Efficient Algorithms for Set-Valued Prediction in Multi-Class Classification

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Abstract

In cases of uncertainty, a multi-class classifier preferably returns a set of candidate classes instead of predicting a single class label with little guarantee. More precisely, the classifier should strive for an optimal balance between the correctness (the true class is among the candidates) and the precision (the candidates are not too many) of its prediction. We formalize this problem within a general decision-theoretic framework that unifies most of the existing work in this area. In this framework, uncertainty is quantified in terms of conditional class probabilities, and the quality of a predicted set is measured in terms of a utility function. We then address the problem of finding the Bayes-optimal prediction, i.e., the subset of class labels with highest expected utility. For this problem, which is computationally challenging as there are exponentially (in the number of classes) many predictions to choose from, we propose efficient algorithms that can be applied to a broad family of utility scores. Two of these algorithms make use of structural information in the form of a class hierarchy, which is often available in prediction problems with many classes. Our theoretical results are complemented by experimental studies, in which we analyze the proposed algorithms in terms of predictive accuracy and runtime efficiency.

1 Introduction

In probabilistic multi-class classification, one often encounters situations in which the classifier is uncertain about the class label for a given instance. In such cases, instead of predicting a single class, it might be beneficial to return a set of classes as a prediction, with the idea that the correct class should at least be contained in that set. For example, in medical diagnosis, when not being sure enough about the true disease of a patient, it is better to return a set of candidate diseases. Provided this set is sufficiently small compared to the total number of diagnoses, it can still be of great help for a medical doctor, because only the remaining candidate diseases need further investigation.

Formally, we assume training examples \( \{(x_i, y_i)\}_{i=1}^N \) from a distribution \( P(x, y) \) on \( \mathcal{X} \times \mathcal{Y} \), with \( \mathcal{X} \) some instance space (e.g., images, documents, etc.) and \( \mathcal{Y} = \{c_1, \ldots, c_K\} \) an output space.
consisting of $K$ classes. In the context of set-valued prediction, we will consider a prediction $\hat{Y}$ from the power set of $\mathcal{Y}$, i.e., predictions are (non-empty) subsets of $\mathcal{Y}$, or more formally, $\hat{Y} \in 2^\mathcal{Y} \setminus \{\emptyset\}$. The quality of the prediction $\hat{Y}$ can be expressed by means of a set-based utility score $u(c, \hat{Y})$, where $c$ corresponds to the ground-truth class and $\hat{Y}$ is the predicted set.

Multi-class classifiers that return set-valued predictions have been considered by several authors under different names. In [Coz et al., 2009], the notion of non-deterministic classification is introduced, and the performance of set-valued classifiers is assessed using set-based utility scores from the information retrieval community, such as precision, recall, and the $F_1$-measure. Unlike typical top-$t$ prediction in information retrieval, the cardinality $t$ of the set varies over instances in set-valued prediction, depending on the uncertainty about the class label for an instance. Other researchers call the same setting credal or cautious classification. In a series of papers, they analyze several set-based utility scores that reward abstention in cases of uncertainty [Corani and Zaffalon, 2008, 2009, Zaffalon et al., 2012, Yang et al., 2017b]. The framework of conformal prediction also produces set-valued predictions, albeit with a focus on confidence (the set covers the true class with high probability) and less on utility [Shalit and Vovk, 2008]. Furthermore, set-valued prediction can be seen as a generalization of multi-class classification with a reject option [Ramaswamy et al., 2015a], where one either predicts a single class or the complete set of classes.

In this paper, we introduce Bayes-optimal algorithms for maximizing set-based utility scores $u(c, \hat{Y})$. To this end, we will consider a decision-theoretic framework, where we estimate a probabilistic model, followed by an inference procedure at prediction time. In a probabilistic multi-class classification framework, we estimate the conditional probability distribution $P(\cdot | x)$ over $\mathcal{Y}$:

$$\forall c \in \mathcal{Y}: 0 \leq P(c | x) \leq 1, \quad \sum_{c \in \mathcal{Y}} P(c | x) = 1. \quad (1)$$

This distribution can be estimated using several types of probabilistic methods (see further below). At prediction time, the goal is to find the Bayes-optimal solution $\hat{Y}_u^*$ by expected utility maximization:

$$\hat{Y}_u^*(x) = \arg \max_{\hat{Y} \in 2^{\mathcal{Y}} \setminus \{\emptyset\}} \mathbb{E}_{P(c | x)}[u(c, \hat{Y})] = \arg \max_{\hat{Y} \in 2^{\mathcal{Y}} \setminus \{\emptyset\}} \sum_{c \in \mathcal{Y}} u(c, \hat{Y}) P(c | x) = \arg \max_{\hat{Y} \in 2^{\mathcal{Y}} \setminus \{\emptyset\}} U(\hat{Y}, P, u), \quad (2)$$

where we introduce the shorthand notation $U(\hat{Y}, P, u)$ for the expected utility. The above problem is a non-trivial optimization problem, as a brute-force search requires checking all subsets of $\mathcal{Y}$, resulting in an exponential time complexity. However, we will be able to find the Bayes-optimal prediction more efficiently. As our main contribution, we present several algorithms that solve (2) in an efficient manner. Applying additional search space restrictions, those algorithms will typically exhibit a trade-off between runtime and predictive performance.

In Section 2 we discuss essential properties of the utility scores we consider, and review existing scores covered by our framework. In Section 3 we present two theoretical results as essential building blocks for solving (2), followed by three algorithms in Section 4. We first introduce a simple algorithm (Section 4.1) that makes $K$ queries to the conditional distribution $P(c | x)$ (with $K$ the number of classes). In Section 4.2 we introduce an algorithm that makes less than $K$ calls to $P(c | x)$, provided the conditional class probabilities are modelled with hierarchical models (e.g. hierarchical softmax). In Section 4.3 we claim that the Bayes-optimal predictor can be computed even more efficiently when a restriction is made to sets of classes that occur as nodes in a predefined hierarchy. In Section 5 we further discuss the trade-offs between runtime and predictive performance of the different algorithms by means of experiments on benchmark datasets.

2 Utility scores for set-valued prediction

The inference algorithms that we introduce can be applied to a general family of set-based utility functions $u : \mathcal{Y} \times 2^\mathcal{Y} \setminus \{\emptyset\} \rightarrow [0,1]$ given as follows:

$$u(c, \hat{Y}) = \begin{cases} 0 & \text{if } c \notin \hat{Y}, \\ g(|\hat{Y}|) & \text{if } c \in \hat{Y}, \end{cases} \quad (3)$$

where $|\hat{Y}|$ denotes the cardinality of the predicted set $\hat{Y}$. This family is parametrized by a sequence $(g(1), \ldots, g(K)) \in [0,1]^K$ that should obey the following properties:
1. \( g(1) = 1 \), i.e., the utility \( u(c, \hat{Y}) \) should be maximal when the classifier returns the true class label as a singleton set;

2. \( g(s) \) should be non-increasing, i.e., the utility \( u(c, \hat{Y}) \) should be higher if the true class is contained in a smaller set of predicted classes;

3. \( g(s) \geq 1/s, i.e., the utility \( u(c, \hat{Y}) \) of predicting a set containing the true and \( s-1 \) additional classes should not be lower than the expected utility of randomly guessing one of these \( s \) classes. This requirement formalizes the idea of risk-aversion: in the face of uncertainty, abstaining should be preferred to random guessing (see e.g. [Zaffalon et al., 2012]).

Many existing set-based utility scores are recovered as special cases of \( u(c, \hat{Y}) \), including the three classical measures from information retrieval adopted in [Coz et al., 2009]: precision with \( g_P(s) = 1/s \), recall with \( g_R(s) = 1 \), and the F1-measure with \( g_{F1}(s) = 2/(1 + s) \). Other utility functions with specific choices for \( g \) are studied in the literature on credal classification [Corani and Zaffalon, 2008][Zaffalon et al., 2012][Yang et al., 2017][Nguyen et al., 2018], such as

\[
g_{\delta, \gamma}(s) = \frac{\delta}{s} - \frac{\gamma}{s^2}, \quad g_{\exp}(s) = 1 - \exp\left(-\frac{\delta}{s}\right), \quad g_{\log}(s) = \log\left(1 + \frac{1}{s}\right).
\]

Especially \( g_{\delta, \gamma}(s) \) is commonly used in this community, where \( \delta \) and \( \gamma \) can only take certain values to guarantee that the utility is in the interval \([0, 1]\). Precision (here called discounted accuracy) corresponds to the case \( (\delta, \gamma) = (1, 0) \). However, typical choices for \( (\delta, \gamma) \) are \((1.6, 0.6)\) and \((2.2, 1.2)\) [Nguyen et al., 2018], implementing the idea of risk aversion. The measure \( g_{\exp}(s) \) is an exponentiated version of precision, where the parameter \( \delta \) also defines the degree of risk aversion.

