

A Simple Algorithm for Optimal Search Trees with Two-Way Comparisons *

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Abstract

We present a simple $O(n^4)$ -time algorithm for computing optimal search trees with two-way comparisons. The only previous solution to this problem, by Anderson et al., has the same running time, but is significantly more complicated and is restricted to the variant where only successful queries are allowed. Our algorithm extends directly to solve the standard full variant of the problem, which also allows unsuccessful queries and for which no polynomial-time algorithm was previously known. The correctness proof of our algorithm relies on a new structural theorem for two-way-comparison search trees.

1 Introduction

Search trees are among the most fundamental data structures for storing and accessing data. *Static* search trees are used in applications where the set of possible queries and their frequencies are known in advance, in which case a single tree can be precomputed and used throughout the application to handle lookup queries. Such a tree is *optimal* if it minimizes the expected search cost. The problem of computing optimal search trees has been studied extensively in various forms since the 1960s. Perhaps the most famous example is Knuth’s $O(n^2)$ -time algorithm [19], which is widely considered one of the gems of algorithmics and has inspired the discovery of general techniques for speeding up dynamic-programming algorithms [3, §7.1].

But most optimal-search-tree results, including Knuth’s, consider only trees based on three-way comparisons [19]. In contrast, standard high-level programming languages implement two-way comparisons (e.g., $=, \leq, <$). As pointed out by Knuth himself in the second edition of “*The Art of Computer Programming*”, it is desirable to understand search trees that use only two-way comparisons [20, §6.2.2 ex. 33]. Yet they are still not well understood: there is only one published proof that optimal two-way-comparison trees can be computed in polynomial time, given decades after Knuth’s result, in a breakthrough by Anderson et al. [1], who gave an $O(n^4)$ -time

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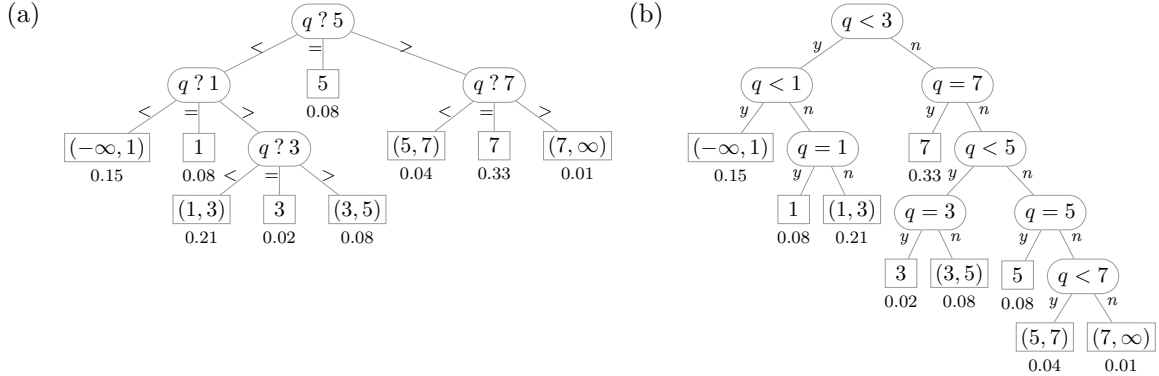


Figure 1: (a) A *three-way-comparison* search tree and (b) a *two-way-comparison* tree. Both trees have keys $\{1, 3, 5, 7\}$. The number below each leaf represents its frequency. The cost of tree (a) is 2.23, the cost of tree (b) is 2.8.

algorithm for the *successful-queries* variant, in which only searches for keys stored in the tree are supported. Their work was motivated by an application to efficient message dispatching in object-oriented programming languages, addressed earlier by Chambers and Chen [4] (see also [21]) who provided an $O(n^2)$ -time heuristic (non-optimal) algorithm for constructing two-way-comparison trees. Independently, Andersson [2] had earlier looked at speeding up search trees by replacing three-way comparisons with two-way ones.

Difficulties introduced by two-way comparisons. Given a query q , the search for q in a search tree starts at the root and traces a path to a leaf, at each node comparing q to the node's key, then following the edge corresponding to the outcome. A *three-way* comparison has three possible outcomes: the query is less than, equal to, or greater than the node's key. In any three-way-comparison tree, the set of queries reaching any internal node N is an open interval between some two keys. Each subtree solves a subproblem defined by some such inter-key interval. This leads to a simple dynamic program with $O(n^2)$ subproblems and to a simple $O(n^3)$ -time algorithm, the derivation of which is a standard exercise [10, §15.5], [11, Ex. 6.20]. Knuth's celebrated result improves the running time to $O(n^2)$.

In contrast (as noted e.g. in [1]), algorithms for *two-way-comparison* search trees face the following obstacle. After a few equality tests, the subproblem that remains is defined by some inter-key interval with *holes* — each hole corresponding to an earlier equality test. (For example, in tree (b) of Figure 1, the set of queries reaching node $\langle q < 5 \rangle$ is $[3, \infty) - \{7\}$.) The resulting dynamic-programming formulation can have $\Theta(2^n)$ subproblems, as the query sets that can arise can contain any subset of the keys.

