An efficient algorithm for optimal pruning of decision trees

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Abstract

Pruning decision trees is a useful technique for improving the generalization performance in decision tree induction, and for trading accuracy for simplicity in other applications. In this paper, a new algorithm called OPT-2 for optimal pruning of decision trees is introduced. The algorithm is based on dynamic programming. In its most basic form, the time and space complexities of OPT-2 are both $\Theta(nC)$, where $n$ is the number of test nodes in the initial decision tree, and $C$ is the number of leaves in the target (pruned) decision tree. This is an improvement over the recently published OPT algorithm of Bohanec and Bratko (which is the only known algorithm for optimal decision tree pruning) especially in the case of heavy pruning and when the tests of the given decision tree have many outcomes. If so desired, the space required by OPT-2 can further be reduced by a factor of $r$ at the cost of increasing the execution time by a factor that is bounded above by $(r + 1)/2$ (this is a considerable overestimate, however). From a practical point of view, OPT-2 enjoys considerable flexibility in various aspects, and is easy to implement.

1. Introduction

Pruning a decision tree, $DT$, is the process of replacing some of the subtrees of $DT$ by leaves. In machine learning research, pruning is a widely used technique for avoiding overfitting of the training data. It is well known that, in noisy domains, pruning usually leads to decision trees with better generalization performance.

Another important motivation of pruning is "trading accuracy for simplicity" as discussed by Bohanec and Bratko [1]. They note that, in many situations, a simple,
comprehensible, but only approximate description of a concept may be more useful than a completely accurate description that involves a lot of details. They illustrate this idea by considering a rule that decides the legality of a white-to-move chess position (the KKK concept of [5]). They show that in representing this rule, (i) a decision tree with 11 leaves gives a completely accurate description, (ii) a pruned tree with only 4 leaves is 98.45% accurate, and (iii) a pruned tree with only 5 leaves is 99.57% accurate. Thus, more than half of the size of the completely accurate tree accounts for less than 0.5% of the accuracy. Pruning is helpful in such situations when the goal is to produce a compact concept description that is sufficiently accurate.

In the context of pruning, it is convenient to view the initial decision tree as a completely accurate one. The accuracy of a pruned decision tree then only indicates how close the pruned tree is to the initial tree. A common practice when pruning a given decision tree, $DT$, with $s$ leaves is to progressively replace various subtrees of $DT$ by leaves leading to a sequence

$$DT_s, DT_{s-1}, DT_{s-2}, \ldots, DT_1$$

of pruned decision trees such that each $DT_i$ has at most $i$ leaves. Viewing the error as the difference from the original tree $DT$, such trees are of increasing error. In an actual application, the best tree is to be selected from the above sequence of pruned trees based on some appropriate criteria, where the goal is to strike a good balance between the size of the tree and its accuracy.

In optimal pruning, it is required that the error of each $DT_i$ in the sequence be minimum over all pruned trees of $i$ (or less) leaves. Although decision tree pruning has been studied by many researchers (e.g., [2, 4, 6]), the only work that addressed optimal pruning so far is the recent paper of Bohanec and Bratko [1]. In their work, they show that previous methods lead to suboptimal solutions, and introduce an algorithm (which they call OPT) that guarantees optimality. Based on dynamic programming, OPT produces the above sequence of pruned trees in time $O(s^2)$, where $s$ is the number of leaves of the initial decision tree.

This paper introduces a new algorithm, OPT-2, that also performs optimal pruning. An important feature of this new algorithm is its considerable flexibility. Unlike OPT, which generates the whole sequence of pruned trees simultaneously, the new algorithm works sequentially generating the trees of the sequence one after the other in increasing order of the number of leaves—that is, in the order $DT_1, DT_2, DT_3, \ldots$. One can argue that generating the whole sequence is often unnecessary, since, eventually, only one tree will be chosen from the sequence as the final result of pruning. Using OPT-2 gives the user the freedom to terminate the sequence generation quite early (and thus, saving unneeded computations) as soon as a tree that satisfies the criteria at hand is found.

Given that trees $DT_1, DT_2, \ldots, DT_{i-1}$ have already been generated, OPT-2 finds $DT_i$ in time $\Theta(n)$, where $n$ is the number of internal nodes (tests) of the initial decision tree. Thus, if the number of leaves of the target tree is $C$, then the total running time of OPT-2 will be $\Theta(nC)$. Usually, $C$ is much smaller than $s$, since the goal is to prune

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1 Of course, under other definitions of accuracy (e.g. generalization performance in inductive learning), a pruned tree may even be more accurate than the initial tree.
the tree. Moreover, \( n \) is also smaller than \( s \) especially in the case of tests with many outcomes (namely, \( s = (k - 1)n + 1 \) in a \( k \)-ary tree). Therefore, OPT-2 is usually more efficient than OPT in terms of execution time. In the extreme case, however, when the whole sequence of pruned decision trees has to be generated, and when the tests of the decision tree are binary, OPT-2 will exhibit the same time complexity as OPT.

