ON THE VC-DIMENSION OF UNIVARIATE DECISION TREES

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Abstract: In this paper, we give and prove lower bounds of the VC-dimension of the univariate decision tree hypothesis class. The VC-dimension of the univariate decision tree depends on the VC-dimension values of its subtrees and the number of inputs. In our previous work (Aslan et al., 2009), we proposed a search algorithm that calculates the VC-dimension of univariate decision trees exhaustively. Using the experimental results of that work, we show that our VC-dimension bounds are tight. To verify that the VC-dimension bounds are useful, we also use them to get VC-generalization bounds for complexity control using SRM in decision trees, i.e., pruning. Our simulation results shows that SRM-pruning using the VC-dimension bounds finds trees that are more accurate as those pruned using cross-validation.

1 INTRODUCTION

In pattern recognition the knowledge is extracted as patterns from a training sample for future prediction. Most pattern recognition algorithms such as neural networks (Bishop, 1995) or support vector machines (Vapnik, 1995) make accurate predictions but are not interpretable, on the other hand decision trees are simple and easily comprehensible. They are robust to noisy data and can learn disjunctive expressions. Whatever the learning algorithm is, the main goal of the learner is to extract the optimal model (the model with least generalization error) from a training set. In the penalization approaches, the usual idea is to define the generalization error in terms of the training error and the complexity of the model.

One problem in estimating the generalization error is to specify the number of free parameters h when the estimator is not linear. In the statistical learning theory (Vapnik, 1995), Vapnik-Chervonenkis (VC) dimension is a measure of complexity defined for any type of estimator. VC dimension for a class of functions $f(x,\alpha)$ where α denotes the parameter vector is defined to be the largest number of points that can be shattered by members of $f(x,\alpha)$. A set of data points is *shattered* by a class of functions $f(x,\alpha)$ if for each possible class labeling of the points, one can find a member of $f(x,\alpha)$ which perfectly separates them. For example, the VC dimension of the linear estimator class in d dimensions is $d+1$ which is also the number of free parameters.

Structural risk minimization (SRM) (Vapnik, 1995) uses the VC dimension of the estimators to select the best model by choosing the model with the smallest upper bound for the generalization error. In SRM, the possible models are ordered according to their complexity

$$M_0 \subset M_1 \subset M_2 \subset \ldots \quad (1)$$

For example, if the problem is selecting the best degree of a polynomial function, M_0 will be the polynomial with degree 0, M_1 will be the polynomial with degree 1, etc. For each model, the upper bound for its generalization error is calculated. For binary classification, the upper bound for the generalization error is (Cherkassky and Mulier, 1998)

$$E_g = E_t + \frac{\varepsilon}{2}\left(1+\sqrt{1+\frac{4E_t}{\varepsilon}}\right) \quad (2)$$

and ε is given by the formula

$$\varepsilon = a_1 \frac{V[\log(a_2 N/V)+1]-\log(\nu)}{N} \quad (3)$$

where V represents the VC dimension of the model, ν represents the confidence level, and E_t represents the training error. It is recommended to use $\nu = \frac{1}{\sqrt{N}}$ for large sample sizes.

In this work, we use decision trees as our hypothesis class. In a univariate decision tree (Quinlan, 1993), the decision at internal node m uses only one attribute, i.e., one dimension of x, x_j. If that attribute is discrete, there will be L children (branches) of each internal node corresponding to the L different outcomes of the

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decision. ID3 is one of the best known univariate decision tree algorithm with discrete features (Quinlan, 1986).

As far as our knowledge, there is no explicit formula for the VC-dimension of a decision tree. Although there are certain results for the VC-dimension of decision trees such as (i) it is known that the VC dimension of a binary decision tree with N nodes and dimension d is between $\Omega(N)$ and $O(N \log d)$ (Mansour, 1997) (ii) it is shown that the VC dimension of the set of all boolean functions on N boolean variables defined by decision trees of rank at most r is $\sum_{i=0}^{r} \binom{n}{i}$ (Simon, 1991), the bounds are structure independent, that is, they give the same bound for all decision trees of size N.

