A High Quartets Distance Construction

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Abstract

Given two binary trees on N labeled leaves, the *quartet distance* between the trees is the number of disagreeing quartets. By permuting the leaves at random, the expected quartets distance between the two trees is $\frac{2}{3}\binom{N}{4}$. However, no strongly explicit construction reaching this bound asymptotically was known.

We consider complete, balanced binary trees on $N = 2^n$ leaves, labeled by n long bit sequences. Ordering the leaves in one tree by the prefix order, and in the other tree by the suffix order, we show that the resulting quartet distance is $\left(\frac{2}{3} + o(1)\right)\binom{N}{4}$, and it always exceeds the $\frac{2}{3}\binom{N}{4}$ bound.

1 Background

Given a set of taxa (a group of related biological species), the goal of phylogeny reconstruction is to build a tree which best represents the course of evolution for this set over time. The leaves of the tree are labeled with the given, extant taxa. Internal nodes correspond to hypothesized, extinct taxa. There are numerous phylogeny reconstruction approaches [9]. One approach of interest is building unrooted, resolved (or binary) trees from quartets, where a quartet is an unrooted tree on 4 leaves. We note that for a given set of 4 leaves there are 3 quartets topologies. The input is a set of (possibly weighted) quartets, and the goal is to build a tree which would agree with the maximum number of input quartets (maximum weighted sum, correspondingly) [4, 5, 10, 12]. It is known that this problem is computationally hard [11].

Various combinatorial problems related to quartets have also been studied extensively. In this paper, we are especially interested in the *quartet distance* problem [7]. Let T_1, T_2 be two resolved (binary) trees on the same set of N labeled leaves. Every set of the same 4 leaves induces two quartets, one in T_1 and the other in T_2. The topologies of the two quartets could either agree or disagree. The quartet distance between T_1, T_2 is the number of disagreeing quartets. Notice that the identity of a quartet in a given binary tree is well defined, regardless of the placement of the root. Thus the quartet distance between T_1, T_2 is invariant under different rootings of T_1, T_2, and under making one or both

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trees unrooted. We remark that there are efficient algorithms to compute the quartet distance of two trees. The most efficient one, by Brodal, Fagerberg, and Pedersen, runs in $O(N \log N)$ time [6].

Bandelt and Dress [3] conjectured that the maximum quartet distance between any two resolved (binary) trees on N leaves is at most $\left(\frac{2}{3} + o(1)\right) \cdot \binom{N}{4}$. Taking two binary trees T_1, T_2 on the same set of N leaves, and assigning labels to the leaves at random, the probability that any quartet will agree equals exactly 1/3. This implies that the expected value of the quartet distance is exactly $\frac{2}{3} \cdot \binom{N}{4}$. This simple probabilistic argument can be de-randomized using standard de-randomization methods. We will further refer to the result of such de-randomization in the context of our work in Section 6.

Alon, Snir, and Yuster [2] showed that the random labeling method implies the existence of trees with quartet distance strictly greater than $\frac{2}{3} \cdot \binom{N}{4}$. They also proved a $\frac{9}{10} \cdot \binom{N}{4}$ asymptotic upper bound on the quartet distance. Finally, using the technique of flag algebra, Alon, Naves, and Sudakov [1] have shown a $(0.69 + o(1)) \cdot \binom{N}{4}$ upper bound on the normalized quartet distance (for large enough number of leaves, N).

No strongly explicit construction attaining the $\frac{2}{3} \cdot \binom{N}{4}$ lower bound asymptotically is known (the notions of explicit and strongly explicit constructions are defined and discussed in Section 6). We consider complete, balanced binary trees on $N = 2^n$ leaves, labeled by n long bit sequences. Ordering the leaves in one tree by the **prefix** (or lexicographic) order, and in the other tree by the **suffix** (or co-lexicographic) order, we show that the resulting quartet distance is $\left(\frac{2}{3} + o(1)\right) \cdot \binom{N}{4}$, and furthermore, the distance exceeds the $\frac{2}{3} \cdot \binom{N}{4}$ bound for all N. An important part of our proof is counting the number of binary strings whose longest common prefixes (or suffixes) are of given lengths.

2 High Level View

Denote by $Pref_n$ the complete, balanced binary tree with leaves labeled by $\{0,1\}^n$ and ordered by prefix (or lexicographic) order, and by $Suff_n$ the complete, balanced binary tree on the same set of leaves, ordered by suffix (or co-lexicographic) order. Consider an ordered 4-tuple of distinct binary sequences (x_0, x_1, x_2, x_3), $x_i \in \{0,1\}^n$ (these are the labels of leaves in our two trees). For every pair of indices $0 \le i < j \le 3$, let $P_{i,j}(x_0, x_1, x_2, x_3)$ be the event "the common prefix of x_i, x_j is not shorter than the other five common prefixes". Likewise, we define the event $S_{i,j}(x_0, x_1, x_2, x_3)$, referring to suffixes. For sake of brevity, we will use $P_{i,j}, S_{i,j}$ to denote $P_{i,j}(x_0, x_1, x_2, x_3), S_{i,j}(x_0, x_1, x_2, x_3)$, correspondingly.