The most-likely-key property. To achieve their polynomial-time algorithm for two-way comparison trees, Anderson et al. circumvent this obstacle in two steps. First, using an elegant *side-weights* argument, they show that every instance has an optimal tree T with what we call the *most-likely-key property*:

(MLK) *In each equality-test node N in T , the test is to some key of maximum weight among keys reaching N .*

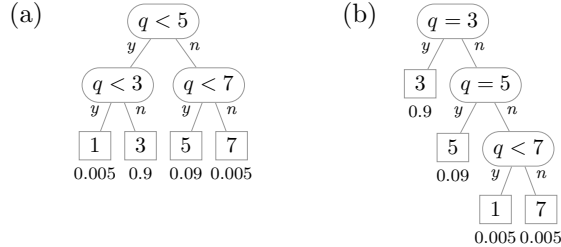


Figure 2: Optimal two-way-comparison trees for the *successful-queries* variant (a) using only inequalities, and (b) when ‘=’s are also permitted. Both trees have key set $\{1, 3, 5, 7\}$. The number below each leaf represents its frequency. The cost of tree (a) is 2, the cost of tree (b) is 1.11.

Their proof is for the successful-queries variant but extends directly to the unrestricted variant. The result implies that it suffices to consider only trees with the MLK property.

If all key weights are distinct, then, at any node N in such a tree T , the set of queries that reach N is an inter-key interval with the g heaviest keys removed, for some $g \in \{0, 1, \dots, n\}$. There are $O(n^3)$ such query sets (intervals with such keys removed) so this yields a dynamic program with $O(n^3)$ subproblems, and a simple $O(n^4)$ -time algorithm for instances with distinct weights.

When the weights are not distinct, however, the MLK property gives no guidance about how to break ties. Even in trees with the MLK property, exponentially many distinct query sets can arise, so the dynamic program still has exponential size. To work around this counter-intuitive obstacle, Anderson et al. then resort to a lengthy argument that establishes “thresholds on the frequency of an item that can occur as an equality comparison at the root of an optimal tree.” This significantly complicates their analysis and their algorithm.

New results. Our first result is a structural theorem (Theorem 1), which implies that there is an optimal tree with what we call the *refined MLK property*:

(RMLK) *In each equality-test node N in T , the test is to the key k_b of maximum weight among keys reaching N , breaking ties by maximizing the index b .*

Breaking ties by the index b (above) is for convenience, in fact any tie-breaking rule will work.

The precise statement of Theorem 1 is somewhat delicate. For example, it is *not* the case that any tree with an equality test at the root can be converted into an equally good tree with an equality test to any given maximum-weight key. (See the remarks following the proof of the theorem.) But, with the correct theorem statement in hand, the proof is straightforward, by augmenting the side-weights argument of Anderson et al. with a perturbation argument.

The theorem implies that, whether or not the weights are distinct, it suffices to consider trees with the RMLK property. Restricting to such trees yields a simple dynamic program with $O(n^3)$ subproblems, each solvable in $O(n)$ time, yielding an $O(n^4)$ -time algorithm (Corollary 1). The algorithm is essentially the algorithm for distinct-weights instances, modified to break ties arbitrarily. Our formulation is simple and easy to implement — Appendix C gives a twenty-two-line implementation in Python. This is the first polynomial-time algorithm to be proven correct for the unrestricted variant.

Other related work. In 1994, Spuler [22, 23] suggested an algorithm for computing optimal two-way comparison trees, based on a result by Huang et al. [17] for a different type of search tree.

But Huang et al.’s related result, and the recurrences underlying Spuler’s proposed algorithm, are demonstrably wrong [6]. Independently, Spuler also conjectured that optimal trees have the MLK property, and based on that conjecture proposed an additional algorithm, without proof of correctness, running in time $O(n^5)$. As discussed earlier, in 2002 Anderson et al. proved the conjecture for the successful-queries variant and obtained an $O(n^4)$ -time algorithm for it. To our knowledge, this is the only previously published proof of correctness for any polynomial-time algorithm for optimal two-way-comparison search trees, for any variant with equality tests and inequality comparisons.

The technical obstacle introduced by non-distinct weights also arises in finding optimal so-called *binary split trees*: for distinct-weight instances, an optimal binary split tree can be found in $O(n^4)$ time, but for arbitrary instances the best bound known is $O(n^5)$ [14]. For *generalized binary split trees* (see [17, 6]) no correct polynomial-time algorithm is yet known.

There are various other models for comparison-based search trees in the literature. As one example, one can consider only inequality comparisons. In trees with three-way comparisons that would correspond to giving every key weight zero (so only non-key queries have positive probability). As noted by Knuth, this model is equivalent to alphabetic coding, solved by Gilbert and Moore in $O(n^3)$ time [13], later improved to $O(n \log n)$ time by Hu and Tucker [15] and, independently, by Garsia and Wachs [12]. As noted by Anderson et al. this is also equivalent to finding the optimal two-way-comparison tree in the successful-queries case that only uses “<” comparisons. For more background information on different models and algorithms (including approximations) for search trees we refer the reader to the 1997 tutorial by Nagaraj [21].

Formal problem statement. Let k_1, k_2, \dots, k_n denote the n given keys, in increasing order. Let $\beta_b \geq 0$, for $b = 1, 2, \dots, n$, be the weight of key k_b and $\alpha_a \geq 0$, for $a = 0, 1, \dots, n$, be the weight of interval (k_a, k_{a+1}) , where for convenience k_0 and k_{n+1} (which are not keys) represent $-\infty$ and ∞ . In standard applications the weights represent query frequencies or probabilities. Here each weight can be an arbitrary non-negative number.

As illustrated in Figure 1(b), a *two-way-comparison search tree* for the instance is a rooted binary tree T , where each non-leaf node N represents a comparison ($=$ or $<$)¹ to some key k_b . T has $2n + 1$ leaves, n of which are associated one-to-one with the keys k_b and the remaining $n + 1$ with the intervals (k_a, k_{a+1}) . Given any value q , the search for q in T must correctly *identify* q , in the following sense. The search starts at the root and proceeds down the tree, following the edges corresponding to the outcomes of the comparisons, and it terminates either at the leaf associated with a key k_b , if $q = k_b$, or at the leaf associated with the interval (k_a, k_{a+1}) containing q , if q is not a key.

