# Selective Augmented Bayesian Network Classifiers Based on Rough Set Theory

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Abstract. The naive Bayes classifier is widely used in interactive applications due to its computational efficiency, direct theoretical base, and competitive accuracy. However, its attribute independence assumption can result in sub-optimal accuracy. A number of techniques have explored simple relaxations of the attribute independence assumption in order to increase accuracy. TAN is a state-of-the-art extension of naive Bayes, that can express limited forms of inter-dependence among attributes. Rough sets theory provides tools for expressing inexact or partial dependencies within dataset. In this paper, we present a variant of TAN using rough sets theory and compare their tree classifier structures, which can be thought of as a selective restricted trees Bayesian classifier. It delivers lower error than both pre-existing TAN-based classifiers, with substantially less computation than is required by the SuperParent approach. Keywords: Naive Bayes, Bayesian Network, Machine Learning,

## 1 Introduction

A classification task in data mining is to build a classifier which can assign a suitable class label to an unlabelled instance described by a set of attributes. Many approaches and techniques have been developed to create a classification model. The naive Bayesian classifier is one of the most widely used in interactive applications due to its computational efficiency, competitive accuracy, direct theoretical base, and its ability to integrate the prior information with data sample information [1,7,3,5,18,15,14]. It is based on Bayes' theorem and an assumption that all attributes are mutually independent within each class. Assume X is a finite set of instances, and  $A = \{A_1, A_2, \cdots, A_n\}$  is a finite set of n attributes. An instance  $x \in X$  is described by a vector  $\{a_1, a_2, \cdots, a_n\}$ , where  $a_i$  is a value of attribute  $A_i$ . C is called the class attribute. Prediction accuracy will be maximized if the predicted class

$$L(x) = argmax_c(P(c \mid \langle a_1, a_2, \cdots, a_n \rangle). \tag{1}$$

Unfortunately, unless the vector occurs many times within X, it will not be possible to directly estimate  $P(c \mid \langle a_1, a_2, \dots, a_n \rangle)$  from the frequency with which

each class  $c \in C$  co-occurs with  $\langle a_1, a_2, \dots, a_n \rangle$  within the training instances. Bayes' theorem provides an equality that might be used to help estimate the posterior probability  $P(c_i \mid x)$  in such a circumstance:

$$P(c_i \mid x) = \alpha \cdot P(c_i) \cdot P(\langle a_1, a_2, \cdots, a_n \rangle \mid c_i)$$
(2)

where  $P(c_i)$  is the prior probability of class  $c_i \in C$ ,  $P(\langle a_1, a_2, \dots, a_n \rangle | c_i)$  is the conditional probability of  $x \in T$  given the class  $c_i$ , and  $\alpha$  is a normalization factor. According to the chain rule, equation 2 can be written as:

$$P(c_i \mid x) = \alpha \cdot P(c_i) \cdot \prod_{k=1}^{n} P(a_k \mid a_1, a_2, \dots, a_{k-1}, c_i)$$
 (3)

Therefore, an approach to Bayesian estimation is to seek to estimate each  $P(a_k \mid a_1, a_2, \dots, a_{k-1}, c_i)$ .

If the n attributes are mutually independent within each class value, then the conditional probability can be calculated in the following way:

$$P(\langle a_1, a_2, \dots, a_n \rangle | c_i) = \prod_{k=1}^n P(a_k | c_i).$$
 (4)

Classification selecting the most probable class as estimated using formulae 2 and 4 is the well-known naive Bayesian classifier.