Another example appears in the literature on multi-class classification with reject option [Ramaswamy et al., 2015a]. In this case, the prediction can only be a singleton or the full set \( Y \) containing \( K \) classes. The first case typically gets a reward of one, while the second case should receive a lower reward, e.g. \( 1 - \alpha \). This second case corresponds to abstaining, i.e., not predicting any class label, and the (user-defined) parameter \( \alpha \) specifies a penalty for doing so, with the requirement \( 0 < \alpha < 1 - 1/K \) to be risk-averse. To include sets of any cardinality \( s \), the utility could be generalized as follows:

\[
g_{\alpha, \beta}(s) = 1 - \alpha \left(\frac{s - 1}{K - 1}\right)^\beta,
\]

with the same interpretation for \( \alpha \), and \( \beta \in [0, \infty] \) a second parameter that defines whether \( g(s) \) is convex or concave. While convexity (like in most of the above utility functions) appears natural in most applications, a concave utility might be useful when predicting a large set is tolerable. In the limit, when \( \beta \to 0 \), we obtain the simple utility function for classification with reject option. In the supplementary material (Fig. 1), we plot \( g(s) \) for some of the above parameterizations.

Set-valued predictions are also considered in hierarchical multi-class classification, mostly in the form of internal nodes of the hierarchy [Alex Freitas, 2007][Rangwala and Naik, 2017][Yang et al., 2017a]. Compared to the “flat” multi-class case, the prediction space is thus restricted, because only sets of classes that correspond to nodes of the hierarchy can be returned as a prediction. Some of the above utility scores also appear here. For example, [Yang et al., 2017a] evaluate various members of the \( u_{\delta, \gamma} \) family in a framework where hierarchies are considered for computational reasons, while [Oh, 2017] optimizes recall by fixing \( |\hat{Y}| \) as a user-defined parameter. Popular in hierarchical multi-label classification is the tree-distance loss, which could also be interpreted as a way of evaluating set-valued predictions (see e.g. [Bi and Kwok, 2015]). This loss is not a member of the family \((3)\), however. Besides, from the perspective of abstention in case of uncertainty, it is a useless loss function (see supplementary material).

### 3 Theoretical results

In this section, we present two theoretical results as building blocks of the algorithms that we consider later on. The formulation in (2) seems to suggest that all subsets of \( \mathcal{Y} \) need to be analyzed to find the Bayes-optimal solution, but a first result shows that this is not the case.

**Theorem 1.** The exact solution of (2) can be computed by analyzing only \( K \) subsets of \( \mathcal{Y} \).
Proof. With \( P(\hat{Y} \mid x) = \sum_{c \in \hat{Y}} P(c \mid x) \), the expected utility can be written as

\[
U(\hat{Y}, P, u) = \sum_{c \in \hat{Y}} u(c, \hat{Y}) P(c \mid x) = \sum_{c \in \hat{Y}} u(c, \hat{Y}) P(c \mid x) + \sum_{c' \notin \hat{Y}} u(c', \hat{Y}) P(c' \mid x)
\]

\[
= \sum_{c \in \hat{Y}} g(\hat{Y}) P(c \mid x) = g(\hat{Y}) P(\hat{Y} \mid x),
\]

(5)

where the last summation in the second equality cancels out since \( u(c', \hat{Y}) = 0 \). Let us decompose (2) into an inner and an outer maximization step. The inner maximization step then becomes

\[
\hat{Y}^{ss} = \arg \max_{\hat{Y} \mid |\hat{Y}| = s} g(s) P(\hat{Y} \mid x) = \arg \max_{\hat{Y} \mid |\hat{Y}| = s} P(\hat{Y} \mid x),
\]

(6)

for \( s = \{1, \ldots, K\} \). This step can be done very efficiently, by sorting the conditional class probabilities, as for a given \( s \), only the subset with highest probability needs to be considered. The outer maximization simply consists of computing \( Y^s_u(x) = \arg \max_{\hat{Y} \in \{\hat{Y}^{s+1}_u, \ldots, \hat{Y}^{s+k}_u\}} g(|\hat{Y}| P(\hat{Y} \mid x) \), which only requires the evaluation of \( K \) sets.

So, one only needs to evaluate \( Y^{s+1}_u, \ldots, Y^{s+k}_u \) to find the Bayes-optimal solution, which already limits the search to \( K \) subsets. Can one do even better? It turns out that by restricting \( g \), we can assure that the sequence \( U(Y^{s+1}_u, P, u), \ldots, U(Y^{s+k}_u, P, u) \) is unimodal. The restriction required for \( g \) is \((1/x)\)-convexity, i.e., convexity after a \((1/x)\) transformation.

**Definition 1.** A sequence \( g(1), g(2), \ldots, g(K) \) is \((1/x)\)-convex if

\[
\frac{1}{g(s+1)} \leq \frac{1/g(s) + 1/g(s+2)}{2} \quad \text{for all} \quad s \in \{1, \ldots, K-2\}.
\]

(7)

**Theorem 2.** Let \( g(1), g(2), \ldots, g(K) \) be a \((1/x)\)-convex sequence and let \( U(Y^{s+1}_u, P, u) > U(Y^{s}_u, P, u) \) for a given \( s \in \{1, \ldots, K-1\} \). Then \( U(Y^{s+1}_u, P, u) > U(Y^{s+i}_u, P, u) \) for all \( i \in \{1, \ldots, K-s\} \).

We refer to the supplementary material for a proof. Actually, \((1/x)\)-convexity is a rather weak restriction. One can easily prove that every decreasing, concave sequence is \((1/x)\)-convex (see Theorem 7 in the supplementary material). Many (but not all) convex sequences are also \((1/x)\)-convex. In particular, precision, recall, the F-measure, as well as the \( u_{\alpha, \beta} \) and \( u_{\delta, \gamma} \) families for practically useful values of \( \alpha, \beta, \delta \) and \( \gamma \), are all utilities with associated \((1/x)\)-convex sequences. Precision with \( g_P(s) = 1/s \) in fact defines “how convex” a sequence is allowed to be, because (7) is satisfied as an equality in that boundary case. At the same time, precision is also a boundary case for the properties of \( u(c, \hat{Y}) \) discussed in Section 2.

## 4 Algorithmic results

In this section, we introduce three approaches for solving (2), each consisting of a learning and an inference algorithm. To analyze their complexity, we use a framework similar to learning reductions [Beygelzimer et al. 2016]. We assume that, during prediction, we can query the conditional class distribution \( P \) for a given \( x \). For each approach, we define a class of queries of \( O(1) \) complexity (e.g., in our first approach, one query consists of computing \( P(c \mid x) \) for a particular class \( c \), which for linear models boils down to computing a dot product between model weights and a feature vector). The motivation for this framework is that query operations significantly dominate all other steps of the presented algorithms. For example, although the inference algorithms of all three approaches have an \( O(K \log K) \) time complexity, they will exhibit clear differences in runtime.

We obtain the distribution \( P \) by running a learning algorithm on the training data. To analyze the complexity of this learning algorithm, we also define a basic operation of \( O(1) \) cost per single training example (e.g., one stochastic gradient update for a class). To simplify the analysis, we ignore the accuracy of the distribution \( P \) compared to the true underlying distribution.
Algorithm 1 (UBOP) – input: $g(\cdot), \mathbf{x}, \mathbf{Y} = \{c_1, \ldots, c_K\}, P$

1: $\hat{Y} \leftarrow \emptyset, p_{\hat{Y}} \leftarrow 0, U^* \leftarrow 0$ \hspace{1em} \triangleright Initialize the current best solution, its probability and utility
2: $Q \leftarrow \emptyset$ \hspace{1em} \triangleright Initialize a priority queue that sorts decreasingly the classes by $P(c | \mathbf{x})$
3: for $c \in \mathbf{Y}$ do \hspace{1em} \triangleright For all classes
4: \hspace{1em} $p_c \leftarrow P(c | \mathbf{x}), Q.add((c, p_c))$ \hspace{1em} \triangleright Query the distribution $P$ to get $P(c | \mathbf{x})$
5: $Q.sort()$ \hspace{1em} \triangleright Sort the list decreasingly according $P(c | \mathbf{x})$
6: while $Q \neq \emptyset$ do \hspace{1em} \triangleright Loop until the list of sorted classes is empty
7: \hspace{2em} $(c, p_c) \leftarrow Q.pop()$ \hspace{1em} \triangleright Pop the first element from $Q$
8: \hspace{2em} $\hat{Y} \leftarrow \hat{Y} \cup \{c\}, p_{\hat{Y}} \leftarrow p_{\hat{Y}} + p_c$ \hspace{1em} \triangleright Update the current solution and its probability
9: \hspace{2em} $U_{\hat{Y}} \leftarrow p_c \times g(\hat{Y})$ \hspace{1em} \triangleright Compute $U(\hat{Y}, P, u)$ according to Eq. (3)
10: if $U_{\hat{Y}} \leq U_u$ then \hspace{1em} \triangleright If the utility of the current solution is greater than the best solution so far
11: \hspace{3em} $\hat{Y}_u \leftarrow \hat{Y}, U^* \leftarrow U_{\hat{Y}}$ \hspace{1em} \triangleright Replace the current best solution
12: else \hspace{1em} \triangleright If there is no improvement
13: \hspace{4em} break \hspace{1em} \triangleright break the while loop according to Theorem 2
14: return $\hat{Y}_u$ \hspace{1em} \triangleright Return the set of classes with the highest utility

