A Geometric Algorithm for Learning Oblique Decision Trees

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Abstract. In this paper we present a novel algorithm for learning oblique decision trees. Most of the current decision tree algorithms rely on impurity measures to assess goodness of hyperplanes at each node. These impurity measures do not properly capture the geometric structures in the data. Motivated by this, our algorithm uses a strategy, based on some recent variants of SVM, to assess the hyperplanes in such a way that the geometric structure in the data is taken into account. We show through empirical studies that our method is effective.

1 Introduction

Decision tree is a well known and widely used method for classification and regression. The popularity of decision tree is because of its simplicity. In this paper we deal with oblique decision trees. These are binary decision trees where each non-leaf node is associated with a hyperplane (also called a split rule) and each leaf with a class label. To classify a pattern we follow a path in the tree by going down the left or right subtree at each node based on whether the pattern is on the positive or negative side of the hyperplane associated with the node; when we reach the leaf the pattern gets assigned the label of the leaf. Most approaches for learning decision trees are recursive algorithms for building the tree in a top down fashion. At each stage, we need to find a hyperplane to associate with the current node which is done by searching for a hyperplane which minimizes some impurity measure. Gini index and entropy are frequently used impurity measures. CART-LC [2], OC1 [8] are few examples of decision tree approaches which learn oblique decision trees by optimizing such impurity measures. All decision tree algorithms employ greedy search and hence a hyperplane assigned to a node once, is never changed. If a bad hyperplane is learnt at some node, it can not be rectified anymore and the effect of it may be a large tree which, in turn, may lead to poor generalization error.

A problem with all impurity measures is that they depend only on the number of (training) patterns of either class on each side of the hyperplane. If we change the class regions without changing the effective areas of class regions on either side of the hyperplane, the impurity measure will not change. Thus the impurity measures do not really capture the geometric structure of class distributions. In this paper we present a new decision tree learning algorithm which is based

on the idea of capturing the geometric structure. For this we borrow ideas from some recent variants of the SVM method which are quite good at capturing (linear) geometric structure of the data. The Proximal SVM [5] finds two parallel clustering hyperplanes, one for each class, and takes the hyperplane situated in the middle of the two as the classifying hyperplane. However, often the points of the two classes are not clustered around parallel hyperplanes. Multisurface Proximal SVM [6] finds two clustering hyperplanes, one for each class, which are not necessary parallel, and the data is classified based on the nearness to the hyperplanes. Many times the class distribution is such that just one pair of hyperplanes is not good enough for classification. For such cases, they [6] extend this idea using the kernel trick of (effectively) learning the pair of hyperplanes in a high dimensional space to which the patterns are transformed.

Motivated by Proximal SVM, we derive our decision tree approach as follows. At each node, we use the idea of Multisurface Proximal SVM to find the linear tendencies in the data by learning hyperplanes around which the data of different classes are clustered. After finding these hyperplanes, the natural guess for a split rule at this node is the angle bisector of the two hyperplanes. This allows us to capture geometry of the classification boundary to some extent. Then, in the usual style of decision tree algorithms, we split the data based on this angle bisector and recursively learn the left and right subtrees of this node. Since, in general, there will be two angle bisectors, we select the one which is better based on an impurity measure. In this paper we discuss the algorithm for only two class classification problem. Since our decision tree approach is motivated by the geometry of the classification problem, we call it **Geometric Decision Tree** (Geometric DT).

2 The Algorithm

For a general decision tree algorithm, the main computational task is: given a set of data, find the best hyperplane to split the data. Let S^t be the set of points falling at node t . Let n_+^t and n_-^t denote the number of patterns of the two classes (say, '+1' and '-1') at that node. Let d be the data dimension. Let $A \in \mathbb{R}^{n_+^t \times d}$ be the matrix representing points of class +1 as row vectors at node t . A_i is the i th row of A which is a row vector in $\mathbb{R}^d$. Similarly $B \in \mathbb{R}^{n_-^t \times d}$ be the matrix whose rows contain points of class -1 at node t . Let $h_1 : \mathbf{w}_1^t \mathbf{x} + b_1 = 0$ and $h_2 : \mathbf{w}_2^t \mathbf{x} + b_2 = 0$ be two clustering hyperplanes, one for each class. As mentioned before we use Multisurface Proximal SVM [6], also called Generalized Proximal SVM (GEPSVM), to find the two clustering hyperplanes. The hyperplane h_1 is closest to all points of class +1 and farthest from class -1. Similarly the hyperplane h_2 is closest to all points of class -1 and farthest from class +1. Then the optimization problems for finding $(\mathbf{w}_1, b_1)$ and $(\mathbf{w}_2, b_2)$ can be written as [6]

