Tree Kernel Usage in Naïve Bayes Classifiers

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Abstract

We present a novel approach in machine learning by combining naïve Bayes classifiers with tree kernels. Tree kernel methods produce promising results in machine learning tasks containing tree-structured attribute values. These kernel methods are used to compare two tree-structured attribute values recursively. Up to now tree kernels are only used in kernel machines like *Support Vector Machines* or *Perceptrons*.
In this paper, we show that tree kernels can be utilized in a naïve Bayes classifier enabling the classifier to handle tree-structured values. We evaluate our approach on three datasets containing tree-structured values. We show that our approach using tree-structures delivers significantly better results in contrast to approaches using non-structured (flat) features extracted from the tree. Additionally, we show that our approach is significantly faster than comparable kernel machines in several settings which makes it more useful in resource-aware settings like mobile devices.

Naïve Bayes Classifier; Tree Kernel; Lazy Learning; Tree-structured Values

1 Introduction

Naïve Bayes classifiers are well-known machine learning techniques. Based on the Bayes theorem the naïve Bayes classifiers deliver very good results for many machine learning tasks in practical use.
Many machine learning techniques like *Support Vector Machines* (SVMs) or *Decision Trees*, for instance, are suffering from a complex training phase. Naïve Bayes classifiers do not have this disadvantage because the training phase just consists of storing the training data efficiently. In this way a naïve Bayes classifier memorizes the training data by calculating probabilities using the observed values of the training data. Machine learning techniques which memorize the training data instead of creating an optimized decision model are called lazy learners. In contrast to lazy learners like *k-NN*, for instance, naïve Bayes classifiers do not memorize the complete training data. Nevertheless, naïve Bayes classifiers create a condensed set of the training data which is not optimized. Although, naïve Bayes classifiers are not optimized, they deliver good results. Their ability to deliver good results while not needing exhaustive training makes naïve Bayes classifiers to be preferred in resource-aware settings like mobile devices [Fricke *et al.*, 2010; Morik *et al.*, 2010].

Unfortunately, memorizing specially shaped attribute values is not as trivial as it is for numerical or nominal attribute values. Tree-structured values for instance are frequently occurring in natural language processing or document classification tasks. Figure 1 shows a constituent parse tree of a sentence. This structured attribute might be helpful to detect and classify relations in this sentence. But it is not useful to store all trees seen in the training set. On the one hand the storage needs are too high, and on the other hand it is very unlikely that an exactly equal tree occurs in training and test phase.

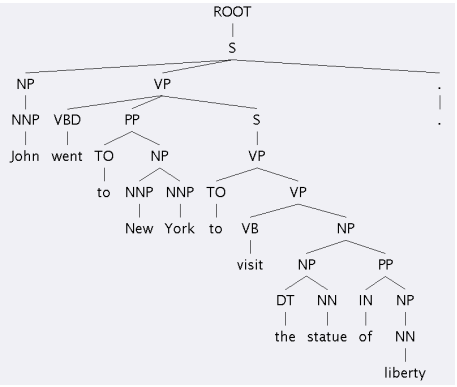


Figure 1: A constituent parse tree

Tree kernels (see Section 3) allow a more flexible calculation of similarities for trees. Current machine learning approaches which respect tree-structured attribute types by using tree kernels are based on kernel machines. Suffering from relatively complex training, these techniques are not useful in resource-aware settings like mobile devices, for instance. Our contribution in this paper is threefold: we show how to embed tree kernels into naïve Bayes classifiers. We present many options to handle the tree kernel values in a naïve Bayes classifier, and we evaluate our tree kernel naïve Bayes approach on three real-world datasets.

We will present already existing related work in this field of research in Section 2. Section 3 describes the handling of tree-structured values by using special kernels in kernel methods. In Section 4 we will show how a naïve Bayes classifier is working. And in Section 5 we will show how to efficiently embed tree kernels in a naïve Bayes classifier. In Section 6 we will demonstrate the experiments we made on three datasets containing tree-structured attribute values. Section 7 sums up our paper.

2 Related Work

To the best of our knowledge tree kernels never have been embedded in naïve Bayes classifiers before. In the following we will show in which domains tree kernels have been used in SVMs to solve many diverse problems.

Tree kernels are very popular in relation extraction [Zhang *et al.*, 2006; Zhou *et al.*, 2007; Nguyen *et al.*, 2009]. Pairs of named entities are representing relation candidates which have to be classified by machine learning techniques. Tree kernels are used in this task to evaluate the parse tree structure spanning the context of both entities in the corresponding sentence. [Bloehdorn and Moschitti, 2007] have used tree kernels for text classification. They tested their approach on question classification and clinical free text analysis. Both are tasks which have formerly mostly been processed by using the bag of word (BOW) representation. BOW is a representation which destroys the structure of the text, and machine learning methods cannot benefit from the structure anymore.