OPT-2 is also efficient in terms of space complexity. In its simplest form, the space required by the algorithm is \( \Theta(nc) \). However, if one is willing to trade time for space, the required space can easily be reduced by a factor of \( r \) at the cost of increasing the execution time by a factor of much less than \( (r + 1)/2 \). The space complexity of OPT-2 can be reduced in this manner down to \( \Theta(nd_{\text{max}}) \), where \( d_{\text{max}} \) is the maximum degree of the tree. The exact space complexity of OPT, on the other hand, is not clear. It can best be upper bounded by \( O(s^2) \) although it may actually require a little less space than that [Bohanec. Private Communication, August, 1994].

In addition to the above advantages, the OPT-2 algorithm is also very easy to implement since (as will be seen later) it only involves simple computations over a two-dimensional array of positive numbers.

Although both OPT and OPT-2 are based on dynamic programming, the two algorithms differ substantially in the way the problem is divided into subproblems. The approach adopted in OPT is usually viewed as a "bottom-up" approach [3]. The idea there is to compute solutions for the subtrees rooted at the lowest level of the tree. Then from these, solutions at the nodes of the next upper level are computed. This process is repeated until the root of the initial tree is reached. A fundamental property of this bottom-up approach is that the trees \( DT_i \) of the pruning sequence are computed simultaneously while we are approaching the root. None of these pruned trees is final unless we reach the root, but once we are at the root the whole sequence becomes available at once. This consequence of the bottom-up approach is not desirable since it is rarely the case that the whole pruning sequence is needed.

In contrast, the OPT-2 algorithm enjoys more flexibility in that it produces the pruned trees one after the other, enabling the user to stop the process at any point as desired. This algorithm is a derivative of a dynamic programming method given by Johnson and Niemi for solving "tree knapsack" problems [3]. As will be seen from the description of the algorithm, processing in OPT-2 is done in a "left-to-right" fashion. Given that we have already computed trees \( DT_1, DT_2, \ldots, DT_{i-1} \), and that necessary intermediate results from these computations are kept in memory, the OPT-2 algorithm finds \( DT_i \) from these through a linear left-to-right pass over the tree. This left-to-right approach, therefore, makes it possible to terminate the process once a satisfactory tree, say \( DT_i \), is found—avoiding unneeded computation of trees \( DT_{i+1} \) through \( DT_{s-1} \).

The rest of this paper is organized as follows. We start in the next section with a formal description of the problem of optimal pruning of decision trees. The OPT-2 algorithm is then described in Sections 3 and 4. Space and time complexity analyses are given in Sections 5 and 6. We conclude with a summary and suggestions for future research in Section 7.

\[ \text{The degree of a test node is the number of its children.} \]
2. The problem

Let $DT$ be a decision tree. Each internal node in $DT$ is labeled with a test $t_i$, and each outgoing edge from that node corresponds to a possible outcome of that test. Each leaf is labeled with some class. The class at a given leaf indicates the "action" to be taken for cases that satisfy the tests along the branches from the root of the tree to that leaf.

For convenience, we will always assume that the test nodes are labeled $t_1, t_2, t_3, \ldots, t_n$ (where $n$ denotes the number of test nodes) according to the depth-first traversal of the tree. (See Fig. 1.) The degree of a node $t_i$, denoted $d(t_i)$, is the number of children of $t_i$.

For a test node $t_i$, let $E_i$ be the set of cases that satisfy the tests along the branches from the root to $t_i$. The majority class at $t_i$ is the most frequent class in $E_i$. Pruning a test node $t_i$ means replacing the subtree of $DT$ rooted at $t_i$ by a leaf labeled with the majority class at $t_i$. A decision tree $DT'$ generated by pruning one or more nodes from $DT$ in this manner is a predecessor-closed subtree of $DT$ in the sense that for each test node $t_j \in DT'$, the parent of $t_j$ is also in $DT'$.

By $error(t_i)$, we denote the number of cases in $E_i$ that are incorrectly classified if the test node $t_i$ is pruned. In other words, if $a$ is the number of cases in $E_i$ labeled with the majority class, then $error(t_i) = E_i - a$.\(^3\) By $error(DT)$, we denote the number of cases that are incorrectly handled by $DT$. This is equivalent to $\sum_{t \in \ell} error(t)$, where $\ell$ is the set of the leaves of $DT$. The size of $DT$, denoted $s(DT)$, is the number of leaves in $DT$. The base-error is the error when the whole tree is replaced with a single leaf. Thus, the base-error is just $error(t_1)$.