$$(\mathbf{w}_1, b_1) = \operatorname{argmin}_{(\mathbf{w}, b) \neq 0} \frac{\|A\mathbf{w} + b\mathbf{e}_{n_+^t}\|^2}{\|B\mathbf{w} + b\mathbf{e}_{n_-^t}\|^2} \quad (1)$$

$$(\mathbf{w}_2, b_2) = \operatorname{argmin}_{(\mathbf{w}, b) \neq 0} \frac{\|B\mathbf{w} + b\mathbf{e}_{n_-^t}\|^2}{\|A\mathbf{w} + b\mathbf{e}_{n_+^t}\|^2} \quad (2)$$

Where $\|\cdot\|$ denotes the standard euclidean norm, $\mathbf{e}_{n_+^t}$ is $(n_+^t \times 1)$ vector of ones and $\mathbf{e}_{n_-^t}$ is $(n_-^t \times 1)$ vector of ones. These optimization problems can be further reduced to [6]

$$\tilde{\mathbf{w}}_1 = \operatorname{argmin}_{\tilde{\mathbf{w}} \neq 0} \frac{\tilde{\mathbf{w}}^T G \tilde{\mathbf{w}}}{\tilde{\mathbf{w}}^T H \tilde{\mathbf{w}}} \quad (3)$$

$$\tilde{\mathbf{w}}_2 = \operatorname{argmin}_{\tilde{\mathbf{w}} \neq 0} \frac{\tilde{\mathbf{w}}^T H \tilde{\mathbf{w}}}{\tilde{\mathbf{w}}^T G \tilde{\mathbf{w}}} \quad (4)$$

where $\tilde{\mathbf{w}} = (\mathbf{w}, b)$, $G = [A \mathbf{e}_{n_+^t}]^T [A \mathbf{e}_{n_+^t}]$ and $H = [B \mathbf{e}_{n_-^t}]^T [B \mathbf{e}_{n_-^t}]$. This problem of finding the two clustering hyperplanes $(\mathbf{w}_1, b_1)$ and $(\mathbf{w}_2, b_2)$ gets reduced [6] to finding the eigenvectors corresponding to the maximum and minimum eigenvalue of the following generalized eigenvalue problem

$$H \tilde{\mathbf{w}} = \gamma G \tilde{\mathbf{w}} \quad (5)$$

Once we find these hyperplanes, the hyperplane we associate with the current node will be one of the angle bisectors of these two hyperplanes because it divide the space in such a way that on one side points of one class are clouded and on the other side points of second class are clouded. Let the hyperplanes $\mathbf{w}_3^t \mathbf{x} + b_3 = 0$ and $\mathbf{w}_4^t \mathbf{x} + b_4 = 0$ be the angle bisectors of $\mathbf{w}_1^t \mathbf{x} + b_1 = 0$ and $\mathbf{w}_2^t \mathbf{x} + b_2 = 0$, then

$$\tilde{\mathbf{w}}_3 \triangleq (\mathbf{w}_3, b_3) = \left(\frac{\mathbf{w}_1}{\|\mathbf{w}_1\|} - \frac{\mathbf{w}_2}{\|\mathbf{w}_2\|}, \frac{b_1}{\|\mathbf{w}_1\|} - \frac{b_2}{\|\mathbf{w}_2\|} \right) \quad (6)$$

$$\tilde{\mathbf{w}}_4 \triangleq (\mathbf{w}_4, b_4) = \left(\frac{\mathbf{w}_1}{\|\mathbf{w}_1\|} + \frac{\mathbf{w}_2}{\|\mathbf{w}_2\|}, \frac{b_1}{\|\mathbf{w}_1\|} + \frac{b_2}{\|\mathbf{w}_2\|} \right) \quad (7)$$