4.1 Unrestricted Bayes-optimal prediction (UBOP)

In the first approach, we assume that a single query to $P$ yields $P(c | \mathbf{x})$ for a particular class $c$. To train $P$ to answer such queries, we usually use an example from class $c$ to also train conditional probabilities for the other classes (e.g., in the 1-vs-all approach). Therefore, the learning complexity with respect to a single training example is $O(K)$. By combining Theorems 1 and 2, we get the inference procedure presented in Algorithm 1. We start by querying the distribution $P$ to get $K$ conditional class probabilities $P(c | \mathbf{x})$ and sort them in decreasing order. Then, the algorithm computes $U(\hat{Y}_{u+1}, P), \ldots, U(\hat{Y}_{u^*}, P)$ in a sequential way, till the stopping criterion of Theorem 2 is satisfied. In step $s$, $\hat{Y}_u$ is found by adding the class with $s$-highest conditional class probability to the predicted set, starting from the solution obtained in the previous step. The algorithm is a generalization of an algorithm introduced by Coz et al. (2009) for optimizing the $F_\beta$-measure in multi-class classification. There is also a strong correspondence with certain $F_\beta$-maximization algorithms in multi-label classification (see e.g., Jansche (2007), Ye et al. (2012), Waegeman et al. (2014)). To be compliant with the other algorithms, we state a simple result that obviously follows from sorting the conditional class probabilities.

Theorem 3. Algorithm 1 finds the Bayes-optimal solution $\hat{Y}_{u^*}$ with $K$ queries to the distribution $P$.

4.2 Unrestricted Bayes-Optimal prediction with class hierarchy (UBOP-CH)

Algorithm 1 is simple and elegant, but needs $K$ queries to the distribution $P$. As only classes with high probability mass are required, one may think of designing a procedure that queries the top classes one by one, without the need of computing conditional probabilities for all classes. To accomplish this, one could for example adapt specialized data structures used for the approximate nearest neighbors problem (Yagnik et al., 2011; Shrivastava and Li, 2014; Johnson et al., 2017). Instead, we factorize the distribution $P(c | \mathbf{x})$ in a hierarchical way, leading to a tree structure that allows for efficient querying. Factorizing the distribution has the additional advantage of an improved training time. This approach in fact underlies many popular algorithms, such as nested dichotomies (Fox, 1997), Frank and Kramer (2004), conditional probability estimation trees (Beygelzimer et al., 2009), probabilistic classifier trees (Dembczynski et al., 2016), or hierarchical softmax (Morin and Bengio, 2005), often used in neural networks as the output layer.

Let us consider a hierarchical structure over the classes, denoted $T$. Let $V_T$ be the set of nodes. In this structure, each node $v \in V_T$ corresponds to a particular non-empty subset of $\mathbf{Y}$, the root $r_T$ represents the complete set $\mathbf{Y}$, and the leaves are individual classes, i.e., singleton sets. For a given node $v$, let $C(v)$ be a set of its children and $\pi(v)$ its parent. We have that $v \subseteq \pi(v)$. Let us also define $L(v)$ as the set of leaves of the subtree rooted in $v$. The degree of node $v$, denoted by $\deg_v$, is the number of children of that node. The depth of node $v$, denoted by $\text{depth}_v$, is the number of edges on a path from $v$ to the root. By $\deg_T$ and $\text{depth}_T$, we denote, respectively, the degree and the depth of $T$, i.e., $\deg_T = \max_{v \in V_T} \deg_v$ and $\text{depth}_T = \max_{v \in V_T} \text{depth}_v$. 

\[ \text{Algorithm 1 (UBOP)} \]

\[
\begin{align*}
1: & \quad \hat{Y} \leftarrow \emptyset, p_{\hat{Y}} \leftarrow 0, U^* \leftarrow 0 \\
2: & \quad Q \leftarrow \emptyset \\
3: & \quad \text{for } c \in \mathbf{Y} \text{ do} \\
4: & \quad \quad p_c \leftarrow P(c | \mathbf{x}), Q.add((c, p_c)) \\
5: & \quad Q.sort() \\
6: & \quad \text{while } Q \neq \emptyset \text{ do} \\
7: & \quad \quad (c, p_c) \leftarrow Q.pop() \\
8: & \quad \quad \hat{Y} \leftarrow \hat{Y} \cup \{c\}, p_{\hat{Y}} \leftarrow p_{\hat{Y}} + p_c \\
9: & \quad \quad U_{\hat{Y}} \leftarrow p_c \times g(\hat{Y}) \\
10: & \quad \quad \text{if } U_{\hat{Y}} \leq U_u \text{ then} \\
11: & \quad \quad \quad \hat{Y}_u \leftarrow \hat{Y}, U^* \leftarrow U_{\hat{Y}} \\
12: & \quad \quad \text{else} \\
13: & \quad \quad \quad \text{break} \\
14: & \quad \text{return } \hat{Y}_u
\end{align*}
\]
We can express the conditional probability of \( v \in V_T \) recursively by using the chain rule of probability in the following way:

\[
P(v \mid x) = \begin{cases} 
1 & \text{if } v = r_T, \\
Q(v \mid \pi(v), x)P(\pi(v) \mid x) & \text{otherwise},
\end{cases}
\]

in which \( Q(v \mid \pi(v), x) \) depicts the probability of choosing node \( v \) in the parent node \( \pi(v) \), with the property that \( \sum_{v' \in C(\pi(v))} Q(v' \mid \pi(v), x) = 1 \). Remark that, for the leaf nodes, we obtain \( P(\{c\} \mid x) = P(c \mid x), c \in \mathcal{Y} \), i.e., the conditional probabilities of classes.

With such a tree, we assume that queries correspond to probabilities \( Q(v \mid \pi(v), x) \), in contrast to Section 4.1, where queries corresponded to the probabilities \( P(c \mid x) \). As before, the time complexity of the query is \( \mathcal{O}(1) \). The learning algorithm uses a training example whenever it is helpful for training \( Q(v \mid \pi(v), x) \), i.e., when the class \( c \) of the example is in \( \pi \). Since the number of child nodes can be greater than 2, this leads to a multi-class problem. A training example is used in all such problems on the path from the root to the leaf corresponding to \( c \). The final cost of training for a single training example is thus \( \mathcal{O}(\text{deg}_T \cdot \text{depth}_T) \). For balanced trees of a constant degree, this gives a logarithmic complexity in the number of classes.

The tree structure combined with Theorem 2 leads to the inference procedure given as Algorithm 2. This \( A^* \)-style algorithm is closely related to search methods used with probabilistic tree classifiers [Dembczyński et al., 2012]. The algorithm computes \( \hat{Y}_u^1, \ldots, \hat{Y}_u^* \), till the stopping criterion in Theorem 2 is reached. By traversing the tree recursively from the root, we only visit the most promising nodes while pruning a large part of the tree. The algorithm uses a priority queue \( Q \) to store all previously visited nodes in descending order of their probabilities \( P(v \mid x) \), computed via (8). In each step, the node with the highest probability is popped from the list and its child nodes are evaluated. This implies that the leaves are visited in decreasing order of \( P(c \mid x) \). Each time a leaf is visited, the expected utility is determined on the set of classes that correspond to the leaves that are visited so far.

Prior to the main theorem (as a counterpart to Theorem 3), we present the following lemma.

**Lemma 1.** To visit \( v \in V_T \) (i.e., pop the node from queue \( Q \)), with probability \( P(v \mid x) \), Algorithm 2 requires at most \( \lceil 1/P(v \mid x) \rceil \cdot \text{deg}_T \cdot \text{depth}_T \) queries to \( P \).

The proof (see Appendix A) relies on an analysis of the number of nodes in the subtree of \( T \) that consists of nodes with probabilities greater than or equal to \( P(v \mid x) \). The key insight is that the number of leaves in this subtree is upper bounded by \( \lceil 1/P(v \mid x) \rceil \).

**Theorem 4.** Algorithm 2 finds the Bayes-optimal solution \( \hat{Y}_u^* \) with at most \( \lceil 1/p \rceil \cdot \text{deg}_T \cdot \text{depth}_T \) queries to distribution \( P \), where \( p = (1 - P(\hat{Y}_u^*)/(K - |\hat{Y}_u^*|)) \).

