Combining Predictions under Uncertainty: The Case of Random Decision Trees

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Abstract. A common approach to aggregate classification estimates in an ensemble of decision trees is to either use voting or to average the probabilities for each class. The latter takes uncertainty into account, but not the reliability of the uncertainty estimates (so to say, the “uncertainty about the uncertainty”). More generally, much remains unknown about how to best combine probabilistic estimates from multiple sources. In this paper, we investigate a number of alternative prediction methods. Our methods are inspired by the theories of probability, belief functions and reliable classification, as well as a principle that we call evidence accumulation. Our experiments on a variety of data sets are based on random decision trees which guarantees a high diversity in the predictions to be combined. Somewhat unexpectedly, we found that taking the average over the probabilities is actually hard to beat. However, evidence accumulation showed consistently better results on all but very small leaves.

Keywords: Random Decision Trees · Ensembles of Trees · Aggregation · Uncertainty.

1 Introduction

Ensemble techniques, such as bagging or boosting, are popular tools to improve the predictive performance of classification algorithms due to diversification and stabilization of predictions [5]. Beside learning the ensemble, a particular challenge is to combine the estimates of the single learners during prediction. The conventional approaches for aggregation are to follow the majority vote or to compute the average probability for each class. More sophisticated approaches are to use classifier fusion [14], stacking [18] or mixture of experts [19]. Most of these approaches mainly aim to identify strong learners in the ensemble, to give them a higher weight during aggregation. However, this ignores the possibility that the predictive performance of each learner in the ensemble may vary depending on the instance to be classified at hand. To take these differences into account, we argue that considering the certainty and uncertainty of each individual prediction might be a better strategy to appropriately combine the estimates.
This should be particularly the case for ensembles generated using randomization techniques since this potentially leads to many unstable estimates.

A popular and effective strategy is to randomize decision trees. The prediction of a single decision tree is usually based on statistics associated with the leaf node to which a test instance is forwarded. A straightforward way of assessing the reliability of a leaf node’s estimate is to consider the number of instances which have been assigned to the node during learning. For example, imagine a leaf containing 4 instances of class A and 0 of B, and another leaf with 10 instances in class A and 40 in class B. The first source of prediction has considerably less evidence to support its prediction in contrast to the second leaf. If both leaves need to be combined during prediction, it seems natural to put more trust on the second leaf and, therefore, one may argue that class B should be preferred though the average probability of 0.6 for A tells us the opposite. However, one may argue for A also for another reason, namely the very high confidence in the prediction for A, or put differently, the absence of uncertainty in the rejection of B. The certainty of the prediction is also known as commitment in the theory of belief functions. In this work, we will review and propose techniques which are grounded in different theories on modelling uncertainty and hence take the support and strength of evidence differently into account.

More specifically, Shaker and Hülkermeier [16] introduced a formal framework which translates observed counts as encountered in decision trees into a vector of plausibility scores for the binary classes, which we use for the prediction, and scores for aleatoric and epistemic uncertainty. While aleatoric uncertainty captures the randomness inherent in the sample, the latter captures the uncertainty with regard to the lack of evidence. The theory of belief functions [15] contributes two well-founded approaches to our study in order to combine these uncertainties. In contrast to the theory of belief functions, in probability theory the uncertainty is usually expressed by the dispersion of the fitted distribution. We introduce a technique which takes advantage of the change of the shape of the distribution in dependence of the sample size. And finally, apart from combining the probabilities themselves, one can argue that evidence for a particular class label should be properly accumulated, rather than averaged across the many members of the ensemble. In this technique, we measure the strength of the evidence by how much the probabilities deviate from the prior probability.

As an appropriate test bed for combining uncertain predictions, we choose to analyse these methods based on random decision trees (RDT) [6]. In contrast to other decision tree ensemble learners, such as random forest, RDT do not optimize any objective function during learning, which results in a large diversity of class distributions in the leaves. This puts the proposed methods specifically to the test in view of the goal of the investigation and makes the experimental study independent of further decisions such as the proper selection of the splitting criterion. We have compared the proposed techniques on 21 standard binary classification data sets. Surprisingly, our experimental evaluation showed that methods, which take the amount of evidence into consideration, did only improve over the simple averaging baseline in some specific cases. However, we could
observe an advantage for the proposed approach of evidence accumulation which takes the strength of the evidences into account.