In this work, we first focus on the easiest case of univariate trees with binary features and we prove that the VC-dimension of a univariate decision tree with binary features depends on the number of binary features and the tree structure. As a next step, we generalize our work to the univariate decision tree hypothesis class, where a decision node can have L children depending on the number of values of the selected feature. We show that the VC-dimension of L-ary decision tree is greater than or equal to the VC-dimension of its subtrees. Based on this result, we give an algorithm to find a lower bound of the VC-dimension of a L-ary decision tree. We use these VC-dimension bounds in pruning to validate that they are indeed tight bounds.

This paper is organized as follows: In Section 2, we give and prove the lower bounds of the VC-dimension of the univariate decision trees with binary features. We generalize our work to L-ary decision trees in Section 3. We give experimental results in Section 4 and conclude in Section 5.

2 VC-DIMENSION OF THE UNIVARIATE DECISION TREES WITH BINARY FEATURES

We consider the well-known supervised learning setting where the decision tree algorithm uses a sample of m labeled points $S = ((\mathbf{x}^{(1)}, y^{(1)}), \ldots, (\mathbf{x}^{(m)}, y^{(m)}) \in (X \times Y)^m$, where X is the input space and Y the label set, which is $\{0,1\}$. The input space X is a vectorial space of dimension d, the number of features, where each feature can take values from $\{0,1\}$. From this point on, we refer only internal nodes of the decision tree as node(s).

Theorem 1. *The VC-dimension of a single decision node univariate decision tree that classifies d dimensional data is* $\lfloor \log_2(d+1) \rfloor + 1$.

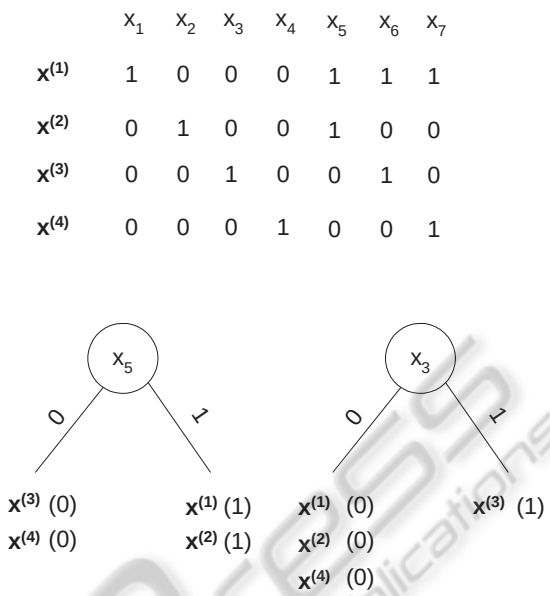


Figure 1: Example for Theorem 1 with $d = 7$ and $m = 4$. If the class labeling of S is $\{1, 1, 0, 0\}$ we select feature 5 (left decision tree). If the class labeling of S is $\{0, 0, 1, 0\}$ we select feature 3 (right decision tree).

Proof. To show the VC-dimension of the single decision node univariate decision tree is at least m, we need to find such a sample S of size m that, for each possible class labelings of these m points, there is an instantiation h of our single node decision tree hypothesis class H that classifies it correctly. We construct the sample S such that each feature x_i corresponds to a distinct possible class labeling of m points, implying a one-to-one mapping between class labelings and features (namely identity function since both features and class labelings come from the same set). So for each possible class labeling, we will choose the decision tree hypothesis h which has the corresponding feature as the split feature (See Figure 1 for an example). A sample with m examples can be divided into two classes in $2^{m-1}-1$ different ways. If we set the number of features to that number:

$$\begin{aligned} d &= 2^{m-1}-1 \\ d+1 &= 2^{m-1} \\ \log_2(d+1) &= m-1 \\ m &= \log_2(d+1)+1 \end{aligned}$$

□

Theorem 2. *The VC-dimension of a degenerate univariate decision tree with N nodes that classifies d dimensional data is at least* $\lfloor \log_2(d-N+2) \rfloor + N$.