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\(^3\) As far as the presented algorithm is concerned, the error can be any non-negative value (not necessarily the error frequency) such that the error at a given node is greater than or equal to the sum of the errors at the children of that node.
The problem of optimal pruning can be stated as an optimization problem as follows:

Given a decision tree $DT$ and a positive integer $C$, find a pruned decision tree $DT'$ from $DT$ such that $s(DT) \leq C$ and $\text{error}(DT)$ is minimized.

As in [1], we assume that the error at each test node is given (see Fig. 1). Obviously, solving the problem as stated above is sufficient to generate the pruning sequence as mentioned in the previous section.

3. The method

Pruning can be viewed as deciding for each node $t_i$ in the initial decision tree whether or not that node is to be included in the final tree. Consider the decision tree of Fig. 2(a) which is generated by pruning the decision tree of Fig. 1 at nodes $t_2$, $t_6$, $t_7$ and $t_8$. Assume that, in addition to the test nodes of this tree, we decided to include node $t_2$ as well. This leads to the tree shown in Fig. 2(b) in which the left-most child of $t_1$ has been replaced by node $t_2$ with two leaves as its children. This move, which can be viewed as “leaf-expansion”, reduces the error of the tree from 6 to 5. The number of the leaves, however, increases from 5 to 6. Similarly, if we further choose to expand, for example, the leaf appearing as the right child of $t_2$ in Fig. 2(b), then the error will decrease to 4, but the total number of leaves will now be 8.

In this paper, the reduction in error which results from expanding a leaf is viewed as “profit”, while the associated increment in the size of the tree is viewed as “cost”. Now, given a decision tree $DT$ that we would like to prune, consider generating another tree, $T$, by doing the following:

- Add a new node, $t_0$, as the parent of $t_1$ (the root of $DT$). This new node, thus, becomes the root of $T$.
- For each node $t_i$ in $T$, $1 \leq i \leq n$, let
  \[ \text{cost}(t_i) = d(t_i) - 1 \]
  and let $\text{cost}(t_0) = 1$. 

For each node $t_i$ in $T$, $1 \leq i \leq n$, let

$$\text{profit}(t_i) = \text{error}(t_i) - \sum_{a: \text{child of } t_i} \text{error}(a)$$

and let $\text{profit}(t_0) = 0$.

- Delete all the leaves of $DT$.

We will call the tree $T$ constructed as above the cost-profit (CP) tree of $DT$. Fig. 3 shows the CP tree that corresponds to the decision tree of Fig. 1.

Note that there is a one-to-one correspondence between the set of all pruned subtrees of a decision tree $DT$, and the set of all predecessor-closed subtrees of the CP tree $T$ obtained from $DT$. Namely, a predecessor-closed subtree, $T'$, of the CP tree $T$ corresponds to the pruned decision tree $DT'$ in which each subtree of $DT$ rooted at a node $t_i \notin T'$ is replaced by a leaf.

For a predecessor-closed subtree $T'$, let us denote by $\text{cost}(T')$, the total cost, and by $\text{profit}(T')$, the total profit of the nodes of $T'$. The reader may confirm that if $DT'$ is the pruned decision tree which corresponds to $T'$, then

- $\text{cost}(T') = s(DT')$, and
- $\text{profit}(T') = \text{base-error} - \text{error}(DT')$.

As an example, let $T'$ be the subtree of the cost-profit tree shown in Fig. 3 induced by the nodes $\{t_0, t_1, t_2, t_4, t_5\}$. The corresponding pruned decision tree $DT'$ in this case is obtained by replacing the test nodes $\{t_3, t_6, t_7, t_8\}$ in the decision tree of Fig. 1 by leaves. The cost of $T'$ is 8, which is equivalent to the number of leaves in $DT'$. The profit of $T'$ is 7. This is equivalent to the difference between the base-error, which is 11, and the error of $DT'$, which is 4.
With the above transformation from a decision tree \( DT \) to a CP tree \( T \), the optimal pruning problem addressed here can be restated as follows:

Given a CP tree \( T \), and a positive integer \( C \), find a predecessor-closed subtree \( T' \) of \( T \) such that \( \text{profit}(T') \) is maximized and \( \text{cost}(T') \leq C \).

**Notation.** For a node \( t_i \) in a CP tree \( T \) and an integer \( j \), \( 0 \leq j \leq d(t_i) \), let us denote by \( T'_j \) the subtree of \( T \) induced by

1. the nodes \( t_0, t_1, t_2, t_3, \ldots, t_{i-1}, t_i \) (which are the nodes visited in a depth-first traversal of the tree up to \( t_i \)), and
2. the first \( j \) children of \( t_i \) and all their successors.