2 Preliminaries

This section briefly introduces RDT, followed by a short discussion on previous work which is relevant to us. Throughout the paper, we put our focus on binary classification which is the task of learning a mapping $f : \mathcal{X}^m \rightarrow y$ between an instance $x \in \mathcal{X}^m$ with $m$ numerical and/or nominal features and a binary class label $y \in \{\ominus, \oplus\}$ through a finite set of observations $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

2.1 Random Decision Trees

Introduced by Fan et al. [6], the approach of RDT is an ensemble of randomly created decision trees which, in contrast to classical decision tree learners and random forest [2], do not optimize a objective function during training. More precisely, the inner tests in the trees are chosen randomly which reduces the computational complexity but still achieves competitive and robust performance.

Construction. Starting from the root node, inner nodes of a single random tree are constructed recursively by distributing the training instances according to the randomly chosen test at the inner node as long as the stopping criterion of a minimum number of instances for a leaf is not fulfilled. Discrete features are chosen without replacement for the tests in contrast to continuous features, for which additionally a randomly picked instance determines the threshold. In case that no further tests can be created, a leaf will be constructed in which information about the assigned instances will be collected. For binary classification, the number of positive $w_\oplus$ and negative $w_\ominus$ class labels are extracted. Hence, a particular leaf can be denoted as $\mathbf{w} = [w_\oplus, w_\ominus]$ where $\mathbf{w} \in \mathcal{W}$ and $\mathcal{W} = \mathbb{N}^2$.

Prediction. For each of the $K$ random trees in the ensemble, the instance to be classified is forwarded from the root to a leaf node passing the respective tests in the inner nodes. The standard approach mainly used in the literature to aggregate the assigned leaf nodes $\mathbf{w}_1, \ldots, \mathbf{w}_K$ is to first compute the probability for the positive class on each leaf which is then averaged across the ensemble.

2.2 Related Work

A very well known approach used for improving the probability estimates of decision trees is Laplace smoothing, which essentially incorporates epistemic uncertainty through a prior. However, whereas Provost and Domingos [12] showed a clear advantage over using the raw estimates for single decision trees, Bostrom [1] observed that for random forest better estimates are achieved without smoothing. Apart from that correction, the reliability of the individual predictions in
decision trees is usually controlled via pruning or imposing leaf sizes [12, 20]. While the common recommendation is to grow trees in an ensemble to their fullest extent, Zhou and Mentch [20] argue that depending on the properties of the underlying data greater leafs and hence more stable predictions are preferable. With respect to RDT, Kulessa and Loza Mencía [8] reward predictions with higher confidence in the ensemble using the inverted Gini-index. However, their weighting approach has not been directly evaluated.

The Dempster-Shafer theory of evidence, or theory of belief functions, [15] is also concerned with the strength of the confidences. The general framework for combining prediction of Lu [9] is based on this theory and the study showed that the proposed technique can improve upon the Bayesian approach. Raza et al. [13] similarly combined outputs of support vector machines but only compared to a single classifier in their evaluation. Nguyen et al. [10] take uncertainties in an alternative way into account by computing interval-based information granules for each classifier. They could improve over common ensemble techniques, however, their approach requires additional optimization during learning and during classification. As already discussed in Section 1, meta and fusion approaches also often require additional learning steps and ignore the uncertainty of individual predictions. Costa et al. [3] also ignore the uncertainties but propose interesting alternative aggregations for ensembles based on generalized mixture functions.

\section{Aggregation of Scores from Leafs}

Based on the leaf nodes \(w_1, \ldots, w_K\) to which an instance has been assigned to during prediction, the concept explained in this section is to first convert the leafs into scores which are then combined using aggregation functions.

\subsection{Scoring Methods}

In this section, the scoring methods are introduced of which most are designed to take the uncertainty of the leafs into account. We denote \(p: \mathcal{W} \to \mathbb{R}\) as the function which assigns a score \(v = p(w)\) to a leaf \(w \in \mathcal{W}\) where \(w = (w^+, w^-)\). All scoring methods proposed in this work are designed such that the sign of the resulting score indicates whether the positive or the negative class would be predicted. In order to understand how the scoring methods deal with uncertainty, we introduce an approach to visualize and compare them in Figure 1.