We choose the angle bisector which has lower impurity. In our work we use *gini* index to measure impurity. Let $\tilde{\mathbf{w}}_t$ be a hyperplane which is used for dividing the set S^t in two parts S^{t_l} and S^{t_r} . Let $n_+^{t_l}$ and $n_-^{t_l}$ denote the number of patterns of the two classes in the set S^{t_l} and $n_+^{t_r}$ and $n_-^{t_r}$ denote the number of patterns of the two classes in the set S^{t_r} . Then *gini* index of hyperplane $\tilde{\mathbf{w}}_t$ is given by,

$$gini(\tilde{\mathbf{w}}_t) = \frac{n^t}{n^t} \left[1 - \left(\frac{n_+^{t_l}}{n^{t_l}} \right)^2 - \left(\frac{n_-^{t_l}}{n^{t_l}} \right)^2 \right] + \frac{n^{t_r}}{n^t} \left[1 - \left(\frac{n_+^{t_r}}{n^{t_r}} \right)^2 - \left(\frac{n_-^{t_r}}{n^{t_r}} \right)^2 \right] \quad (8)$$

where $n^t = n_+^t + n_-^t$ is the number of points in S_t . Also $n^{t_l} = n_+^{t_l} + n_-^{t_l}$ is the number of points falling in the set S^{t_l} and $n^{t_r} = n_+^{t_r} + n_-^{t_r}$ is the number of points falling in the set S^{t_r} . We choose $\tilde{\mathbf{w}}_3$ or $\tilde{\mathbf{w}}_4$ to be the split rule for S^t based on which of the two gives lesser value of *gini* index given by Eq.(8). Algorithm. 2 describes the complete decision tree learning algorithm.

3 Experiments

To test the effectiveness of Geometric DT we test its performance on several synthetic and real world data sets. We consider three synthetic problems

Algorithm 1. Geometric DT

Input: Sample $S = \{(\mathbf{x}_i, y_i)\}_{i=1\dots n}$, Max-Depth, ϵ_1 **Output:** Pointer to the root of a decision tree**begin** Root = *growTree*(S); **return** Root;**end****Procedure** *growTree*(S^t) **Input:** Set of patterns at node t , S^t **Output:** Pointer to a subtree **begin**

1. – Find matrices A and B using the set S^t of patterns at node t .
 – Find $\tilde{\mathbf{w}}_1$ and $\tilde{\mathbf{w}}_2$ according to Eq.(3),(4).
 – Compute angle bisectors $\tilde{\mathbf{w}}_3$ and $\tilde{\mathbf{w}}_4$ using Eq.(6),(7).
 – Calculate the *gini* index (Eq.(8)) for both the angle bisectors $\tilde{\mathbf{w}}_3$ and $\tilde{\mathbf{w}}_4$.
 – Choose the one which gives lesser value of *gini* index. Call it $\tilde{\mathbf{w}}^*$.
 – Let $\tilde{\mathbf{w}}_t$ denote the split rule at node t . Assign $\tilde{\mathbf{w}}_t \leftarrow \tilde{\mathbf{w}}^*$.
2. Let $S^{t_l} = \{\mathbf{x}_i \in S^t | \tilde{\mathbf{w}}_t^T \tilde{\mathbf{x}} < 0\}$ and $S^{t_r} = \{\mathbf{x}_i \in S^t | \tilde{\mathbf{w}}_t^T \tilde{\mathbf{x}} \geq 0\}$
 Define $\eta(S^t) = \frac{\text{\#points of minority class at node } t}{\text{\#points at node } t}$.
3. **if** ($\eta(S^{t_l}) < \epsilon_1$) **or** (*Tree-Depth*=*Max-Depth*) **then**
 get a node t_l and make t_l a leaf node and assign appropriate class label to t_l ;
 else $t_l = \text{growTree}(S^{t_l})$;
 make t_l left child of t ;
4. **if** ($\eta(S^{t_r}) < \epsilon_1$) **or** (*Tree-Depth*=*Max-Depth*) **then**
 get a node t_r and make t_r a leaf node and assign appropriate class label to t_r ;
 else $t_r = \text{growTree}(S^{t_r})$;
 make t_r right child of t ;
5. **return** t ;