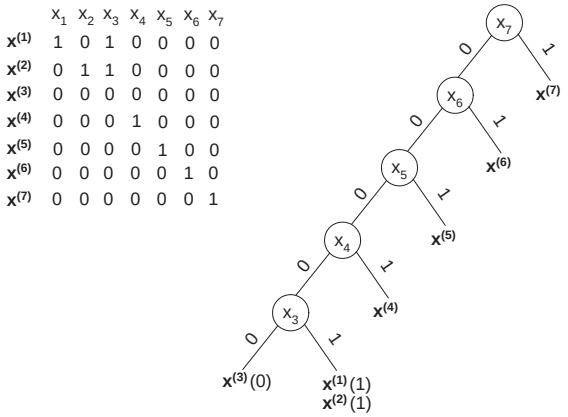


Figure 2: Example for Theorem 2 with $d = 7$ and $m = 7$. If the class labeling of S is {1, 1, 0, *x*, *x*, *x*, *x*} we select feature 3 in the bottom node. The labelings of the last four examples do not matter since they are alone in the leaves they reside.

In a degenerate decision tree each node (except the bottom one) has a single child node.

Proof. Similar to the Theorem 1, we produce a sample S such that, for each possible class labelings of this sample, there is an instantiation h of our degenerate decision tree hypothesis class H that classifies the sample correctly. We proceed in a bottom-up fashion. The bottom node can classify m examples by setting up $2^{m-1}-1$ features to produce a one-to-one mapping between class labelings and those features (See Theorem 1). We also add one feature and one example for each remaining node, where the value of the new feature is 1 for the corresponding example and 0 for the remaining examples (See Figure 2 for an example). The classification of the sample goes as follows: $N-1$ nodes (which have a single child node) will select the new $N-1$ features respectively as the split features so that each added example will be forwarded to the leaf of the corresponding node alone. The remaining m examples will be forwarded to the bottom node, where the decision node can classify those examples whatever their class combination is. The number of features is,

$$\begin{aligned} d &= 2^{m-1}-1+N-1 \\ d-N+2 &= 2^{m-1} \\ m &= \log_2(d-N+2)+1 \end{aligned}$$

So the VC-dimension of the degenerate decision tree is at least $(m+N-1)$, that is $\lfloor \log_2(d-N+2) \rfloor + N$. □

Theorem 3. *The VC-dimension of a full univariate decision tree of height h that classifies d dimensional data is at least* $2^{h-1}(\lfloor \log_2(d-h+2) \rfloor + 1)$. *In a full decision tree each node has two child nodes.*

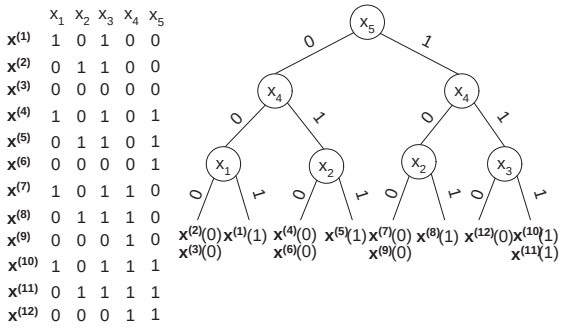


Figure 3: Example for Theorem 3 with $d = 5$ and $m = 12$. Using feature 5 in the first level and feature 4 in the second level, one divides the class labelings into 4 subproblems of $m = 3$. Each subproblem can then be shattered with a single node.

Proof. Similar to the Theorem 2 we proceed in a bottom up fashion. Each bottom node (For this case, there are 2^{h-1} of them) can classify m examples by setting up $2^{m-1}-1$ features to produce a one-to-one mapping between class labelings and those features (See Theorem 1). We also add $h-1$ features to the sample, where the first feature will be used in the first level, the second feature will be used in the second level, etc. (See Figure 3 for an example). This way each bottom node can be labeled as a $h-1$ digit binary number, which corresponds to the values of the new $h-1$ features of the examples forwarded to that node. For example, the values of the first, second, ..., $h-1$'th features (added features) of the examples forwarded to leftmost bottom node will be 0. On the other hand, the values of the first, second, ..., $h-1$'th features of examples forwarded to the rightmost bottom node will be 1. Given such a setup, one can produce a full decision tree which can classify $2^{h-1}m$ points for each possible class labeling. The number of features is,

$$\begin{aligned} d &= 2^{m-1}-1+h-1 \\ d-h+2 &= 2^{m-1} \\ m &= \log_2(d-h+2)+1 \end{aligned}$$