Fig. 4 shows two examples. \( T^0_5 \) is the subtree induced by node \( t_5 \) and all nodes of lower indices. None of the children of \( t_5 \) is included because the superscript in \( T^0_5 \) is 0. Likewise, \( T^2_1 \) is the subtree induced by node \( t_1 \) and its first two children and their successors (which are \( \{t_2, t_3, t_4, t_5, t_6, t_7\} \)), and node \( t_0 \) since it has a lower index.

**Notation.** Note that any \( T^j_i \) is itself a cost-profit tree. For some positive integer \( c \) and some \( T^j_i \), let \( \text{Solution}[T^j_i, c] \) denote a maximum profit predecessor-closed subtree of \( T^j_i \) that contains \( t_i \) and whose cost is less than or equal to \( c \). By \( P[T^j_i, c] \) we will denote the profit of that solution, i.e., \( \text{profit}(\text{Solution}[T^j_i, c]) \).
For example, consider the subtree $T_f^2$ of Fig. 4. If the maximum allowed cost is 7, then the subtree induced by nodes $\{t_0, t_1, t_5, t_6, t_7\}$ gives the highest possible profit which is 7. Therefore, $P[T_f^2, 7] = 7$ in this case.\footnote{Note that other solutions with the same profit also exist. When there are multiple solutions, finding one will be considered sufficient in this work.}

With the above notation, our goal becomes to find $\text{Solution}[T_0^i, C]$, where $C$ is the target tree size. It should be noted that, even though some subtrees such as $T_f^2$ and $T_g^2$ are equivalent, a solution for $T_g^2$ has to include $t_5$ whereas a solution for $T_f^2$ does not. The reader may check, for example, that $P[T_f^2, 6]$ is 7 while $P[T_g^2, 6]$ is only 6.

Normally, $P[T_i^j, c]$ takes non-negative values. However, since Solution$[T_i^j, c]$ has to contain $t_i$ and all its predecessors (this is because the solution subtree has to be predecessor-closed), no solution exists if $c$ is less than the total cost of these nodes. In this case, we let $P[T_i^j, c] = -\infty$. For example, for $T_g^2$ of Fig. 4, there exists no solution of cost 4, and thus, $P[T_g^2, 4] = -\infty$.

The pruning algorithm introduced in this paper is based on the following three rules:

- **Rule 1:**
  
  \[ P[T_0^i, c] = 0. \]

- **Rule 2:** Let $t_i$ be the $k$th child of $t_r$. Then
  
  \[ P[T_i^j, c] = \begin{cases} 
  P[T_{r-1}^i, c - \text{cost}(t_i)] + \text{profit}(t_i), & \text{if } c - \text{cost}(t_i) \geq 1, \\
  -\infty, & \text{otherwise.} 
  \end{cases} \]

- **Rule 3:** Let $t_i$'s $j$th child be $t_k$. Then
  
  \[ P[T_i^j, c] = \max \left\{ P[T_{k}^{d(t_k)}, c], P[T_{i-1}^j, c] \right\}. \]

The correctness of these rules is not difficult to confirm:

- Rule 1 is trivial.
- For Rule 2, the situation is depicted in Fig. 5. Note that $T_0^i$ contains no children of $t_i$, and that, by definition, a solution for $T_0^i$ must contain $t_i$. Therefore, given that $t_i$ is the child number $k$ of $t_r$, a solution within cost $c$ has to be the node $t_i$ along with a solution for $T_{k-1}^i$ within cost $c - \text{cost}(t_i)$. But, of course, if $c - \text{cost}(t_i) \leq 0$, then no solution exists for $T_0^i$ within cost $c$, and thus, $P = -\infty$ in this case.
- For Rule 3, note that both $T_i^j$ and $T_k^{d(t_k)}$ denote the same subtree. However, by definition, any solution for $T_k^{d(t_k)}$ has to include $t_k$. To find a solution for $T_i^j$, we have two choices, either to include $t_k$ (possibly with some of its descendants) or not to include it. Not including $t_k$ means just finding a solution for $T_i^{j-1}$ (the tree $T_i^j$ with $t_k$ and all its descendants removed), while including $t_k$ means finding a solution for $T_i^{d(t_k)}$. The rule states that we are to choose one of these two solutions, whichever gives higher profit.

Our goal, that of computing $\text{Solution}[T_i^j, C]$ for some target tree size $C$, can be achieved by repeated application of the above rules. Even though the above rules only compute the profit of the solution for a given cost (and not the solution itself), it turns
out that the actual solution can be easily computed from these numbers. This will be explained in the next section.

To be able to apply the rules, the computations have to be done in a proper order so that the \( P \) values on the right-hand side of a rule are computed before we attempt to apply that rule. For this purpose, we order the subtrees \( T_i \)'s of \( T \) such that

1. \( T_i \) precedes \( T_{i+1} \).
2. If \( t_k \) is the \( j \)th child of \( t_i \), then \( T_{i-1} \) precedes \( T_k \) and \( T_{d(t_k)} \) precedes \( T_{i-1} \).