# 2 Approaches of Improving Naive Bayesian Method

In real world problems, the performance of a naive Bayesian classifier is dominated by two explicit assumptions: the attribute independence assumption and the probability estimation assumption. Of numerous proposals to improve the accuracy of naive Bayesian classifiers by weakening its attribute independence assumption, both Tree Augmented Naive Bayes(TAN) [4, 3, 5] and Lazy Bayesian Rules(LBR) [18] have demonstrated remarkable error performance [14]. Friedman, Geiger and Goldszmidt presented a compromise representation, called treeaugmented naive Bayes (TAN, simply called the basic TAN), in which the class node directly points to all attributes' nodes and an attribute node can have only at most one additional parent to the class node. Keogh & Pazzani took a different approach to constructing tree-augmented Bayesian networks [5] (simply called SuperParent or SP). The two methods mainly differ in two aspects. One is the criterion of attribute selection used to select dependence relations among the attributes while building a tree-augmented Bayesian network. Another is the structure of the classifiers. The first one always tends to construct a tree including all attributes, the second one always tends to construct a tree with fewer dependence relations among attributes and better classification accuracy. Zheng and Webb proposed a lazy Bayesian rule (LBR) learning technique [18]. LBR can be thought of as applying lazy learning techniques to naive Bayesian rule induction. Both LBR and TAN can be viewed as variants of naive Bayes that relax the attribute independence assumption [14].

In this paper, however, we concentrate on the eager strategy, which holds a computational advantage when a single model can be applied to classify many instances. First of all, we mainly analyze the implementations of two different TAN classifiers and their tree classifier structures, and experimentally show how different dependence relations impact on the accuracy of TAN classifiers. Second, based on the definition of dependence in the basic rough set theory, we propose a definition of dependence measurement given the class variable, and use it to build a new dependence relation matrix. We believe that the directions of dependence relations are very important for performance of a classifier. Using this kind of definition, we can actually gain a directed-graph description. Third, we present a new algorithm for building selective augmented Bayesian network classifiers, which reduce error relative to the TAN classifiers, and has similar computational overheads. Experimental results also show that can deliver some improvements on performance, while requiring substantially less computation.

## 3 Some Issues in the Implementations

Now, we discuss some extended issues in the implementations of the TAN classifiers. First of all, the problem is related to the probability estimation assumption. In the basic TAN, for each attribute we assess the conditional probability given the class variable and another attribute. This means that the number of instances used to estimate the conditional probability is reduced as it is estimated from the instances that share three specific values (the class value, the parent value and the child value). Thus it is not surprising to encounter unreliable estimates, especially in small datasets. Friedman, Geiger and Goldszmidt dealt with this problem by introducing a smoothing operation [3]. There is a problem with this strategy when attribute value a does not occur in the training data (this situation can occur during cross validation testing), the value of the estimate will be zero. In our implementation, we use both these smoothing adjustments to estimate any conditional probability with  $|\pi(a)| = 2$ , i.e.,

$$\widehat{P}(a \mid \pi(a)) = \frac{counts(a, \pi(a)) + N^0 \cdot \frac{counts(a) + 1}{|T| + |A|}}{counts(\pi(a)) + N^0}.$$
 (5)

where |A| is the number of values for attribute A. We use Laplace estimation to estimate any other probability. In Keogh and Pazzani's SuperParent algorithm, they replace zero probabilities with a small epsilon (0.0001). Kohavi, Becker and Sommerfield [8] have shown that different methods for estimating the base probabilities in naive Bayes can greatly impact upon its performance. Similarly, different estimation methods will gain different effects on the same TAN classification model. We think that estimation methods should depend on the distribution of variables, as well as the number of training instances to support these kinds of estimation methods. Estimation methods should be independent of classification models for the same probability. In order to compare

the performances of classification models, we use the same method to estimate probabilities. In all the algorithms mentioned in our experiments, we always use formular 5 to estimate any conditional probability with  $|\pi(a)| = 2$  and only standard Laplace estimation applied to any other probability.

