On the Optimality of Trees Generated by ID3

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Abstract

Since its inception in the 1980s, ID3 has become one of the most successful and widely used algorithms for learning decision trees. However, its theoretical properties remain poorly understood. In this work, we analyze the heuristic of growing a decision tree with ID3 for a limited number of iterations $t$ and given that nodes are split as in the case of exact information gain and probability computations. In several settings, we provide theoretical and empirical evidence that the TopDown variant of ID3, introduced by Kearns and Mansour (1996), produces trees with optimal or near-optimal test error among all trees with $t$ internal nodes. We prove optimality in the case of learning conjunctions under product distributions and learning read-once DNFs with 2 terms under the uniform distribution. Using efficient dynamic programming algorithms, we empirically show that TopDown generates trees that are near-optimal ($\sim \%1$ difference from optimal test error) in a large number of settings for learning read-once DNFs under product distributions.

1 Introduction

Decision tree algorithms are widely used in various learning tasks and competitions. The most popular algorithms, which include ID3 (Quinlan, 1986) and its successors C4.5 and CART, use a greedy top-down approach to grow trees. In each iteration, ID3 chooses a leaf and replaces it with an internal node connected to two new leaves. This splitting operation is based on a splitting criterion, which promotes reduction of the training error. The popularity of this algorithm stems from its simplicity, interpretability and good generalization performance.

Despite its success in practice, the theoretical properties of trees generated by ID3 are not well understood. For example, consider the heuristic of running ID3 for a limited number of iterations $t$. In this case, the best guarantee one can get is that the generated tree has the lowest test error among all trees with $t$ internal nodes. ID3 may not generate an optimal tree with $t$ internal nodes. For example, this holds for learning the parity function under the uniform distribution (Kearns, 1996). However, to the best of our knowledge, there are no results which show under which conditions ID3 does generate a bounded-size tree whose error is close to the error of an optimal tree with the same number of internal nodes. The empirical success of ID3 may suggest that such conditions exist.

In this work, we analyze the optimality of the trees generated by TopDown (Kearns & Mansour, 1999), a variant of ID3, after running for $t$ iterations. TopDown is an implementation of ID3, where in each iteration the leaf that it chooses to split is the one with the largest gain reduction weighted by the probability to reach the leaf. We provide theoretical and empirical evidence, that in the case of exact gain and probability computations, TopDown does generate optimal or near-optimal trees in several settings.

On the theory side, we consider two settings for which we show that for all $t$, TopDown generates the tree with optimal test error among all trees with $t$ internal nodes. We show this for learning

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See Remark 3.1 for a discussion on this assumption.

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conjunctions under product distributions and learning read-once DNFs with two terms under the uniform distribution. Empirically, we devise efficient dynamic programming algorithms to calculate the optimal trees for a large number of settings for learning read-once DNF under product distributions. For each DNF, we calculate the average of the difference between the test error of the generated tree and the optimal tree, across $t$. We show that for all DNFs this average is $\sim 1\%$.

Our results suggest that for product distributions, the TopDown algorithm is a good choice for learning read-once DNFs using bounded-size decision trees. Surprisingly, to the best of our knowledge, TopDown is not widely used in practice. Rather, a similar variant (Shi, 2007), which we denote BestFirst, is used. For instance, it is used in WEKA (Hall et al., 2009). In each iteration, BestFirst chooses to split the leaf with the largest gain reduction without taking into account the probability to reach the leaf. TopDown is a more natural choice than BestFirst, because in each iteration it induces a larger reduction on an upper bound on the training error. We further corroborate this in our settings and show in theory and experiments that TopDown has a clear advantage in performance over BestFirst.

2 Related Work

The ID3 algorithm was introduced by Quinlan (1986). There are a few papers which study its theoretical properties. The main difference between our work and previous ones, is that we provide test guarantees for trees of practical size by analyzing trees generated by ID3 in each iteration. In contrast, previous works provide guarantees for ID3 in the cases of building a large tree which implements the target function exactly or a tree with a very large polynomial size.

The most related to our work, is Fiat & Pechyon (2004), which show that ID3 can learn read-once DNF and linear functions under the uniform distribution in polynomial time. They also show that ID3 builds the tree with minimal size among all trees that implement the ground-truth function. Their results require ID3 to build a tree which implements the ground-truth exactly. This can result in a very large tree.

In a concurrent work, Brutzkus et al. (2019) use smoothed analysis to show that ID3 can learn $\log(n)$-juntas over $n$ variables under product distributions in polynomial time. Their result requires to build a tree with a large polynomial size that implements the target function exactly. Furthermore, their analysis and techniques are different from ours. The paper is given in the supplementary material.

Another related work is Kearns & Mansour (1999), which introduce the TopDown variant of ID3. They show that TopDown is a boosting algorithm under the assumptions that there is a weak approximation of the target function in each node. To get a test error guarantee of $\epsilon$, there result requires to build a tree with at least $(\frac{1}{\epsilon})^{128}$ nodes, which is highly non-practical. Other works study learnability of decision trees through algorithms which are different from algorithms used in practice (O’Donnell & Servedio, 2007; Kalai & Teng, 2008; Bshouty & Burroughs, 2003; Bshouty et al, 2005; Ehrenfeucht & Haussler, 1989; Chen & Moitra, 2018) or show hardness results for learning decision trees (Rivest, 1987; Hancock et al., 1996).

3 Preliminaries

**Distributional Assumptions:** Let $X = \{0, 1\}^n$ be the domain and $Y = \{0, 1\}$ be the label set. Let $D$ be a product distribution on $X \times Y$ realizable by a read-once DNF. Namely, for $(x, y) \sim D$ it holds that $x \sim \prod_{i=1}^n \text{Bernoulli}(p_i)$ where $p_1, ..., p_n \in (0, 1)$ and $y = f(x)$ for a read-once DNF $f: X \rightarrow Y$. Recall that a read-once DNF is a DNF where each variable appears at most once, e.g., $f(x) = (x_1 \land x_2 \land x_3) \lor (x_4 \land x_5)$.

**Decision Trees:** Let $T$ be any decision tree whose internal nodes are labeled with features $\{x_i\}_{i=1}^n$. For a node in the tree $v$, we let $p_T(v)$ be the probability that a randomly chosen $x$ reaches $v$ in $T$ and let $q_T(v)$ be the probability that $f(x) = 1$ given that $x$ reaches $v$. For convenience, we will usually omit the subscript $T$ from the latter definitions when the tree used is clear from the context. Let $\ell(T)$ be the set of leaves of $T$ and $I(T)$ be the set of internal nodes (non-leaves). We assume that each leaf is labeled $1$ if $q(l) \geq \frac{1}{2}$ and $0$ otherwise. If $l \in \ell(T)$ we let $T(l, i)$ be the same as the tree $T$.\footnote{See Section 3 for further details.}
The TopDown algorithm introduced by Kearns & Mansour (1999) is a variant of ID3 where

\begin{algorithm}[H]
\textbf{Algorithm TopDown}_{D}(t)
\begin{enumerate}
\item Initialize $T$ to be a single leaf labeled by the majority label with respect to $D$.
\item while $T$ has less than $t$ nodes:
\begin{enumerate}
\item $\Delta_{best} \leftarrow 0$.
\item for each pair $l \in \ell(T)$ and $i \in F_l$:
\begin{enumerate}
\item $\Delta \leftarrow H(T) - H(T(l, i))$.
\item if $\Delta \geq \Delta_{best}$ then:
\begin{enumerate}
\item $\Delta_{best} \leftarrow \Delta$; $l_{best} \leftarrow l$; $i_{best} \leftarrow i$.
\end{enumerate}
\end{enumerate}
\item $T \leftarrow T(l_{best}, i_{best})$.
\end{enumerate}
\end{enumerate}
\end{algorithm}


Figure 1: TopDown algorithm.

except that the leaf $l$ is replaced with an internal node labeled by $x_i$ and connected to two leaves $l_0$ and $l_1$. The leaf $l_j$ corresponds to the assignment $x_i = j$ and each leaf is labeled according to the majority label with respect to $D$ conditioned on reaching the leaf. For a leaf $l \in \ell(T)$, let $F_l$ be the set of features that are not on the path from the root to $l$.

Let $E(T) = \mathbb{P}_D[T(x) \neq f(x)]$ be the error of the tree $T$. Then it holds that, $E(T) = \sum_{l \in \ell(T)} p(l) C(q(l))$ where $C(x) = \min(x, 1 - x)$. Let $H(x) = -x \log(x) - (1 - x) \log(x)$ be the entropy function, where the log is base 2, and define the entropy of $T$ to be $H(T) = \sum_{l \in \ell(T)} p(l) H(q(l))$ which satisfies $E(T) \leq H(T)$.