In addition, tree kernels have been used addressing another interesting and currently popular topic: sentiment analysis [Jiang *et al.*, 2010]. Like for relation extraction two entities were used for this approach. The first entity is an opinion and the second entity is a product. The parse tree spanning the context of both entities is used to classify the corresponding pair. [Moschitti and Basili, 2006] used tree kernels for question answering. [Bockermann *et al.*, 2009] used tree kernels to classify *SQL*-requests. The *SQL*-requests were parsed to get an *SQL*-tree which can be used for classifying those requests.

But SVMs are not the only machine learning technique tree kernels were used in. [Aiolli *et al.*, 2007] showed that tree kernels can be efficiently embedded into perceptrons which can be used for online-learning.

3 Tree Kernels

Tree kernels are creating a mapping of examples into a tree kernel space providing a kernel function to compute the inner product of two tree elements. Tree kernels offer some sort of distance measure for trees delivering a real valued output given two trees. The usage of tree kernel methods delivers best results in classification tasks offering tree-structured values like relational learning [Zhou *et al.*, 2007; Zhang *et al.*, 2006].

The work of [Zhou *et al.*, 2007; Zhang *et al.*, 2006] is based on the convolution kernel presented by [Haussler, 1999] for discrete structures. To make the structural information of a parse tree applicable by a machine learning technique a kernel for the comparison of two parse trees is used. This kernel compares two parse trees and delivers a real-valued number which can be used by machine learning techniques. [Collins and Duffy, 2001] define a treekernel as written in eq. (1), where T_1 and T_2 are trees. N_1 and N_2 are the amounts of nodes of T_1 and T_2. Each node n of a tree is the root of a (smaller) subtree of the original tree. $I_{subtree_i}(n)$ is an indicator-function that returns 1 if the root of subtree i is at node n. $\mathcal{F}$ is the amount of all subtrees which are apparent in the trees of the training data.

$$K(T_1, T_2) = \sum_{n_1 \in N_1} \sum_{n_2 \in N_2} \sum_{i}^{|\mathcal{F}|} I_{subtree_i}(n_1) I_{subtree_i}(n_2) \quad (1)$$

$$= \sum_{n_1 \in N_1} \sum_{n_2 \in N_2} C(n_1, n_2) \quad (2)$$

Creating the amount $\mathcal{F}$ is very complex. The question arises, if the computation of the eq. 1 could be done more efficiently. Instead of summing over the complete amount of subtrees $\mathcal{F}$ $C(n_1, n_2)$ is used in eq. 2. $C(n_1, n_2)$ represents the number of common subtrees at node n_1 and n_2. The number of common subtrees finally represents a syntactic similarity measure and can be calculated recursively starting at the leaf nodes in $\mathcal{O}(|N_1||N_2|)$. Summing over both trees ends up in a runtime of $\mathcal{O}((|N_1||N_2|)^2)$.

During this recursive calculation three cases are being respected:

1. If the productions at n_1 and n_2 are different, $C(n_1, n_2) = 0$
2. If the productions at n_1 and n_2 are the same and if n_1 and n_2 are preterminals, $C(n_1, n_2) = 1$
3. Else if the productions at n_1 and n_2 are the same and if n_1 and n_2 are not preterminals, $C(n_1, n_2) = \prod_j (\sigma + C(n_{1_j}, n_{2_j}))$, where n_{1_j} is the j-th children of n_1 (in a uniform manner for n_2) and $\sigma \in \{1, 0\}$.

The σ-value is used to switch between the subset tree kernel (SST) [Collins and Duffy, 2001; **?**] and the subtree kernel (ST) [Vishwanathan and Smola, 2002; **?**]. By using $\sigma = 1$ the SST is calculated, whereas for $\sigma = 0$ the ST is calculated. Trees containing few nodes by definition only result in small kernel-outputs. In contrast, larger trees can achieve larger kernel-outputs. To avoid this bias, [Collins and Duffy, 2001] established a scaling factor $0 < \lambda \leq 1$ which is used in two of the three cases for the kernel calculation:

2. If the productions at n_1 and n_2 are the same and if n_1 and n_2 are preterminals, $C(n_1, n_2) = \lambda$
3. Else if the productions at n_1 and n_2 are the same and if n_1 and n_2 are not preterminals, $C(n_1, n_2) = \lambda \left(\prod_j (\sigma + C(n_{1_j}, n_{2_j})) \right)$.

4 Naïve Bayes Classifier

The naïve Bayes classifier (NBC) [Hastie *et al.*, 2003] assigns labels $y \in Y$ to examples $\mathbf{x} \in X$. Each example is a vector of m attributes written here as x_i, where $i \in \{1, ..., m\}$. The probability of a label given an example according to the Bayes Theorem is shown in eq. (4). Domingos and Pazzani [Domingos and Pazzani, 1996] rewrite eq. (4) by assuming that the attributes are independent given the category (Bayes assumption). They define the *Simple Bayes Classifier* (SBC) shown in eq. (5). The classifier delivers the most probable class $y \in Y$ for a given example $\mathbf{x} = x_1, \ldots, x_m$, formally described in eq. (5).