Secondly, regarding the problem of missing values, in both the basic TAN classifiers and SuperParent classifiers, instances with missing values were deleted from the set of training instances. We keep all the instances, but ignore missing values from the counts for missing attribute values. Also, when we estimate a conditional probability  $P(a_k \mid c_i)$ , for a prior probability of class value  $c_i$  we exclude the occurrences of class value  $c_i$  with missing values on attribute  $A_k$ . Obviously, this makes the estimation of the condition more reliable while estimating any conditional probability.

Thirdly, although the choice of root variable does not change the log-likelihood of the basic TAN network, we have to set the direction of all edges for classification. When each edge (Ai, Aj) is added to the current tree structure, we always set the direction from Ai to Aj (i < j) at once. In Keogh and Pazzani's SuperParent classifiers, the direction of an arc is always from the super parent node to the favorite child node. That means that when an dependence relation is singled out, it always has the specific direction.

## 4 Selective Augmented Bayesian Classifiers

There are further factors that influence the performance of an augmented naive Bayesian classifier. The first one is the criterion for selecting dependence relations among the attributes. The second one is the criterion of terminating the selection. In this section, we describe our new algorithm for selective augmented Bayesian classifiers, explain how it works and is different from the basic TAN classifiers and SuperParent classifiers, and experimentally show its better performance and preferable computational profile.

#### 4.1 Dependence Relation Matrix Based on Rough Set Theory

Friedman, Geiger and Goldszmidt explain why they use the conditional mutual information as the criterion of selecting dependence relations among the attributes [3, 4]. One problem with this criterion, as mentioned above, is how to decide the directions of dependence relations. Keogh and Pazzani use leave-one-out cross-validation to handle this problem in the process of building a classifier [5, 6]. When the best super parent and its favorite child are found, the dependence relation between them is naturally from the best super parent to its favorite child, i.e., the favorite child is depends on the corresponding best super parent. For each arc to be added into the structure, SuperParent needs many times to execute leave-one-out cross-validations on the whole set of training instances. Although they proposed some shortcuts to speed up the process of evaluating many classifiers, the algorithm is still very time consuming. In our algorithm, we will use a dependence measurement based on rough sets theory.

Rough set [11] provides, in particular, tools for expressing inexact or partial dependencies within dataset. Given a dataset of some description or measurements concerning available instances, rough set methods enable to extract dependence relations between corresponding attributes or variables. These dependence relations can be applied to inductive reasoning about new, so far unseen cases, in a way well understandable for the user. Above advantages, as well as very effective computational framework for extraction of the most interesting dependencies from real-life data, cause a rapid development of applications of rough sets to more and more scientific fields and practical tasks [13].

According to the values of class variable, we define a new dependence relation matrix, in which each item of conditional dependence relation,  $D(A_i, A_j \mid C)$ , can be described as follows:

$$D(A_i, A_j \mid C) = \sum_{A_i, A_j, Y_c} \frac{|POS_{A_i}^{Y_c}(A_j)|}{counts(Y_c)}$$
(6)

where  $POS_{A_i}^{Y_c}(A_j)$  represents the positive region of attribute  $A_j$  relative to attribute  $A_i$  within the class value  $Y_c$  [11]. Using this kind of definition, we can actually gain a directed-graph description. Each item not only reflects the degree of the dependence between two attributes, but also tells us the direction of the dependence relation.

#### 4.2 A New Selective Augmented Bayesian Algorithm

In an augmented Bayesian classifier, the second important issue is how to decide the candidate dependence set and when terminate the the selection. There are n(n-1) different dependence relations among n attributes. When there are n-1 or no any edge with the conditional mutual information more than 0, a basic TAN structure will have n-1 arcs. We also try to add n-1 arcs to our augmented Bayesian classifier, but the candidate set is different from the basic TAN. Because the way of weighting a candidate arc and the way of setting the direction of an arc are different from the basic TAN structure, the candidate arc set is different.

Based on above discussions, we can describe our selective augmented Bayesian algorithm, simply called *Select* in all tables, as follows.