For each node N in T , let T_N denote the subtree rooted at N . The *weight of subtree* T_N , denoted w_N , is the total weight of the keys k_b and intervals (k_a, k_{a+1}) in the set of queries reaching N (these are the keys and intervals associated with the leaves of T_N).

The *cost* of T is the weighted depth of its leaves, that is:

$$\text{cost}(T) = \sum_{\ell \in \text{leaves}(T)} \text{depth}_T(\ell) \times w_\ell = \sum_{N \in T - \text{leaves}(T)} w_N, \quad (1)$$

where $\text{leaves}(T)$ is the set of leaves in T and $\text{depth}_T(\ell)$ is the number of edges on the path from the root to ℓ in T .

¹For simplicity of presentation, we don’t allow the $>$ (or equivalently \leq) comparison. See the discussion below.

A search tree T is called *optimal* for a given instance if it has minimum **cost** among all search trees for the given instance. The objective is to compute such an optimal tree.

The successful-queries variant. The problem definition above is for the “full” variant, with unrestricted queries. In the *successful-queries* variant, illustrated in Figure 2, only queries to the given keys k_1, k_2, \dots, k_n are allowed. An instance is specified by just those keys and their frequencies $\beta_1, \beta_2, \dots, \beta_n$, and the problem is to find the minimum cost of any tree that handles $\mathcal{S} = \{k_1, \dots, k_n\}$. (Section 2 formally defines “handles”.) While our algorithm’s description in Section 2 assumes the full variant, it can be adapted directly to the successful-queries variant, retaining its running time of $O(n^4)$, by a straightforward modification of the dynamic program². This adapted algorithm has the same asymptotic running time as Anderson et al.’s (who considered only the successful case), but is much simpler.

Other comparison operators. Similarly, for the sake of exposition, and following the model in [1], we allow only the two comparison operators $\{<, =\}$. As explained later (see the end of Section 2), our algorithm and its analysis extend naturally to the model with comparison set $\{<, \leq, =\}$. Due to symmetries and equivalences, this is the only other set of operators of interest for the full variants of the problem (allowing unsuccessful queries) that include equality comparisons. For example, operator \geq can be replaced by operator $<$ by swapping the subtrees of each node with the \geq comparison. We note, in passing, that Hu and P. A. Tucker [16] have shown that the full variant with only comparison operators in $\{<, \leq\}$ allowed can be solved in time $O(n \log n)$ by reducing it to an instance of alphabetic coding with $2n + 1$ keys and applying the algorithm of Hu and A. C. Tucker [15].

2 The Dynamic-Programming Algorithm

Within any tree having the RMLK property, at any node N , the set \mathcal{S} of queries reaching N has the following form: \mathcal{S} consists of the queries lying in some inter-key interval, minus some number of heaviest keys removed. The algorithm will solve one subproblem for each set \mathcal{S} of this form. Next we explicitly define these sets and their subproblems.

Fix a permutation $k_{\pi(1)}, k_{\pi(2)}, \dots, k_{\pi(n)}$ of the keys that orders them by nondecreasing weight, breaking ties arbitrarily. For each key $k_{\pi(r)}$, call r the *rank* of the key. A set \mathcal{S} is *valid* if either (i) \mathcal{S} is a singleton key, of the form $\mathcal{S} = \{k_b\}$, or (ii) \mathcal{S} is an inter-key interval with some largest-rank keys removed — that is, for some $i, j \in \{0, 1, \dots, n + 1\}$ with $i < j$, and $h \in \{0, 1, \dots, n\}$, the set \mathcal{S} equals $S(i, j, h)$, defined as

$$S(i, j, h) = [k_i, k_j] - \{k_{\pi(h+1)}, k_{\pi(h+2)}, \dots, k_{\pi(n)}, k_0\}.$$

(These sets are not necessarily distinct — for example, it is possible that $S(i, j, h) = S(i, j, h')$ even though, say, $h \neq h'$. Removing k_0 is needed only to deal with the case when $i = 0$.)

Note that $S(i, j, h)$ is a union of some keys and “failure” intervals (k_a, k_{a+1}) . Let $w(S(i, j, h))$ denote the total weight of these keys and intervals. Given a search tree T , if those keys and intervals

²Note that the successful-queries variant is *not* a special case of the full variant, since, by definition, any search tree for this variant must contain leaves representing all inter-key intervals (k_a, k_{a+1}) , even though their probabilities α_a are 0.

are also the ones associated with T 's leaves, say that T handles $S(i, j, h)$ (so, for each $q \in S(i, j, h)$, the tree correctly identifies q). Define $\text{opt}(i, j, h)$ to be the minimum cost of any tree that handles $S(i, j, h)$. Note that $S(0, n+1, n) = (-\infty, +\infty)$, so the goal is to return $\text{opt}(0, n+1, n)$. (If desired, an optimal tree can also be constructed in the standard fashion.)