For example, the \( T_i \)'s of the CP tree shown in Fig. 3 are ordered as \( T_0, T_1, T_2, T_3, T_4, T_5, T_6, T_7, T_8, T_9, T_10, T_11, T_12, T_13, T_14, T_15, T_16, T_17 \).

Notation. \( T(k) \) will be used to denote the subtree number \( k \) in the above-mentioned ordering. Moreover, for any \( j \geq 1 \), \( T_{i-1} \) will be called the *elder sibling* of \( t_i \). If \( T_{i-1} \) is the \( k \)th subtree, and \( T_j \) is the \( y \)th subtree in the ordering, then we write \( ES(y) = k \).

It is obvious that \( ES(y) \) is always less than \( y \).

For the CP tree of Fig. 3, \( T(3) = T_0, T(5) = T_1 \) and \( T(7) = T_2 \), and thus, \( ES(5) = 3 \) and \( ES(7) = 5 \).

Note that, for any \( i \geq 1 \), if \( T_i \) is the \( y \)th subtree in our ordering, and \( t_i \) is the \( k \)th child of \( t_r \), then \( T_{k-1} \) is the \((y-1)\)th subtree in the ordering. Therefore, using the above notation, Rule 2 can be restated as follows:

- **Rule 2**: If \( T(y) = T_i \) for \( 1 \leq i \leq n \), then

\[
P[T(y), c] = \begin{cases} 
P[T(y-1), c - \text{cost}(t_i)] + \text{profit}(t_i), & \text{if } c - \text{cost}(t_i) \geq 1, \\
\infty, & \text{otherwise.} \end{cases}
\]
Table 1
The P values for the CP tree given in Fig. 3; "*" indicates \(-\infty\); ES indicates the elder sibling information; the underlined values are the values referenced when constructing a solution of total cost 10

| y | \(T(y)\) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | ES |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | \(T_1^0\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | \(
| 2 | \(T_2^0\) | * | * | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 3 | \(T_3^0\) | * | * | * | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| 4 | \(T_4^0\) | * | * | * | * | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 3 |
| 5 | \(T_5^0\) | * | * | * | 6 | 6 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 3 | 3 |
| 6 | \(T_6^0\) | * | * | * | * | 7 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| 7 | \(T_7^0\) | * | * | 6 | 7 | 7 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 5 | 5 | 5 | 5 | 5 |
| 8 | \(T_8^0\) | * | 5 | 6 | 6 | 7 | 7 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 2 | 2 | 2 | 2 |
| 9 | \(T_9^0\) | * | * | * | 5 | 6 | 7 | 7 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| 10 | \(T_{10}^0\) | * | * | * | * | 6 | 7 | 7 | 8 | 8 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 |
| 11 | \(T_{11}^0\) | * | * | * | 5 | 6 | 7 | 7 | 8 | 8 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 |
| 12 | \(T_{12}^0\) | * | * | * | 5 | 6 | 7 | 8 | 8 | 9 | 9 | 9 | 9 | 10 | 10 | 10 | 10 | 10 | 10 |
| 13 | \(T_{13}^0\) | * | * | * | 5 | 6 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 14 | \(T_{14}^0\) | * | * | 5 | 6 | 6 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 15 | \(T_{15}^0\) | * | * | * | 5 | 6 | 6 | 7 | 7 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 16 | \(T_{16}^0\) | * | * | * | 5 | 6 | 7 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 17 | \(T_{17}^0\) | * | * | * | 5 | 6 | 7 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 18 | \(T_{18}^0\) | * | 5 | 6 | 6 | 7 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| 19 | \(T_{19}^0\) | 0 | 0 | 5 | 6 | 6 | 7 | 7 | 8 | 8 | 9 | 10 | 10 | 10 | 10 | 10 | 10 | 10 | 10 |
| Error | 11 | 11 | 6 | 5 | 5 | 4 | 4 | 3 | 3 | 2 | 2 | 1 | 1 | 1 | 1 | 0 |

Likewise, for \(j \geq 1\), if \(T_j^i\) is the \(y\)th subtree, and \(t_k\) is the \(j\)th child of \(t_i\), then \(T_{k(j)}^i\) is just \(T(y-1)\), and \(T_{k-1}^i\) is just \(T(ES(y))\). Therefore, Rule 3 can be restated as follows:

- Rule 3: If \(T(y) = T_j^i\) for some \(j \geq 1\), then

\[
P[T(y), c] = \max \{P[T(y - 1), c], P[T(ES(y)), c]\}.
\]

The reader can confirm that computing \(P[T(y), c]\) can be done by two nested loops for \(c = 1, 2, 3, \ldots\) as the outer loop and for \(y = 1, 2, 3, \ldots\) as the inner one. Thus, performing the computation in the above sequence not only enables the use of the rules, but also makes the algorithm quite easy to implement.