**Algorithm:** The TopDown algorithm introduced by Kearns & Mansour (1999) is a variant of ID3 (Quinlan, 1986). For our analysis we assume that TopDown can compute exact probabilities and information gain computations in each iteration. Thus, WLOG, we can assume that it has access to the distribution $D$.

The main difference between TopDown and ID3 is the choice of the splitting node in each iteration. TopDown chooses the node which maximally decreases $H(T)$ and therefore hopefully reduces $E(T)$ as well. Formally, in each iteration, it chooses a leaf $l$ and feature $x_i$, where $i \in F_l$, which maximize:

\[
H(T) - H(T(l, i)) = p(l) (H(q(l)) - (1 - \tau_i)H(q(l_0)) - \tau_iH(q(l_1)))
\]

(1)

where $\tau_i$ is the probability that $x_i = 1$ given that $x$ reaches $l$. We let $T_t$ be the tree computed by TopDown at iteration $t$. The algorithm is given in Figure [1]

**Remark 3.1.** In this work we focus on the optimality of trees that TopDown generates in each iteration. In practice, the number of iterations of algorithms such as TopDown are limited to avoid overfitting. Ultimately, we would like the algorithm to choose the leaf and feature in each iteration as in the case of exact gain and probability calculations. This case may occur in practice for a bounded-size tree where in each split there is sufficient data for accurate estimation. Thus, it is desirable to provide guarantees in this case and we assume that this holds in our analysis. Notice that our analysis is different from the standard PAC setting where sample complexity guarantees are given.

### 4 Conjunctions and Product Distributions

In this section we consider learning a conjunction on $k$ out of $n$ bits with TopDown under a product distribution. We will show that in the case of exact information gain computations, for each number of iterations $1 \leq t \leq k$, TopDown generates the tree with the best test error among all trees with at most $t$ internal nodes.

#### 4.1 Setup and Additional Notations

Let $J \subseteq [n]$ be a subset of indexes such that $|J| = k$. In this section we assume a target function $f_J(x) = \bigwedge_{i \in J} x_i$. Note that $f_J$ is realizable by a depth $k$ tree. Let $D$ be the product distribution on
$\mathcal{X} \times \mathcal{Y}$ defined in Section 3. We assume, without loss of generality, that $0 < p_1 \leq p_2 \leq \cdots \leq p_n < 1$ and denote $q_i = 1 - p_i$. Denote $J = \{i_1, \ldots, i_k\}$ where $p_{i_1} \leq p_{i_2} \leq \cdots \leq p_{i_k}$ and define $J_t = \{p_{i_1}, p_{i_2}, \ldots, p_{i_t}\}$ for any $1 \leq t \leq k$ and $J_0 := \emptyset$.

For any tree $T$ let $I_T$ be the set of features that appear in all of its nodes. We let $T_t$ be the set of all decision trees with $t$ internal nodes. For simplicity, we define $I_t$ to be the set of features of the tree $T_t$ and let $I_0 := \emptyset$. We say that a binary tree is right-skewed if the left child of each internal node is a leaf with label 0. We denote by $\mathcal{A}_t$ the set of all right-skewed trees $R \in T_t$ such that $I_R \subseteq J$.

### 4.2 Main Result

In this section we will provide a partial proof of the following theorem. The remaining details are deferred to the supplementary material.

**Theorem 4.1.** Assume that ID3 runs for $1 \leq t \leq k$ iterations. Then it outputs the tree with optimal test error among all trees in $T_t$.

For the proof we will need the following key lemma which is used throughout our analysis. The proof is given in the supplementary material.

**Lemma 4.2.** Let $0 < y < 1$ and $0 < x_1 \leq x_2 \leq 1$. Then:

1. $x_1 H(y|x_2) \leq x_2 H(y|x_1)$ and this inequality is strict if $x_1 < x_2$.

2. $x_1 C(y|x_2) \leq x_2 C(y|x_1)$.

The proof outline of Theorem 4.1 goes as follows. First, we show that the set of optimal trees in $T_t$ intersects with the set $\mathcal{A}_t$ (Lemma 4.3). Then we will show that TopDown chooses features in $J$ in ascending order of $p_i$ (Lemma 4.4). In Lemma 4.5 we will prove that the tree found by TopDown has the best test error in the set $\mathcal{A}_t$. By combining all of these facts together we get the theorem.

**Lemma 4.3.** For any $1 \leq t \leq k$ there exists a right-skewed tree $R \in T_t$ such that $I_R \subseteq J$ and $R$ has the lowest test error among all trees in $T_t$.

The proof idea is to use Lemma 4.2 to show that any tree in $T_t$ can be converted to a right-skewed tree $R \in T_t$ such that $I_R \subseteq J$, without increasing the test error. The full proof appears in the supplementary material.

The next lemma shows that ID3 chooses features in $J$ in ascending order of $p_i$ using Lemma 4.2. The proof is given in the supplementary material.

**Lemma 4.4.** Assume that ID3 runs for $1 \leq t \leq k$ iterations. Then $T_t$ is right-skewed, $I_t = J_t \subseteq J$ and $T_t$ has test error $\prod_{i \in J_t} p_i C\left(\prod_{i \in J \setminus J_t} p_i\right)$.

The next lemma shows that the test error of the tree generated by ID3 at iteration $t$, is the lowest among all test errors of trees in $\mathcal{A}_t$.

**Lemma 4.5.** The following equality holds:

$$\min_{|I| = t, J \subseteq J_t} \prod_{i \in I} p_i C\left(\prod_{i \in J \setminus I} p_i\right) = \prod_{i \in J_t} p_i C\left(\prod_{i \in J \setminus J_t} p_i\right).$$

**Proof.** Define $g(K) = \prod_{i \in K} p_i C\left(\prod_{i \in J \setminus J_t} p_i\right)$. Let $K_1 \subseteq J$ such that $K_1 \neq J_t$ and $|K_1| = t$. By definition of $K_1$, there exists $j \in K_1$ and $l \in J \setminus K_1$ such that $p_j \geq p_l$. Define $K_2 = (K_1 \setminus \{j\}) \cup \{l\}$. It suffices to prove that $g(K_1) \geq g(K_2)$. Denote $z = \prod_{i \in K_1 \setminus \{j\}} p_i$ and $y = \prod_{i \in J \setminus (K_1 \cup \{l\})} p_i$. It holds that $g(K_1) = z p_j C(y p_j)$ and $g(K_2) = z p_l C(y p_l)$. Since $p_j \geq p_l$, $z > 0$ and $0 < y < 1$, we conclude that $g(K_1) \geq g(K_2)$ by Lemma 4.2.

We are now ready to prove the theorem.

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*In the case that there are features $i_{l_1}, i_{l_2} \in J$ with $p_{i_{l_1}} = p_{i_{l_2}}$ and $l_1 < l_2$, we assume, without loss of generality, that TopDown chooses feature $i_{l_1}$ before $i_{l_2}$.}
We assume a boolean target function \( f : \{0, 1\}^n \rightarrow \{0, 1\} \), where \( f(x) = (x_l \land \cdots \land x_j) \lor (x_j \land \cdots \land x_{j_m}) \) where \( 1 \leq l \leq m \) and all literals are of different variables.

We state our main result in the following theorem:

We will show that for each number of iterations \( t \), TopDown generates a tree with the best test error among all trees with at most \( t \) internal nodes. However, in this case the analysis is more involved.

5 Read-Once DNF with 2 Terms and Uniform Distribution

In this section, we analyze the TopDown algorithm for learning read-once DNFs with 2 terms under the uniform distribution. Similarly to the previous section, we show that for each iteration \( t \), TopDown generates a tree with the best test error among all trees with at most \( t \) internal nodes. However, in this case the analysis is more involved.

5.1 Setup and Additional Notations

**Learning Setup:** We assume a boolean target function \( f : \{0, 1\}^n \rightarrow \{0, 1\} \), where \( f(x) = (x_l \land \cdots \land x_j) \lor (x_j \land \cdots \land x_{j_m}) \) where \( 1 \leq l \leq m \) and all literals are of different variables. WLOG, we only consider literals which are variables and not their negations. By symmetry, our analysis holds for all literal configurations. We assume that \( D \) is a uniform distribution over \( \{0, 1\}^n \).

For convenience, we will denote \( f(x) = (x_1 \land x_2 \land \cdots \land x_l) \lor (y_1 \land y_2 \land \cdots \land y_m) \), where each variable in this formula corresponds to an entry of \( x \). We say that the \( x_i \) are \( x \)-variables and similarly define \( y \)-variables.