$$p(y|x_1, ..., x_m) = \frac{p(y)p(x_1, ..., x_m|y)}{p(x_1, ..., x_m)} \quad (3)$$

$$p(y|x_1, ..., x_m) = \frac{p(y)}{p(x_1, ..., x_m)} \prod_{j=1}^{m} p(x_j|y) \quad (4)$$

$$\arg\max_y p(y|x_1, ..., x_m) = \frac{p(y)}{p(x_1, ..., x_m)} \prod_{j=1}^{m} p(x_j|y) \quad (5)$$

The term $p(x_1, ..., x_m)$ can be neglected in eq. (5) because it is a constant for every class $y \in Y$. The decision for the most probable class y for a given example $\mathbf{x}$ just depends on $p(y)$ and $p(x_i|y)$ for $i \in \{1, \ldots, m\}$. One is using the expected values for the probabilities calculated on the training data. The values can be calculated after one run on the training data. The training runtime is $\mathcal{O}(n)$, where n is the number of examples in the training set. The number of probabilities to be stored during

training are $|Y| + \left(\sum_{j=1}^{m} |X_j||Y|\right)$ for nominal attributes, where $|Y|$ is the number of classes and $|X_j|$ is the number of different values of the jth attribute. If the attributes are numerical, just a value for mean and standard deviation have to be stored resulting in $\mathcal{O}(m|Y|)$ probabilities.

Most implementations of naïve Bayes classifiers deliver the class y which results in the greatest outcome for eq. (5) for a given example $\mathbf{x}$. It is not stringently required to use values between 0 and 1. This becomes important in Section 5.3. It has often been shown that SBC or NBC perform quite well for many data mining tasks [Domingos and Pazzani, 1996; Huang *et al.*, 2003].

5 Tree Kernel Naïve Bayes Classifier

In Section 4 it became clear that the important parameters for the naïve Bayes classifier are $p(y)$ and $p(x_i|y)$. $p(y)$ is not affected by attribute-values and therefore is not affected by tree-structured attributes, too. $p(x_i|y)$ is the crucial parameter which should be regarded in the following. We distinguish three types of attribute value types: nominal, numerical and tree-structured value types.

For nominal attribute value types x_i, $p(x_i|y)$ is calculated by simply counting the occurrences of the particular values of x_i for each class $y \in Y$. For numerical attribute value types x_i, the mean (μ_i) and the standard-deviation (σ_i) of the attribute are used to calculate the probability density function for every class $y \in Y$ as seen in eq. (6). A Gaussian normal distribution is expected, here.

$$p(x_i|y) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{-\frac{1}{2}\left(\frac{x_i-\mu_i}{\sigma_i}\right)^2} \tag{6}$$

The calculation of the probability for tree-structured attribute values is not that trivial. A simple approach would be just to store each unique tree-structured value and count its occurrences like for nominal attributes. But this approach is not promising as it is too coarse. It is not very probable that many examples are containing exactly the same tree-structured value. We are presenting a more flexible approach which uses tree kernels for the calculation of the conditional probabilities $p(x_i|y)$ for tree-structured attribute values:

If an attribute x_i is tree-structured the tree kernel-value v_y for class y is calculated by applying a tree kernel on x_i and on every tree-structure x_j been seen in the training-set S together with class y as shown in eq. (7).

$$v_y = f_y(x_i) = \sum_{x_j \in \mathbf{x}' | (\mathbf{x}', y') \in S, y' = y} K(x_i, x_j) \tag{7}$$

This value could be used like every numerical value (see Section 5.2). To calculate this sum of kernel calculations all the tree-structures which have been seen in the training set have to be taken into account. But storing every tree-structure ever seen in the training-phase on its own in a list for instance has two major drawbacks: The storage needs and the numbers of kernel calculations are very high. To lower the storage needs and the number of kernel-calculations we use the approach presented by [Aiolli *et al.*, 2007] to store all tree-structured values in a compressed manner.

5.1 Efficient tree access

A minimal directed acyclic graph (DAG) containing a minimal number of vertices is used to store all the tree-structures, having seen in the training set for a particular attribute and class, together. This leads to an amount of $|Y|$ DAGs, where $|Y|$ is the number of classes. The DAG $G = (V, E)$ contains a set of vertices V consisting of a *label* on the one hand and a *frequency* value on the other hand. And the DAG contains a set of directed edges E connecting some of the vertices.