**Probability and Laplace.** Computing the probability \(p_{prob}(w)\) is the conventional approach to obtain a score from a leaf. Hence, it will serve as a reference point in this work. In addition, we include the Laplace smoothing \(p_{lap}(w)\) which corrects the estimate for uncertainty due to a lack of samples.

\[
p_{prob}(w) = \frac{w^+}{w^+ + w^-} - 0.5 \quad p_{lap}(w) = \frac{w^+ + 1}{w^+ + w^- + 2} - 0.5
\]

In Figure 1 we can see how both \(p_{prob}\) and \(p_{lap}\) converge to the same score for larger leafs but that \(p_{lap}\) has much less extreme predictions for small leafs.
**Plausibility.** The idea of this approach is to measure the uncertainty in terms of aleatoric and epistemic uncertainty. In order to define the uncertainty, Shaker and Hüllemeier \[16\] introduces the degree of support for the positive class $\pi(\oplus|w)$ and the negative class $\pi(\ominus|w)$ which can be calculated for a leaf $w$ as follows:

$$
\pi(\oplus|w) = \sup_{\theta \in [0,1]} \min \left( \left( \theta \frac{w^\oplus}{w^\oplus + w^\ominus} \right)^{w^\oplus} \left( \frac{1 - \theta}{\frac{w^\ominus}{w^\oplus + w^\ominus}} \right)^{w^\oplus}, 2\theta - 1 \right),
$$

$$
\pi(\ominus|w) = \sup_{\theta \in [0,1]} \min \left( \left( \theta \frac{w^\ominus}{w^\oplus + w^\ominus} \right)^{w^\ominus} \left( \frac{1 - \theta}{\frac{w^\ominus}{w^\oplus + w^\ominus}} \right)^{w^\ominus}, 1 - 2\theta \right).
$$

Based on this *plausibility* the epistemic uncertainty $u_e(w)$ and the aleatoric uncertainty $u_a(w)$ can be defined as:

$$
u_e(w) = \min \left[ \pi(\oplus|w), \pi(\ominus|w) \right] \quad u_a(w) = 1 - \max \left[ \pi(\oplus|w), \pi(\ominus|w) \right]
$$

Following Nguyen et al. \[11\], the degree of preference for the positive class $s_{\oplus}(w)$ can be calculated as

$$
s_{\oplus}(w) = \begin{cases} 
1 - (u_a(w) + u_e(w)) & \text{if } \pi(\oplus|w) > \pi(\ominus|w), \\
1 - (u_a(w) + u_e(w)) / 2 & \text{if } \pi(\oplus|w) = \pi(\ominus|w), \\
0 & \text{if } \pi(\oplus|w) < \pi(\ominus|w)
\end{cases}
$$

and analogously for the negative class. We use the trade-off between the degrees of preference as our score:

$$
p_{\text{plas}}(w) = s_{\oplus}(w) - s_{\ominus}(w).
$$

With respect to Figure 1 we can observe that the plausibility approach models the uncertainty similarly to the Laplace method but also preserves a high variability for small leaf sizes. From that point of view, it could be seen as a compromise between the Probability and the Laplace method.

![Fig. 1. Evolution of the scores (y-axis) for each scoring method based on simulating a leaf to which random samples are added (x-axis) with a probability of 75% for the positive class. This Bernoulli trial is repeated 100 times (cyan lines). The average over the trials scores is depicted by the red line and the 10%, 25%, 75% and 90% quantiles by the green and purple line, respectively.](image-url)
Confidence Bounds. Another possibility to consider uncertainty is to model the probability of the positive and the negative class each with a separate probability distribution and to compare these. In this work, we use a beta-binomial distribution parameterized with \( w^+ \) number of tries, \( \alpha = w^+ + 1 \), and \( \beta = w^- + 1 \) to model the probability of the positive class, analogously for the negative class. To get a measure \( c(w) \) of how well both classes are separated, we take the intersection point in the middle of both distributions, normalized by the maximum height of the distribution, and use this as in the following:

\[
p_{cb}(w) = (1 - c(w)) \left( \frac{w^-}{w^+ + w^-} - 0.5 \right)
\]

Hence, \( c(w) \) generally decreases with 1) increasing class ratio in the leaf, or 2) with more examples, since this leads to more peaky distributions. In contrast to Laplace and Plausibility in Figure 1, the scores of confidence bounds are increasing more steadily which indicates a weaker consideration of the size of the leaves than the aforementioned methods.

### 3.2 Aggregation Functions

In a final step the scores \( v_1, \ldots, v_K \), where \( v_i = p(w_i) \), need to be combined using an aggregation function \( h : \mathbb{R}^K \rightarrow \mathbb{R} \). Due to space restrictions, we limit our analysis in this work to the arithmetic mean and 0-1-voting

\[
h_{\text{avg}}(v) = \frac{1}{K} \sum_{i=1}^{K} v_i \quad \quad h_{\text{vote}}(v) = \frac{1}{K} \sum_{i=1}^{K} \text{sgn}(v_i > 0)
\]

with \( \text{sgn}(\cdot) \) as the sign function. We consider \( h_{\text{vote}} \) as a separate method in the following, since all presented scoring methods change their sign equally. Note that \( p_{\text{prob}} \) in combination with \( h_{\text{avg}} \) corresponds to what is known as weighted voting, and \( p_{cb} \) an instantiation of weighted averaging over \( p_{\text{prob}} \).