end

and two real world data sets from UCI ML repository [1]. First two synthetic problems are rotated 2×2 and 4×4 checkerboard data sets in two dimensions. The third problem is in $\mathbb{R}^{10}$. We sample points uniformly from $[-1 \ 1]^{10}$. Let $\tilde{\mathbf{w}}_1 = [1, 1, 0, 1, 0, 0, 1, 0, 0, 1, 0]^T$, $\tilde{\mathbf{w}}_2 = [1, -1, 0, 0, 1, 0, 0, 1, 0, 0, 0]^T$ and $\tilde{\mathbf{w}}_3 = [0, 1, -1, 0, -1, 0, 1, 1, -1, 1, 0]^T$ be three hyperplane parameters in $\mathbb{R}^{10}$. Now the points are labeled +1 or -1 based on the following rule

$$y = \begin{cases} 1, & \text{if } (\tilde{\mathbf{w}}_1^t \tilde{\mathbf{x}} \geq 0 \ \& \ \tilde{\mathbf{w}}_2^t \tilde{\mathbf{x}} \geq 0 \ \& \ \tilde{\mathbf{w}}_3^t \tilde{\mathbf{x}} \geq 0) \parallel \\ & (\tilde{\mathbf{w}}_1^t \tilde{\mathbf{x}} \leq 0 \ \& \ \tilde{\mathbf{w}}_2^t \tilde{\mathbf{x}} \leq 0 \ \& \ \tilde{\mathbf{w}}_3^t \tilde{\mathbf{x}} \geq 0) \parallel \\ & (\tilde{\mathbf{w}}_1^t \tilde{\mathbf{x}} \leq 0 \ \& \ \tilde{\mathbf{w}}_2^t \tilde{\mathbf{x}} \geq 0 \ \& \ \tilde{\mathbf{w}}_3^t \tilde{\mathbf{x}} \leq 0) \parallel \\ & (\tilde{\mathbf{w}}_1^t \tilde{\mathbf{x}} \geq 0 \ \& \ \tilde{\mathbf{w}}_2^t \tilde{\mathbf{x}} \leq 0 \ \& \ \tilde{\mathbf{w}}_3^t \tilde{\mathbf{x}} \leq 0) \parallel \\ -1, & \text{else} \end{cases}$$

For each synthetic problem 2000 points were sampled for training set and 1000 for testing set. To evaluate the performance of the algorithm on real dataset we use Breast Cancer Data set and Bupa Liver Disorder Data set [1]. Breast

Cancer Data set is a 10 dimensional binary classification problem. It has total 683 instances, out of which we use 500 for training and 183 for testing. Bupa Liver Disorder Data set is a 6-dimensional binary classification problem. It has a total 345 instances, out of which we use 200 for training and 145 for testing. We compare performance of our approach with several algorithms, namely, CART-LC [2], OC1-AP, OC1(Oblique) [8], Support Vector Machine (SVM) [3] and GEPSVM [6]. For OC1 and CART-LC we use the downloadable [7] package. For SVM we use libsvm [4] code. Geometric DT is implemented in MATLAB. For GEPSVM also we wrote MATLAB code. We compare the performances on several measures like training time, training accuracy, test accuracy, number of leaves and depth of the tree. In the SVM method we used Gaussian kernel to capture non-linear classification boundaries. In case of GEPSVM also we used Gaussian kernel for all problems except the first problem where a pair of hyperplanes is good enough for classification. Best parameters for kernel were found by using 10-fold cross validation. The comparison results are shown in Table.1 (For OC1 and CART-LC which are randomized algorithms we show mean and standard deviation of results on 10 runs.) From Table. 1 we see that, over all the problems, Geometric DT performs better than all the other decision tree approaches in test accuracy, tree size and number of leaves. GEPSVM with linear kernel performs same as Geometric DT for the 2×2 checkerboard problem