Figure 2 shows three trees which might occur during training for a specific class. A DAG containing all information being existent in these trees is shown in Figure 3. The algorithm to create a minimal DAG out of multiple trees is given in Algorithm **??**. This algorithm converts ev-

Algorithm 1 Creating a minimal DAG out of a forest of trees by [Aiolli *et al.*, 2007]

procedure CREATE MINIMAL DAG(A TREE FOREST $F = x_{i_1}, ..., x_{i_n}$)
  Initialize an empty DAG D
  for $int\ j = 1; j <= n; j++$ **do**
    vertex_list $\leftarrow$ invTopOrder(x_{i_j})
    for all $v \in$vertex_list **do**
      if $\exists u \in D | dag(u) \equiv dag(v)$ **then**
        $f(u) += f(v)$
      else
        add node w to D with $l(w) = l(v)$ and $f(w) = f(v)$
        for all $ch_i[v]$ **do**
          add arc (w, c_i) to D where $c_i \in$ Nodes(D)
          and $dag(c_i) \equiv dag(ch_i[v])$
        end for
      end if
    end for
  end for
  Return D
end procedure

ery tree into its inverse topological ordered list of vertices. The first elements of the list are vertices with zero outdegree. After that vertices containing at most children with zero outdegree are contained in the list, and so on. The vertices are formally sorted in ascending order by the length of the longest path from each vertex to a leaf. The tree shown in Figure 2 a) becomes list $\{D, E, F, B, C, A\}$, the tree shown in Figure 2 b) becomes $\{D, E, B, F, A\}$, and finally, the tree shown in Figure 2 c) becomes $\{B, F, A\}$.

After that, the lists are processed and for every vertex it will be checked if it is already existent in the DAG or if it is not. The formalism $dag(u) \equiv dag(v)$ checks wether the DAG rooted at vertex u is equivalent to the DAG rooted at vertex v. If a particular (sub-) DAG already is available in the DAG the frequency of the corresponding root node in the DAG is raised by the frequency of the vertex to be inserted. Otherwise, a node containing *label* and *frequency* of the vertex is created in the DAG. After that all the corresponding children of the new node are connected by edges. The fact, that the vertices of the trees are sorted is very important because it is guaranteed that the children of a newly created node are already present in a DAG (if the created node has any). Using this DAG to store all tree-structured values avoids the calculation of a sum of kernel-calculations. One kernel value v_y now is calculated for each class resulting in just $|Y|$ kernel calculations: $v_y = f_y(x_i) = K(x_i, D_y)$

A DAG is handled like a tree in the tree kernel calculation (see Section 3). There is just one difference: instead of

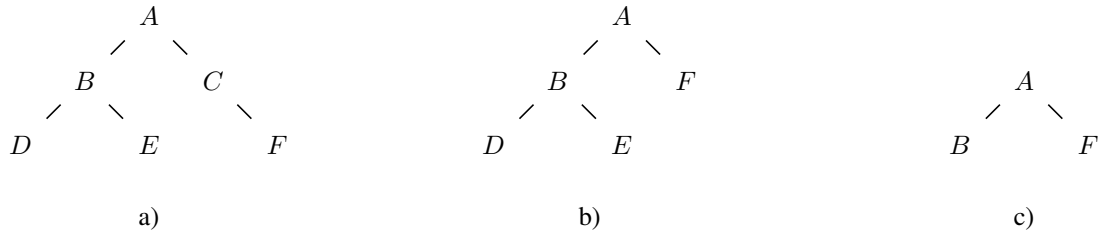


Figure 2: Three tree-structures

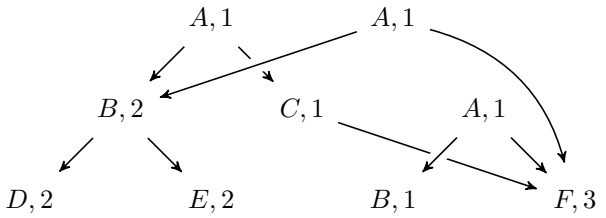


Figure 3: A DAG containing the information given by the tree-structures shown in Fig. 2

calculating $C(n_1, n_2)$ we calculate $C'(n_1, n_2)$, where n_2 is a vertex of a DAG.

1. If the productions at n_1 and n_2 are different, $C'(n_1, n_2) = 0$
2. If the productions at n_1 and n_2 are the same and if n_1 and n_2 are preterminals, $C'(n_1, n_2) = \lambda$
3. Else if the productions at n_1 and n_2 are the same and if n_1 and n_2 are not preterminals, $C'(n_1, n_2) = \lambda \left(\prod_j (\sigma + \text{freq}_{n_2} \left(C(n_{1_j}, n_{2_j}) \right) \right)$.

$C(n_{1_j}, n_{2_j})$ in the last item of the enumeration, again, is the recursive calculation of $C(n_{1_j}, n_{2_j})$ as already used in Section 3. Our approach is different from the one presented by [Aiolli *et al.*, 2007] because they used the DAG representation inside of a perceptron. The perceptron is a binary machine learning method and therefore cannot be used for multi-class problems, easily. Our approach is directly usable for multi-class problems. [Aiolli *et al.*, 2007] are using just one DAG in a binary setting. The trees of the negative class are put into the DAG using a negative frequency, and trees of the positive class are put into the DAG using a positive frequency. This makes the DAG decide wether an example is of the negative class or of the positive class. Our approach would use two DAGs in a binary setting.