Similarly to Costa et al. [3], we found in preliminary experiments that alternative approaches, including the median, maximum and a variety of generalized mixture functions [7], could be beneficial in some cases, but did not provide meaningful new insights in combination with the explored scoring functions.

### 4 Integrated Combination of Leafs

In contrast to the aggregation of scores, the integrated combination of leaves skips the intermediate step of score generation and directly combines the statistics of the leaves \( g : W^K \rightarrow \mathbb{R} \) to form a prediction for the ensemble. Through this approach the exact statistics of the leaves can be considered for the aggregation which would otherwise be inaccessible using scores. In contrast to Figure 1, Figure 2 depicts the outputs of 100 simulated ensembles.
Pooling. The basic idea of pooling is to reduce the influence of leaves with a low number of instances which otherwise would obtain a high score either for the positive or the negative class. Therefore, this approach first sums up the leaf statistics and then computes the probability which can be defined as:

\[
g_{\text{pool}}(w_1, w_2, \ldots, w_K) = \frac{\sum_{i=1}^{K} w_i^\oplus}{\sum_{i=1}^{K} (w_i^\oplus + w_i^\ominus)} - 0.5
\]

With respect to Figure 2, we can observe that pooling behaves similarly to the probability approach. The reduced variability is mainly caused due to the simulation of more leaves.

Dempster. Based on the Dempster-Shafer framework, leaf aggregation can also be performed using the theory of belief functions [15]. For our purpose the states of belief can be defined as \( \Omega = \{\oplus, \ominus\} \), where \( \oplus \) represents the belief for the positive and \( \ominus \) represents the belief for the negative class. A particular mass function \( m : 2^\Omega \rightarrow [0, 1] \) assigns a mass to every subset of \( \Omega \) such that \( \sum_{A \subseteq \Omega} m(A) = 1 \). Based on the plausibility (c.f. Section 3.1), we define the mass function for a particular leaf \( w \) as follows:

\[
\begin{align*}
m_w(\emptyset) &= 0 \\
m_w(\{\oplus\}) &= s_\oplus(w) \\
m_w(\{\ominus\}) &= s_\ominus(w) \\
m_w(\{\oplus, \ominus\}) &= u_e(w) + u_a(w).
\end{align*}
\]

In order to combine the predictions of multiple leaves, the mass functions can be aggregated using the (unnormalized) Dempster’s rule of combination:

\[
(m_{w_1} \oplus m_{w_2})(A) = \sum_{B \cap C = A} m_{w_1}(B)m_{w_2}(C) \quad \forall A \subseteq \Omega
\]

Hence, for the ensemble we can define the following belief function:

\[
m_{\text{dempster}}(A) = (m_{w_1} \oplus (m_{w_2} \oplus (\ldots \oplus m_{w_K}))) (A)
\]

which can be used to form a score for the positive class as follows:

\[
g_{\text{dempster}}(w_1, w_2, \ldots, w_K) = m_{\text{dempster}}(\{\oplus\}) - m_{\text{dempster}}(\{\ominus\})
\]

Fig. 2. Evolution of the scores (y-axis) for each combination method based on simulating 100 ensemble’s final predictions (cyan lines) based each on 100 leafs sampled like in Figure 1.
A particular drawback of Dempster’s rule of combination is that it requires independence among the combined mass functions which is usually not true for classifiers in an ensemble which have been trained over the same data. The independence assumption can be omitted by using the cautious rule of combinations \[4\]. The idea behind the cautious rule is based on the Least Commitment Principle \[17\] which states that, when considering two belief functions, the least committed one should be preferred. Following this principle, the cautious rule $\wedge$ can be used instead of Dempster’s rule of combination $\cap$. For more information we refer to Denœux \[4\]. Hence, for the ensemble we can define the following belief function

$$m_{\text{cautious}}(A) = (m_{w_1} \wedge (m_{w_2} \wedge \ldots \wedge m_{w_K}))(A)$$

which can be transformed to a score for the positive class as follows:

$$g_{\text{cautious}}(w_1, w_2, \ldots, w_K) = m_{\text{cautious}}(\{\oplus\}) - m_{\text{cautious}}(\{\ominus\})$$

We use a small value ($10^{-5}$) as the minimum value for certain steps during the calculation to deal with numerical instabilities for both Dempster and Cautious.