The algorithm computes $\text{opt}(0, n+1, n)$ using the following recurrence relation:

- (a) If $j = i + 1$ and $k_i \notin S(i, j, h)$, then $S(i, j, h) = (k_i, k_{i+1})$ so $\text{opt}(i, j, h) = 0$.
- (b) If $h > 0$ and $k_{\pi(h)} \notin S(i, j, h)$, then $S(i, j, h) = S(i, j, h-1)$, so $\text{opt}(i, j, h) = \text{opt}(i, j, h-1)$.
- (c) Else, $\text{opt}(i, j, h) = w(S(i, j, h)) + \min \begin{cases} \text{opt}(i, j, h-1) & (\text{if } h > 0, \text{ else } +\infty), \\ \min \{ \text{opt}(i, b, h) + \text{opt}(b, j, h) : i < b < j \}. \end{cases}$

Correctness. For any tree T that handles $S(i, j, h)$, note that $\text{cost}(T)$ is zero if T is a leaf, and otherwise $\text{cost}(T) = w(S(i, j, h)) + \text{cost}(T_L) + \text{cost}(T_R)$, where T_L and T_R are the left and right subtrees.

By inspection, the cases in the recurrence relation are exhaustive. Likewise, Cases (a) and (b) are correct. For Case (c), the two terms in the right-hand side correspond to creating a tree whose root does either (i) an equality-test with key $k_{\pi(h)}$ (if $h > 0$ so that $S(i, j, h)$ contains some keys, with $k_{\pi(h)}$ being the one of largest rank), or (ii) an inequality comparison with some key k_b . By Theorem 1 in Section 3 there is an optimal tree of this form that handles $S(i, j, h)$, so the recurrence is correct in Case (c). (Note that if $j = i + 1$, the range of the minimum in the second term is empty, and there no trees of type (ii) above. In this case, we take the minimum to be infinite, so the recurrence remains correct.)

Running time. The number of subproblems $S(i, j, h)$ is $O(n^3)$. For each subproblem, by inspection of the recurrence, $\text{opt}(i, j, h)$ can be computed in $O(n)$ time. Thus the running time is $O(n^4)$. This proves Corollary 1:

Corollary 1. *There is an $O(n^4)$ -time algorithm for computing optimal two-way-comparison search trees (with unrestricted queries).*

Extension to operators $\{=, <, \leq\}$. The algorithm and its proof of correctness extend naturally to the model with three comparison operators, $\{=, <, \leq\}$, potentially allowing lower tree costs (even for the case $n = 1$). The overall principle of the algorithm remains the same, although the presence of two inequality operators introduces minor technical complications. The modified algorithm will have four types of subproblems that correspond to four types of inter-key intervals: (k_i, k_j) , $[k_i, k_j)$, $(k_i, k_j]$, and $[k_i, k_j]$, each with some number h of holes. In the recurrence for each type of subproblem, the minimum in (c) will have three choices that correspond to operators $=, <$ and \leq . As for the correctness proof, the statement of Lemma 1 needs to be modified to say in part (b) that ‘‘The root of T does an inequality comparison’’. The proofs of Lemma 1, Lemma 2, and Theorem 1 apply as presented.

3 Statement and Proof of Theorem 1

Fix the keys k_1, k_2, \dots, k_n and their associated weights. Let \mathcal{S} be any valid set, and consider the subproblem of finding a minimum-cost (two-way-comparison) tree that handles \mathcal{S} .

Theorem 1. *Fix any key k_b of largest weight among keys in \mathcal{S} . Then some optimal tree T satisfies one of the following three conditions:*

- (i) *T consists of a single leaf.*
- (ii) *The root of T does a less-than comparison.*
- (iii) *The root of T does an equality test to k_b .*

(See also the stronger Theorem 2 in Appendix B, with a different proof.)

Proof. The rest of this section gives the proof. It uses the following lemma as a black box.

Lemma 1. *Some optimal tree T satisfies one of the following three conditions:*

- (a) *T consists of a single leaf.*
- (b) *The root of T does a less-than comparison.*
- (c) *The root of T does an equality test to some key k_b of maximum weight among keys in \mathcal{S} .*

(Anderson et al. prove essentially the same lemma (their Corollary 3), but for the successful-queries variant. Their proof uses their side-weights technique and extends essentially unchanged to our setting. For completeness we include the proof in Appendix A.)

The idea of the proof is to infinitesimally perturb the weights to make k_b the uniquely largest-weight key in \mathcal{S} . Lemma 1 implies that there is a tree T that is optimal for the perturbed instance and has one of the Properties (a)–(c), which (given the perturbation) implies that T has one of the Properties (i)–(iii). The perturbation is sufficiently small so that any optimal tree (T , in particular) for the perturbed instance must also be optimal for the original instance. (Similar arguments have been used for other problems, such as the Minimum Spanning Tree problem, to extend algorithms for distinct-weights instances to algorithms for general instances, see e.g. [18, §4.5].) Here are the details.

For each integer $i \geq 1$, define a new instance with the same set of keys but with the weight of key k_b increased by $1/i$. That is, let $\beta_b^i = \beta_b + 1/i$ and $\beta_a^i = \beta_a$ for all $a \neq b$. By Lemma 1, there is an optimal tree T^i for the modified instance such that T^i satisfies one of (a)–(c) of Lemma 1 for the modified instance, and therefore satisfies one of (i)–(iii) of the theorem for the original instance. Let tree T be such that $T = T^i$ for infinitely many i . (Such a T must exist, because the possible trees for each modified instance are the same, and there are finitely many of them.) Then T is a possible tree for the original instance and has one of Properties (i)–(iii), as desired. To finish we show that T is optimal for the original instance.