The theorem is proven by using Lemma 1 and noticing that the inference procedure stops after visiting a leaf with the highest probability, whose class is not included in \( \hat{Y}_u^* \) (see Appendix A). In the worst case, the number of calls to \( P \) can be as high as \( 2 \cdot K - 2 \), but it will usually be much smaller than \( K \). More precisely, for \( p > \text{deg}_T \cdot \text{depth}_T/K \), the number of queries is less than \( K \). For example, this boils down to \( p > 2 \log_2 K/K \) for complete binary trees.

### 4.3 Restricted Bayes-optimal prediction with class hierarchy (RBOP-CH)

This approach uses the same distribution \( P \) as in the previous section. Therefore, the training complexity as well as the complexity of a single query are the same. However, we slightly change the definition of the problem by restricting the set of possible set-valued predictions to the nodes in \( V_T \), i.e., \( \hat{Y} \in V_T \). This further improves the complexity of Algorithm 2. In addition to runtime gains, limiting the search to sets that naturally appear as nodes in the hierarchy also greatly reduces the “semantic complexity” for problems where a correctly specified hierarchy exists. When a domain expert constructs a hierarchy, he/she is often only interested in analyzing those sets, which correspond to groups of classes that belong together, and therefore have a clear interpretation. This is a second motivation for restricting the search to particular subsets.

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1. A similar inference algorithm could be used with the distribution \( P \) considered in Section 4.1 by first getting \( P(c \mid x) \) for all \( c \in \mathcal{Y} \) and then computing the node probabilities by simple summation. This approach, however, uses \( K \) queries to the distribution.
Algorithm 2 (UBOP-CH) – input: \( g(\cdot), x, Y = \{c_1, \ldots, c_K\}, P, T \)

1: \( \hat{Y} \leftarrow \emptyset, \ P_{\hat{Y}} \leftarrow 0, U^* \leftarrow 0 \) \hspace{1cm} \triangleright \text{Initialize the current best solution, its its probability and utility}
2: \( Q \leftarrow \emptyset \) \hspace{1cm} \triangleright \text{Initialize a priority queue that sorts decreasingly the nodes by } P(v | x) \n3: \( Q.\text{add}((r_T, 1)) \) \hspace{1cm} \triangleright \text{Add the root node with probability 1 to the queue}
4: \text{while } Q \neq \emptyset \text{ do} \hspace{1cm} \triangleright \text{While the queue is not empty}
5: \( (v, p_v) \leftarrow Q.\text{pop}() \) \hspace{1cm} \triangleright \text{Pop the first node in } Q
6: \text{if } |v| = 1 \text{ then} \hspace{1cm} \triangleright \text{If the node is the leaf (i.e., the corresponding set of classes is a singleton}
7: \( \hat{Y} \leftarrow \hat{Y} \cup v, p_{\hat{Y}} \leftarrow p_{\hat{Y}} + p_v \) \hspace{1cm} \triangleright \text{Update the current solution and its probability}
8: \( U_{\hat{Y}} \leftarrow p_{\hat{Y}} \times g(|\hat{Y}|) \) \hspace{1cm} \triangleright \text{Compute } U(\hat{Y}, P, u) \text{ according to Eq. (5)}
9: \text{if } U^* \leq U_{\hat{Y}} \text{ then} \hspace{1cm} \triangleright \text{If the utility of the current solution is better than the previous ones}
10: \( \hat{Y}^* \leftarrow \hat{Y}, U^* \leftarrow U_{\hat{Y}} \) \hspace{1cm} \triangleright \text{Replace the current best solution}
11: \text{else} \hspace{1cm} \triangleright \text{If there is no improvement}
12: \text{break} \hspace{1cm} \triangleright \text{break the while loop according to Theorem 5}
13: \text{else} \hspace{1cm} \triangleright \text{If the node is the internal node}
14: \text{for } v' \in C(v) \text{ do} \hspace{1cm} \triangleright \text{For each child node}
15: \( q_{v'} \leftarrow Q(v' | v, x) \) \hspace{1cm} \triangleright \text{Query the distribution } P \text{ to get } Q(v' | v, x)
16: \( Q.\text{add}((v', q_{v'} \times p_v)) \) \hspace{1cm} \triangleright \text{Add the child node with } P(v | x) \text{ to the queue}
17: \text{return } \hat{Y}^*_u \hspace{1cm} \triangleright \text{Return the set of classes with the highest utility}

Algorithm 3 (RBOP-CH) – input: \( g(\cdot), x, Y = \{c_1, \ldots, c_K\}, P, T \)

1: \( \hat{Y} \leftarrow \emptyset, \ P_{\hat{Y}} \leftarrow 0, U^* \leftarrow 0 \) \hspace{1cm} \triangleright \text{Initialize the current best solution, its its probability and utility}
2: \( Q \leftarrow \emptyset \) \hspace{1cm} \triangleright \text{Initialize a priority queue that sorts decreasingly the nodes by } P(v | x) \n3: \( Q.\text{add}((r_T, 1)) \) \hspace{1cm} \triangleright \text{Add the root node with probability 1 to the queue}
4: \text{while } Q \neq \emptyset \text{ do} \hspace{1cm} \triangleright \text{While the queue is not empty}
5: \( (v, p_v) \leftarrow Q.\text{pop}() \) \hspace{1cm} \triangleright \text{Pop the first node in } Q
6: \( \hat{Y} \leftarrow v, p_{\hat{Y}} \leftarrow p_v \) \hspace{1cm} \triangleright \text{Update the current solution and its probability}
7: \( U_{\hat{Y}} \leftarrow p_{\hat{Y}} \times g(|\hat{Y}|) \) \hspace{1cm} \triangleright \text{compute } U(\hat{Y}, P, u) \text{ according to Eq. (5)}
8: \text{if } U^* \leq U_{\hat{Y}} \text{ then} \hspace{1cm} \triangleright \text{If the utility of the current solution is better than the previous ones}
9: \( \hat{Y}^* \leftarrow \hat{Y}, U^* \leftarrow U_{\hat{Y}} \) \hspace{1cm} \triangleright \text{Replace the current best solution}
10: \text{if } |v| = 1 \text{ then} \hspace{1cm} \triangleright \text{If the node is the leaf (i.e., the corresponding set of classes is a singleton}
11: \text{break} \hspace{1cm} \triangleright \text{break the while loop according to Theorem 5}
12: \text{else} \hspace{1cm} \triangleright \text{If the node is the internal node}
13: \text{for } v' \in C(v) \text{ do} \hspace{1cm} \triangleright \text{For each child node}
14: \( q_{v'} \leftarrow Q(v' | v, x) \) \hspace{1cm} \triangleright \text{Query the distribution } P \text{ to get } Q(v' | v, x)
15: \( Q.\text{add}((v', q_{v'} \times p_v)) \) \hspace{1cm} \triangleright \text{Add the child node with } P(v | x) \text{ to the queue}
16: \text{return } \hat{Y}^*_u \hspace{1cm} \triangleright \text{Return the set of classes with the highest utility}

Adopting the same reasoning as in \( \boxed{5} \), the utility maximization problem now becomes

\[
\hat{Y}_u^T(x) = \operatorname{arg\:max}_{\hat{Y} \in V_T} U(\hat{Y}, P, u) = \operatorname{arg\:max}_{\hat{Y} \in V_T} g(|\hat{Y}|) P(\hat{Y} | x). \tag{9}
\]

Algorithm \( \boxed{3} \) solves this restricted optimization problem in an exact manner. It modifies Algorithm \( \boxed{2} \) with regard to two aspects: (a) After popping a node from \( Q \), it immediately evaluates the expected utility of the subset that corresponds to that node, and (b) it stops as soon as it encounters a leaf. Due to modification (a), only sets of classes that are associated with the nodes in \( V_T \) are considered as candidate predictions. The second modification explains why Algorithm \( \boxed{3} \) should be faster than Algorithm \( \boxed{2} \). The following result states the correctness of the algorithm and an upper bound of the number of queries to the distribution \( P \), which in many cases is significantly lower than \( K \).

**Theorem 5.** Algorithm \( \boxed{3} \) finds the Bayes-optimal solution \( \hat{Y}_u^T(x) \) to the restricted maximization problem in \( \boxed{2} \) with at most \( \lceil 1/p_{\max} \rceil \cdot \deg_T \cdot \text{depth}_T \) queries to the distribution \( P \) to find \( \hat{Y}_u^T(x) \), where \( p_{\max} = \max_{c \in Y} P(c | x) \).