3.1. Example

Table 1 shows all the P values for the CP tree of Fig. 3. For a given target tree size \(C\), columns are computed from left to right for \(c = 1, 2, \ldots, C\). Within each column, computation is done from top to bottom. When computing \(P[T_j^i, c]\), Rule 1 is applied if \(i = j = 0\), and Rule 2 is applied if \(i \neq 0\) but \(j = 0\). Rule 3 is applied otherwise.

For Rule 2, suppose \(T_j^0\) is the \(y\)th subtree in our ordering. To compute \(P[T_j^0, c]\) (which is the entry on row \(y\), column \(c\)), all we need to do is to add \(profit(t_i)\) to the
entry at row $y - 1$ and column $c - \text{cost}(t_i)$. For example, let us see how to compute
the entry at row 6, column 9, which is $P[T_4^0, 9]$. The profit of $t_4$ is 1 and the cost is 2.
Therefore, this entry is given by $P[T(5), 9 - 2] + 1 = 8$.

For Rule 3, suppose $T_i^y$ is the $y$th subtree in our ordering. To compute $P[T_i^y, c]$ (which
is the entry on row $y$, column $c$), we need to compare the entries $P[T(y - 1), c]$ and
$P[T(ES(y))_1, c]$, and take the larger of these. As an example, let us compute the entry
at row 18, column 10, which is $P[T_3^3, 10]$. The first term is $P[T(17), 10] = 8$. Since
$ES(18) = 14$, the second term is $P[T(14), 10] = 9$. Taking the maximum of these,

Computation of the $P$ values is terminated after computing column $C$ and $P[T^0, C]$ (the
value at the bottom of column $C$) is taken as the final solution. For example, when
the target tree size is 10, the maximum profit is 9. The row at the bottom of Table 1
indicates the error of the corresponding pruned tree. It says, in this case, that the best
tree of size 10 has error

$$\text{base-error} - P[T_0^0, 10] = 11 - 9 = 2.$$ 

4. Constructing actual solutions

Once the $P$ values have been computed up to column $C$, where $C$ is the target tree
size, the following three rules can be applied to find $\text{Solution}[T_i^y, c]$ for any $T_i^y$ and
$c < C$:

- **Rule 1'**: 
  $$\text{Solution}[T_0^0, c] = \{t_0\}.$$ 

- **Rule 2'**: Let $T_i^0$ be the $y$th subtree in the ordering. Then
  $$\text{Solution}[T(y), c] = \begin{cases} \{t_i\} \cup \text{Solution}[T(y - 1), c - \text{cost}(t_i)], & \text{if } P[T(y), c] \geq 0, \\ \text{no solution exists, otherwise.} & \end{cases}$$

- **Rule 3'**: Let $T_i^y$ be the $y$th subtree in the ordering. Then
  $$\text{Solution}[T(y), c] = \begin{cases} \text{Solution}[T(y - 1), c], & \text{if } P[T(y), c] = P[T(y - 1), c], \\ \text{Solution}[T(ES(y)), c], & \text{otherwise.} \end{cases}$$

The correctness of these rules can be verified following the same logic of the three rules
of the previous section.

4.1. Example—revisited

For target tree size 10, let us see how we can actually construct a minimal error
tree within this size after the first 10 columns of Table 1 have been computed. Our
goal is, thus, to compute $\text{Solution}[T(19),10] = \text{Solution}[T(18),10]$. This can be done using the three rules given above as follows: (i) By Rule 3', since $P[T(19),10] = P[T(18),10]$, the desired solution is equal to $\text{Solution}[T(18),10]$. (ii) By Rule 3', since $P[T(18),10] > P[T(17),10]$ and since $ES(18) = 14$, the desired solution is equal to $\text{Solution}[T(14),10]$. (iii) By Rule 3', since $P[T(14),10] = P[T(13),10]$, the solution is again equal to $\text{Solution}[T(13),10]$. (iv) Again, $P[T(13),10] = P[T(12),10]$ and thus the desired solution is just $\text{Solution}[T(12),10]$. (v) $T(12) = T_0^0$, and therefore, Rule 2' is the one to be applied this time (since the superscript is 0). Given that $\text{cost}(t_7) = 1$, the desired solution is the union of $\{t_7\}$ and $\text{Solution}[T(11),9]$. Continuing in this manner (see Fig. 6), we find that the final solution is $\{t_7,t_6,t_5,t_4,t_2,t_1,t_0\}$.