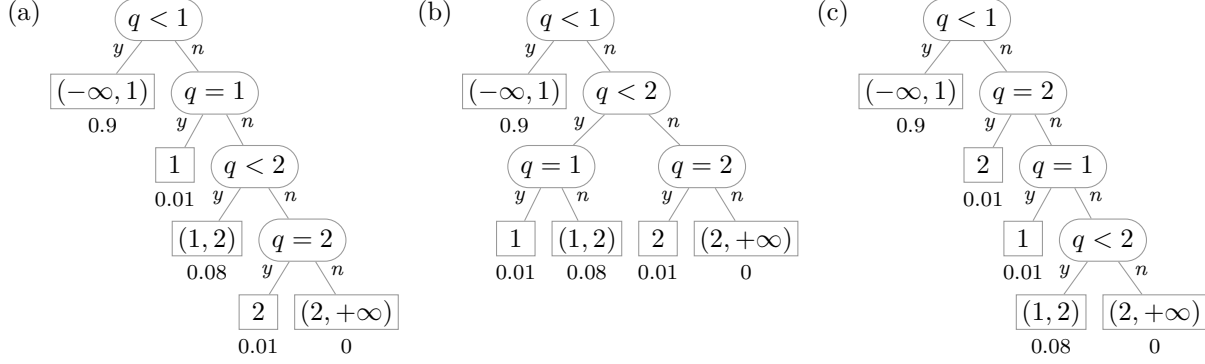


Figure 3: Trees for a full instance with $\mathcal{K} = \{1, 2\}$, $(\beta_1, \beta_2) = (0.01, 0.01)$ and $(\alpha_0, \alpha_1, \alpha_2) = (0.9, 0.08, 0)$. As discussed in the remarks, the subproblem with valid set $\mathcal{S} = [1, \infty)$ has an optimal solution with an equality test to key 1, but none with an equality test to key 2, even though $\beta_1 = \beta_2$.

Let T^* be an optimal tree for the original instance. For all i such that $T = T^i$,

$$\begin{aligned}
\text{cost}(T, \beta) &= \text{cost}(T, \beta^i) - \text{depth}_T(k_b)/i && \text{by definition of } \beta_a^i \text{'s and Equation (1)} \\
&\leq \text{cost}(T, \beta^i) \\
&= \text{cost}(T^i, \beta^i) && \text{because } T = T^i \text{ for this } i \\
&\leq \text{cost}(T^*, \beta^i) && \text{because } T^i \text{ is optimal for } \beta_a^i \text{'s} \\
&= \text{cost}(T^*, \beta) + \text{depth}_{T^*}(k_b)/i && \text{by definition of } \beta_a^i \text{'s and Equation (1)}.
\end{aligned}$$

(In this derivation, arguments β or β^i in the cost function indicate which key weights are used to compute it.) This holds as $i \rightarrow \infty$, so $\text{cost}(T, \beta) \leq \text{cost}(T^*, \beta)$, and thus T is also optimal for the original instance. \square

Remarks. The correct statement of Theorem 1 is somewhat delicate. Consider the following statement: *If there is an optimal tree whose root does an equality test, then, for any maximum-weight key k in \mathcal{S} , there is an optimal tree whose root does an equality test to k .* This seemingly similar statement is false. Figure 3 gives a counterexample.

In that figure, keys 1 and 2 both have maximum weight among keys reaching the right child of the root. Trees (a) and (b) are optimal. In (a), the right child of the root does an equality test to key 1, but no optimal subtree for that subproblem (the subproblem with valid set $\mathcal{S} = [1, \infty)$) has an equality test to key 2 at the root — tree (c) has minimum cost among trees with such a subtree. This counter-example also holds in the problem variant where all comparisons in $\{<, \leq, =\}$ are allowed.³

The proof of Theorem 1 perturbs the weights infinitesimally, giving k_b the unique largest weight and (via Lemma 1) forcing any root equality test to be to key k_b . It then observes that, because the minimum tree cost is a continuous function of the weights, any tree that is optimal for the (infinitesimally!) perturbed instance must also be optimal for the original instance. This infinitesimal

³For the successful-queries variant no such counter-example is possible. By Theorem 2 in Appendix B, if some optimal tree has an equality test at the root, then for *any* maximum-weight key there is an optimal tree that uses this key in the equality-test at the root. This stronger property, however, does not seem to have any algorithmic implications.

perturbation can make *all* previously optimal trees with equality tests at the root non-optimal. (For example, in Figure 3, after an infinitesimal increase in β_2 , only tree (b) would be optimal.)

The RMLK property from the introduction is a corollary of the theorem. To prove it, let T be the optimal tree for \mathcal{S} , with root as specified in the theorem. Then (using induction on n) replace each of the two subtrees by an optimal one (for its subproblem) having the RMLK property. The resulting tree T' is also an optimal tree for \mathcal{S} , and has the RMLK property.

In fact, there must be an optimal tree with the following stronger property. *At any node N that does an equality test, if there are d largest-weight keys in the search space reaching N , then the top d nodes on the right spine in T_N do equality tests to those d keys in some order (and permuting that order arbitrarily preserves optimality).* See Corollary 2 in Appendix B.

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Appendices

A Proof of Lemma 1

This appendix proves Lemma 1. First we state Anderson et al.'s side-weights lemma [1, Lemma 2], and prove it in our setting. (The proof is identical.) Fix the keys k_1, k_2, \dots, k_n and associated weights. Let \mathcal{S} be any valid set and consider the problem of finding a minimum-cost tree among trees that handle \mathcal{S} . Let T be any optimal tree for this problem.