To show the correctness, our proof (Section \( \boxed{7} \) in the Appendix) makes use of a decomposition into an inner and outer maximization, similar to Theorem \( \boxed{1} \). The key observation is that, among the nodes with the same number of classes, the algorithm always visits a node with highest probability first. To show the upper bound for the number of queries, we use Lemma \( \boxed{4} \) and the fact that the algorithm
Table 1: Performance versus runtime for restricted (UBOP, UBOP-CH) and unrestricted (RBOP-CH) classifiers, tested on seven benchmark datasets. Notation: $K$ – number of classes, $N$ – number of samples, ACC – top-1 accuracy, $u$ – average utility score, $|Y|$ – average prediction size, $t$ – CPU time in seconds

| Dataset   | Classifier | $t_{train}$ | $t_{test}$ | $u_{\alpha=1,\beta=0.1}$ | $|Y|$ | $t_{test}$ | $u_{\alpha=1,\beta=0.5}$ | $|Y|$ | $t_{test}$ |
|-----------|------------|-------------|------------|---------------------------|------|------------|--------------------------|------|------------|
| VOC2006, $K = 10$ | UBOP | 7.5 | 5.3 | 90.72 | 1.0 | 5.5 | 91.33 | 1.1 | 5.8 | 93.07 | 1.1 | 5.5 |
| $N_{train}$ = 1508 | UBOP-CH | 6.3 | 89.98 | 5.0 | 5.0 | 90.64 | 1.1 | 4.9 | 94.25 | 1.2 | 5.0 |
| $N_{test}$ = 1477 | RBOP-CH | 6.3 | 89.98 | 5.0 | 4.9 | 90.32 | 1.0 | 5.0 | 91.70 | 1.1 | 5.0 |
| VOC2007, $K = 20$ | UBOP | 23.9 | 88.28 | 12.8 | 88.28 | 1.0 | 12.3 | 89.53 | 1.1 | 12.4 | 92.72 | 1.3 | 13.8 |
| $N_{train}$ = 2638 | UBOP-CH | 17.3 | 87.82 | 10.8 | 87.82 | 1.0 | 11.2 | 89.00 | 1.1 | 11.2 | 92.34 | 1.3 | 11.2 |
| $N_{test}$ = 2841 | RBOP-CH | 17.3 | 87.82 | 10.8 | 88.23 | 1.0 | 10.8 | 89.97 | 1.0 | 10.7 | 89.97 | 1.3 | 10.6 |
| CAL101, $K = 97$ | UBOP | 234.9 | 95.14 | 42.1 | 95.14 | 1.0 | 48.7 | 96.73 | 1.2 | 63.5 | 98.55 | 1.5 | 45.6 |
| $N_{train}$ = 4338 | UBOP-CH | 47.3 | 92.95 | 23.2 | 92.95 | 1.0 | 23.0 | 94.88 | 1.3 | 27.8 | 97.35 | 1.8 | 27.1 |
| $N_{test}$ = 4339 | RBOP-CH | 47.3 | 92.95 | 23.2 | 92.95 | 1.0 | 23.1 | 95.73 | 1.5 | 27.5 | 94.22 | 2.3 | 27.7 |
| CAL256, $K = 256$ | UBOP | 2226 | 80.82 | 333.6 | 80.82 | 1.0 | 337.6 | 88.07 | 2.2 | 365.0 | 93.42 | 3.7 | 317.3 |
| $N_{train}$ = 14890 | UBOP-CH | 360.7 | 70.73 | 98.0 | 70.73 | 1.0 | 116.4 | 79.73 | 2.4 | 134.0 | 86.69 | 4.0 | 152.1 |
| $N_{test}$ = 14890 | RBOP-CH | 360.7 | 70.73 | 98.0 | 70.73 | 1.0 | 101.9 | 72.38 | 3.7 | 102.4 | 75.20 | 6.6 | 101.9 |
| PROTEIN, $K = 3486$ | UBOP | 774.5 | 55.82 | 1294 | 56.71 | 60.0 | 1002 | 70.24 | 341.4 | 947 | 78.94 | 504.6 | 927 |
| $N_{train}$ = 12206 | UBOP-CH | 738.5 | 57.17 | 38 | 57.86 | 2.0 | 50 | 78.36 | 13.9 | 81 | 87.43 | 33.8 | 116 |
| $N_{test}$ = 9803 | RBOP-CH | 738.5 | 57.17 | 38 | 57.76 | 8.2 | 38 | 73.15 | 69.5 | 38 | 83.66 | 125.5 | 38 |
| LSHTC1, $K = 12204$ | UBOP | 60398 | 39.64 | 6749 | 11.23 | 3663 | 6751 | 39.10 | 4466 | 6762 | 56.30 | 5272 | 6776 |
| $N_{train}$ = 309905 | UBOP-CH | 76077 | 33.20 | 58 | 36.40 | 57 | 87 | 65.73 | 154 | 158 | 76.56 | 286 | 206 |
| $N_{test}$ = 34905 | RBOP-CH | 76077 | 33.20 | 58 | 33.69 | 182 | 58 | 52.23 | 700 | 58 | 63.58 | 932 | 58 |
| Dmoz, $K = 27874$ | UBOP | 9.1 | 10 | 17.35 | 4×10^4 | 11.46 | 8063 | 4×10^4 | 39.79 | 9899 | 4×10^4 | 57.33 | 11670 | 4×10^4 |
| $N_{train}$ = 304760 | UBOP-CH | 9.1 | 10 | 17.35 | 4×10^4 | 11.46 | 8063 | 4×10^4 | 39.79 | 9899 | 4×10^4 | 57.33 | 11670 | 4×10^4 |
| $N_{test}$ = 104263 | RBOP-CH | 9.1 | 10 | 17.35 | 4×10^4 | 11.46 | 8063 | 4×10^4 | 39.79 | 9899 | 4×10^4 | 57.33 | 11670 | 4×10^4 |
| $N_{max} = 10$ | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 | 104263 |

Steps after reaching the first leaf. Notice that the ratio of costs between Algorithm 3 and Algorithm 2 can be characterized by the ratio between $p_{max}$ and $p$ from Theorem 4. Moreover, in the worst case, the number of queries of Algorithm 3 is $2 \cdot K − 2$.

5 Empirical results

We experimentally compare the UBOP, UBOP-CH, and RBOP-CH approaches on seven benchmark datasets with a predefined hierarchy over the classes, because RBOP-CH is only useful when such a hierarchy exists. We analyze four image classification datasets: VOC 2006, VOC 2007, Caltech-101, and Caltech-256, two large-scale text classification datasets LSHTC1 and DMOZ, and two large-scale protein datasets. Hidden representations for the image and protein datasets are obtained by using convolutional neural nets, implemented in Python (PyTorch library [Paszke et al., 2017]) and trained end-to-end on a GPU. For text classification, we use bag-of-words hidden representations assumed to be fixed and given throughout the experiments. For training the probabilistic model, we well for the implementation of the inference algorithms, we use C++ (Liblinear library [Fan et al., 2008]) to assure a fair comparison between all classifiers. We estimate the probabilistic model in (6) by means of a hierarchical softmax layer that utilizes the predefined hierarchy. A more in-depth description of the experimental setup can be found in Section C in the supplementary material.

In Table 1, we report results for UBOP, UBOP-CH, and RBOP-CH, optimized on three convex utility scores, listed in decreasing order of convexity: $u_{\alpha=1,\beta=0.1}$, $u_{\alpha=1,\beta=0.5}$, and $u_{\alpha=1,\beta=1}$. We report the predictive performance, the runtime and the size of the predicted sets for these utility scores. All scores are averages over the test set. We also perform inference for the mode of $P(c|x)$ as a reference, and report top-1 accuracy in that case. In addition, we show some relevant statistics regarding the benchmark datasets, such as the number of classes and sample sizes.

Unsurprisingly, imposing a hierarchy over the classes leads to a clear gain in training time, due to factorizing the distribution $P$. In addition, clear test time gains are observed when using UBOP-CH, which is in accordance with our theoretical results. Moreover, the efficiency becomes even higher when further restricting the search space. For RBOP-CH, the test time is identical to inference for the mode, with small differences due to separate runs.

However, imposing a hierarchy comes at the expense of top-1 accuracy for most datasets. In case of less convex utility scores, the algorithms typically return bigger prediction sets, resulting in a higher recall for all algorithms. This clearly illustrates the trade-off between precision and correctness that

2The multi-label VOC datasets are preprocessed by removing instances with more than one label.
comes with set-based predictions. When comparing the classifiers with a hierarchical probabilistic model, it is clear that restricting the search space during inference (RBOP-CH) results in predictive performance drops. For the image datasets, UBOP seems to yield the best predictive performance. This can be attributed to several factors, such as the relatively low number of classes, informative hidden representations that facilitate the classification tasks, or the use of less meaningful hierarchies. In contrast, UBOP-CH and RBOP outperform UBOP on the datasets with large $K$. In these cases, rather simple hidden representations, together with a high class imbalance, make the classification problem much harder. Here, factorizing the probability distribution by means of a meaningful hierarchy is beneficial. In Section F of the supplementary material, we present additional theoretical results that shed more light on the price one might pay by factorizing the probability distribution.

6 Conclusion

We introduced a decision-theoretic framework for a general family of set-based utility functions, including most of the measures used in the literature so far, and developed three Bayes-optimal inference algorithms that exploit specific assumptions to improve runtime efficiency. Depending on the concrete dataset, those assumptions may or may not affect predictive performance.