So the VC-dimension of the full decision tree is at least $2^{h-1}m$, that is $2^{h-1}(\lfloor \log_2(d-h+2) \rfloor + 1)$. □

Theorem 4. *The VC-dimension of a univariate decision tree with binary features that classifies d dimensional data is at least the sum of the VC-dimensions of its left and right subtrees those classifying* $d-1$ *dimensional data.*

Proof. Let the VC-dimension of two decision trees (DT_1 and DT_2) be VC_1 and VC_2 respectively. Under this assumption, those trees can classify VC_1 and VC_2 examples under all possible class labelings of those

```
VCDimension LB(DT, d)
1  if DT is a leaf node
2      return 1
3  if left and right subtrees of DT are leaves
4      return ⌊log2(d+1)⌋+1
5  DT_L = Left subtree of DT
6  DT_R = Right subtree of DT
7  return LB(DT_L, d−1) + LB(DT_R, d−1)
```

Figure 4: The pseudocode of the recursive algorithm for finding a lower bound of the VC-dimension of univariate decision tree with binary features: DT: Decision tree hypothesis class, d: Number of inputs

examples. Now we form the following tree: We add a new feature to the dataset and use that feature on the root node of the new decision tree, which has its left and right subtrees DT_1 and DT_2 respectively. The value of the new feature will be 0 for those instances forwarded to the left subtree (DT_1), 1 for those instances forwarded to the right subtree (DT_2). Now the new decision tree can classify at least $VC_1 + VC_2$ examples for all possible class labelings of those examples. □

Figure 4 shows the recursive algorithm that calculates a lower bound for the VC-dimension of an arbitrary univariate decision tree using Theorems 1 and 4. There are two base cases; (i) the decision tree is a leaf node whose VC-dimension is 1, (ii) the decision tree is a single node decision tree whose VC-dimension is given in Theorem 1.

3 GENERALIZATION TO L-ARY DECISION TREES

Until now, we considered the VC-dimension of univariate decision trees with binary features. In this section, we generalize our idea to univariate decision trees with discrete features. In a univariate decision tree generated for such a dataset, there will be L children (branches) of each internal node corresponding to the L different outcomes of the decision. For this case, the input space X is a vectorial space of dimension d, the number of features, where each feature X_i can take values from discrete set $\{1,2,\ldots,L_i\}$.

Theorem 5. *The VC-dimension of a single node L-ary decision tree that classifies d dimensional data is* $\lfloor \log_2(\sum_{i=1}^{d}(2^{L_i-1}-1)+1)\rfloor+1$.

Theorem 6. *The VC-dimension of L-ary decision tree that classifies d dimensional data is at least the sum of the VC-dimensions of its subtrees those classifying* $d-1$ *dimensional data.*

```
VCDimension LB-L-ary(DT, d)
1  if DT is a leaf node
2      return 1
3  if all subtrees of DT are leaves
4      return ⌊log2(Σ_{i=1}^{d}(2^{L_i−1}−1)+1)⌋+1
5  sum = 0
6  for i = 1 to number of subtrees
7      sum += LB-L-ary(DT_i, d−1)
8  return sum
```

Figure 5: The pseudocode of the recursive algorithm for finding a lower bound of the VC-dimension of L-ary decision tree: DT: Decision tree hypothesis class, d: Number of inputs

The proofs are similar to the proofs of Theorems 1 and 4. We omit them due to lack of space.