5. Time complexity

A formal description of the OPT-2 algorithm is shown in Figs. 7, 8, 9 and 10. All the variables are assumed global unless declared otherwise. A CP tree is assumed given in which nodes are labeled $t_0,t_1,t_2,\ldots,t_n$ in depth-first ordering. Each node $t_i$ has cost and profit values accessible by calling $\text{cost}(i)$ and $\text{profit}(i)$. 
Procedure DepthFirstPreprocessing(Tree)
begin
  Y = Y + 1
  NodeOf[Y] = root of Tree
  ChildNo[Y] = 0
  es = Y /* es is a local variable !! */
  for i = 1 to d(root of Tree) /* for all children of root */
    DepthFirstPreprocessing(i-th subtree of Tree)
  Y = Y + 1
  NodeOf[Y] = root of Tree
  ChildNo[Y] = i
  ElderSibling[Y] = es
  es = Y
end

Fig. 8. Initialization routine.

Procedure ComputeP(c)
begin
  for y = 1 to Y
    if NodeOf[y] = 0 and ChildNo[y] = 0 then P[y,c]=0 /*Rule1*/
    else if ChildNo[y] = 0 then /*Rule2*/
      if c - cost(NodeOf[y]) > 0 then
        P[y,c] = P[y-1,c-cost(NodeOf[y])]+profit(NodeOf[y])
      else P[y,c] = - infinity
    else P[y,c] = max{P[y-1,c],P[ElderSibling[y],c]} /*Rule3*/
end

Fig. 9. Computation of the $P$ values.

The two arrays NodeOf[] and ChildNo[] store the subtree information. If subtree $T_i^j$ is the $y$th subtree in the ordering, then NodeOf[y] = i and ChildNo[y] = j. The two-dimensional array $P[,,]$ is used to store the $P$ values, as illustrated in Table 1. Thus, entry $P[y,c]$ is just $P[T(y),c]$.

The array ElderSibling[] is used to store the elder sibling information. Thus, if $T_{i-1}^j$ is the $x$th subtree and $T_i^j$ is the $y$th array in the ordering, we let ElderSibling[y] = x.

As shown in Fig. 7, the algorithm starts by calling the initialization procedure DepthFirstPreprocessing (Fig. 8). This procedure initializes the arrays NodeOf[], ChildNo[] and ElderSibling[] by performing a depth-first traversal of the given CP tree. The algorithm then starts computing the $P[y,c]$ entries for increasing values of $c$ until some stopping criterion is reached. The computation of $P[y,c]$ is done by the procedure ComputeP(c) (Fig. 9), which implements the three rules given in Sec-
Procedure FindActualSolution(c)
local variable y: integer
begin
    y = Y
    if P[y, c] < 0 then
        output('No Solution')
    else
        while y > 1 do
            if ChildNo[y] = 0 then
                output(NodeOfCyl)
                c = c - cost(NodeOf[y])
                y = y - 1
            else if P[y, c] = P[y-1, c] then y = y - 1
            else y = ElderSibling[y]
        end
end

Fig. 10. Computing actual solutions.

tion 3. Actual solutions can be generated from the array P[,] by calling the procedure FindActualSolution.

Let us now analyze the time complexity of OPT-2. Let n and s be the number of internal nodes (tests) and the number of leaves (respectively) in the original decision tree. The number of nodes in the corresponding cost-profit tree is then n + 1. The number of leaves, C, in the target decision tree, can be any integer between 1 and s. In most cases, however, C is significantly smaller than s since the goal is to prune the tree.

The number of T_i's (which is the variable Y in the algorithm) is exactly 2n + 1. The procedure DepthFirstPreprocessing simply fills in the entries NodeOf[y], ChildNo[y] and ElderSibling[y] for y from 1 up to Y, and thus, this initialization step runs in time Θ(n).

The time needed to execute each iteration in ComputeP() is bounded by a constant. Therefore, a call to ComputeP() runs in time Θ(n).

Finally, the last step of computing the actual solution obviously takes time Θ(n) in the worst case. Summing up, the overall running time of the algorithm is Θ(nC).

6. Space complexity

It is interesting to note that, unlike OPT, actual solutions in OPT-2 are never stored explicitly in memory but only computed when needed. The space required by the algorithm as described so far is dominated by the array P[,] whose size is Θ(nC). This is usually reasonable for practical purposes. However, in some situations, reducing the amount of space is given high priority even if it may cause some increase in the execution time. Trading time for space can easily be achieved in OPT-2. The idea is based on the following observations:
Given that the maximum degree over all the nodes of the initial decision tree is \( d_{\text{max}} \), the maximum cost over all the nodes of the corresponding CP tree is \( d_{\text{max}} - 1 \). Therefore, applying Rule 2 when computing say column number \( c \) of the \( P[,,] \) matrix never requires accessing any of the columns \( 1 \) through \( c - d_{\text{max}} \).