In order to provide a more intuitive explanation, consider the following three estimates to combine: $s_{\oplus}(w_1) = s_{\oplus}(w_2) = 0.4$ and $s_{\ominus}(w_3) = 0.4$. Dempster would consider that there are two estimates in favor of the positive class and hence predicts it, whereas Cautious ignores several preferences for the same class, since they could result from dependent sources, and would just take the stronger one. Hence, Cautious would produce a tie (but high weights for $\emptyset$ and $\{\oplus, \ominus\}$).

This behaviour can also be observed in Figure 2 where the plot for Cautious resulted very similar to that of the maximum operator (not shown due to space restrictions). For Dempster, in contrast, the majority of leaves confirming the positive class very quickly push the prediction towards the extreme. Consider for that the following scenario, which also visualizes the behaviour under conflict. For $s_{\oplus}(w_1) = s_{\oplus}(w_2) = 0.8$ and $s_{\ominus}(w_3) = 0.98$ Dempster’s rule would prefer the negative over the positive class, but already give a weight of 0.94 to neither $\oplus$ nor $\ominus$, whereas Cautious would prefer the negative class with a score of 0.20 and 0.78 for $\emptyset$.

**Evidence accumulation.** In the presence of uncertainty, it may make sense to reach a decision not by combining individual recommendations themselves, but by accumulating the evidence underlying each recommendation. This motivates a new combining rule, here called EVA (EVidence Accumulation).

To get the intuition behind the idea, consider a police inspector investigating a crime. It is perfectly possible that no clue by itself is convincing enough to arrest a particular person, but jointly, they do. This effect can never be achieved by expressing the evidence as probabilities and then averaging. E.g., assume there are 5 suspects, $A, B, C, D, E$; information from Witness $w_1$ rules out $D$ and $E$, and information from Witness $w_2$ rules out $A$ and $B$. Logical deduction leaves $C$ as the only possible solution. Now assume $w_1$ and $w_2$ express their
knowledge as probabilities: \( w_1 \) returns \( (0.33, 0.33, 0.33, 0, 0) \) (assigning equal probabilities to A, B and C and ruling out D and E), and \( w_2 \) returns \( (0, 0, 0.33, 0.33, 0.33) \). Averaging these probabilities gives \( (0.17, 0.17, 0.33, 0.17, 0.17) \), when logic tells us it should be \( (0, 0, 1, 0, 0) \). Note that 1 is out of the range of probabilities observed for C: no weighted average can yield 1. Somehow the evidence from different sources needs to be accumulated.

In probabilistic terms, the question boils down to: How can we express \( P(y \mid \bigwedge_i w_i) \) in terms of \( P(y \mid w_i) \)? Translated to our example, how does the probability of guilt, given the joint evidence, relate to the probability of guilt given each individual piece? There is not one way to correctly compute this: assumptions need to be made about the independence of these sources. Under the assumption of class-conditional independence (as made by, e.g., Naive Bayes), we can easily derive a simple and interpretable formula:

\[
P(y \mid \bigwedge_i w_i) \sim P(y \mid w_i) \prod_i P(w_i \mid y) = P(y) \prod_i \frac{P(y \mid w_i)}{P(y)}
\]

Thus, under class-conditional independence, evidence from different sources should be accumulated by multiplying the prior \( P(Y) \) with a factor \( P(y \mid w_i)/P(y) \) for each source \( w_i \). That is, if a new piece of information, on its own, would make \( y \) twice as likely, it also does so when combined with other evidence. In our example, starting from \( (0.2, 0.2, 0.2, 0.2, 0.2) \), \( w_1 \) multiplies the probabilities of A, B, C by 0.33/0.2 and those of D, E by 0, and \( w_2 \) lifts C, D, E by 0.33/0.2 and A, B by 0; this gives \( (0, 0, 0.54, 0, 0) \) which after normalization becomes \( (0, 0, 1, 0, 0) \).

Coming back to the binary classification setting, we compute

\[
g_{eva}(w_1, w_2, \ldots, w_K) = P(\oplus) \prod_i \frac{P(\oplus \mid w_i)}{P(\oplus)} - P(\ominus) \prod_i \frac{P(\ominus \mid w_i)}{P(\ominus)}
\]

where \( P(\oplus) \) and \( P(\ominus) \) is estimated by the class distribution on the training data and \( P(y \mid w_i) \) essentially comes down to \( p_{prob}(w_i) \). We apply similar tricks as in Naive Bayes for ensuring numerical stability such as a slight Laplace correction of 0.1 in the computation of \( P(y \mid w_i) \).