- 1. Compute the dependence relation matrix conditional mutual information using formula 6.
- 2. Select an arc using a near maximum branching directed arborescence alogorithm [10], based on the dependence relation matrix.
- 3. Use leave-one-out cross-validation to evaluate the current set of arborescences to decide whether this arc should be added into the current structure or not, adding it only if doing so reduces cross-validation error.
- 4. Repeat the previous iteration n-1 times, or until no more arcs can be tested.

An important difference from the basic TAN algorithm is that this algorithm tries to build a maximum directed branch or arborescence [10], not a maximum

undirected spanning tree. We believe that the direction of dependence relations is a critical issue to minimizing error. In the procedure of building an augmented Bayesian classifier the network is always a directed structure.

### 5 Experimental Results

There are thirty-two natural domains used in our experiments, shown in Table 1. Twenty-nine of these are totally drawn from the previous research paper [18]. The other three (Satellite, segment, and Shuttle) are larger datasets. " $S\sharp$ " means the number of instances. " $C\sharp$ " means the number of values of a class attribute. " $A\sharp$ " means the number of attributes, not including the class attribute. All the experiments were performed in the Weka system [17]. The error rate of each classification model on each domain is determined by running 10-fold cross-validation on a dual-processor 1.7Ghz Pentium 4 Linux computer with 2Gb RAM. We use the default discretization method "weka.filters.DiscretizeFilter" as the discretization method for continuous values, which is based on Fayyad and Irani's method [2].

Table 1 also shows the error rates of naive Bayes classifier (NB), the basic TAN classifier, the SuperParent clssifier (SP), and our selective augmented Bayesian classifier (Select) on each domain, respectively. The last row contains the mean error rates for each column. The best one for a given dataset is shown in bold text. It shows the selective augmented Bayesian classifier has the lowest mean error rate. Table 2 presents the WIN/LOSS/DRAW records for comparing with all other classifiers. This is a record of the number of data sets for which the nominated algorithm achieves lower, higher, and equal error to the comparison algorithm, measured to two decimal places. The table also includes the outcome of a two-tailed binomial sign test. This indicates the probability that the observed outcome or more extreme should occur by chance if wins and losses were equiprobable. The selective augmented Bayesian classifier demonstrates the best performance. In the thirty-two databases, there are nineteen databases which the selective augmented Bayesian classifier has higher classification accuracy than Naive Bayes, twenty-one databases than the basic TAN classifier, sixteen databases than the SuperParent classifier. It is remarkable that there are eighteen databases which the basic TAN classifier has higher classification accuracy than Naive Bayes, and twelve datasets worse than Naive Bayes.

This suggests that selective augmented Bayesian classifier has similar error to the SuperParent classifier, but the selective augmented Bayesian classifier is much more efficient than the SuperParent classifier. Table 3 shows the time of building each classifier. On the most of domains, the selective augmented Bayesian classifier is much faster than the SuperParent classifier.

Table 4 shows the number of arcs in the Bayesian network built by the SuperParent classifier (SP), the basic TAN classifier, and our (Select) on each domain, respectively. These experimental results show that the basic TAN always tends to construct a tree including all attributes, the SP always tends to construct a tree with fewer dependence relations among attributes and better