Define the *side-weight* of any node N in T , denoted $\text{sw}(N)$, as follows. If N is a leaf, then $\text{sw}(N) = 0$. If N does an equality test to a key, then $\text{sw}(N)$ is the weight of that key. Otherwise (N is an inequality-comparison node) $\text{sw}(N) = \min\{w_L, w_R\}$, where L and R are N 's left and right children. The utility lemma states that side-weights are monotone along paths from the root:

Lemma 2 ([1, Lemma 2]). *If P is the parent of N in T , then $\text{sw}(P) \geq \text{sw}(N)$.*

Proof. If N is a leaf, it has side-weight 0 and the property holds, so assume that N is not a leaf. There are four cases according to whether at each of P or N the comparison done is an equality or an inequality. Recall that T is an optimal tree.

Case 1: *Both P and N are inequality comparisons.* Assume without loss of generality that N is the right child of P . Let T_1 be the subtree rooted at the child of P that is not N . Let T_2 and T_3 be the subtrees rooted, respectively, at the left and right children of N . Let μ_i denote the weight of T_i (for $i \in \{1, 2, 3\}$). Then $\text{sw}(P) = \min\{\mu_1, \mu_2 + \mu_3\}$ and $\text{sw}(N) = \min\{\mu_2, \mu_3\}$. Now do a left rotation at P , so that N takes the place of P , P becomes N 's left child, and T_2 becomes the right subtree of P . While T_2 stays at the same depth, T_1 moves down and T_3 moves up, each by one level. The increase in cost is $\mu_1 - \mu_3$. This must be non-negative, as T is optimal, so $\mu_1 \geq \mu_3$. This implies $\min\{\mu_1, \mu_2 + \mu_3\} \geq \min\{\mu_2, \mu_3\}$, that is, $\text{sw}(P) \geq \text{sw}(N)$.

Case 2: *Node P is an inequality comparison and N is an equality comparison.* Let T_1 , of weight, say, μ_1 , be the subtree rooted at the child of P which is not N . Let μ_2 be the weight of the left subtree, say T_2 , of N (consisting of a leaf for the equality-test key of N). Let μ_3 be the weight of the right subtree, say T_3 of N . We have $\text{sw}(P) = \min\{\mu_1, \mu_2 + \mu_3\}$ and $\text{sw}(N) = \mu_2$. Modify T by moving the equality test at N just above P . Tree T_1 moves down one level, T_3 stays at the same level, yet T_2 , of weight μ_2 , moves up one level. The net increase in cost is $\mu_1 - \mu_2$. Since T is optimal, this is non-negative, so $\mu_1 \geq \mu_2$. Thus $\min\{\mu_1, \mu_2 + \mu_3\} \geq \mu_2$. That is, $\text{sw}(P) \geq \text{sw}(N)$.

Case 3: *Both P and N are equality comparisons.* Swap the comparisons in P and N . The increase in cost is $\text{sw}(P) - \text{sw}(N)$. Since T is optimal, this is non-negative, so $\text{sw}(P) \geq \text{sw}(N)$.

Case 4: *Node P is an equality comparison and N is an inequality comparison.* Let μ_1 be the weight of P 's left-subtree T_1 (consisting of a leaf for the equality-test key of P). Let T_2 and T_3 of weight μ_2 and μ_3 , respectively, be the subtrees hanging off N . Move the equality-test node P down just above the appropriate child of N . Then exactly one of T_2 and T_3 moves up while T_1 moves down. The increase in cost is either $\mu_1 - \mu_2$ or $\mu_1 - \mu_3$. Since T is optimal, the increase is non-negative, so $\mu_1 \geq \min\{\mu_2, \mu_3\}$. That is, $\text{sw}(P) \geq \text{sw}(N)$. \square

Next is the proof of Lemma 1. The proof is essentially the same as Anderson et al.'s proof of [1, Corollary 3], which is for successful-queries instances but extends directly to our setting.

Lemma 1. *Some optimal tree T satisfies one of the following three conditions:*

- (a) T consists of a single leaf.
- (b) The root of T does a less-than comparison.
- (c) The root of T does an equality test to some key k_b of maximum weight among keys in \mathcal{S} .

Proof. Let T be an optimal tree with root N . In the case that N does an inequality comparison, we are done. So assume N does an equality test to some key k_b , necessarily in \mathcal{S} . Let k_a be any largest-weight key in \mathcal{S} . The parent of the leaf for k_a is some node P in T . First, if P doesn't do an equality test to k_a , replace the comparison at P by an equality test to k_a , without otherwise changing T . This preserves correctness and optimality. Now, in the case that P is the root N , we are done. In the remaining case, by Lemma 2, along the path from N to P , the side-weights are non-increasing, so $\beta_b = \text{sw}(N) \geq \text{sw}(P) = \beta_a$, and k_b is a largest-weight key in \mathcal{S} . \square

B A stronger alternative to Theorem 1

The results in this section do not appear in the ACM TALG journal version of this paper [9].

Fix an instance of either the full variant or the successful-queries variant (as described in the introduction and illustrated in Figure 2(b)). Consider the subproblem of finding a minimum-cost (two-way-comparison) tree that handles any given valid set \mathcal{S} . (The terms *valid* and *handles* are defined in Section 2.)

Theorem 2. *For either problem variant, at least one of the following conditions holds:*

- (i) *The optimal tree consists of a single leaf.*
- (ii) *There is an optimal tree whose root does an inequality comparison.*
- (iii) *For any ordering of the max-weight keys in \mathcal{S} , there is an optimal tree that starts by doing equality tests to each of those keys in that order (before doing any inequality tests or equality tests to keys of lesser weight).*

For the successful-queries variant, if any optimal tree does an equality test at the root, then either Condition (iii) above holds, or all keys in \mathcal{S} have the same weight and, for any ordering of those keys, there is an optimal tree that consists solely of equality tests (in the given order) to all but the last of those keys. In the latter case, either all keys have weight 0, or $n \leq 3$.