**Additional Notations and Definitions:** Let \( T \) be any decision tree. Let \( r_T \) be the root of \( T \) and \( T_L \) and \( T_R \) be the left and right sub-trees of \( r_T \), respectively. For a node \( v \), let \( d(v) \) be its depth in the tree, where \( d(r_T) = 0 \). We let \( F(v) \) be the DNF formula corresponding to the node \( v \). This is the ground truth DNF \( f \) conditioned on all variables and assignments in the path from the root to \( v \). If a node \( v \) is split with respect to an \( x \)-variable then we say that \( v \) is an \( x \)-node. Similarly, we define \( y \)-nodes. We define all nodes which are not \( x \)-nodes or \( y \)-nodes as \( o \)-nodes. From now on, we consider trees whose nodes are one of the latter 3 types.

Let \( T_t \) be the set of all trees with \( t \) nodes. For a node \( v \), consider its split with respect to the variable with maximal information gain. Let \( v_0 \) be its left child and \( v_1 \) its right child after the split. We define the weighted gain of \( v \) as \( W(v) = p(v) (H(q(v)) - \frac{1}{2} H(q(v_0)) - \frac{1}{2} H(q(v_1))) \).

In each iteration, TopDown chooses the leaf \( l \) for which \( W(l) \) is maximal. Equivalently, this is the leaf which maximally decreases \( H(T) \). We also define the error reduction of the node \( v \) to be \( C(v) = C(q(v)) - \frac{1}{2} C(q(v_0)) - \frac{1}{2} C(q(v_1)) \) and \( C(T) = \sum_{v \in T} p(v) C(v) \) the error reduction of \( T \). In each iteration, in which a node \( v \) is split, the test error is decreased by \( p(v) C(v) \). Therefore, we get the following identity:

\[
E(T) = C(\mathbb{P}_D [f(x) = 1]) - C(T)
\]  

By Equation 2, we can reason about \( E(T) \) through \( C(T) \). For \( E(T) \) to be minimal we need \( C(T) \) to be maximal.

For a tree \( T \) we define its right-path to be the nodes in its right-most path. If the right-path consists only of \( x \)-nodes, we say that it is a right \( x \)-path. Similarly, we define a right \( y \)-path. We define \( C_1 \) to be the set of all trees that consist only of a right-path where the nodes are either all \( x \) nodes or all \( y \) nodes. We also say that these trees are right-paths. We define \( C_2 \) to be the set of all trees such that for each node in the right-path the following holds. If it is an \( x \)-node, then its left sub-tree is a tree in \( C_1 \) with \( y \)-nodes. Similarly, if it is a \( y \)-node, then its right sub-tree is a tree in \( C_1 \) with \( x \)-nodes. In Figure 2, we illustrate these sets of trees. For a tree \( T \in C_1 \) such that \( F(r_T) = y_1 \land y_2 \land \cdots \land y_m \) we say that \( T \) is a full right \( y \)-path if \( T \) has \( m \) \( y \)-nodes.

5.1.1 Main Result

We will show that for each number of iterations \( t \), TopDown builds a tree, which we denote by \( B_t \), and this tree has the best test error among all trees with at most \( t \) internal nodes. Formally, \( B_t \) is a tree of size \( t \) in \( C_2 \) whose right-path consists only of \( x \)-nodes. The left sub-tree of each \( x \)-node is in \( C_1 \) and consists only of \( y \)-nodes. Furthermore, for any two \( x \)-nodes \( v_1 \) and \( v_2 \) in the right-path such that \( v_2 \) is deeper than \( v_1 \), the following holds. The left sub-tree of \( v_2 \) is not a leaf only if the left sub-tree of \( v_2 \) is a full right \( y \)-path. Figure 3 shows \( B_t \) for the formula \((x_1 \land x_2) \lor (y_1 \land y_2 \land y_3)\).

We state our main result in the following theorem:
Theorem 5.1. Let \( t \geq 1 \). Then, \( T_t = B_t \) and \( T_t \) is a tree with the optimal test error in \( \mathcal{T}_t \).

5.1.2 Proof Sketch of Theorem 5.1

The proof proceeds as follows. In the first part we show that for each iteration \( t \), TopDown outputs the tree \( B_t \), i.e., \( T_t = B_t \) (Proposition 5.2). In the second part, we show that for any \( t \), \( B_t \) has minimum test error among all trees in \( \mathcal{T}_t \) (Proposition 5.3). These two parts together prove Theorem 5.1.

We begin with the first part:

Proposition 5.2. Assume TopDown runs for \( t \) iterations. Then \( T_t = B_t \).

The proof uses a result of [Fiat & Pechyon 2004], which show that in the setting of this section, for each node \( v \) that ID3 splits, it chooses a variable in \( F(v) \) which is in a minimal size term. For example, if \( F(v) = (x_1 \land x_2) \lor (x_3 \land x_4 \land x_5) \), then ID3 chooses either \( x_1 \) or \( x_2 \) (they have the same gain due to the uniform distribution assumption). Then, the proof follows by several inequalities involving the entropy function. These inequalities arise from comparing the weighted gain of pairs of nodes and showing that their correctness implies that \( T_t = B_t \). We defer the proof to the supplementary material.

Next, we show the following proposition.

Proposition 5.3. Let \( t \geq 1 \). Then, \( B_t \) is a tree with optimal test error among all trees in \( \mathcal{T}_t \).

The idea of the proof is to first show by induction on \( t \) that there exists an optimal tree in \( C_2 \). Then, the proof proceeds by showing that any tree in \( C_2 \) with \( t \) internal nodes can be converted to \( B_t \) without increasing the test error. To illustrate the latter part with a simple example, consider the case where \( f(x) = (x_1 \land x_2) \lor (y_1 \land y_2 \land y_3) \). In this case the tree in Figure 2a, which we denote by \( T_1 \), is equal to \( B_5 \), whereas the tree in Figure 2b, which we denote by \( T_2 \), is a tree in \( C_2 \) with 5 internal nodes which is not \( B_5 \). In this example, by direct calculation it can be shown that \( E(T_1) < E(T_2) \). However, to illustrate our proof in the general case, let \( v_1 \) be the left child of the root in \( T_1 \) and let \( v_2 \) be the left child of the root in \( T_2 \). Then \( C(v_1) = C(v_2) \), but \( p(v_1) > p(v_2) \). Therefore, \( p(v_1)C(v_1) > p(v_2)C(v_2) \). By continuing this way for the rest of the nodes on the left sub-trees, we get \( C(T_1) > C(T_2) \). This implies by equation 2 that \( E(T_1) < E(T_2) \). This technique of comparing error reduction of nodes allows us to handle more complex cases, e.g., to show that the tree in Figure 2b is not optimal. The full proof is given in the supplementary material.

6 Empirical Results

In this section we present dynamic programming algorithms that allow us to calculate optimal trees efficiently in a large number of settings. We will need the following notations for this section. For any \( t \), let \( OPT(F, t) \) be the minimal test error of all trees of with \( t \) internal nodes, over \( D \) with ground-truth DNF \( F \). For any \( t \) we let \( E(T_t, F) \) be the test error of the tree TopDown outputs after \( t \) iterations assuming ground-truth \( F \). We define \( \Delta_{F,t} = E(T_t, F) - OPT(F, t) \), \( m_F = 1/100 \sum_{t=1}^{100} \Delta_{F,t} \) and \( \sigma_F = \sqrt{1/100 \sum_{t=1}^{100} (\Delta_{F,t} - m_F)^2} \).
Figure 3: Bt examples for DNF \((x_1 \land x_2) \lor (y_1 \land y_2 \land y_3)\). x-nodes are in blue, y-nodes in green and leaves in red. (a) \(t = 2\). (b) \(t = 5\). (c) \(t = 6\). (d) \(t = 8\). This tree has 0 test error.

6.1 Uniform Distribution

In this section we assume that \(D\) is the uniform distribution. Let \(F\) be a read-once DNF with \(k\) terms \(c_1, \ldots, c_k\). We refer to \(F\) as a set over the terms. For a term \(c\), let \(c^-\) be a term with \(|c^-| = |c| - 1\). Let \(A\) be the set of all read-once DNFs over the uniform distribution with at most 8 terms and most 8 literals in each term. We use the following relation to compute optimal trees:

\[
\text{OPT}(F, t) = \min_{1 \leq i \leq k, 0 \leq j \leq t - 1} \left\{ \frac{1}{2} \text{OPT}(F \setminus \{c_i\}, j) + \frac{1}{2} \text{OPT}(F \setminus \{c_i\} \cup c_i^-, t - 1 - j) \right\}
\]

The correctness of the formula follows since \(D\) is a product distribution and a sub-tree of an optimal tree is optimal. See supplementary for details.