Table 1. Comparison results on synthetic and real world data sets

		Geometric DT	OC1(AP)	OC1 (Oblique)	CART-LC	SVM	GEPSVM
2×2 Checker-board	TrTime(sec)	0.064	0.031	3.112±0.83	1.049±0.8	0.132	.004
	TrAcc	99.70	99.34±0.3	99.40±0.92	98.57±1	99.25	99.70
	TesAcc	99.90	97.45±0.55	98.52±1.17	96.98±0.94	99.5	99.90
	# leaves	4	39±5.83	17.8±6.84	22±8.1	-	-
	Depth	2	11.8±1.93	8.4±3.24	9.6±2.8	-	-
4×4 Checker-board	TrTime(sec)	0.062	0.047	4.247±0.53	2.029±0.98	0.154	451.86
	TrAcc	97.75	98.28±0.4	98.78±0.76	98.08±0.71	98.10	90.70
	TesAcc	98.50	92.48±0.86	94.65±0.91	92.53±0.9	97.50	89.80
	# leaves	16	18.4±15.08	82.7±21.96	104.4±19.18	-	-
	Depth	4	16.3±2	14.6±2.32	15.4±2.46	-	-
10 Dimensional Dataset	TrTime(sec)	0.1192	0.249±0.02	18.37±1.73	31.54±9.67	1.048	384.10
	TrAcc	85.20	72.10±2.88	74.76±3.64	61.83±1.54	98.65	92.20
	TesAcc	84.60	60.40±1.86	63.50±0.74	61.29±1.46	74.60	67.30
	# leaves	26	55.8±15.27	31.7±12.81	16.3±7.6	-	-
	Depth	7	11.3±1.57	9.7±2.11	7.9±1.79	-	-
Breast Cancer	TrTime(sec)	0.0145	0.011±0.001	1.41±0.42	0.10±0.02	0.061	9.63
	TrAcc	96.4	97.30±1.03	97.02±0.76	95.14±1.65	100	100
	TesAcc	100	96.77±0.91	97.27±1.15	93.34±3.18	77.05	77.05
	# leaves	3	7.9±4.68	4.9±2.33	2.8±1.32	-	-
	Depth	2	4±1.63	2.9±1.29	1.7±1.06	-	-
Bupa Liver Disorder	TrTime(sec)	0.0137	0.008	0.74±0.15	0.06±0.01	0.018	0.83
	TrAcc	77	81.3±6.71	84.2±5.15	80.9±6.38	100	79.00
	TesAcc	72.41	59.3±2.28	60.76±2.67	59.66±2.33	73.1	71.72
	# leaves	11	11.5±6.45	12.9±5.51	12.5±7.09	-	-
	Depth	7	7±3.13	7.6±3.17	6.7±3.13	-	-

because for this problem the two approaches work in a similar way. But when there are more than two hyperplanes required, GEPSVM with Gaussian kernel performs worse than our decision tree approach. For example, for 4×4 checkerboard example, GEPSVM can achieve only about 89.8% test accuracy while our decision tree gives about 98.5% test accuracy. Moreover, with Gaussian kernel, GEPSVM solves the generalized eigenvalue problem of the size of number of points, whereas our decision tree solves the generalized eigenvalue problem of the dimension of the data (which is the case with GEPSVM only when it uses linear kernel). This gives us an extra advantage in computational cost over GEPSVM.

In 10-dimensional problem, both in test accuracy and training time, Geometric DT performs better than all the other approaches. This shows that our algorithm scales with data dimension. For the real world problems also Geometric DT performs well. It gives highest test accuracy with Breast Cancer Data set. For Liver Disorder Data set also it performs better than all other decision tree approaches and the test accuracy of SVM is marginally better.

In Figure. 1 we show the effectiveness of our algorithm in terms of capturing the geometric structure of the classification problem. We show the first few hyperplanes generated by our approach and OC1(oblique) for 2×2 and 4×4 checkerboard data. We see that our approach learns the correct geometric structure of the classification boundary, whereas the OC1(oblique), which uses the *gini* index as impurity measure, does not capture that.

Fig. 1. Comparisons of Geometric DT with OC1(Oblique) on rotated 2×2 and 4×4 checkerboard data: (a) Hyperplane at root node learnt using Geometric DT on rotated 2×2 checkerboard data; (b) Hyperplane at left child of root node learnt using Geometric DT on rotated 2×2 checkerboard data; (c) Hyperplane at root node learnt using OC1(Oblique) DT on rotated 2×2 checkerboard data; (d), (e) and (f) show the hyperplanes for 4×4 checkerboard data in a similar way

4 Conclusions

In this paper we presented a new algorithm for learning oblique decision trees. The novelty is in learning hyperplane that captures the geometric structure of the data using the GEPSVM idea. Through empirical studies we showed that the method performs better than the other approaches and also captures the geometric structure well. Though we consider only the 2-class problems here, the approach can easily be generalized to multiclass problems by learning a split rule, at each node, to separate the majority class from the rest. We will be explaining this in our future work.

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