Corollary 2. *For any ordering π of the keys, there is an optimal tree T such that each subtree T_N either starts with an inequality comparison, or starts with equality tests to all max-weight keys that reach the root N of T_N , doing the tests in the order in which those keys occur in π .*

The corollary follows from the first part of Theorem 2. (Let T be any optimal tree that, for the subproblem arising at each node, uses a subtree that satisfies Condition (iii) of the theorem whenever possible, and otherwise uses a subtree that satisfies Condition (i) or (ii).)

Proof of Theorem 2. Assume that there is an optimal tree whose root does an equality test. (Otherwise the theorem holds trivially.) Among such trees, let T be one that maximizes the number of equality tests to max-weight keys, breaking ties as follows. For the full variant, break ties by choosing a tree that maximizes the number of *inversions*, where an inversion is a pair of nodes such that

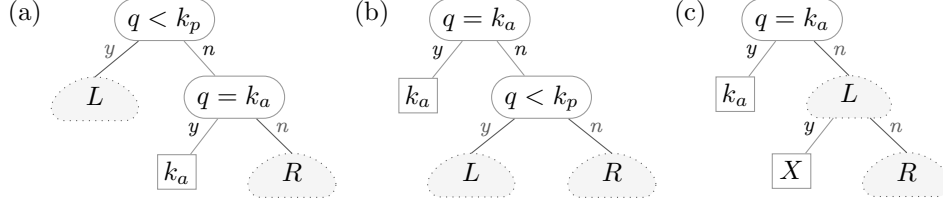


Figure 4: For Case 1 of the proof of Theorem 2.

one is an ancestor of the other, with the ancestor doing an inequality test and the descendant doing an equality test to a max-weight key. For the succesful-queries variant, break ties by *minimizing* the number of inversions.

Let $\beta_{\max} = \max_i \beta_i$. We will use the following utility lemma:

Lemma 2. *For every maximum-weight key k_a , along the path traversed by a search for k_a from the root, each non-leaf node has side-weight β_{\max} .*

Proof. Let k_a be any max-weight key. The parent of the leaf of k_a does an equality-test to a max-weight key (otherwise replacing the comparison at the parent by an equality test to k_a would preserve optimality and increase the number of equality tests to max-weight keys, contradicting the choice of T). The side-weight of the parent is therefore β_{\max} . By Lemma 2, along the path from the parent to the root, the side-weights are non-decreasing. On the other hand, the root does an equality test, so its side-weight (which equals its key's weight) can't exceed β_{\max} . So every node on the path must have side-weight β_{\max} . \square

The body of the proof has four cases.

Case 1: *Suppose that this is a succesful-queries instance, and there is an inequality test on the search path to some max-weight key k_b .*

Let N_b be the parent of k_b 's leaf, and consider the path from the root to N_b . The parent N_b does an equality test to a max-weight key (otherwise replacing N_b by an equality test to k_b would give an optimal tree with more equality tests to max-weight keys, contradicting the choice of T). So some inequality test on the path is followed by an equality test. Let $\langle q < k_p \rangle$ and $\langle q = k_a \rangle$ be such a parent and child. Assume that $\langle q = k_a \rangle$ is the right child of $\langle q < k_p \rangle$ (the other case is symmetric). As shown in Figure 4(a), let L be the left subtree of $\langle q < k_p \rangle$ and let R be the right subtree of $\langle q = k_a \rangle$. By Lemma 2, both nodes have side-weight β_{\max} . By definition, this means that k_a has weight β_{\max} , and the minimum of the weights of $\langle q < k_p \rangle$'s two subtrees is β_{\max} .

Case 1.1: *Suppose that the weight of L equals β_{\max} .* Moving the node $\langle q = k_a \rangle$ just above $\langle q < k_p \rangle$, as shown in Figure 4(b), increases the depth of L by one but reduces the depth of k_a 's leaf by one, so preserves the cost and yields another optimal tree T' . But T' has the same number of equality tests to max-weight keys (including one at the root), and one less inversion than T . This contradicts the choice of T , so Case 1.1 cannot happen.

Case 1.2: *Otherwise the weight of L strictly exceeds β_{\max} .* Recalling that the side-weight of $\langle q < k_p \rangle$ equals β_{\max} , this implies that the weight of $\langle q < k_p \rangle$'s right subtree equals β_{\max} , which (given that the subtree contains R and the key k_a of weight β_{\max}) implies that all keys in R have weight zero.

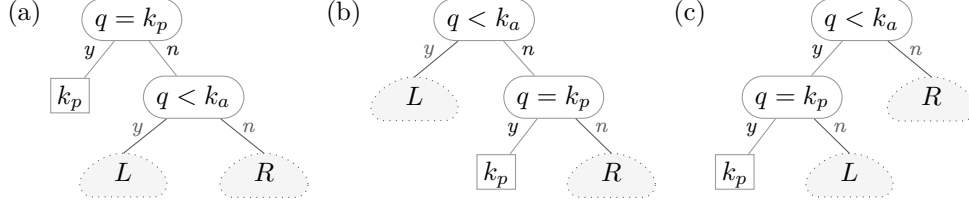


Figure 5: For Case 2 of the proof of Theorem 2.

Now consider the following modification to T . Replace the subtree rooted at $\langle q < k_p \rangle$ by a subtree (as shown roughly in Figure 4(c)) with root $\langle q = k_a \rangle$, whose left child is the leaf of k_a , and whose right subtree L' is obtained from L as follows.

