	1	6	3	2	5	4

Table 6 The ranking based on classification accuracy of six datasets of αRSC , K-NN, decision tree (J48), NBTree, NB and NNge using average results of 30 different runs on χ^2 , IG and RL

The best results for each dataset regardless of cut-off points are shown in Tables 7, 8 and 9. In these tables we want to show which is the best performing classifier for each dataset since each classifier may perform badly on some cut-off while better on others. In addition, the main target of any classifiers is to find the best accuracy over a set of cut-offs. We also show Friedman mean ranks for each attribute filtering method. The tables show that αRSC ranked 1st for the χ^2 , 2nd for RL and 3rd for the Information gain filtering methods.

Table 7The best test set accuracy (in %) of αRSC , K-NN, decision tree (J48), NBTree, NB and
NNge using average results of 30 different runs on χ^2

Dataset	αRSC	NBTree	K-NN	NB	NNge	DT
BreastCancer	77.58	76.16	75.35	71.11	71.01	72.42
Prostate	91.01	90.87	94.35	70.00	89.35	90.22
Lungcancer	99.13	99.23	99.07	100.00	99.95	95.63
Ovarian	98.86	97.96	99.33	98.59	98.55	97.10
ColonTumor	85.24	88.10	84.29	87.46	84.29	83.81
CentralNervous	80.33	80.67	78.83	78.17	74.00	76.67
Mean rank	4.67	4.50	4.08	3.50	2.42	1.83
Ranks	1	2	3	4	5	6

Dataset	NB	αRSC	K-NN	NNge	NBTree	DT
BreastCancer	81.62	77.37	80.40	73.84	74.65	71.52
Prostate	76.09	91.96	95.07	87.75	89.13	89.71
Lungcancer	99.29	99.23	98.31	99.07	98.69	95.96
Ovarian	98.78	97.88	99.18	98.59	97.84	97.10
ColonTumor	85.08	86.03	80.79	82.7	82.86	79.68
CentralNervous	78.33	77.17	76.83	70.83	70.67	71.17
Mean rank	4.83	4.67	4.17	2.83	2.67	1.83
Ranks	1	2	3	4	5	6

Table 8The best test set accuracy (in %) of αRSC , K-NN, Decision tree (J48), NBTree, NB and
NNge using average results of 30 different runs on RL

Table 9The best test set accuracy (in %) of αRSC , K-NN, decision tree (J48), NBTree, NB and
NNge using average results of 30 different runs on IG

Dataset	K-NN	NBTree	αRSC	NNge	NB	DT
BreastCancer	75.35	76.87	78.38	69.90	69.9	72.63
Prostate	90.51	88.99	89.49	87.61	67.25	89.71
Lungcancer	99.18	99.67	99.34	100.00	100.00	95.63
Ovarian	99.53	98.04	98.90	98.59	98.59	97.06
ColonTumor	85.40	86.51	85.87	84.92	84.44	82.22
CentralNervous	77.83	82.83	74.00	75.33	75.67	74.50
Mean ranks	4.50	4.33	4.00	3.08	2.92	2.17
Ranks	1	2	3	4	5	6

The overall ranking results of the three attribute filtering methods is calculated by summing the mean ranks of the three tables as shown in Table 10. αRSC has ranked first while K-NN ranked 2nd. These results show that αRSC is a good classifier for these gene expression datasets, and that it works well with attribute filters.

Classifiers	Sum ranks	All ranks
αRSC	13.33	1
K-NN	12.75	2
NBTree	11.50	3
NB	11.25	4
NNge	8.33	5
DT	5.83	6

Table 10 All ranks over the three attribute filtering methods

5.5 Experiment 4: bias/variance decomposition of αRSC

For these experiments, we employ ten different datasets, four synthetic (clouds, concentric, twonorm and ringnorm) and the remaining datasets are taken from the UCI repository. In bias/variance decomposition, small training set and large test sets are used to perform the evaluation of bias and variance. For both synthetic and real datasets we used bootstrapping to replicate the data. In both cases we computed the mean prediction, bias, unbiased and biased variance, net-variance according to the procedures found in Valentini and Dietterich (2004). That is, the data is divided into a training set T_r and a test set T_s . The training bootstrap samples are much smaller than $|T_s|$. That is,

200 datasets are made from T_r , each one consisting of 200 examples uniformly drawn with replacement from T_r . Except for two datasets twonorm and waveform, we used 300 training datasets each made of 300 examples.