Table 1. Descriptions of Data and Average Error Rates

	Domain	S#	C#	Α♯	Μ	NB	SP	TAN	Select
1	Anealing	898	6	38	Y	5.46	3.3	4.34	4.12
2	Audiology	226	24	69	Y	29.20	27.88	27.43	26.55
3	Breast Cancer	699	2	9	Y	2.58	2.58	5.01	2.58
4	Chess(kr-vs-kp)	3169	2	39	Ν	12.36	5.19	6.54	8.01
5	Credit	69	2	15	Y	15.07	15.22	14.93	15.23
6	Echocardiogram	131	2	6	Y	27.48	29.01	35.88	28.24
7	Glass	214	7	9	N	41.12	41.59	37.85	35.98
8	Heart	270	2	13	Ν	15.19	16.30	20.74	17.04
9	Hepatitis	155	2	19	Y	16.13	16.13	11.61	14.84
10	Horse Colic	368	2	21	Y	20.11	19.29	19.84	19.02
11	House Votes 84	435	2	16	N	9.89	6.67	7.59	9.20
12	Hypothyroid	3163	2	25	Y	2.94	2.81	2.66	2.75
13	Iris	150	3	4	N	6.00	6.67	5.33	8.00
14	Labors	57	2	16	Y	3.51	3.51	12.28	3.51
15	LED	1000	10	7	N	26.20	26.60	25.90	26.70
16	Bupa	345	2	6	N	36.81	38.84	37.68	39.13
17	Lung Cancer	32	3	56	Y	46.88	50.00	46.88	43.75
18	Lymphography	148	4	18	Ν	14.19	14.86	18.92	12.84
19	PID	768	2	8	N	25.00	25.52	25.00	24.74
20	Post Operative	90	3	8	Y	28.89	31.11	35.56	30.00
21	Primary Tumor	339	22	17	Y	48.97	51.15	54.28	50.15
22	Promoters	106	2	57	Ν	8.49	8.48	16.04	11.32
23	Satellite	6435	6	36	N	18.90	12.18	12.29	12.15
24	Segment	2310	7	19	N	11.08	7.01	6.15	$\bf 5.54$
25	Shuttle	58000	7	9	Ν	10.07	5.09	8.06	6.95
26	Solarflare	1389	3	10	Ν	3.89	1.08	1.08	1.87
27	Sonar	208	2	60	N	25.48	25.96	29.33	23.08
28	Soybean	683	19	35	Y	7.17	6.59	10.98	6.44
29	Splice	3177	3	60	Ν	4.66	4.50	4.60	4.41
30	TTT	958	2	9	N	29.54	27.45	26.10	29.54
31	Wine	178	3	13	Ν	3.37	3.37	3.93	2.81
32	Zoology	101	7	16	N	5.94	6.93	4.95	6.93
	Error Mean					17.58	16.93	18.11	16.67

classification accuracy. In order to show the candidate arc set and the structure are different from the basic TAN classifier, we give an example produced by the basic TAN algorithm, the SuperParent algorithm, and our selective augmented Bayesian algorithm on dataset Soybean respectively. The basic TAN algorithm produced a tree with n-1 arcs (n=35), shown in figure 1, where a node which parent is node 0 and has no any child is omitted for simplicity. This tree includes all the attribute nodes. The selective augmented Bayesian algorithm produced eight arcs in four branches, shown in figure 2. The structure of this Bayesian classifier is a forest, where some of arcs belong to the TAN structure,

Table 2. Comparison of Select to others

	WIN	LOSS	DRAW	P
Naive Bayes	19	10	3	0.1360
SuperParent	16	11	5	0.4420
TAN	21	11	0	0.1102