Let Q be the set of queries in \mathcal{S} whose searches in T reach the root of R . Because of the node $\langle q < k_p \rangle$, each value in Q is at least k_p . On the other hand, all comparison keys used by nodes in L are strictly less than k_p (as all queries routed through L are less than k_p , and T has no “redundant” nodes). So no comparison made in L can distinguish between different queries in Q . So all queries in Q , if searched for in L , reach the same leaf, say X , in L . (In the current case, X is the leaf at the end of the right spine.)

Since this is a successful-queries instance, the leaf X has a single key. Obtain L' from X by replacing X by a new equality test to X 's key, giving the new node left child X and right subtree R . In the modified tree, any query in Q reaches the root of L , is then routed through L to R , and then is routed through R just as it was in T , to an appropriate leaf. Queries not in Q are still handled correctly (although the query to X 's leaf has one extra equality test).

As for cost, the modification decreases the depth of the leaf of k_a by one, while increasing the depth X 's leaf by one. The resulting tree cannot be cheaper than T , so X 's key must also be a max-weight key. But then the modified tree has the same cost but more equality tests to max-weight keys, contradicting the choice of T . So Case 1 cannot happen.

Case 2: Suppose that this is a full instance, and there is an inequality test on the search path to some max-weight key. Let $\langle q < k_a \rangle$ be the first inequality-test node on the search path. As shown in Figure 5(a), let $\langle q = k_p \rangle$ be the parent of $\langle q < k_a \rangle$, let L and R be the subtrees of $\langle q < k_a \rangle$. Consider moving the node $\langle q = k_p \rangle$ just below $\langle q < k_a \rangle$, either just above R (Figure 5(b)) or just above L (Figure 5(c)). One of these modifications preserves correctness (the first if $k_p \geq k_a$, otherwise the second). Both increase the depth of k_p by one, but decrease the depth of L or R by one. By Lemma 2, the side-weight of each node is β_{\max} , so the weight of k_p is β_{\max} , and the weights of L and R are both at least β_{\max} . So the resulting tree T' is also optimal. It has as many equality tests to max-weight keys as T , and one more inversion, so (by the choice of T) the modified tree T' cannot have an equality test at the root. So Condition (ii) holds. By the assumption that this is a full instance, this suffices to prove the theorem in Case 2.

Case 3: Suppose that T starts by doing equality tests to all the max-weight keys in \mathcal{S} in any order. Exchanging any two of the equality-test nodes to the max-weight keys preserves optimality. By repeated exchanges, we can modify T to do the equality tests to the max-weight keys in any order. So Condition (iii) holds, proving the theorem in Case 3.

Case 4: In the remaining case, along every search path to every max-weight key all tests are equality tests, but T doesn't start by doing equality tests to all the max-weight keys in some order. Let k_a be a max-weight key with maximum leaf depth. Let N_a be the parent of k_a 's leaf. Every node on

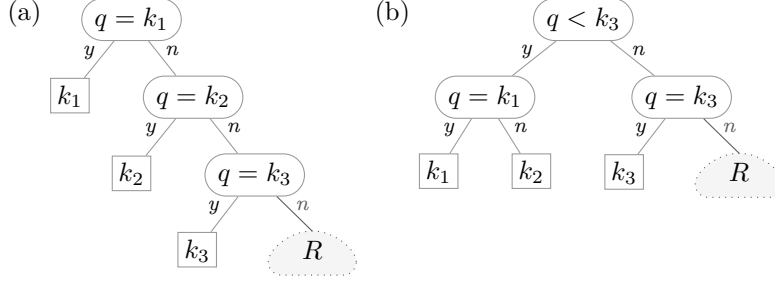


Figure 6: For Case 4 of the proof of Theorem 2.

the path P_a from the root to N_a does an equality test, necessarily (by Lemma 2) to a max-weight key. Assume without loss of generality that the equality test at N_a is to k_a (otherwise take k_a to be the key that N_a does an equality test to, which has the same leaf depth). Let Q be the set of queries that don't have equality tests along the path P_a . By the condition for Case 4, Q contains at least one max-weight key, say k_b . The search path for each query in Q reaches the right child of N_a , but (by the choice of k_a) the search for k_b must end at that child, so that child must be the leaf for k_b . Hence (for the tree to be correct) Q can contain only k_b . It follows that T is just a path of equality tests, one for every key except k_b . It follows that this is a successful-queries instance, and every key has weight β_{\max} .

Suppose for contradiction that $\beta_{\max} > 0$ and $n \geq 4$. Replacing T 's equality-test keys appropriately yields another optimal tree T' that starts with equality tests to k_1 , k_2 , and k_3 in that order. Let R be the right subtree of $\langle q = k_3 \rangle$, as shown in Figure 6(a). Let T'' be the tree shown in Figure 6(b). The weights of keys k_1 and k_3 are equal, and (as $n \geq 4$) the weight of R is positive, implying that T'' is strictly cheaper than T' . This contradicts the optimality of T' . So $n \leq 3$ or $\beta_{\max} = 0$, proving the theorem. \square

C Source code (Python)

See Figure 7.

```

1  #!/usr/bin/env python3.9
2  from math import inf # infinity
3  from functools import lru_cache
4  memoize = lru_cache(maxsize=None)
5
6
7  def opt_cost(K, alpha, beta):
8      'Return min cost of any 2-way-comparison tree for (K, alpha, beta).'

```

Figure 7: Python code for the algorithm for the full variant. (Technical note: the memoization decorator uses a dictionary. To achieve a truly faithful implementation, it should be replaced by a three-dimensional array.)