In future work, we plan to extend our decision-theoretic framework toward uncertainty representations more general than standard probability, for example taking up a distinction between so-called aleatoric and epistemic uncertainty recently put forward by several authors [Senge et al., 2014, Kendall and Gal, 2017, Depeweg et al., 2018, Nguyen et al., 2018].

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Supplementary material for “Efficient Algorithms for Set-Valued Prediction in Multi-Class Classification”

A Interpretation of different utility scores

In this section we provide a tabular overview of the different utility scores discussed in the main paper, with an indication of the corresponding form for \( g \). In Figure 1 we also plot \( g \) for the different utility scores.

| Name              | Utility \( u(c, \hat{Y}) \)                                                                 | \( g \)       |
|-------------------|------------------------------------------------------------------------------------------|---------------|
| Precision [Coz et al. 2009] | \[
\begin{align*}
    u_{\text{P}}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    \frac{1}{|\hat{Y}|} & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\text{P}}(s) &= \frac{1}{s}
\end{align*}
\] |               |
| Recall [Coz et al. 2009]       | \[
\begin{align*}
    u_{\text{R}}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    1 & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\text{R}}(s) &= 1
\end{align*}
\] |               |
| F1-measure [Coz et al. 2009]   | \[
\begin{align*}
    u_{\text{F1}}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    \frac{2}{1 + |\hat{Y}|} & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\text{F1}}(s) &= \frac{2}{1 + s}
\end{align*}
\] |               |
| Credal Utility [Zaffalon et al. 2012] | \[
\begin{align*}
    u_{\delta,\gamma}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    \delta & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\delta,\gamma}(s) &= \delta - \frac{\gamma}{s}
\end{align*}
\] |               |
| Exp. Utility [Zaffalon et al. 2012] | \[
\begin{align*}
    u_{\exp}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    1 - \exp\left(-\frac{\delta}{|\hat{Y}|}\right) & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\exp}(s) &= 1 - \exp\left(-\frac{\delta}{s}\right)
\end{align*}
\] |               |
| Log. Utility [Zaffalon et al. 2012] | \[
\begin{align*}
    u_{\log}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    \log\left(1 + \frac{1}{|\hat{Y}|}\right) & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\log}(s) &= \log(1 + \frac{1}{s})
\end{align*}
\] |               |
| Reject Option [Ramaswamy et al. 2015a] | \[
\begin{align*}
    u_{\alpha}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    1 & \text{if } \hat{Y} = \{c\}, \\
    1 - \alpha & \text{if } \hat{Y} = \hat{Y},
    \end{cases} \\
    g_{\alpha}(s) &= \begin{cases} 
    1 & \text{if } s = 1, \\
    1 - \alpha & \text{if } s = K.
    \end{cases}
\end{align*}
\] |               |
| Gen. Reject Option (Eq. 4) | \[
\begin{align*}
    u_{\alpha,\beta}(c, \hat{Y}) &= \begin{cases} 
    0 & \text{if } c \notin \hat{Y}, \\
    1 - \alpha \left(\frac{|\hat{Y}| - 1}{N - 1}\right)^{\beta} & \text{if } c \in \hat{Y},
    \end{cases} \\
    g_{\alpha,\beta}(s) &= 1 - \alpha \left(\frac{s - 1}{N - 1}\right)^{\beta}
\end{align*}
\] |               |

B Additional discussion on the tree distance loss

The tree distance loss \( \ell_T(c, \hat{Y}) \) is defined as the path distance between the true class \( c \) and the prediction \( \hat{Y} \) in the hierarchy. In the main text we claim that the Bayes-optimal predictor for the tree distance loss always returns the smallest subtree with probability at least 0.5. This result was proven by [Ramaswamy et al. 2015b], albeit for a slightly different framework, where the ground truth \( c \) can also be an internal node of the hierarchy. Below we show that the same result also applies to our framework. Consequently, the tree distance loss is not appealing from an abstention perspective, because it does not have a mechanism for controlling the size of a set \( \hat{Y} \). In general, this loss will return rather large sets as prediction.

For the theorem and the proof we use some of the notations that are introduced in the main paper. Let us additionally define the Bayes-optimal prediction \( \hat{Y}^* \) for the tree-distance loss \( \ell_T \) as the minimizer of the expected risk:

\[
\hat{Y}^* = \arg \min_{\hat{Y} \in V_T} R(\hat{Y}, P, \ell_T),
\]  

(10)

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Figure 1: A visualization of $g(|\hat{Y}|)$ for different values of $|\hat{Y}|$ and different set-based utility functions. Top: $K = 10$, Bottom: $K = 100$.

where the expected risk is given by

$$R(\hat{Y}, P, \ell_T) = \sum_{c \in \mathcal{Y}} \ell_T(c, \hat{Y}) P(c | x).$$

**Theorem 6.** The solution of optimization problem (10) is the prediction $\hat{Y}^*_\ell \in V_T$ that satisfies the following two properties:

1. $P(\hat{Y}^*_\ell | x) \geq 0.5,$
2. $\forall \hat{Y} \in C(\hat{Y}^*_\ell) : P(\hat{Y} | x) < 0.5.$

**Proof.** Assume that we search for the node $\hat{Y} \in V_T$ for which $|L(\hat{Y})|$ is minimal and having $P(\hat{Y} | x) \geq 0.5$. This subtree will be denoted $\hat{Y}_{0.5}$. It can be found by greedy search, using an approach that is very similar to Algorithm 2, starting from the root of the hierarchy. If $\hat{Y}_{0.5} = \hat{Y}^*_\ell$, then the theorem trivially holds. Therefore, assume $\hat{Y}_{0.5} \neq \hat{Y}^*_\ell$. We will prove that this leads to a contradiction. To this end, let us denote the regret of $\hat{Y}_{0.5}$, w.r.t. the tree-distance loss $\ell_T$, by:

$$\Delta(\hat{Y}_{0.5}) = R(\hat{Y}^*_\ell, P, \ell_T) - R(\hat{Y}_{0.5}, P, \ell_T),$$

and let $D(\hat{Y})$ be the set of descendants of node $\hat{Y}$. Now, let us consider three cases:
Case 1: \( \hat{Y}_\ell^* \notin D(\hat{Y}_{0.5}) \)

\[
\Delta_\ell(\hat{Y}_{0.5}) = \sum_{\hat{Y} \in L(\hat{Y}_{0.5})} (\ell_T(\hat{Y}, \hat{Y}_\ell^*) - \ell_T(\hat{Y}, \hat{Y}_{0.5})) P(\hat{Y} \mid x) \\
+ \sum_{\hat{Y} \in L(\hat{Y}_{0.5})} (\ell_T(\hat{Y}', \hat{Y}_\ell^*) - \ell_T(\hat{Y}', \hat{Y}_{0.5})) P(\hat{Y}' \mid x),
\]

\[
= \sum_{\hat{Y} \in L(\hat{Y}_{0.5})} \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_{0.5})} (\ell_T(\hat{Y}', \hat{Y}_\ell^*) - \ell_T(\hat{Y}', \hat{Y}_{0.5})) P(\hat{Y}' \mid x),
\]

\[
\geq \sum_{\hat{Y} \in L(\hat{Y}_{0.5})} \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_{0.5})} -\ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}' \mid x),
\]

\[
= \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}_{0.5} \mid x) - \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5})(1 - P(\hat{Y}_{0.5} | x)),
\]

\[
= \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}_{0.5} \mid x)(2P(\hat{Y}_{0.5} \mid x) - 1),
\]

\[
\geq 0,\]

and, hence, giving a contradiction.

Case 2: \( \hat{Y}_\ell^* \in D(\hat{Y}_{0.5}) \setminus C(\hat{Y}_{0.5}) \)

Let \( \hat{Y}_c \) be the child of \( \hat{Y}_{0.5} \) that is an ancestor of \( \hat{Y}_\ell^* \). By construction it holds that \( P(\hat{Y}_c \mid x) \leq 0.5 \), such that

\[
\Delta_\ell(\hat{Y}_{0.5}) = \sum_{y \in L(\hat{Y}_c)} (\ell_T(\hat{Y}, \hat{Y}_\ell^*) - \ell_T(\hat{Y}, \hat{Y}_{0.5})) P(\hat{Y} \mid x) \\
+ \sum_{\hat{Y} \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_c)} (\ell_T(\hat{Y}', \hat{Y}_\ell^*) - \ell_T(\hat{Y}', \hat{Y}_{0.5})) P(\hat{Y}' \mid x),
\]

\[
= \sum_{\hat{Y} \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_c)} (\ell_T(\hat{Y}, \hat{Y}_\ell^*) - \ell_T(\hat{Y}, \hat{Y}_{0.5})) P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_c)} \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}' \mid x),
\]

\[
\geq \sum_{\hat{Y} \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_c)} -\ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_c)} \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}' \mid x),
\]

\[
= -\ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5}) P(\hat{Y}_c \mid x) \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5})(1 - P(\hat{Y}_c \mid x)),
\]

\[
= \ell_T(\hat{Y}_\ell^*, \hat{Y}_{0.5})(1 - 2P(\hat{Y}_c \mid x)),
\]

\[
\geq 0,\]

again yielding a contradiction.