We calculated \(\text{OPT}(F, t)\) for all \(1 \leq t \leq 100\) and for all \(F \in A\). For each \(F \in A\) we calculated \(m_F\) and \(\sigma_F\). Empirically, we got \(\max_{F \in A} m_F < 0.018\) and \(\max_{F \in A} \sigma_F < 0.017\). In Figure 4a we plot \(m_F\) for all \(F \in A\). These results show that for many read-once DNFs and number of iterations \(t\), TopDown is near-optimal with difference from optimal error roughly 1%.

6.2 Product Distributions

In this section we assume that the distribution \(D\) over variables is a product distribution where each variable has distribution Bernoulli\((p_1)\) or Bernoulli\((p_2)\) for \(0 < p_1, p_2 < 1\). We experimented with the pairs \((p_1, p_2) \in \{(0.3, 0.7), (0.4, 0.6), (0.2, 0.9)\}\). Let \(F\) be a read-once DNF with \(k\) terms \(c_1, \ldots, c_k\). We refer to \(F\) as a set over the terms. For each term \(c\), let \(n_{c,1}\) be the number of variables with distribution Bernoulli\((p_1)\) and similarly define \(n_{c,2}\). Denote by \(c(n_1, n_2)\) a term with \(n_1\) variables with distribution Bernoulli\((p_1)\) and \(n_2\) variables with distribution Bernoulli\((p_2)\). Let \(B\) be the set of all read-once DNFs over \(D\) with at most 4 terms and at most 5 literals, where each literal is a variable (not its negation) which has distribution Bernoulli\((p_1)\) or Bernoulli\((p_2)\).

We use the following relation to compute optimal trees:

\footnote{Note that we do not need to consider trees with variables that are not in the DNF. See supplementary for details.}
We calculated $OPT$ where TopDown will generate the tree in Figure 3b and this is the optimal tree with 5 internal nodes. However, The BestFirst algorithm (Shi, 2007), is similar to TopDown but with a different policy to choose leaves in each iteration. A version of BestFirst is used in WEKA (Hall et al., 2009). Instead of choosing the leaf and feature with maximal weighted gain (equation 1), it chooses the leaf $l$ and feature $i$ with maximal gain, i.e, which maximize $H(q(l)) - (1 - \tau_j) H(q(l_0)) - \tau_j H(q(l_1))$. This can degrade the performance compared to TopDown. For example, consider learning the formula $(x_1 \land x_2) \lor (y_1 \land y_2 \land y_3)$ under the uniform distribution. As shown in Section 5, TopDown will generate the tree in Figure 3b and this is the optimal tree with 5 internal nodes. However, it can be shown that BestFirst can generate the tree in Figure 2a after 5 iterations (see supplementary material for details). As shown in Section 5.1.2, the latter tree is sub-optimal. Empirically, we ran the experiments of Section 6.2 with BestFirst and $(p_1, p_2) \in \{(0.3, 0.7), (0.4, 0.6)\}$. Figure 4c and 4d show that the trees generated by BestFirst can be far from optimal.

7 Comparison with BestFirst

The BestFirst algorithm (Shi, 2007), is similar to TopDown but with a different policy to choose leaves in each iteration. A version of BestFirst is used in WEKA (Hall et al., 2009). Instead of choosing the leaf and feature with maximal weighted gain (equation 1), it chooses the leaf $l$ and feature $i$ with maximal gain, i.e, which maximize $H(q(l)) - (1 - \tau_j) H(q(l_0)) - \tau_j H(q(l_1))$. This can degrade the performance compared to TopDown. For example, consider learning the formula $(x_1 \land x_2) \lor (y_1 \land y_2 \land y_3)$ under the uniform distribution. As shown in Section 5, TopDown will generate the tree in Figure 3b and this is the optimal tree with 5 internal nodes. However, it can be shown that BestFirst can generate the tree in Figure 2a after 5 iterations (see supplementary material for details). As shown in Section 5.1.2, the latter tree is sub-optimal. Empirically, we ran the experiments of Section 6.2 with BestFirst and $(p_1, p_2) \in \{(0.3, 0.7), (0.4, 0.6)\}$. Figure 4c and 4d show that the trees generated by BestFirst can be far from optimal.

8 Conclusion

In this work we analyze the optimality of trees generated by the TopDown algorithm. We show through theory and experiments that in a large number settings for learning read-once DNFs under product distributions, TopDown generates trees with optimal or near-optimal test error. There are many interesting directions for future work. First, it would be interesting to close the gap between our theory and experiments. We conjecture that in most cases, TopDown generates near-optimal trees for learning read-onces DNF under product distributions. It would be interesting to consider other distributions with dependencies between variables and other DNFs. Providing theoretical guarantees for random forests and gradient boosting is a challenging direction for future work. Following the results in Section 7, it would be interesting to see if TopDown can be used to improve performance in practical applications.
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A Proofs for Section 4

A.1 Proof of Lemma 4.2

1. Define \( f(x) = xH(yx_1) - x_1H(yx) \). Then \( f(x_1) = 0 \) and by the fact that \( H'(x) = -\log \left( \frac{x}{1-x} \right) \), we get for \( x_1 \leq x \leq 1 \):

\[
f'(x) = -yx_1 \log(yx_1) - (1 - yx_1) \log(1 - yx_1) + yx_1 \log \left( \frac{yx}{1-yx} \right)
\]

\[= -\log(1 - yx_1) + yx_1 \log \left( \frac{yx(1-yx_1)}{yx_1(1-yx)} \right) > 0\]

where the last inequality follows since \( 0 < x_1 \leq x \) and \( 0 < yx_1 < 1 \). This completes the proof.

2. We will consider several cases. If \( yx_1 \geq \frac{1}{2} \) then \( x_1C(yx_2) \leq x_2C(yx_1) \) holds iff \( x_1(1-yx_2) \leq x_2(1-yx_1) \) which is equivalent to \( x_1 \leq x_2 \). If \( yx_2 \geq \frac{1}{2} \) then \( C(yx_1) = yx_1 \) and \( C(yx_2) = yx_2 \) and the claim holds. Finally, if \( yx_1 \leq \frac{1}{2} \leq yx_2 \) then the desired inequality is equivalent to \( x_1(1-yx_2) \leq x_2yx_1 \) which holds since \( yx_2 \geq \frac{1}{2} \).
We will now show that with feature $j$ in $S$ in the tree $T$, we can add $l$ to $T$ as a right child of the right leaf in $T$. Denote by $T'$ the resulting tree.

Then, $E(T) = \prod_{j \in T} p_j C \left( \prod_{j \notin T} p_j \right)$ because any right-skewed tree $T$ with $I_T \subseteq J$, can only err in the case that $x_j = 1$ for all $j \in I_T$. Similarly, $E(T') = \prod_{j \in I_T \cup \{1\}} p_j C \left( \prod_{j \notin I_T \cup \{1\}} p_j \right)$.

Let $z = \prod_{j \in I_T} p_j$, $y = \prod_{j \notin I_T \cup \{1\}} p_j$, $x_1 = p_t$ and $x_2 = 1$. Then, by Lemma 4.2, we have $zx_1 C(y x_2) \leq z x_2 C(y x_1)$, which is equivalent to $E(T') \leq E(T)$. Therefore, we can get the desired tree $T'$.

Now assume that $S$ contains a node with a feature in $[n] \setminus J$. Let $i$ be such a node for which the tree rooted at $i$ contains, besides $i$, only nodes with features in $J$. Denote this sub-tree by $S_i$. Then $S_i$ has the following structure. Without loss of generality, the right sub-tree and the left sub-tree of $i$ are both right-skewed (because otherwise we can replace each with a right leaf with label 0 without increasing the test error). Consider the following modification to $S_i$. Connect the left sub-tree of $i$ to the right-most leaf of $S_i$, remove the node $i$ and replace it with its right child. Let $v_i$ be the new right leaf in the tree (that was previously the right leaf of the left sub-tree of $i$). Choose the label for $v_i$ which results in lowest test error. Finally, remove nodes such that for each feature, there is at most one node with that feature in the path from the root to $v_i$. Let $T'$ be the tree obtained by this modification to $S_i$. Then $T'$ has one less node with feature in $[n] \setminus J$ compared to $S_i$. It remains to show that $E(T') \leq E(S_i)$. This will finish the proof, because we can apply this modification multiple times until we have only features with nodes in $J$. Then we can use the previous argument in the case that $I_S \subseteq J$.