With respect to Figure 2 we can observe an even stronger decrease of the absolute score with increasing leaf size than for Cautious. This indicates that the output of EVA can be highly influenced by smaller leaves which are more likely to carry more evidence than larger leaves, in the sense that their estimates are more committed.

5 Evaluation

A key aspect of our experimental evaluation is to compare our proposed methods for combining predictions with respect to the conventional approaches of voting and averaging probabilities. In order to put the combination strategies to the test, our experiments are based on random decision trees which, in contrast to other tree ensembles, guarantee a high diversity of estimates in the ensemble.
Table 1. Binary classification datasets and statistics.

| name        | #instances | #features | class ratio | name       | #instances | #features | class ratio |
|-------------|------------|-----------|-------------|------------|------------|-----------|-------------|
| scene       | 2407       | 299       | 0.18        | sonar      | 208        | 60        | 0.47        |
| webdata     | 36974      | 123       | 0.24        | mushroom   | 8124       | 22        | 0.48        |
| transfusion | 748        | 4         | 0.24        | vehicle    | 98528      | 100       | 0.50        |
| biodeg      | 1055       | 41        | 0.34        | phishing   | 11055      | 30        | 0.56        |
| telescope   | 19020      | 10        | 0.35        | breast-cancer | 569      | 30        | 0.63        |
| diabetes    | 768        | 8         | 0.35        | ionosphere | 351        | 34        | 0.64        |
| voting      | 435        | 16        | 0.39        | tic-tac-toe | 958       | 9         | 0.65        |
| spambase    | 4601       | 57        | 0.39        | particle   | 130064     | 50        | 0.72        |
| electricity | 45312      | 8         | 0.42        | skin       | 245057     | 3         | 0.79        |
| banknote    | 1372       | 4         | 0.44        | climate    | 540        | 20        | 0.91        |
| airlines    | 539383     | 7         | 0.45        |            |            |           |             |

5.1 Experimental Setup

Our evaluation is based on 21 datasets for binary classification shown in Table 1, which we have chosen in order to obtain diversity w.r.t. the size of dataset, the number features and the balance of the class distribution. To consider a variety of scenarios for combining unstable predictions, we have performed all of our evaluations with respect to an ensemble of 100 trees and minimum leaf sizes 1, 2, 3, 4, 8 or 32. Note that a single RDT ensemble for each leaf size configuration is enough in order to obtain the raw counts $w_i$ and hence produce the final predictions for all methods. We used 5 times two fold cross validation in order to decrease the dependence of randomness on the comparability of the results.

For measuring the performance, we have computed the area under receiver operating characteristic curve (AUC) and the accuracy. For a better comparison we have computed average ranks across all datasets. As an additional reference points to our comparison, we added the results of a single decision tree and a random forest ensemble. Note that though imposing an equal tree structure, these trees were trained with the objective of obtaining a high purity of class distributions in their leaves. Therefore, we did not expect to reach the performance w.r.t. classification but it was intended to show to what degree advanced combination strategies are able to close the gap between using tree models resulting merely from the data distribution and tree models specifically optimized for a specific task.

5.2 Results

Figure 3 shows a comparison between all methods with respect to different tree structures. The first observation is that most of the methods perform around the baseline of taking the average probability. Exceptions are evidence accumulation, which is on top of the remaining approaches especially in terms of accuracy.
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Fig. 3. Comparison of the average ranks with respect to the 11 methods and the 6 leaf configurations (worst rank is $6 \cdot 11 = 66$). Left: AUC. Right: Accuracy.

Fig. 4. Heatmap of pairwise comparisons. Each row and each column belongs to a method in the order $p_{\text{prob}}, p_{\text{lap}}, p_{\text{pls}}, p_{\text{cb}},$ and $g_{\text{eva}}$ and the number and color indicates how often the method in the row had a better AUC score than the method in the column. $\bullet$, $\Diamond$ and $\star$ indicate a significant difference according to the Bonferroni corrected Wilcoxon signed-rank test with $\alpha = 0.05$, 0.01 and 0.001, respectively.

and the approaches based on the theory of belief functions, which especially exhibit problems in producing rankings (AUC). Nonetheless, Dempster rule of combination has an advantage over the other methods for middle to large sized leafs in terms of accuracy. Figure 4 shows again how close the methods are together (Dempster, Cautious, Pooling and Voting were left out). We can see that $p_{\text{lap}}$ always is worse than $p_{\text{prob}}$, regardless of the leaf size. While $p_{\text{pls}}$ is not much worse than the best method ($p_{\text{prob}}$) on small leafs, it falls behind with increasing leaf size. Without $g_{\text{eva}}, p_{\text{cb}}$ would be the best method on medium sized or larger leafs but $g_{\text{eva}}$ has even better results there. Overall, $p_{\text{prob}}$ most often has the best results on very small leafs, but for not much larger leafs, $p_{\text{prob}}$ starts falling behind $g_{\text{eva}}$.