Case 3: \( \hat{Y}_\ell^* \in C(\hat{Y}_{0.5}) \)

By construction it holds that \( P(\hat{Y}_\ell^* \mid x) \leq 0.5 \).

\[
\Delta_\ell(\hat{Y}_{0.5}) = \sum_{\hat{Y} \in L(\hat{Y}_\ell^*)} (\ell_T(\hat{Y}, \hat{Y}_\ell^*) - \ell_T(\hat{Y}, \hat{Y}_{0.5})) P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_\ell^*)} (\ell_T(\hat{Y}', \hat{Y}_\ell^*) - L_T(\hat{Y}', \hat{Y}_{0.5})) P(\hat{Y}' \mid x),
\]

\[
= \sum_{\hat{Y} \in L(\hat{Y}_\ell^*)} -P(\hat{Y} \mid x) + \sum_{\hat{Y}' \in L(\hat{Y}_{0.5}) \setminus L(\hat{Y}_\ell^*)} P(\hat{Y}' \mid x),
\]

\[
= 1 - 2P(\hat{Y}_\ell^* \mid x),
\]

\[
\geq 0,
\]

and, finally, also leading to a contradiction. \(\square\)

### C Additional discussion on Theorem 2

In this section we provide more background on Theorem 2 from the main paper.
We are now ready to prove Theorem 2 from the main paper.

**Definition 1.** A sequence \( g(1), g(2), \ldots, g(K) \) is \((1/x)\)-convex if
\[
1/g(s + 1) \leq \frac{1/g(s) + 1/g(s + 2)}{2} \quad \text{for all } s \in \{1, \ldots, K - 2\}. \tag{7}
\]

As claimed in the main paper, we show that every decreasing, concave sequence is \((1/x)\)-convex.

**Definition 2.** A sequence \( g(1), g(2), \ldots, g(K) \) is concave if
\[
g(s + 1) \geq \frac{g(s) + g(s + 2)}{2} \quad \text{for all } s \in \{1, \ldots, K - 2\}
\]

**Theorem 7.** Let \( g(1), g(2), \ldots, g(K) \) be a concave, decreasing sequence. Then \( g(1), g(2), \ldots, g(K) \) is also \((1/x)\)-convex.

**Proof.** Let us first observe the following equivalence.
\[
1/g(s + 1) \leq \frac{1/g(s) + 1/g(s + 2)}{2} \tag{8}
\]
\[
\iff 2 \leq \frac{g(s + 1)}{g(s)} + \frac{g(s + 1)}{g(s + 2)} \tag{9}
\]
\[
\iff g(s)g(s + 1) + g(s + 2)g(s + 1) \geq 2g(s)g(s + 2) \tag{10}
\]
\[
\iff g(s)[g(s + 1) - g(s + 2)] \geq g(s + 2)[g(s) - g(s + 1)] \tag{11}
\]

If \( g(1), g(2), \ldots, g(K) \) is decreasing it holds that \( g(s) \geq g(s + 2) \). If \( g(1), g(2), \ldots, g(K) \) is concave it also holds that
\[
g(s + 1) - g(s + 2) \geq g(s) - g(s + 1).
\]
Combining those two inequalities lets us conclude that the sequence must be \((1/x)\)-convex. \( \square \)

We are now ready to prove Theorem 2 from the main paper.

**Theorem 2.** Let \( g(1), g(2), \ldots, g(K) \) be a \((1/x)\)-convex sequence and let \( U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \) for a given \( s \in \{1, \ldots, K - 1\} \). Then \( U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \) for all \( i \in \{1, \ldots, K - s\} \).

**Proof.** Starting from (11), as an equivalence for \((1/x)\)-convexity of a sequence, we derive a couple of additional equivalences.
\[
g(s)[g(s + 1) - g(s + 2)] \geq g(s + 2)[g(s) - g(s + 1)] \tag{12}
\]
\[
\iff \frac{g(s)}{g(s) - g(s + 1)} \geq \frac{g(s + 2)}{g(s + 1) - g(s + 2)} \tag{13}
\]
\[
\iff \frac{g(s + 1)}{g(s) - g(s + 1)} + 1 \geq \frac{g(s + 2)}{g(s + 1) - g(s + 2)} \tag{14}
\]

Let us assume that for a given \( s \) it holds that \( U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \). We need to prove that \( U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \) for all \( i \in \{1, \ldots, K - s\} \). Let \( p_i = P(c_i | x) \) and let us first observe that the following equivalences hold.
\[
U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \iff g(s) \sum_{i=1}^{s} p_i > g(s + 1) \sum_{i=1}^{s+1} p_i \tag{15}
\]
\[
\iff (g(s) - g(s + 1)) \sum_{i=1}^{s} p_i > g(s + 1)p_{s+1} \tag{16}
\]
\[
\iff \sum_{i=1}^{s} p_i > \frac{g(s + 1)}{g(s) - g(s + 1)} p_{s+1} \tag{17}
\]
To prove that \( U(\hat{Y}_u^{s*}, P, u) > U(\hat{Y}_u^{s+i}, P, u) \) for all \( i \in \{1, \ldots, K - s\} \) we prove that
\[
U(\hat{Y}_u^{s+i}, P, u) > U(\hat{Y}_u^{s+i+1}, P, u) \tag{18}
\]
and use mathematical induction to complete the proof. To prove (14) observe that from (12) and (13) it follows that

\[ \sum_{i=1}^{s+1} p_i > \frac{g(s + 1)}{g(s) - g(s + 1)} p_{s+1} + p_{s+1} \]  
\[ \iff \sum_{i=1}^{s+1} p_i > \left( \frac{g(s + 1)}{g(s) - g(s + 1)} + 1 \right) p_{s+1} \]  
\[ \Rightarrow \sum_{i=1}^{s+1} p_i > \frac{g(s + 2)}{g(s + 1) - g(s + 2)} p_{s+2} \]  
\[ \iff U(\hat{Y}_{s+1}, P, u) > U(\hat{Y}_{s+2}, P, u) \]  
\[ \square \]

D Proofs of results concerning UBOP-CH

Lemma 1. To visit \( v \in V_T \) (i.e., pop the node from queue \( Q \)), with probability \( P(v \mid x) \), Algorithm 2 requires at most \( [1/P(v \mid x)] \cdot \deg_T \cdot \text{depth}_T \) queries to \( P \).

Proof. First notice that the number of queries to \( P \) is equivalent to the number of insertions of nodes to \( Q \). Next, consider a subtree \( T' \) that consists of nodes of \( T \) such that for each \( v' \in T' \) we have \( P(v' \mid x) \geq P(v \mid x) \). Obviously \( T' \) contains the node \( v \). Since for each \( v \in V_T \) we have \( \sum_{v' \in C(v)} Q(v') \pi(v') = 1 \), this tree cannot have more than \( [1/P(v \mid x)] \) leaves. Notice however that some internal nodes of \( T' \) can be of degree 1. Taking this into account \( T' \) consists of at most \( [1/P(v \mid x)] \cdot \text{depth}_T \) nodes, i.e., we count here all nodes on paths from leaves to the root assuming the depth of each leave to be equal \( \text{depth}_T \). From the construction of Algorithm 2 we observe that all nodes from \( T' \) will be visited (popped from queue \( Q \)) before approaching any node with probability less than \( P(v \mid x) \). The final bound is obtained by observing that for each visited node from \( T' \) distribution \( P \) is queried at most \( \deg_T \) times. \( \square \)

Theorem 4. Algorithm 2 finds the Bayes-optimal solution \( \hat{Y}_u^* \) with at most \( [1/p] \cdot \deg_T \cdot \text{depth}_T \) queries to distribution \( P \), where \( p = (1 - P(\hat{Y}_u^*)/(K - |\hat{Y}_u^*|)) \).