We will now show that $E(T') \leq E(S_i)$. Let $V_i$ be the set of nodes in the path from the root to node $i$ in the tree $S_i$, excluding $i$. Let $V_2$ be the internal nodes in the right sub-tree of $i$ and $V_3$ be the internal nodes in the left sub-tree of $i$. Recall that the left and right sub-tree are right-skewed. For any node with feature $j$ in $V_i$ let $t_j \in \{p_j, q_j\}$ be the corresponding probability according to the label of $j$ in the path. Then we get the following:

$$E(S_i) - E(T') = p_i D_1 + q_i D_2 - D_3$$  \hspace{1cm} (4)

where

$$D_1 = \prod_{j \in V_1} t_j \prod_{j \in V_2} p_j C \left( \prod_{j \notin J \setminus (V_1 \cup V_2)} p_j \right)$$

$$D_2 = \prod_{j \in V_1} t_j \prod_{j \in V_3} p_j C \left( \prod_{j \notin J \setminus (V_1 \cup V_3)} p_j \right)$$

$$D_3 = \prod_{j \in V_1} t_j \prod_{j \in V_2 \cup V_3} p_j C \left( \prod_{j \notin J \setminus (V_1 \cup V_2 \cup V_3)} p_j \right)$$

This follows since $p_i D_1$ is the error of the path in $S_i$ from the root to the right most leaf in the right sub-tree of node $i$. Similarly, $q_i D_2$ is the error of the path from the root to the right most leaf in the left sub-tree of node $i$ and $D_3$ is the error in the path in $T'$ from the root to the new right leaf.

Let $z = \prod_{j \in V_1} t_j \prod_{j \in V_2} p_j$, $y = \prod_{j \notin J \setminus (V_1 \cup V_2 \cup V_3)} p_j$, $x_1 = \prod_{j \in V_1 \setminus V_2} p_j$ and $x_2 = 1$. By Lemma 4.2, it holds that $zx_1 C(y x_2) \leq z x_2 C(y x_1)$, or equivalently, $D_3 \leq D_1$. Similarly, we have $D_3 \leq D_2$. Hence, by Equation (4), we conclude that $E(T') \leq E(S_i)$.
A.3 Proof of Lemma 4.4

We will first prove by induction that \( I_k = J_k \). For the base case \( I_0 = J_0 = \emptyset \). Assume that up until iteration \( 0 \leq t < k \), ID3 chose the features \( I_t = J_t \). First we note that since feature \( i \notin J \) is independent of features in \( J \), and \( f_j \) depends only on features in \( J \), it follows that for any iteration, the gain of feature \( i \) is zero.

Now, for any \( l > t \) the gain of feature \( i_t \in J \) is

\[
H \left( \prod_{j \in J \setminus J_t} p_j \right) - p_{i_t} H \left( \prod_{j \in J \setminus (J_t \cup \{i_t\})} p_j \right) + q_{i_t} H(0)
\]

\[
= H \left( \prod_{j \in J \setminus J_t} p_j \right) - p_{i_t} H \left( \prod_{j \in J \setminus (J_t \cup \{i_t\})} p_j \right) > 0
\]

where the last inequality follows from the concavity of \( H \) and the fact that \( p_{i_t} > 0 \). Therefore, if \( t + 1 = k \) we are done because TopDown will choose feature \( i_k \) which has the only non-zero gain.

If \( t + 1 < k \) then let \( t + 1 < r \leq k \). By setting \( y = \prod_{j \in J \setminus (J_t \cup \{i_{t+1}, i_r\})} p_j \), \( x_1 = p_{i_{t+1}} \), \( x_2 = p_{i_r} \) and applying Lemma 4.2 we have \( x_1 H(y|x_2) \leq x_2 H(y|x_1) \), or equivalently, \( p_{i_{t+1}} H \left( \prod_{j \in J \setminus (J_t \cup \{i_{t+1}\})} p_j \right) \leq p_{i_r} H \left( \prod_{j \in J \setminus (J_t \cup \{i_r\})} p_j \right) \) and the inequality is strict if \( p_{i_{t+1}} < p_{i_r} \). Therefore, \( i_{t+1} \) has the largest gain in iteration \( t + 1 \) and TopDown will choose it.

Finally, we note that the latter proof shows that TopDown builds a right-skewed tree. It follows that the test error of \( T_t \) is \( \prod_{i \in I_t} p_i C \left( \prod_{i \in J \setminus I_t} p_i \right) \).

B Proofs for Section 5

B.1 Proof of Proposition 5.2

We first prove several inequalities which involve the entropy function.

**Lemma B.1.** Let \( 0 < a < \frac{1}{2} \), then

\[
2H(3a) - 3H(a) + H(2a) - H(5a) > 0
\]

**Proof.** Define \( g(a) = 2H(3a) - 3H(a) + H(2a) - H(5a) \). Since \( g(0) = 0 \), it suffices to prove that \( g'(a) > 0 \) for \( 0 < a < \frac{1}{2} \). We have,

\[
g'(a) = -6 \log \left( \frac{3a}{1-3a} \right) + 3 \log \left( \frac{a}{1-a} \right) - 2 \log \left( \frac{2a}{1-2a} \right) + 5 \log \left( \frac{5a}{1-5a} \right)
\]

\[
= \log \left( \frac{(1-3a)^6(1-2a)^2(5a)^5}{(3a)^6(1-a)^3(2a)^2(1-5a)^5} \right)
\]

First, we notice that \( a^3(5a)^5 > (3a)^6(2a)^2 \). Therefore, we are left to show that

\[
\frac{(1-3a)(1-2a)}{(1-a)^2(1-5a)^5} > 1
\]

By the following 2 inequalities:

1. \( (1-3a)(1-2a) > (1-a)(1-5a) \).
2. \( (1-3a)^2 > (1-a)(1-5a) \).

proving Equation \ref{eq:inequality} reduces to showing that \( \frac{(1-3a)^2}{(1-5a)^5} > 1 \), which is true, as desired.
Lemma B.2. Let $0 < a = \frac{1}{\pi^2}, k \geq 2$ and $H(x) = -x \log(x) - (1 - x) \log(1 - x)$. Then,

$$2H(3a - 2a^2) - 3H(a) + H(2a) - H(5a - 4a^2) > 0$$

Proof. Define $g(a) = 2H(3a - 2a^2) - 3H(a) + H(2a) - H(5a - 4a^2)$. We will prove that the inequality holds for all $0 < a \leq \frac{1}{512}$. The inequality can be proved to hold for the cases $2 \leq k \leq 8$ by calculating $g(a)$ with sufficiently high precision.

Since $g(0) = 0$. It suffices to show that $g'(a) > 0$ for $0 < a \leq \frac{1}{512}$. We have,

$$g'(a) = -2(3 - 4a) \log \left( \frac{3a - 2a^2}{1 - (3a - 2a^2)} \right) + 3 \log \left( \frac{a}{1-a} \right) - 2 \log \left( \frac{2a}{1-2a} \right) + (5-8a) \log \left( \frac{5a - 4a^2}{1 - (5a - 4a^2)} \right)$$

$$= \log \left( \frac{(1-a)(1-2a)^{6-8a}(1-a)^2(5a - 4a^2)^5-8a}{3a - 2a^2} \right) \log \left( \frac{(1-a)^3(2a)^2((1-a)(1-4a))^{5-8a}}{4(3a - 2a)^{6-8a}(1-a)^2(1-4a)^{5-8a}} \right)$$

Define

$$\Delta = (1-2a)^{5-8a}(5-4a)^{5-8a} - 4(3-2a)^{6-8a}(1-a)^2(1-4a)^{5-8a}$$

It suffices to show that $\Delta > 0$. Define $h_1(x) = (3-2x)^{6-8x}$ and $h_2(x) = -5120x + 3^6$. It holds that $h_1(0) = h_2(0) = 3^6$ and $h_2 \left( \frac{1}{512} \right) = 719 > 3^6 \cdot \frac{1}{512} > h_1 \left( \frac{1}{512} \right)$. Furthermore, $h_1(x)$ is convex for $0 \leq x \leq \frac{1}{512}$, because in this case:

$$\frac{\partial^2 h_1}{\partial x^2} (x) = (3-2x)^{6-8x} \left( \frac{72-32x}{(3-2x)^2} + \left( -8 \ln(3-2x) - \frac{2(6-8x)}{3-2x} \right)^2 \right) > 0$$

It follows that $h_2(x) > h_1(x)$ for all $0 \leq x \leq \frac{1}{512}$. Therefore, we get:

$$\Delta > (1-2a)^{7.5} \left( 5 - \frac{1}{128} \right)^{5-\frac{1}{128}} - 4(-5120a + 3^6)$$

$$> (1-15a)(4 \cdot 3^6 + 100) - 4(-5120a + 3^6)$$

$$> 0$$

where the second inequality follows by Bernoulli’s inequality and the last follows by the assumption $a \leq \frac{1}{512}$. \qed