Applying Rule 3 when computing column number \( c \) is done by accessing the \( P \) values in column \( c \) only.

We can, therefore, implement the \( P[,,] \) matrix as a "circular array" keeping only the most recent \( d_{\text{max}} \) columns, and thus, making the required space as low as \( O(nd_{\text{max}}) \). Constructing actual solutions will, however, need some of the "forgotten" \( P \) values, and thus, these have to be recomputed. Consider now the following observation:

When computing \( \text{Solution}[T(y), c] \), all the \( P \) values needed are in the portion of the \( P[,,] \) matrix confined between \( P[1,1] \) and \( P[y-1,c] \).

These observations suggest the following strategy: Let \( k \) be any fixed integer greater than or equal to \( d_{\text{max}} \). We start by computing the \( P \) matrix column by column such that when the \( c \)th column is being computed, only the \( k \) most recent columns (i.e., the columns \( c, c-1, \ldots, c-k \)) are kept in memory. When we reach the target tree size \( C \), we trace the \( P \) values back in order to construct an actual solution (as done in the procedure \( \text{FindActualSolution} \)). Suppose that, during this trace, an unavailable entry, say \( P[y_1,c_1] \), such that \( c_1 < c - k \), is needed. At this point, we stop the tracing temporarily and start recomputing the \( P[,,] \) matrix, but this time only up to row \( y_1-1 \), and column \( c_1 \). Again, only the most recent \( k \) columns are kept during the computation. We then continue tracing back to construct the solution. Tracing and recomputing is done alternately in this manner until the whole solution is generated.

For example, consider again the \( P \) values given in Table 1. Let \( k \) be 5, and suppose the target tree size is 10. For this case, we first compute the columns \( 1 \) through \( 10 \) of the table. However, at the time we finish computing column \( 10 \), only columns \( 6, 7, 8, 9, \) and \( 10 \) are available in memory. In order to find \( \text{Solution}[T(19), 10] \), we trace the \( P \) values back as shown in Fig. 6. After generating some part of the solution (namely, the set \( \{t_7, t_6, t_5, t_4\} \)), we will need to access the entry \( P[5,4] \). This entry is not available, so we recompute the area of the \( P[,,] \) matrix confined between the entry \( P[1,1] \) and \( P[y-1,c] \). We then continue tracing back as done in Fig. 6 until the whole solution is generated.

In the above example, the required space is reduced by a factor of 2, while the number of \( P \) values that have to be computed increases from 190 to 210. If we let \( k \) be 3 for this same example, then recomputation will occur once at the entry \( P[8,6] \) and again at the entry \( P[3,2] \). In this case, the space is cut roughly by a factor of 3, while the number of \( P \) value computations increases from 190 to 244.

It can be verified that if we choose to reduce the required space by a factor of \( r \) (that is to let \( k \approx C/r \), provided that \( k \geq d_{\text{max}} \)), then the increment in the execution time is bounded by a factor of \( (r+1)/2 \). This is, however, a considerable overestimate.

Thus, based on the available resources, the user of OPT-2 can freely adjust the space complexity of the algorithm at any level between \( \Theta(nC) \) and \( \Theta(nd_{\text{max}}) \). The ability to trade time for space and vice versa in this manner gives the user of OPT-2 considerable flexibility to meet his/her requirements.
7. Summary and future research

In this paper, a new algorithm, OPT-2, for optimal pruning of decision trees was introduced. The algorithm is based on dynamic programming. In its most basic form, OPT-2 runs in time $\Theta(n^C)$, and requires space $\Theta(n^C)$, where $n$ is the number of test nodes in the initial decision tree, and $C$ is the number of leaves in the target (pruned) decision tree. If so desired, the space required by the algorithm can be reduced by a factor of $r$ at the cost of increasing the execution time by a factor that is bounded above by $(r + 1)/2$ (this is a considerable overestimate, however). OPT-2 is, therefore, an improvement over the recently published OPT algorithm of Bohanec and Bratko (which is the only known algorithm for optimal decision tree pruning) especially in the case of heavy pruning and when the tests of the given decision tree have many outcomes. Moreover, from a practical point of view, OPT-2 is quite flexible and easy to implement.

An interesting problem for future research is to consider pruning without imposing the requirement of “predecessor-closedness” over the pruned decision trees. In this setting, pruning means that a subtree of the initial decision tree may possibly be replaced by one of its subtrees, and not necessarily by a leaf. The only work that considers this kind of pruning is Quinlan’s C4.5 package [71]. However, pruning is done only heuristically in that work. It is interesting to design a polynomial time algorithm for optimal pruning when pruning is defined in this way and/or to prove results on computational hardness of such a task.

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