5.2 Calculation of probabilities using kernel-values

Tree kernel values are real-valued. The question arises if these values can be used like every other numerical attribute value for the calculation of the conditional probabilities in the naïve Bayes classifier. Eq. (6) shows the calculation of the probability for an attribute value x_i given a particular class $y \in Y$ by using the mean and the standard deviation of the attribute in the training dataset. Using this approach for tree kernel values has a certain shortcoming. Unfortunately, to calculate the mean and standard deviation of the tree kernel values during training, it is necessary to calculate the kernel values for each example in the training set using the DAG which is used during the prediction phase, too. This means that our approach has to perform one run over the training set previously, to create all minimal DAGs. After that, another run over the training set is needed to calculate the kernel values on the training set which are needed to calculate mean and standard deviation. We will evaluate if it is useful to handle tree kernel outcomes like numerical attribute values in this context.

Algorithm 2 Tree kernel naïve Bayes classifier prediction

```
1: procedure TREE KERNEL NAÏVE BAYES PREDICTION( x )
2:     for all x_i ∈ x do
3:         for all possible y ∈ Y do
4:             if x_i is numerical or nominal then
5:                 calculate probabilities p(x_i|y)
6:             else
7:                 if x_i is tree-structured then
8:                     calculate tree kernel-value v_y = f_y(x_i) = K(x_i, D_y)
9:                     calculate the probability p(x_i|y) using v_y
10:                end if
11:            end if
12:        end for
13:    end for
14:    deliver arg max_y p(y) ∏_{j=1}^{m} p(x_j|y)
15: end procedure
```

5.3 Pseudo-probabilities using kernel-values

Algorithm 2 shows our approach of a tree kernel naïve Bayes classifier after being trained. Line 9 has to be replaced by Eq. (6) in order to calculate the probability by expecting a Gaussian normal distribution. The calculation of the mean and standard deviation of the tree kernel-values is very time consuming because the tree kernel has to be applied on every example of the training set with each DAG. This results in $n|Y|$ kernel calculations, where n is the number of examples in the training set. We try to overcome this computational complexity by not calculating the mean and standard deviation of the tree-structured values. We are using various normalization methods to create pseudo-probabilities which are used like probabilities in case of predictions in the classifier, directly. These values are not between 0 and 1, of necessity. We are replacing the calculation of the probability in line 9 of Algorithm 2 by various normalization methods. In this paper, we present six normalization methods which are finally evaluated on three real-world datasets:

none: The calculated tree kernel value v_y is used directly as a probability

$$p(x_i|y) = v_y$$

normalize by DAG frequency: The calculated tree kernel value v_y is normalized by the sum of all frequencies contained in the DAG D_y for class y

$$p(x_i|y) = \frac{v_y}{freq_{D_y}}$$

normalize by tree number: The calculated tree kernel value v_y is normalized by the number of trees contained in the DAG D_y for class y

$$p(x_i|y) = \frac{v_y}{trees_{D_y}}$$

normalize by maximum: The calculated tree kernel value v_y is normalized by the maximum value calculated on the training set by the DAG D_y for class y

$$p(x_i|y) = \frac{v_y}{max\{v_y^j | j \in \{1, \ldots, |S|\}\}}$$

normalize by all: The calculated tree kernel value v_y is normalized by the sum of the values calculated on the training set by the DAG D_y for class y

$$p(x_i|y) = \frac{v_y}{\sum_{j=1}^{|S|} v_y^j}$$

normalize by treesize: The calculated tree kernel value v_y is normalized by the fraction of DAG frequency and tree number for class y

$$p(x_i|y) = \frac{v_y}{\left(\frac{freq_{D_y}}{trees_{D_y}}\right)}$$

normalize by example number: The calculated tree kernel value v_y is normalized by the number of examples given for the particular class

$$p(x_i|y) = \frac{v_y}{|\{(\mathbf{x}', y') \in S | y' = y\}|}$$

6 Experiments

In the following we evaluated our method on three real-world datasets containing tree-structured values. We implemented the presented naïve Bayes tree kernel approach for the opensource datamining toolbox *RapidMiner* [Mierswa *et al.*, 2006]. The state-of-the-art and mostly used implementation of tree kernels in SVMs is the tree kernel implementation of Moschitti[1] which is using the SVM^{light}-implementation of Joachims [Joachims, 1999]. To show the competitiveness of our approach, we compared the runtime of our approach with the runtime of the tree kernel implementation of Moschitti. The runtime presented in Table 1 is measured for a ten-fold cross-validation over the complete dataset. Table 2 contains measured values for a five-fold cross-validation on a 10% sample of the dataset. Although, the tree kernel naïve Bayes approach is faster the true gain in case of runtime can not be evaluated because our approach is implemented in *Java* and the SVM^{light} is implemented in C.