Lemma B.3. Let $0 < a, b < 1$ such that $b \geq 2a$ and $a + 2b < 1$. Then

$$2H(a + b) - 3H(a) + H(2a) - H(a + 2b) > 0$$

Proof. Fix $a < 1$ and define $g(b) = 2H(a + b) - 3H(a) + H(2a) - H(a + 2b)$. By Lemma B.1, we have $g(2a) = 2H(3a) - 3H(a) + H(2a) - H(5a) > 0$. It therefore suffices to show that $g'(b) > 0$ for all $2a \leq b < \frac{1-a}{2}$. We have,

$$g'(b) = -2 \log \left( \frac{a + b}{1 - (a + b)} \right) + 2 \log \left( \frac{a + 2b}{1 - (a + 2b)} \right)$$

$$= 2 \log \left( \frac{(1 - (a + b))(a + 2b)}{(a + b)(1 - (a + 2b))} \right)$$

$$> 0$$

where the inequality follows since

$$(1 - (a + b))(a + 2b) = a + 2b - (a + b)(a + 2b)$$

$$> a + b - (a + b)(a + 2b)$$

$$= (a + b)(1 - (a + 2b))$$

\qed
We first notice that which is true because Therefore, to finish the proof, it suffices to show that

**Lemma B.4.** Let $0 < a, b < 1$ such that $a + 4b < 1$. Then

$$H(a + 2b) - H(a + b) - \frac{1}{4} H(a + 4b) + \frac{1}{4} H(a) > 0$$

*Proof.* Fix $a < 1$ and define $g(b) = H(a + 2b) - H(a + b) - \frac{1}{4} H(a + 4b) + \frac{1}{4} H(a)$. We have

$$g(0) = H(a) - H(a) - \frac{1}{4} H(a) + \frac{1}{4} H(a) = 0$$

and therefore it suffices to show that $g'(b) > 0$ for all $b < \frac{1 - a}{4}$. We have,

$$g'(b) = -2 \log \left( \frac{a + 2b}{1 - (a + 2b)} \right) + \log \left( \frac{a + b}{1 - (a + b)} \right) + \log \left( \frac{a + 4b}{1 - (a + 4b)} \right)$$

$$= \log \left( \frac{(1 - (a + 2b))^2 (a + b)(a + 4b)}{(a + 2b)^2 (1 - (a + b))(1 - (a + 4b))} \right)$$

We first notice that

$$(a + b)(a + 4b) = a^2 + 5ab + 4b^2 > a^2 + 4ab + 4b^2 = (a + 2b)^2$$

Thus, to finish the proof, it suffices to show that

$$\Delta \triangleq (1 - (a + 2b))^2 - (1 - (a + b))(1 - (a + 4b)) > 0$$

which is true because

$$\Delta = 1 - 2a - 4b + a^2 + 4ab + 4b^2 - (1 - 2a - 5b + a^2 + 5ab + 4b^2)$$

$$= b - ab > 0$$

\[\square\]

**Lemma B.5.** Let $0 < a \leq \frac{1}{2}$ and $b = \frac{1}{4} (1 - a)$. Then

$$\Delta = H(a + 2b) - H(a + b) + \frac{1}{4} H(a) > 0$$

*Proof.* Since $H \left( \frac{1}{2} a + \frac{1}{2} \right) = H \left( \frac{1}{2} - \frac{1}{2} a \right)$ and $\frac{1}{2} - \frac{1}{2} a \geq \frac{3}{4} a + \frac{1}{4}$ for $a \leq \frac{1}{2}$, it follows that

$$H \left( \frac{1}{2} a + \frac{1}{2} \right) \geq H \left( \frac{3}{4} a + \frac{1}{4} \right)$$

Therefore,

$$\Delta = H \left( \frac{1}{2} a + \frac{1}{2} \right) - H \left( \frac{3}{4} a + \frac{1}{4} \right) + \frac{1}{4} H(a) \geq \frac{1}{4} H(a) > 0$$

\[\square\]

**Lemma B.6.** Let $x = \frac{1}{m}$ and $y = \frac{1}{lm}$ where $m$ and $l$ are integers such that $1 \leq k < m$. Then the following three inequalities hold.

1. $\frac{1}{2} H(x + y - xy) - \frac{1}{4} H(y) + \frac{1}{4} H(2y) - \frac{1}{4} H(2x + y - 2xy) > 0$.
2. If $k \geq 3$ then $H(2x + y - 2xy) + \frac{1}{4} H(y) - H(x + y - xy) - \frac{1}{4} H(4x + y - 4xy) > 0$.
3. If $k = 2$ then $H(2x + y - 2xy) + \frac{1}{4} H(y) - H(x + y - xy) > 0$.
4. $H(2y) - H(y) - \frac{1}{4} H(4y) > 0$.

*Proof.*

1. For $k < m - 1$ it holds that $x - xy \geq 2y$. Therefore, in this case the identity follows by plugging $a = y$ and $b = x - xy$ in Lemma B.3. If $k = m - 1$ then $x - xy = 2y - 2y^2$ and the identity follows by Lemma B.2.

2. This follows by plugging $a = y$ and $b = x - xy$ in Lemma B.4.
3. This follow by Lemma B.5 with \( a = y \).

4. This follows by plugging \( a = 0 \) and \( b = y \) in Lemma B.4.

We now proceed to show that \( T_i = B_i \). We need to show that TopDown first builds the right-path of the tree and then builds all left sub-trees of nodes in the right-path from top to bottom. The proof has three parts:

Part 1: Let \( v_1 \) and \( v_2 \) be the right child and left child of the root, respectively. We first show that \( W(v_1) \geq W(v_2) \). Recall that by the results in [Fiat & Pechyony 2004], TopDown chooses an \( x \)-variable as its root (this is WLOG if \( l = m \)).

Denote \( x = \frac{1}{2^{l-1}} \) and \( y = \frac{1}{2^{m}}. \) Then,

\[
W(v_1) = \frac{1}{2}H(x+y-xy) - \frac{1}{4}H(y) - \frac{1}{4}H(2x+y-2xy)
\]

and

\[
W(v_2) = \frac{1}{2}H(1-y) - \frac{1}{4}H(1-2y)
\]

Therefore,

\[
W(v_1) - W(v_2) = \frac{1}{2}H(x+y-xy) - \frac{3}{4}H(y) + \frac{1}{4}H(2y) - \frac{1}{4}H(2x+y-2xy)
\]

which is positive by part 1 of Lemma B.6

Part 2: Next, let \( v \) be a node on the right path and let \( u \) be its parent. We will show that \( W(v) \geq W(u) \).

First assume that \( l \geq 3 \). Let \( 1 \leq k \leq l-2 \) be the depth of \( u \), \( x = \frac{1}{2^{l-k}} \) and \( y = \frac{1}{2^{m}}. \) Then

\[
2^k W(v) = \frac{1}{2}H(2x+y-2xy) - \frac{1}{4}H(y) - \frac{1}{4}H(4x+y-4xy)
\]

and

\[
2^k W(u) = H(x+y-xy) - \frac{1}{2}H(y) - \frac{1}{2}H(2x+y-2xy)
\]

Therefore:

\[
2^k W(v) - 2^k W(u) = H(2x+y-2xy) + \frac{1}{4}H(y) - H(x+y-xy) - \frac{1}{4}H(4x+y-4xy)
\]

\[
> 0
\]

by part 2 of Lemma B.6. Therefore, \( W(v) > W(u) \).

If \( l = 2 \) then

\[
2^k W(v) = \frac{1}{2}H(2x+y-2xy) - \frac{1}{4}H(y)
\]

and therefore,

\[
2^k W(v) - 2^k W(u) = H(2x+y-2xy) + \frac{1}{4}H(y) - H(x+y-xy)
\]

\[
> 0
\]

by part 3 of Lemma B.6.

Part 3: Let \( v \) be a non-root node of a left sub-tree of a node in the right-path. Let \( u \) be its parent. Let \( y = \frac{1}{2^{m-k}} \) where \( m \geq 2 \) and \( 0 \leq k \leq m - 2 \) is the depth of \( u \) in the left sub-tree. We have:

\[
2^{d(u)} (W(v) - W(u)) = \frac{1}{2}H(2y) - \frac{1}{4}H(4y) - \left( H(y) - \frac{1}{2}H(2y) \right)
\]

\[
= H(2y) - H(y) - \frac{1}{4}H(4y) > 0
\]
where the inequality follows by part 4 of Lemma B.6. Therefore, \( W(v) > W(u) \).