**Table 3.** Time in CPU Seconds

Table 4. Arcs for each algorithm

Domain	SP	TAN	Select	-	Domain	SP	$\overline{TAN}$	Select
1 Anealing	110.31	0.17	13.95	_	1 Anealing	9	27	12
2 Audiology	530.96	1.79	126.38		2 Audiology	6	61	11
3 Breast Cancer	1.20	0.17	0.40		3 Breast Cancer	0	8	1
4 Chess	662.98	1.14	61.81		4 Chess	8	35	17
5 Credit	5.02	0.14	1.35		5 Credit	4	13	7
6 Echocardiogram	0.07	0.03	0.10		6 Echocardiogram	. 0	5	17
7 Glass	0.37	0.11	0.31		7 Glass	3	5	7
8 Heart	0.31	0.11	0.25		8 Heart	0	10	3
9 Hepatitis	2.13	0.11	1.59		9 Hepatitis	2	18	3
10 Horse Colic	6.78	0.13	1.42		10 Horse Colic	4	18	7
11 House Votes	1.51	0.10	1.50		11 House Votes	1	15	3
12 Hypothyroid	130.58	0.25	28.8		12 Hypothyroid	7	24	14
13 Iris	0.07	0.02	0.07		13 Iris	0	3	1
14 Labor	0.09	0.09	0.17		14 Labor	0	10	3
15  LED	1.48	0.07	1.54		15 LED	1	6	4
16 Bupa	0.24	0.06	0.13		16 Bupa	1	2	1
17 Lung Cancer	7.23	0.14	5.56		17 Lung Cancer	2	19	6
18 Lymphography	0.36	0.10	1.52		18 Lymphography	1	17	4
19 PID	1.37	0.12	1.32		19 PID	1	5	1
20 Post Operative	0.10	0.02	0.11	-	20 Post Operative	2	7	3
21 Ptn	2.63	0.11	5.22	-	21 Ptn	0	16	5
22 Promoters	11.75	0.34	10.77	4	22 Promoters	0	56	4
23 Satellite	6247.56	_	269.66	:	23 Satellite	35	35	35
24 Segment	202.69	1.84		:	24 Segment	13	15	17
25 Shuttle	137.68	5.14	79.82	4	25 Shuttle	2	6	8
26 Solarflare	8.85	0.07	2.56	4	26 Solarflare	6	9	8
27 Sonar	165.06	1.88	22.62	:	27 Sonar	3	56	7
28 Soybean	51.59	0.43	51.63		28 Soybean	2	34	8
29 Splice	1090.46		313.44	4	29 Splice	2	59	7
30  TTT	1.07	0.06	0.53	;	30 TTT	1	8	0
31 Wine	0.17	0.13	0.48	;	31 Wine	0	12	2
32 Zoo	1.80	0.09	0.61	;	31 Zoo	2	15	3

but some others do not belong to the TAN structure. This example also shows our selective augmented Bayesian algorithm produces different results from the sTAN method described by Keogh and Pazzani [6]. In the sTAN model, they only select from those edges that appear in the basic TAN tree structure. The

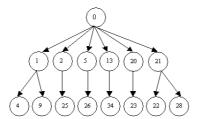


Fig. 1. The Bayesian network of TAN on dataset Soybean

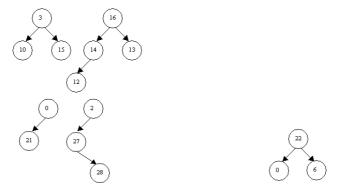


Fig. 2. The Bayesian network of selective augmented TAN on dataset Soybean

**Fig. 3.** The Bayesian network of super parent TAN on dataset Soybean

result of the SuperParent algorithm is shown in figure 3. The SuperParent algorithm only uses leave-one-out cross validation to determine the directions of arcs, but it can not always obtain better performance. For example, on dataset PID, the Bayesian networks built by both the SuperParent algorithm and the selective augmented Bayesian algorithm have only one arc, but the directions are different. The tree structure built by the SuperParent algorithm is only the arc:  $\langle 4,1 \rangle$ , but the selective augmented Bayesian algorithm produces one arc with reverse direction.

#### 6 Conclusion

In this paper we have investigated three issues that affect the quality of TAN classifiers learned from data. The first issue is how to estimate the base probabilities. We conclude that it is important to use a consistent estimation to compare with each other. The second is how to measure dependence relations between two attributes with directions. Based on the definition of dependence degree in the basic rough set theory, we propose a definition of dependence measurement given class variable for building a classification model. Thirdly, we mainly present a selective augmented Bayesian network classifier that reduces error relative to the

original TAN, and with similar computational overheads, but much lower computational overheads than the SuperParent, which is a state-of-the-art variant of the basic TAN classifier. Experimental results show that it can deliver some improvements on performance, while requiring substantially less computation.

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