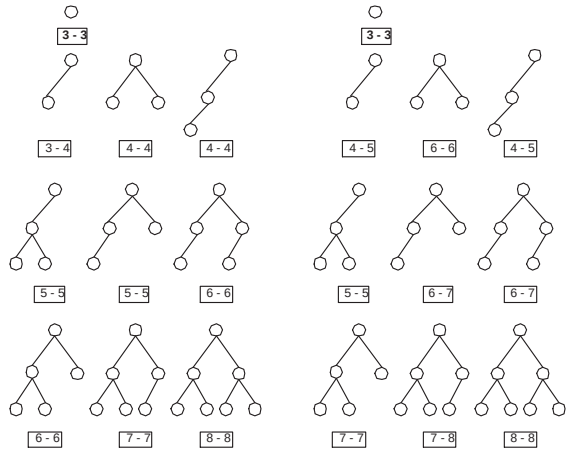
Figure 5 shows the recursive algorithm that calculates a lower bound for the VC-dimension of an arbitrary L-ary decision tree using Theorems 5 and 6. There are two base cases; (i) the L-ary decision tree is a leaf node whose VC-dimension is 1, (ii) the L-ary decision tree is a single node decision tree whose VC-dimension is given in Theorem 5.

4 EXPERIMENTS

4.1 Exhaustive Search Algorithm

To show the bounds found using Theorems 1-4 or using the algorithm in Figure 4 are tight, we run the exhaustive search algorithm explained in our previous work (Aslan et al., 2009) on different decision tree hypothesis classes. Since the computational complexity of the exhaustive search algorithm is exponential, we run the algorithm only on cases with small d and $|H|$.

Figure 6 shows our calculated lower bound and exact VC-dimension of decision trees for datasets with 3 and 4 input features. It can be seen that the VC-dimension increases as the number of nodes in the decision tree increases, but there are exceptions where the VC-dimension remains constant though the number of nodes increases, which shows that the VC-dimension of a decision tree not only depends the number of nodes, but also the structure of the tree. The results show that our bounds are tight: the maximum difference between the calculated lower bound and the exact VC-dimension is 1. Also for most of the cases (70 percent), our proposed algorithm based on lower bounds finds the exact VC-dimension of the decision tree.



(a) (b)

Figure 6: Calculated lower bound and the exact VC-dimension of univariate decision trees for datasets with 3 (a) and 4 (b) input features. Only the internal nodes are shown.

4.2 Complexity Control using VC-Dimension Bounds

In this section to show that our VC-dimension bounds are useful, we use them for complexity control in decision trees. Controlling complexity in decision trees could be done in two ways. We can control the complexities of the decision nodes by selecting the appropriate model for a node (Yıldız and Alpaydın, 2001), or we can control the overall complexity of the decision tree via pruning. Since this paper covers only discrete univariate trees, we take the second approach and use the VC-dimension bounds found in the previous section for pruning.

When we prune a node using SRM (SRMprune), we first find the VC generalization error using Equation 2 where V is the VC-dimension and E_t is the training error of the subtree. Then, we find the training error of the node as if it is a leaf node. Since the VC-dimension of a leaf node is 1, we can find the generalization error of the tree as if it is pruned. If the generalization error of the leaf node is smaller than the generalization error of the subtree, we prune the subtree, otherwise we keep it. We compare SRM based pruning with CVprune, where we evaluate the performance of the subtree with a leaf replacing the subtree on a separate validation set. For the sake of generality, we also include the results of trees before any pruning is applied (NOprune). We use a total of 11 data sets where 9 of them are (*artificial*, *krvskp*, *monks*, *mushroom*, *promoters*, *spect*, *tictactoe*, *titanic*, and *vote*) from UCI repository (Blake and Merz, 2000) and 2 are (*acceptors* and *donors*) bioinformatics datasets. We use 10×10 fold cross-validation to generate training and test sets. For CVprune, 20 percent of the training data is put aside as the pruning set. for SRMprune we did a grid-search on a_1 and a_2 using cross-validation and used $a_1 = 0.1$ and $a_2 = 2.0$.

Table 1: The average and standard deviations of error rates of decision trees generated using NOprune, CVprune, and SRMprune.