Finishing the proof: By part 1 and part 2, TopDown will first grow the right path of the tree before expanding any left sub-tree. To see this, let \( v_1 \) and \( v_2 \) be two left children of nodes in the right-path and \( v_1 \) is in a higher left sub-tree. Note that \( v_1 \) and \( v_2 \) are \( y \)-nodes. Then, it holds that \( W(v_1) > W(v_2) \). Thus, by parts 1 and 2 the weighted gain of any node on the right path is larger than the weighted gain of any left child of a node in the right-path.

Next, after completing the right path, TopDown will expand the left child of the root (and not other roots of left-sub trees by the previous argument). By part 3, it will then expand the highest left sub-tree. By the same argument, it will continue to expand each left sub-tree from top to bottom.

### B.2 Proof of Proposition 5.3

We first need to prove several lemmas.

**Lemma B.7.** For any DNF with at most 2 terms, there exists an optimal tree that consists only of \( x \)-nodes or \( y \)-nodes. Furthermore,

1. In the case of one term, the tree is in \( C_1 \).
2. In the case of 2 terms, the tree is in \( C_2 \).

**Proof.** We prove the claim by induction on \( t + s \) where \( t \) is the size of the tree and \( s \) is the number of literals in the DNF. For \( t = s = 1 \) the claim holds. Assume it holds for \( t + s \). First assume that the DNF has one term with \( y \)-variables. Consider the root of an optimal tree \( T \). If it is not in the DNF, then both \( T_R \) and \( T_L \) correspond to the ground-truth DNF and are of size less than \( t \). By induction, they are WLOG right-paths that consist of only \( y \)-nodes. Assume WLOG that \( E(T_R) \leq E(T_L) \). Then \( E(T) = \frac{1}{2} E(T_L) + \frac{1}{2} E(T_R) \geq E(T_R) \), where the equality follows by the fact that the DNF of the root of \( T_L \) and the DNF of the root of \( T_R \) are equal to the ground-truth DNF, and that the variables are independent. Thus by replacing \( T \) with \( T_R \) we get a new tree in \( C_1 \) with less than \( t \) nodes and did not increase the test error. We can add more nodes to get a tree of size \( t \) and not increase the test error.

If the root node is in the DNF then its left sub-tree is WLOG a leaf, because a single leaf is optimal for a constant function. By induction, its right sub-tree is WLOG a right-path, and therefore the whole tree is in \( C_1 \).

Now, assume that the DNF has two terms. Consider the root of an optimal tree. If it is not in the DNF, then both its right and left sub-tree correspond to the ground-truth DNF and are of size less than \( t \). By induction they are both in \( C_2 \) and consist only of \( x \)-nodes and \( y \)-nodes. Assume WLOG that \( E(T_R) \leq E(T_L) \). Then \( E(T) = \frac{1}{2} E(T_L) + \frac{1}{2} E(T_R) \geq E(T_R) \), where the equality follows by the fact that the DNFs of \( T_L \) and \( T_R \) are the ground-truth DNF. Thus by replacing \( T \) with \( T_R \) we get a new tree in \( C_2 \) with less than \( t \) nodes and did not increase the test error. We can add more nodes to get a tree of size \( t \) and not increase the test error.

If the root is in the DNF, by induction the left sub-tree is in \( C_1 \) and the right sub-tree in \( C_2 \). Therefore, the tree is in \( C_2 \). Furthermore, all nodes are \( x \)-nodes or \( y \)-nodes by induction. \( \square \)

**Lemma B.8.** Let \( v \) be an \( x \)-node with \( F(v) = (x_1 \land x_2 \land \cdots \land x_{k_1}) \lor (y_1 \land y_2 \land \cdots \land y_{k_2}) \). Then the following holds:

1. If \( k_1 = 1, k_2 = 0 \), then \( C(v) = \frac{1}{2} \).
2. If \( k_2 \geq 2, k_1 = 2 \), then \( C(v) = \frac{1}{2^{k_2}} - \frac{1}{2^{k_2+1}} \).
3. If \( k_2 \geq 2, k_1 = 1 \), then \( C(v) = \frac{1}{2} - \frac{1}{2^{k_2+1}} \).
4. If \( k_1 > 1 \) and \( k_2 = 0 \) or \( k_1, k_2 > 2 \), then \( C(v) = 0 \).

**Proof.** By direct calculation we get:

---

8 Analogous claims hold when \( v \) is a \( y \)-node. We also use the notation that for \( k_2 = 0 \) we get a one-term DNF with \( x \)-variables.
1. \( C(v) = C \left( \frac{1}{2} \right) - \frac{1}{2} C(1) - \frac{1}{2} C(0) = \frac{1}{2} \).

2. 
\[
C(v) = C \left( \frac{1}{2^{k_1}} + \frac{1}{2^{k_2}} - \frac{1}{2^{k_1+k_2}} \right) - \frac{1}{2} C \left( \frac{1}{2^{k_1-1}} + \frac{1}{2^{k_2}} - \frac{1}{2^{k_1+k_2-1}} \right) - \frac{1}{2} C \left( \frac{1}{2^{k_2}} \right) \\
= \frac{1}{4} + \frac{1}{2^{k_2}} - \frac{1}{2^{k_1+k_2}} - \frac{1}{2^{k_2+2}} + \frac{1}{2^{k_2+1}} - \frac{1}{4} - \frac{1}{2^{k_2+1}} \\
= \frac{1}{2^{k_2}} - \frac{1}{2^{k_2+1}}
\]

3. 
\[
C(v) = C \left( \frac{1}{2^{k_1}} + \frac{1}{2^{k_2}} - \frac{1}{2^{k_1+k_2}} \right) - \frac{1}{2} C(1) - \frac{1}{2} C \left( \frac{1}{2^{k_2}} \right) \\
= \frac{1}{2^{k_1}} + \frac{1}{2^{k_2}} - \frac{1}{2^{k_1+k_2}} - \frac{1}{2^{k_2+1}} + \frac{1}{2^{k_1+k_2}} - \frac{1}{2^{k_2+1}} \\
= 0
\]

4. In the first case, \( C(v) = C \left( \frac{1}{2^{x_1}} \right) - \frac{1}{2} C \left( \frac{1}{2^{x_1+x}} \right) - \frac{1}{2} C(0) = 0 \)

Proof. If \( t \leq l \), then the optimal tree is a right-path with \( x \)-nodes. This follows since by Lemma B.8, the only nodes with \( C(v) > 0 \) in a tree of size less than \( l \) are the \( l - 1 \) and \( l \) nodes in the right-path.

Assume that \( t > l \). By Lemma B.7, WLOG each left sub-tree of an \( x \)-node in the right-path is a right \( y \)-path. Assume by contradiction that \( T \) has an \( x \)-right-path with less than \( l \) nodes. Then by Lemma B.8 its error reduction is at most
\[
\sum_{i=1}^{l-1} \frac{1}{2^{m+i+1}} + \frac{1}{2^{m+l-1}} = \frac{1}{2^m} - \frac{1}{2^{m+l-1}} + \frac{1}{2^{m+l-1}} = \frac{1}{2^m} \leq \frac{1}{2^l}
\]

where the first summand on the left side is the total test error reduction of all left sub-trees which are right \( y \)-paths. The second summand is the error reduction of the \( l - 1 \) node in the right \( x \)-path of the tree. The right-side of Equation 8 is the error reduction of a full right \( x \)-path. Indeed, by Lemma B.8 this is given by the sum of error reduction of nodes \( l - 1 \) and \( l \) in the path, which is \( \frac{1}{2^{m+l-1}} + \frac{1}{2^{m+l-1}} = \frac{1}{2^l} \). Therefore, a full right \( x \)-path has error reduction at least as any other tree with no full right \( x \)-path. We can thus assume WLOG that the optimal tree has a full right \( x \)-path.

We are left to show that there is no node in a left sub-tree (which is a right \( y \)-path), unless all left sub-trees above it are full right \( y \)-paths. Assume by contradiction that this does not hold and consider a left sub-tree \( T'_L \) which violates this condition. We claim that by moving the nodes of \( T'_L \) to higher left sub-trees can only increase the error reduction. To see this, first consider the case where \( T'_L \) is not full. In this case the error reduction of all its nodes is 0. We can therefore remove them without decreasing error reduction. Placing them in higher left sub-trees can only increase the error reduction.