Proof. From Theorem 2 we can easily observe that the algorithm finds the optimal solutions as it visits the leaf nodes corresponding the classes in the decreasing order of \( P(c \mid x) \). Next, we prove the upper bound for the number of queries to \( P \). Let \( p \) be the highest probability among classes not in \( \hat{Y}_u^* \). Because of the stopping criterion, the algorithm will stop after visiting a leaf with probability \( p \). From Lemma 1 we know that to find a node with probability \( p \) we need at most \( [1/p] \cdot \text{depth}_T \cdot \deg_T \) queries to \( P \). From this we see that we need to find the lowest possible value of \( p \) to get the upperbound of queries needed to get the Bayes optimal solution. It is easy to observe that the lowest \( p \) we obtain for the uniform distribution over the classes outside \( \hat{Y}_u^* \), i.e.,

\[ p = \frac{1 - P(\hat{Y}_u^*)}{K - |\hat{Y}_u^*|}. \]

\( \square \)

E A proof of Theorem concerning RBOP-CH

Theorem 5. Algorithm 3 finds the Bayes-optimal solution \( \hat{Y}_u^T(x) \) to the restricted maximization problem in \( Q \) with at most \( [1/p_{\text{max}}] \cdot \deg_T \cdot \text{depth}_T \) queries to the distribution \( P \) to find \( \hat{Y}_u^T \), where \( p_{\text{max}} = \max_{c \in Y} P(c \mid x) \).
which the lower bound holds. As we make a restriction to binary trees, let us consider when the unrestricted Bayes-optimal prediction is not part of this restricted search space. Such a

The upper bound of the number of queries to distribution $P$ we obtain by applying Lemma 1 and noticing that the algorithm stops after reaching the first leaf, for which we have $p_{\text{max}} = \max_{x \in Y} P(c \mid x)$. \qed

\section{Restricted versus unrestricted Bayes-optimal prediction}

The RBOP-CH algorithm, which restricts the search to nodes in the hierarchy, yields a substantial improvement over the unrestricted Bayes-optimal algorithm in terms of runtime. Do we have to pay a price for restricting the search to sets that occur in some hierarchy? The answer is in general yes, when the unrestricted Bayes-optimal prediction is not part of this restricted search space. Such a situation is not unrealistic, because domain experts not always have predictive performance in mind when they define a hierarchy over classes. This is also observed in the experimental results, where the RBOP-CH algorithm outperforms the unrestricted algorithms on some datasets, while it yields a suboptimal predictive performance on other datasets. So, what’s the worst-case regret one might encounter?

\textbf{Remark 1.} Let $T$ be a binary tree and let $u$ be $u_{\alpha, \beta}$ with $\alpha = 1$ and $\beta = 1$. Then the worst-case regret of $\hat{Y}_u^T$ is lower bounded by 0.5 when $K \to \infty$:

$$\lim_{K \to \infty} \sup_{P,T} \left[ U(\hat{Y}_u^*, P, u_{1,1}) - U(\hat{Y}_u^T, P, u_{1,1}) \right] \geq 0.5. \tag{19}$$

\textbf{Proof.} We provide a constructive proof, by introducing a family of probability distributions for which the lower bound holds. As we make a restriction to binary trees, let us consider $K$ where $K$ is a power of two. For a given instance $x$, assume that the posterior distribution is as follows: $P(c_1 \mid x) = P(c_2 \mid x) = 0.5$ and $P(c_i \mid x) = 0$ for all other $i$. Then, the Bayes-optimal predictor is $\hat{Y}_u^* = \{c_1, c_2\}$ with

$$U(\hat{Y}_u^*, P, u_{1,1}) = 1 - \frac{1}{K-1} = \frac{K-2}{K-1}. \tag{20}$$

Let us now construct the binary tree in such a way that in the root the classes $c_1$ and $c_2$ are sent to the left and right branch, respectively. Then, for $K \geq 4$ we will have tie among $\hat{Y}_u^T = \{c_1\}$ and $\hat{Y}_u^T = \{c_2\}$. In both cases the expected utility will be $U(\hat{Y}_u^T, P, u_{1,1}) = 0.5$. Taking the difference between the two expected utilities then yields:

$$U(\hat{Y}_u^*, P, u_{1,1}) - U(\hat{Y}_u^T, P, u_{1,1}) = \frac{K-2}{K-1} - \frac{1}{2} \tag{21}$$

Taking the limit of $K \to \infty$ then leads to the lower bound mentioned in the theorem. \qed

The remark is formulated for large $K$, but the worst-case regret is already substantially big for small $K$, as can be observed in the proof. Also notice that this remark is a lower bound on the worst-case regret. We are able to construct more complicated probability distributions that result in a higher regret, but such examples are omitted due to space restrictions. Nevertheless, a regret of 0.5 is high and sufficient to substantiate the point we want to make. Such a high regret of course only occurs for very unlucky choices of hierarchies, and in practice the regret will be much smaller, as shown in our experimental results.
Table 2: Additional summary statistics for the image and protein datasets.

|        | n\_TRAIN | n\_VAL  | n\_TEST |
|--------|----------|---------|---------|
| VOC 2006 | 1118     | 280     | 1477    |
| VOC 2007 | 2328     | 582     | 2841    |
| CAL101   | 3254     | 1084    | 4339    |
| CAL256   | 11168    | 3722    | 14890   |
| PROTEIN  | 6103     | 6103    | 9803    |

Figure 2: Architecture for learning hidden representations for the protein dataset.

Under certain conditions the regret will be zero. This happens when the Bayes-optimal prediction is a node of the hierarchy. The combination of the following two conditions is sufficient for this to happen:

(a) the hierarchy is constructed in such a way that for every pair of classes \((c_i, c_j)\), the leaf \(c_i\) is to the left of the leaf \(c_j\) when \(P(c_i | x) > P(c_j | x)\).

(b) in the path from the root to the most left leaf we encounter a node \(\hat{Y}\) for which \(|\hat{Y}| = |\hat{Y}_n^*|\).

However, conditions of this type will in practice be rarely fulfilled for all instances, as a specific hierarchy might be needed for particular instances.

G Experimental setup

For the image and protein datasets, we use convolutional neural networks in order to obtain hidden representations, which serve as input to the probabilistic models in our experiments. The networks are trained and validated, with statistics shown in Table 2. Moreover, for the image datasets, the features are vectors of size \(D_{vgg} = 25088\), obtained by resizing images to 224x224 pixels and passing them through the convolutional part of an entire VGG16 architecture, including a max-pooling operation [Simonyan and Zisserman, 2014]. The weights are set to those obtained by training the network on ImageNet. A custom convolutional neural network is used for the protein dataset as shown in Fig. 2. Protein sequences are truncated to inputs of size 1000 and are passed through a convolutional part. After passing through a fully connected dense part, functional domain encodings, obtained as described in [Li et al., 2018], of the original sequences are then concatenated with the output of the convolutional part. The concatenated outputs are then fed as input to a final dense layer resulting in feature vectors of size \(D_{prot} = 5012\). ReLU activation and batch normalization is used throughout the whole network. The network is trained end-to-end with either a regular or hierarchical softmax layer, depending on the kind of probabilistic model that is considered. Training is done by minimizing the cross-entropy loss, by means of Adam optimization with a learning rate \(\eta = 1 \epsilon - 4\) and a batch size of 32. The number of epochs is set to 100 and early stopping is applied after ten iterations. An overview of the hyperparameters and their corresponding ranges during hyperparameter optimization
Table 3: Optimized hyperparameters with corresponding ranges for the convolutional neural networks applied on the image and protein datasets.

| HYPERPARAMETER | RANGE |
|----------------|-------|
| EPOCHS         | [0,...,100] |
| $\eta$         | \{0.01, 0.001, 0.0001\} |
| $D_{vgg}$      | \{25088\} |
| $D_{prot}$     | \{5012\} |

Table 4: Optimized hyperparameters with corresponding ranges for the Liblinear solver.

| HYPERPARAMETER | RANGE |
|----------------|-------|
| $\epsilon$     | 0.1, 0.001 |
| cost           | \{1, 10\} |

is shown in Table 3. For training the convolutional neural networks we used an infrastructure with the following specifications:

- **CPU**: i7-6800K 3.4 GHz (3.8 GHz Turbo Boost) – 6 cores / 12 threads.
- **GPU**: 2x Nvidia GTX 1080 Ti 11GB + 1x Nvidia Tesla K40c 11GB.
- **RAM**: 64GB DDR4-2666.

Finally, after training of convolutional neural networks, we used obtained hidden representations for the image and protein datasets are obtained by using convolutional neural network and bag-of-words representation for the text datasets to train the probabilistic model using dual version of L2-regularized logistic regression solver from Liblinear [Fan et al., 2008]. Details of the hyperparameters optimize are shown in Table 4. For training and inference of probabilistic models we used infrastructure with the following specifications:

- **CPU**: i7-8559U 2.7 GHz (4.5 GHz Turbo Boost) – 4 cores / 8 threads.
- **RAM**: 16GB DDR4-2133.

G.1 Class hierarchies

We also briefly summarize the predefined hierarchies that are used for the classifiers with class hierarchies:

- **VOC2006 and VOC2007**: hierarchies are based on the given taxonomy in the original Pascal Visual Object Classes paper [Everingham et al., 2007]. The classes can be considered in a taxonomy with four main branches: vehicles, animals, household objects and people and a maximal depth of four.
- **Caltech-101 and Caltech-256**: similar as for the VOC datasets, we use a given taxonomy from the Caltech-256 Object Category Dataset report [Griffin et al., 2007]. Here the taxonomy has a maximal depth of 6 and consists of two main branches: animate and inanimate.
- **Protein**: a natural hierarchy, which is imposed by the Enzyme Commission number classification scheme, is used.
- **LSHTC1 and DMOZ**: for the two datasets a hierarchy file is provided which contains parent-child relations between each category. More information can be found in the LSHTC paper [Partalas et al., 2015].