Set	NOprune	CVprune	SRMprune
Acc	17.1 ± 1.6	$\mathbf{15.5 \pm 2.3}$	15.6 ± 1.6
Art	$\mathbf{0.0 \pm 0.0}$	0.5 ± 1.4	$\mathbf{0.0 \pm 0.0}$
Don	8.0 ± 1.1	7.1 ± 1.1	$\mathbf{6.7 \pm 1.1}$
Krv	$\mathbf{0.3 \pm 0.3}$	1.2 ± 0.7	0.6 ± 0.4
Mon	$\mathbf{4.2 \pm 5.9}$	10.0 ± 7.6	$\mathbf{4.2 \pm 5.9}$
Mus	$\mathbf{0.0 \pm 0.0}$	0.0 ± 0.1	$\mathbf{0.0 \pm 0.0}$
Pro	23.6 ± 12.5	24.7 ± 12.9	$\mathbf{20.6 \pm 12.3}$
Spe	25.4 ± 7.9	$\mathbf{20.9 \pm 3.6}$	22.1 ± 7.1
Tic	$\mathbf{14.2 \pm 3.8}$	18.5 ± 4.2	$\mathbf{14.2 \pm 3.8}$
Tit	$\mathbf{21.0 \pm 1.7}$	21.5 ± 2.1	22.6 ± 2.1
Vot	6.3 ± 3.6	4.4 ± 2.9	$\mathbf{3.9 \pm 3.4}$

Table 2: The average and standard deviations of tree complexities of decision trees generated using NOprune, CVprune, and SRMprune.

Set	NOprune	CVprune	SRMprune
Acc	1015 ± 29	$\mathbf{55 \pm 42}$	838 ± 31
Art	16 ± 0	$\mathbf{15 \pm 2}$	16 ± 0
Don	1489 ± 32	$\mathbf{145 \pm 35}$	910 ± 74
Krv	138 ± 6	$\mathbf{80 \pm 13}$	122 ± 9
Mon	121 ± 50	$\mathbf{57 \pm 17}$	121 ± 50
Mus	43 ± 0	$\mathbf{41 \pm 4}$	43 ± 0
Pro	48 ± 5	$\mathbf{13 \pm 6}$	39 ± 3
Spe	165 ± 9	$\mathbf{5 \pm 10}$	60 ± 16
Tic	437 ± 31	$\mathbf{123 \pm 25}$	436 ± 31
Tit	32 ± 1	16 ± 4	$\mathbf{5 \pm 2}$
Vot	89 ± 8	$\mathbf{9 \pm 8}$	23 ± 8

Tables 1 and 2 show the average and standard deviations of error rates and tree complexities of decision trees generated using NOprune, CVprune, and SRMprune respectively. On four datasets (*artificial*, *monks*, *mushroom*, and *tictactoe*) there is no need to prune, i.e., pruning decreases performance and in this cases, CVprune prunes trees aggressively by sacrificing from accuracy, whereas SRMprune does not prune and gets the best performance with NOprune.

On five datasets (*acceptors*, *donors*, *spect*, *promoters*, and *vote*) pruning helps, i.e., pruning both reduces both the error rate and the tree complexity as needed. For those datasets, on two datasets CVprune is better than SRMprune, whereas on three datasets SRMprune is better than CVprune.

On two datasets (*titanic* and *krvskp*), both

CVprune and SRMprune prune more than needed and therefore can not decrease error rate. In general, CVprune prunes more aggresively than SRMprune which can cause a decrease in performance.

5 CONCLUSIONS

This paper tries to fill the gap in the statistical learning theory, where there is no explicit formula for the VC-dimension of a decision tree. In this work, we first focused on the easiest case of univariate trees with binary features. Starting from basic decision tree with a single decision node, we give and prove lower bounds of the VC-dimension of different decision tree structures. We also prove that the VC-dimension of a univariate decision tree with binary features depends on the number of features and the VC-dimension of the left and right subtrees of it (tree structure).

We use the exhaustive search algorithm given in (Aslan et al., 2009) to calculate the exact VC-dimension of simple trees and compare our bounds with the exact VC-dimension values, where the results show that our bounds are tight. These VC-dimension bounds are then used in pruning using SRM and when compared with cross-validation pruning, we see that SRM pruning using our VC-dimension values work well and find trees that are as accurate as CV pruning without the overhead of cross-validation or needing to leave out some data for training set.

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