If \( T'_L \) is a full right \( y \)-path, let \( T''_L \) be a higher left sub-tree which is not full (it exists by our assumption). By moving nodes from \( T'_L \) to \( T''_L \) we can make \( T''_L \) full. By part 1 of Lemma B.8 the error reduction of the whole tree increases by \( \frac{1}{2^{m+k_2}} - \frac{1}{2^{m+k_2}} > 0 \) where \( k_1 \) and \( k_2 \) are the depths of the last nodes in \( T'_L \) and \( T''_L \), respectively.

\[ \square \]
We now turn to proving the proposition. We prove it by induction on \( t \). For \( t = 1 \), TopDown chooses an \( x \)-node which is \( B_1 \). Assume the claim holds for \( t - 1 \). Let \( T \) be the optimal tree with \( t \) nodes. We have 4 cases:

**Case 1:** The root of \( T \) is an \( x \)-node. By the induction hypothesis, there exists an optimal tree \( T' \) whose right-most path consists only of \( x \)-nodes. This follows since we can replace the right sub-tree of the root of \( T \) with a tree \( B_t' \), where \( t' \) is the number of inner nodes in the right sub-tree, to get the tree \( T' \). By induction, this does not increase the test error. Therefore, by Lemma [B.9] \( B_t \) is optimal.

**Case 2:** The root of \( T \) is a \( y \)-node and \( l = m \). Similarly to the previous case, we get by the induction hypothesis that there exists an optimal tree \( T' \) whose right path consists only of \( y \)-nodes. By Lemma [B.9] applied to the case where \( l = m \) and right \( y \)-path (which by symmetry can be analyzed the same as the case of a right \( x \)-path), \( B_t \) is optimal.

**Case 3:** The root of \( T \) is a \( y \)-node, \( l < m \) and the left sub-tree of the root is a full \( x \)-tree. The following procedure does not decrease the test error reduction and does not increase the size of the tree: Remove root and left sub-tree and add one \( y \)-node to each left sub-tree of \( x \)-node in the right path. Note that there are at most \( l \) \( x \)-nodes in the right path. Add remaining nodes as \( x \)-nodes to right path. We will denote by \( T' \) the new resulting tree.

First, we note that by adding a \( y \)-node to each left sub-tree of an \( x \)-node, the total error reduction of each such left-sub tree does not change. To see this, consider two cases. In the first the left sub-tree of an \( x \)-node is not full. Then its error reduction is 0 and therefore, removing the root cannot decrease its error reduction. Second, if the left sub-tree is full, then the only node with non-zero error reduction is the last node. Its error reduction is \( \frac{1}{2^{l+1}} \). After removing the root and adding a \( y \)-node, the last node still has error reduction of \( \frac{1}{2^{l+1}} \).

By Lemma [B.8] part 1, the error reduction of the left sub-tree of \( T' \) is \( \frac{1}{2^l} \). Denote by \( D \) the difference between the error reduction of the right-path of \( T \) and the error reduction of the right-path of \( T' \). It suffices to show that \( D \geq \frac{1}{2^m} \). Let \( C_r \) be the error reduction of the right-path of \( T \). Since \( T \) has a root \( y \)-node, we get by Lemma [B.8] that \( C_r \leq \frac{1}{2^r} \). By the induction hypothesis and the assumption that the left sub-tree of \( r_T \) is full, \( T' \) has \( l \) \( x \)-nodes on its right-path. Therefore, by Lemma [B.8] we have \( D = \frac{1}{2^l} - C_r \geq \frac{1}{2^m} \), as desired.

**Case 4:** The root of \( T \) is a \( y \)-node, \( l < m \) and the left sub-tree of the root is not a full \( x \)-tree.

Assume that there exists an \( x \)-node in the right-most path whose left-sub tree is a full right \( y \)-path. Then, we can create a new tree by moving nodes from the latter left sub-tree to the left sub-tree of the root, to create a full right \( x \)-path in the left sub-tree of the root. This does not decrease the test error reduction. Then we are in the previous case where the left sub-tree of the root is a full \( x \)-path.

We are left with the case in which there is no \( x \)-node in the right-most path with full left-sub tree. In this case, we can remove the root and its left sub-tree and replace the tree with its right sub-tree. If there is no right sub-tree then we can replace the tree with a single \( x \)-node. The total test error reduction will not decrease. To see this, note that there is no error reduction in left sub-trees of \( x \)-nodes (because they are not full) and the error reduction in the left sub-trees of \( y \)-nodes can only increase because we increase the probability to get to each node.

Finally, the error reduction of the right-path can only increase as well. Note that by induction, WLOG the nodes on the right-path, not including the root, are \( x \)-nodes. If the length of the right-path is less than \( l \), then every node has zero error reduction and this will not change after removal of the root and its left sub-tree. If its length is \( l \), then the only non-zero error reduction is at the last node in the path, denoted by \( v \). This error reduction is \( \frac{1}{2^{l-1}} \frac{1}{2m} = \frac{1}{2^{l+1}} \), by Lemma [B.8] part 2. After the removal of nodes, its error reduction is \( \frac{1}{2^{l-1}} \frac{1}{2m} = \frac{1}{2^{l+1}} \), and therefore does not change. If its length is \( l + 1 \), i.e., it has \( l \) \( x \)-nodes, then the total error reduction before removal is

\[
\frac{1}{2^{l-1}} \frac{1}{2m} + \frac{1}{2} \left( \frac{1}{2} - \frac{1}{2^{l-1}} \right) = \frac{1}{2^{l+1}}
\]
Algorithm BestFirst(T)

Initialize T to be a single leaf labeled by the majority label with respect to D.

while T has less than t nodes:
    \( \Delta_{best} \leftarrow 0 \).
    for each pair \( l \in \ell(T) \) and \( i \in F \):
        \( \Delta \leftarrow H(q(l)) - (1 - \tau_i)H(q(l_0)) - \tau_i H(q(l_1)) \).
        if \( \Delta \geq \Delta_{best} \) then:
            \( \Delta_{best} \leftarrow \Delta; l_{best} \leftarrow l; i_{best} \leftarrow i \).
            \( T \leftarrow T(l_{best}, i_{best}) \).

return T.

Figure 5: BestFirst algorithm.

and after
\[
\frac{1}{2^{t-2}} + \frac{1}{2^{t-1}} - \frac{1}{2^m} = \frac{1}{2^t}
\]
and thus the error reduction increases, which finishes the proof.

C Comparison with BestFirst

Here we show that BestFirst chooses the tree in Figure 2a. Figure 5 shows the pseudo-code for BestFirst, where we use the same notation as in Section 3. By parts 1 and 2 at the end of the proof of Proposition 5.2, BestFirst will first grow the right-path of \( x \)-nodes. Note that in part 2 we show that a node on the right-path has larger weighted gain than its parent. Since it is a deeper node it also has a larger gain. However, the gain of the left childs of the nodes on the right-path are equal. Therefore, it can choose to grow the left child of the second \( x \)-node on the right-path. Then, by part 3 at the end of the proof of Proposition 5.2, it will expand the left sub-tree of the second \( x \)-node before expanding the left child of the first \( x \)-node. Here again, we use the fact that if the weighted gain of a child is larger than the weighted gain of its parent, then also its gain is larger than the gain of its parent.

D Correctness of Dynamic Programming Formulas

First, we will show by induction on \( t \) that there is an optimal tree which all of its nodes are variables in the DNF. In the induction step, if by contradiction there is an optimal tree \( T \) with a root node that is not in the DNF, we can replace it with one of its sub-trees \( T_R \) or \( T_L \) (whose nodes are all in the DNF by the induction hypothesis) without increasing the test error. This follows since the test error of \( T \) is a convex combination of the test errors of \( T_R \) and \( T_L \), by the independence assumption.

We initialized \( OPT(F, 0) \) to be the test error of a single root node with DNF \( F \) and \( OPT(\emptyset, t) = 0 \). Furthermore, in equation 3 we set \( S_c(F, t, j, c) = 1 \) if \( c \) does not have a variable with distribution \( \text{Bernoulli}(p_i) \). Now, consider an optimal tree \( T \) over \( D \) with a ground truth DNF \( F \) and consider WLOG its left sub-tree \( T' \) with \( t \) internal nodes and the DNF \( F' \) which is the DNF \( F \) after conditioning on the assignments from the root of \( T \) to the root of \( T' \) (which is the left child of the root of \( T \)). Then since \( D \) is a product distribution, \( T' \) is the optimal tree with \( t \) internal nodes over \( D \) with a ground-truth DNF \( F' \) (i.e., the same marginal distribution on \( X \) but realizable with \( F' \) and not \( F \)). By considering all possible splitting variables from the DNF and all possible number of internal nodes for the left and right sub-trees, we get the formulas in Section 6.