Figure 5 provides further insights on four selected datasets (single random 50% train/test split). It becomes apparent that the advantage of EVA is also
Fig. 5. Accuracy of selection of five combination strategies and distribution with mean (dashed blue line), 1, 2 and 3 standard deviations (blue shaded areas) over accuracies of the underlying individual trees in the ensemble (turquoise dots).

often substantial in absolute terms. On the other hand, we can also observe cases where EVA falls behind the other approaches (airlines). Interestingly, the accuracy of EVA on webdata increases with increasing leaf size long after the other methods reach their peak, contrary to the general trend.

We can further observe that, as expected, the performances of the proposed methods lay between those of random forests and the single decision tree. However, Figure 6 reveals that an important factor is the class ratio of the classification task. While random forest clearly outperform all other methods for highly imbalanced tasks, the advance is negligible for the balanced problems. This indicates a general problem of RDT with imbalanced data, since it gets less likely on such data to obtain leafs with (high) counts for the minority class.

5.3 Discussion

In the following, we discuss the results of each individual method in more detail.

Probability, Laplace, Voting and Pooling. Computing the expectation over $p_{prob}$ straightforwardly showed to be very effective compared to most of the
Combining Predictions under Uncertainty: Random Decision Trees

Alternative method ideas. Especially when small leaves are involved this behaviour was not expected since we believed that small leaves with overly certain but likely wrong estimates (probabilities 0 and 1) would out-weight the larger leaves which provide more evidence for their smoother estimates. Instead, the results indicate that a large enough ensemble (we used 100 trees) makes up for what we considered too optimistic $p_{\text{prob}}$ leaf predictions [1]. In fact, applying Laplace correction towards uniform distribution was hindering especially for small leaf sizes in our experiments. Voting is able to catch-up with the other methods only for the configuration of trees with very small leaves, where, indeed, the scores to be combined are identical to those of $p_{\text{prob}}$ except for leaves with size greater one. Interestingly, Pooling improves over the other methods on a few datasets as it can be seen for airlines in Figure 5. Nevertheless, the results on most of the datasets indicate that the consideration of the leaf size by this method might be too extreme in most cases, leading generally to unstable results.

**Plausability, Dempster and Cautious.** We expected that a precise computation and differentiation of plausibility and uncertainties would be beneficial in particular for small leaf sizes. However, we were not able to observe a systematic advantage of $p_{\text{plas}}$ over the $p_{\text{prob}}$ baseline in our experiments. Nonetheless, the usage of the uncertainty estimates in Dempster’s rule of combinations shows the potential of having access to such scores. When the data was balanced, Dempster classified as good or better than EVA or even the random forest. The gap w.r.t. AUC demonstrates that the proposed translation of the components of the mass function into one score is not yet optimal. Moreover, the results suggests that the lack of independence is not problematic when combining predictions in RDT, but on the contrary, the way the Cautious rule addressed it caused serious problems.
Confidence Bounds. Among the methods with similar performance to $p_{\text{prob}}$, the approach using confidence bounds exhibits the greatest (but still small) advantage over the baseline for trees with medium to large leaf sizes. For very small leaves, however, the chosen statistical modeling is obviously not ideal, at least for ranking. Also, it might be possible to achieve even better results with the same idea by using distributions or more elaborated strategies which can achieve a better fit.

Evidence Accumulation. Using a small value for Laplace smoothing, $g_{\text{eva}}$ proved to be a very effective prediction strategy across all but the very smallest leaves. This suggests that the assumptions underlying EVA are well-met by RDTs. The randomness of the leaves fits EVA’s independence assumption.

The stronger consideration of the class prior probability than in other methods may also play a role on why EVA works better on unbalanced data, particularly for larger leaf sizes (Figure 6). Remind that EVA relates the estimates for each source to the prior probability and judges the evidence according to how much the leaf distribution deviates from it. Leaves for the minority class might hence have a higher impact on the final prediction than for other methods, where such leaves are more likely to be out-ruled by the average operation and the leaves following the class prior.