6.1 Syskill and Webert Web Page Ratings

The first dataset *Syskill and Webert Web Page Ratings* (SW) is available at the UCI machine learning repository [Frank and Asuncion, 2011]. The dataset originally was used to learn user preferences. It contains websites of four domains, and user ratings on the particular websites are given. We will just focus on the classification of the four domains. We parsed the websites for the construction of a tree-structured attribute value for each website by using a *html*-parser[2]. Unfortunately, the leafs of the resulting *html*-tree contain huge text fragments in some extent. We converted every leaf which contains text into a leaf containing just the word *'leaf'* have only structured information. Unfortunately, the trees still were too huge to be processed by the tree kernel implementation of Moschitti which is restricted to smaller trees in the origin implementation. An analysis of the trees showed that many equally shaped subtrees are contained many times in the trees. We pruned the trees by a very trivial heuristic which just deletes equally shaped subtrees in the trees. A tree which is processed in this way just contains unique subtrees. Using this heuristic shortens the trees making them applicable by the tree kernel implementation of Moschitti.

To compare our approach to traditional naïve Bayes classifiers we converted the string representation[3] of the trees into its BOW representation containing the corresponding *TF-IDF* values. We split the string representation by using spaces and brackets for splitting. In addition, we used the two-grams of this splitted representation as features. This preprocessing finally resulted in 445 attributes including the tree containing attribute. The dataset contains 341 examples of four classes. 136 examples belong to class *BioMedical*, 61 to class *Bands*, 64 to class *Goats* and finally, 70 examples belong to class *Sheep*.

We made a grid-parameter-optimization just by using the tree containing attribute to analyze the best parameter-setting for the tree kernel naïve Bayes approach. We used all seven possible normalization methods. We used σ-values of 0 and 1. We used 21 different λ-values between 0.1 and 10^7, and in half of the settings we handled the kernel values like numerical values expecting a Gaussian normal distribution. On the other half of the settings we expected no gaussian normal distribution and used the (normalized) values directly. This setup results in 588 individual experiment-settings. Each of this setting is evaluated by a ten-fold cross validation. Figure 4 shows the visualization of four of the seven normalization methods. The plots of the missing normalizations are comparable to the plots of Figure 4 a) and c) and they are missing because of space limitations.

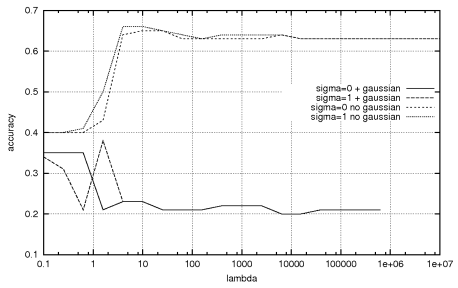
The original tree kernel is restricted to λ-values of $0 < \lambda \leq 1$. But for the tree kernel naïve Bayes approach λ-values greater than 1 are delivering the best results. Another interesting fact is that using the kernel values directly as probabilities – without expecting a normal Gaussian distribution and without normalization – nearly delivers the best results. This is remarkable because expecting a normal Gaussian distribution means to calculate the mean and standard deviation after the construction of the DAGs. Not calculating the mean and standard deviation for the training set results in a more ordinary calculation and finally a better runtime (see Table **??**).

It is remarkable that using tree kernel values like numerical attributes by expecting a Gaussian normal distribution

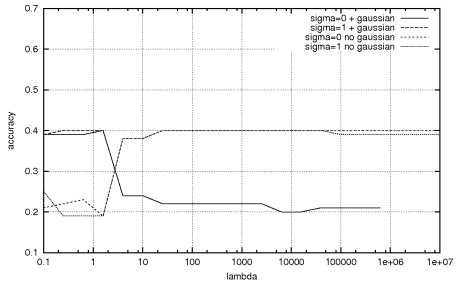
[1] `http://disi.unitn.it/moschitti/Tree-Kernel.htm`

[2] `http://htmlparser.sourceforge.net`

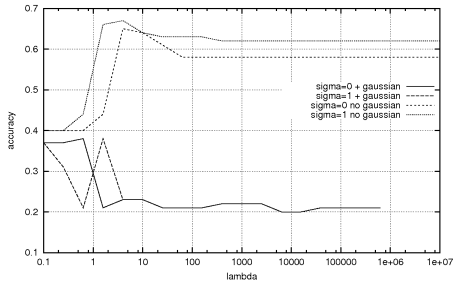
[3] The string representation of the tree shown in Figure 1 is: *(ROOT (S (NP (NNP John)) (VP (VBD went) (PP (TO to) (NP (NNP New) (NNP York))) (S (VP (TO to) (VP (VB visit) (NP (NP (DT the) (NN statue)) (PP (IN of) (NP (NN liberty))))))))) (. .)))*