Dataset	Avg. error	Bias	Net var.	Var. unb.	Var. bias.
Diabetes					
$\alpha = 0$	0.3124	0.2500	0.0624	0.1374	0.0750
$\alpha = 3$	0.2780	0.2367	0.0413	0.1006	0.0594
Diff %	↑ <i>11.01</i>	↑ <i>5.32</i>	↑ <i>33.81</i>	† 26.78	† 20.80
Heart					,
$\alpha = 0$	0.2599	0.1833	0.0765	0.1274	0.0509
$\alpha = 7$	0.2138	0.1667	0.0471	0.0872	0.0400
Diff %	↑ <i>17.74</i>	↑ 9.06	↑ <i>38.43</i>	↑ <i>31.55</i>	↑ <i>21.41</i>
Clouds					,
$\alpha = 0$	0.1613	0.1107	0.0507	0.0812	0.0306
$\alpha = 3$	0.1354	0.1196	0.0158	0.0397	0.0240
Diff %	↑ <i>16.06</i>	↓ 8.04	↑ 68.84	↑ <i>51.11</i>	† 21.5 7
Waveform	·	·	·	·	·
$\alpha = 0$	0.1626	0.0934	0.0692	0.1043	0.0352
$\alpha = 11$	0.1387	0.0961	0.0426	0.0722	0.0296
Diff %	↑ <i>14.70</i>	↓ <i>2.89</i>	↑ 38.44	↑ <i>30.78</i>	↑ <i>15.91</i>
Concentric			·	·	·
$\alpha = 0$	0.0616	0.0131	0.0485	0.0544	0.0059
$\alpha = 5$	0.0630	0.0295	0.0335	0.0453	0.0118
Diff %	↓ 2.27	↓ <i>125.19</i>	↑ <i>30.93</i>	↑ <i>16.73</i>	↓ 100
Twonorm			·		
$\alpha = 0$	0.0730	0.0227	0.0504	0.0586	0.0082
$\alpha = 10$	0.0515	0.0222	0.0293	0.0366	0.0073
Diff %	↑ <i>29.45</i>	† 2.20	↑ <i>41.86</i>	† <i>37.54</i>	↑ <i>10.97</i>
Pendigitis					
$\alpha = 0$	0.1206	0.0355	0.0850	0.0956	0.0106
$\alpha = 1$	0.1398	0.0652	0.0745	0.0913	0.0167
Diff %	↓ <i>15.92</i>	↓ 83.66	↑ <i>12.35</i>	† 4.50	↓ 100
Magic					
$\alpha = 0$	0.2510	0.1751	0.0759	0.1298	0.0539
$\alpha = 4$	0.2151	0.1937	0.0215	0.0556	0.0341
Diff %	↑ <i>14.30</i>	↓ <i>10.62</i>	↑ <i>71.67</i>	↑ <i>57.16</i>	↑ <i>36.73</i>
Yeast					
$\alpha = 0$	0.5360	0.4170	0.1190	0.2045	0.0855
$\alpha = 1$	0.5159	0.4152	0.1007	0.1776	0.0768
Diff %	↑ <i>3.75</i>	↑ 0.43	↑ <i>15.38</i>	↑ <i>10.17</i>	↑ <i>10.01</i>
wdbc					
$\alpha = 0$	0.0978	0.0563	0.0415	0.0580	0.0165
$\alpha = 8$	0.0898	0.0784	0.0114	0.0275	0.0161
Diff %	↑ 8.18	↓ <i>39.25</i>	† 72.53	† <i>52.59</i>	† 2.42

Table 11 Comparing best bias and variance results of αRSC on various datasets

Notes: Var. unb. and var. bias. stand for unbiased and biased variance. Diff stands for the percentage difference between the pruned and unpruned values. The up arrow \uparrow means an increase while a down arrow \downarrow means a decrease.

The results in Table 11 show a pattern on the bias and variance performance of αRSC classifier:

- 1 If pruning improves performance, which it does for the majority of cases in our experiment, there is a substantial decrease in net variance. However, there are two trends in relation to bias.
 - Increase in bias is shown on clouds (8.04%), waveform (2.89%), magic (10.62%), and wdbc (39.25%). However, unbiased variance is significantly decreased in these datasets, as shown on cloud (51.11%), waveform (30.78%), magic (57.16%), and wdbc (52.59%), which explains the decrease in average error.
 - Decrease in bias is shown on diabetes (5.32%), heart (9.06%), twonorm (2.20%), and yeast (0.43%). In all these cases both unbiased and biased variance are both decreased.
- 2 If pruning degrades performance, then we notice an increase in bias. This is shown on Pendigitis dataset with 15.92% increase in average error for $\alpha = 1$, and a substantial increase in bias (83.66%). Pruning, for this dataset, has also increased substantially the biased variance (100%). Similarly, Concentric dataset shows an increase in average error (2.27%) and a massive increase in bias (125.10%). We notice also a big increase for biased variance (100%). This should not be a surprise because Concentric dataset is rather unusual; removing spheres that are close to the decision boundary will significantly underfit the data because no separation exist between the two classes. As for Pendigitis dataset, it is made of ten classes which could be an issue for choosing the same α values for each class. Obviously, for both Concentric and Pendigitis datasets we see a decrease in net variance caused by the decrease in unbiased variance which emphasises the role of pruning in reducing the net variance.

The important observation that can be made from the bias/variance results is that pruning significantly reduces unbiased variance. However, in only a few cases do we notice a small decrease in bias. Therefore, the decrease of αRSC average error is caused mainly by the decrease of unbiased variance resulting in the overall error reduction.

6 Conclusions

The classification accuracy of our proposed randomised classifier is competitive in comparison to various deterministic algorithms. In addition, the classification accuracy is significantly improved by pruning, to the extent that on average it outranks five other classifiers. The reason for this improvement is the result of unbiased variance reduction as demonstrated by the bias/variance experiments. Pruning is only responsible for the reduction of unbiased variance, which indicates that further improvement is possible by reducing bias. Feature selection is known to reduce bias for IBL classifiers. We intend to investigate the effect of attribute selection on αRSC and assess the usefulness of the classifier when used in ensembles. Several variation are possible with the sphere cover classifier. For instance, sphere can be allowed to be inside other spheres, and to find the optimum radius of each sphere. Other possibilities might be investigated in regards to sphere positioning. In the future, we will examine the relationships between

 α , the accuracy and the cardinality of cover using probabilistic bound based on the compression scheme. Manipulating these three quantities in a compression bound should result in an accurate prediction of the true error, which can be used as an efficient model selection technique. In addition, we will investigate whether further compression is better achieved using kernel methods.

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