6 Conclusions

In this work, we proposed methods to combine predictions under uncertainty in an ensemble of decision trees. Uncertainty here refers not only to how uncertain a prediction is, but also to uncertainty about this uncertainty estimate. Our methods include Laplace smoothing, distinguishing between aleatoric and epistemic uncertainty, making use of the dispersion of probability distributions, combining uncertainties under the theory of belief functions, and accumulating evidence. Random decision trees ensured a high diversity of the predictions to combine and a controlled environment for our experimental evaluation. We found that including the support for the available evidence in the combination improves performance over averaging probabilities only in some specific cases. However, we could observe a consistent advantage for the proposed approach of evidence accumulation.

This result suggests that the strength of the evidence might be a better factor than the support for the evidence when combining unstable and diverse predictions from an ensemble. However, the principle of evidence accumulation revealed additional aspects, like the rigorous integration of the prior probability or the multiplicative accumulation of evidence, which might also be relevant for the observed improvement. Moreover, Dempster’s rule showed that combining support (through the plausibilities) and commitment of evidence produces good results when certain conditions, such as even class ratio, are met. We plan to investigate these aspects in future work, e.g. by integrating a prior into Dempster’s
rule or aspects of reliable classification into EVA. Further research questions include which insights can be carried over to random forest ensembles, which are more homogeneous in their predictions, or if the presented strategies have a special advantage under certain conditions, such as small ensembles.

Bibliography

[1] Bostrom, H.: Estimating class probabilities in random forests. In: Sixth International Conference on Machine Learning and Applications, pp. 211–216 (2007)
[2] Breiman, L.: Random forests. Machine Learning 45(1), 5–32 (2001)
[3] Costa, V.S., Farias, A.D.S., Bedregal, B., Santiago, R.H., Canuto, A.M.d.P.: Combining multiple algorithms in classifier ensembles using generalized mixture functions. Neurocomputing 313, 402–414 (2018)
[4] Denœux, T.: The cautious rule of combination for belief functions and some extensions. In: 9th International Conference on Information Fusion, pp. 1–8 (2006)
[5] Dietterich, T.G.: Ensemble methods in machine learning. In: Multiple Classifier Systems, pp. 1–15, Springer Berlin Heidelberg (2000)
[6] Fan, W., Wang, H., Yu, P.S., Ma, S.: Is random model better? On its accuracy and efficiency. In: 3rd IEEE International Conference on Data Mining (2003)
[7] Farias, A.D.S., Santiago, R.H.N., Bedregal, B.: Some properties of generalized mixture functions. In: IEEE International Conference on Fuzzy Systems, pp. 288–293 (2016)
[8] Kulesza, M., Loza Mencía, E.: Dynamic classifier chain with random decision trees. In: Proc. 21st International Conference of Discovery Science, pp. 33–50 (2018)
[9] Lu, Y.: Knowledge integration in a multiple classifier system. Applied Intelligence 6(2), 75–86 (1996)
[10] Nguyen, T.T., Pham, X.C., Liew, A.W.C., Pedrycz, W.: Aggregation of classifiers: a justifiable information granularity approach. IEEE transactions on cybernetics 49(6), 2168–2177 (2018)
[11] Nguyen, V.L., Destercke, S., Masson, M.H., Hüllermeier, E.: Reliable multi-class classification based on pairwise epistemic and aleatoric uncertainty. In: International Joint Conference on Artificial Intelligence, pp. 5089–5095 (2018)
[12] Provost, F., Domingos, P.: Tree induction for probability-based ranking. Machine learning 52(3), 199–215 (2003)
[13] Raza, M., Goudal, I., Green, D., Coppel, R.L.: Classifier fusion using dempster-shafer theory of evidence to predict breast cancer tumors. In: IEEE Region 10 International Conference TENCON, pp. 1–4 (2006)
[14] Ruta, D., Gabrys, B.: An overview of classifier fusion methods. Computing and Information Systems 7, 1–10 (2000)
[15] Shafer, G.: A mathematical theory of evidence, vol. 42. Princeton university press (1976)
[16] Shaker, M.H., Hüllermeier, E.: Aleatoric and epistemic uncertainty with random forests. In: Advances in Intelligent Data Analysis XVIII, pp. 444–456 (2020)
[17] Smets, P.: Belief functions: the disjunctive rule of combination and the generalized bayesian theorem. International Journal of approximate reasoning 9(1), 1–35 (1993)
[18] Wolpert, D.: Stacked generalization. Neural Networks 5(2), 241–259 (1992)
[19] Yuksel, S.E., Wilson, J.N., Gader, P.D.: Twenty years of mixture of experts. IEEE transactions on neural networks and learning systems 23(8), 1177–1193 (2012)
[20] Zhou, S., Mentch, L.: Trees, forests, chickens, and eggs: When and why to prune trees in a random forest. arXiv preprint arXiv:2103.16700 (2021)