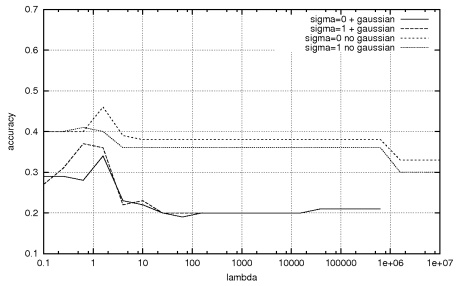
a) No normalization



b) Normalize by maximum



c) Normalize by DAG frequency



d) Normalize by all

Figure 4: Optimization experiments for SW

achieves the worst performance. A reason for this could be outliers contained in the training data. If a tree-structured value contained in the training data delivers a huge tree kernel output the mean and standard deviation might not be correct for later use. Unfortunately, finding outliers in tree-structured attributes is not trivial as first of all, the DAGs have to be constructed. After that all kernel-values have to be calculated. If there are any outliers found, they have to be removed from the DAGs, or the DAGs have to be reconstructed. This is a topic for future work. Another argument for outliers to be contained in the training data is visible in Figure 4 b) and d). It delivers bad results to normalize the tree kernel outcome using the maximum and the sum of the kernel outcomes of the training phase. Outliers could create huge kernel-outcomes which cannot be used for normalization during prediction. We extracted the best parameter setting for the tree kernel naïve Bayes approach using the tree and the BOW features together, too. After that we used the best settings to evaluate the performance of our approach. Table 1 shows the performances (and the standard deviation) concerning accuracy, recall and precision. Those values have been evaluated using a loop of 100 ten-fold cross-validations for the naïve Bayes and tree kernel naïve Bayes approaches. The tree kernel SVM just were evaluated on a ten-fold cross-validation. The results presented for the tree kernel SVM are not statistically significant because we just made one ten-fold cross-validation. But the results show that our naïve Bayes tree kernel approach delivers comparable performance in combination with much shorter runtime, at least.

Using an analysis of variance (ANOVA) test it becomes apparent that using the tree kernel naïve Bayes approach on tree-structured values delivers significantly better results in cases of accuracy and precision than a naïve Bayes approach using no tree-structured values. Using the tree kernel naïve Bayes approach on tree-structured and BOW features delivers slightly better results in cases of accuracy, again.

6.2 SQL

[Bockermann *et al.*, 2009] presented a dataset for intrusion detection. The dataset contains SQL-requests which are parsed to get tree-structured values. The requests are classified as normal request and attack. The relevant class in this binary dataset is relatively rare. The dataset is containing just 15 attacks on 1000 requests. Again, we used the tree-structured attribute and the one- and two-grams of the string representation of the trees resulting in 1695 attributes. [Bockermann *et al.*, 2009] used an SVM with a tree kernel to detect the attacks. To optimize the parameters for our tree kernel naïve Bayes approach, we used the same setting as already described for the SW dataset. The best performance is achieved by using no normalization and some other normalizations achieving 99.2% accuracy. A default learner which just predicts the majority class would achieve 98.5% accuracy. Like for the *Syskill and Webert Web Page Ratings* dataset the normalization methods using the sum or the maximum of the outcome been seen during training are not flexible enough, to achieve good results. They never perform better than the default learner. The remaining normalization methods do not perform better than no normalization. Additionally, the results and the runtime are bad if we are expecting a Gaussian normal distribution on the values calculated on the training set and using this for calculation of the probabilities during prediction.

Table 1 shows the results using the best parameter setting. Using the tree kernel naïve Bayes approach compared to a naïve Bayes approach using no tree-structured values delivers significantly better results in cases of precision and accuracy. All experiments using naïve Bayes approaches were evaluated using a loop of 100 ten-fold cross-validations and calculating the average. The results of the tree kernel SVM are of one ten-fold cross-validation. An interesting fact is that using a tree kernel SVM on the tree-structured values and BOW ends up in shorter runtime than using a tree kernel SVM alone. We suggest that the combination of tree and BOW features results in faster convergence, internally. Using our approach on this dataset delivers better results for all performance measures compared to using a SVM. Especially, the shorter runtime is remarkable.

Method	Accuracy	Recall	Precision	Time (in s)
SW				
Baseline (majority vote)	39.9%	25.0%	10.0%	
Naïve Bayes on BOW	$60.9 \pm 1.5\%$	$63.3 \pm 1.0\%$	$64.2 \pm 0.9\%$	0.2
Tree Kernel Naïve Bayes	$66.5 \pm 0.8\%$	$63.0 \pm 0.8\%$	$70.8 \pm 1.3\%$	1.81
(+ Gaussian)				2.73
Tree Kernel Naïve Bayes & BOW	$66.7 \pm 0.8\%$	$64.2 \pm 0.8\%$	$67.2 \pm 1.4\%$	1.98
Tree Kernel SVM	$60.4 \pm 5.8\%$	$55.7 \pm 5.5\%$	$59.1 \pm 11.7\%$	34
Tree Kernel SVM & BOW	$\mathbf{71.5 \pm 7.3\%}$	$\mathbf{66.7 \pm 8.3\%}$	$\mathbf{72.2 \pm 14.0\%}$	51
SQL				
Baseline (majority vote)	98.5%	50.0%	49.3%	
Naïve Bayes on BOW	$96.6 \pm 0.2\%$	$\mathbf{81.0 \pm 2.2\%}$	$62.3 \pm 1.0\%$	3.12
Tree Kernel Naïve Bayes	$\mathbf{99.3 \pm 0.1\%}$	$79.6 \pm 1.2\%$	$\mathbf{94.3 \pm 1.9\%}$	72.2
(+ Gaussian)				612
Tree Kernel Naïve Bayes & BOW	$96.6 \pm 0.2\%$	$64.9 \pm 4.4\%$	$25.1 \pm 1.9\%$	74.7
Tree Kernel SVM	$98.5 \pm 0.5\%$	$50.0 \pm 0.0\%$	$49.3 \pm 0.3\%$	138
Tree Kernel SVM & BOW	$98.8 \pm 0.8\%$	$62.5 \pm 20.2\%$	$64.4 \pm 23.2\%$	110

Table 1: Results of various machine learning approaches on SW and SQL

Combining the tree-structured values with the BOW features using our tree kernel naïve Bayes approach delivers results which are worse than using the BOW or the tree-structured features exclusively. Developing a smoother combination of both probability distributions inside of the naïve Bayes classifier might overcome this problem.

6.3 ACE 2004

The shared task of the Automatic Content Extraction conference 2004 offered one of the first tasks for relational learning [Lin, 2004]. The dataset contains seven types of relations and one irrelevant (negative) class. The dataset consists of more than 50000 examples of which less than 10% belong to one of the seven relation types. Because of the long runtime seen in Table 2 we extracted a sample of 10% of the dataset to evaluate the best parameter setting. We evaluated the best experiment setting and the performance of the tested methods on that sample like we did for the SW and SQL datasets. To calculate the values for precision and recall, we calculated the average values of the certain values for each of the seven (positive) classes. These seven classes are the relevant ones. The values for precision and recall for the negative examples are good just because of the amount of negative examples. The performance values of the naïve Bayes approaches are evaluated using a loop of 100 five-fold cross-validations. [Zhou *et al.*, 2005] presented many features which can be extracted out of tree-structured values for relational learning. These features are nominal or numerical ones and can be used by machine learning methods which cannot handle tree-structured values. We used the features presented by [Zhou *et al.*, 2005] in several settings shown in Table 2. Again, the tree kernel SVM is a little bit faster if it is applied on a tree-structured attribute together with non-tree-structured attributes. Nevertheless, the tree kernel SVM is much slower than our tree kernel naïve Bayes approach. Although, the results for the tree kernel SVM are not significant the results achieved by the tree kernel naïve Bayes approach are comparable. Using the tree-structured attributes in contrast to just using the features presented by [Zhou *et al.*, 2005] (Zhou-features) results in significantly better results in cases of precision and accuracy. In contrast to the other two datasets we evaluated the f-score, too. The f-score is the harmonic mean of precision and recall and the best result is achieved by the tree kernel naïve Bayes approach together with the Zhou-features.

7 Conclusion and future work

We presented the novel tree kernel naïve Bayes approach which is a naïve Bayes classifier being able to process tree-structured attribute-values. We present the possibilities in handling these attribute values which are absolutely different from traditional attribute value types (nominal and numerical) handled by naïve Bayes classifiers. To memorize the training data we are using directed acyclic graphs which efficiently store the trees apparent in the training set for each class. Different types of handling the tree kernel values are analyzed. Exhaustive experiments on three real-world datasets show that our tree kernel naïve Bayes approach delivers good results, although it is a lazy learning method which is not optimized. We have shown that our tree kernel approach can be an efficient and fast alternative to tree kernels embedded in kernel machines. Possible future work is the detection of outliers in tree-structured attribute values. In addition, the creation of the DAGs could be done more efficiently. Furthermore, the DAGs are still very complex for special datasets. The question arises if it is possible to just use the relevant pieces of a tree for the creation of the DAGs. For the SQL dataset the combination of tree-structured values and the BOW features deliver worse results. Another topic for future work could be to combine the probability values delivered by tree-structured and flat features even smoother.

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Method	**Accuracy**	**Recall**	**Precision**	**F-measure**	**Time** (in s)
Baseline (majority vote)	91.5%	0.0%	0.0%	nan	
NB on Zhou-features	$79.0 \pm 0.2\%$	$\mathbf{56.2 \pm 2.0}\%$	$18.1 \pm 0.6\%$	27.4%	0.07
TKNB	$91.0 \pm 0.2\%$	$15.3 \pm 1.4\%$	$\mathbf{29.7 \pm 2.6}\%$	20.2%	320
(+ Gaussian)					1400
TKNB & Zhou-features	$86.8 \pm 0.3\%$	$48.3 \pm 1.9\%$	$25.7 \pm 1.0\%$	$\mathbf{33.5}\%$	320
TKSVM	$92.5 \pm 0.3\%$	$4.0 \pm 3.8\%$	$13.5 \pm 10.2\%$	6.2%	620
TKSVM & Zhou-features	$\mathbf{93.3 \pm 0.3}\%$	$12.6 \pm 6.8\%$	$27.7 \pm 16.9\%$	17.3%	585

Table 2: Results of various approaches on ACE (the runtime values are rounded (NB = Naïve Bayes, TKNB = Tree Kernel naïve Bayes, TKSVM = Tree Kernel SVM))

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