There are some obvious relations among the $P_{i,j}$ or the $S_{i,j}$. For example $P_{0,1}$, $P_{0,2}$, $P_{0,3}$ are mutually exclusive. More generally, any pair P_{i_1,j_1}, P_{i_2,j_2} sharing exactly one subscript ($i_1 = i_2$ or $j_1 = j_2$) is mutually exclusive. Note, however, that *e.g.* $P_{0,1}$ and $P_{2,3}$ are *not* mutually exclusive. Clearly, the number of ordered binary sequences satisfying $P_{i,j}, S_{i,j}$ is the same for all choices of indices $i < j$.

To determine the quartet distance between our two trees, we will exactly compute the number of length n sequences satisfying various combinations of these events, such as $P_{0,1} \cap P_{2,3}$, $P_{0,1} \cap S_{0,1}$, $P_{0,1} \cap P_{2,3} \cap S_{0,1}$, and $P_{0,1} \cap P_{2,3} \cap S_{0,1} \cap S_{2,3}$. These, in turn, will enable the derivation of the exact and asymptotic quartet distance between the "suffix order" and the "prefix order" binary sequences' trees, using a simple inclusion-exclusion argument.

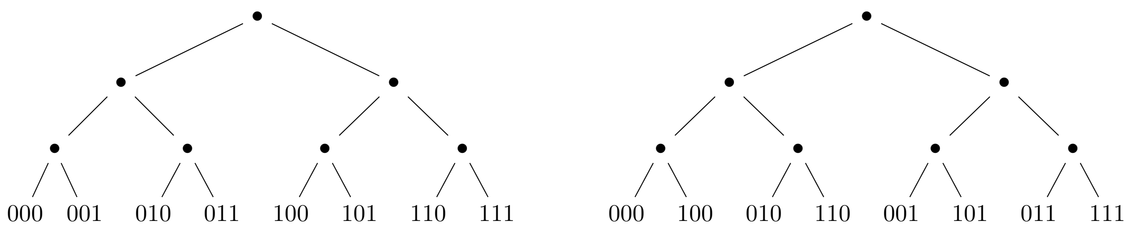


Figure 1: The complete, balanced binary tree for strings of length $n = 3$, with labels in prefix (lexicographic) order on the left, and suffix (co-lexicographic) order on the right.

3 Sequence Counts of Specific Events

For each event we will count the number of four tuples of different *ordered* sequences, (x_0, x_1, x_2, x_3) satisfying it, using simple properties of prefixes and suffixes of n bit long binary sequences. The lengths of common prefixes and suffixes of any pair of binary sequences remains invariant by xoring the sequences to any one sequence (namely computing the bit-wise XOR of the sequences). By xoring the four sequences to x_0, we can thus assume without loss of generality that x_0 is the all 0 sequence, while x_1, x_2, x_3 are three uniformly distributed sequences that are non zero and distinct.

3.1 $P_{0,1} \cap S_{2,3}$

Let us denote the length of the longest common prefix of x_0, x_1 by $\ell, (\ell \le n-1)$, and the length of the longest common suffix of x_2, x_3 by $k, (k \le n-1)$. For $P_{0,1}$, $\ell \ge 1$ should hold, and for $S_{2,3}$, $k \ge 1$ should hold. We treat separately the following three cases:

(1) $\ell + k + 2 \le n$ (the ℓ long prefix plus one bit buffer zone, and the k long suffix plus one bit buffer zone, do not overlap). Note that since $1 \le k$, the value ℓ is bounded by $\ell \le n-3$.

(2) $\ell + k + 1 = n$

(3) $\ell + k \ge n$

We start by analyzing case (1). There is no overlap between the $\ell+1$ long prefixes and the $k+1$ long suffixes. This will enable us to analyze the number of possible prefixes and possible suffixes for x_1, x_2, x_3 separately, thereby facilitatating the counting. Let us start with the prefixes. Given that $x_0 = 0^n$, as the longest common prefix of x_0, x_1 is of length ℓ, the $\ell+1$ long prefix of x_1 must be $0^\ell 1$. The $\ell+1$ long prefix of x_2 must differ from both $0^{\ell+1}$ and $0^\ell 1$ for the event $P_{0,1}$ to hold. Thus, there are $2^{\ell+1} - 2 = 2(2^\ell - 1)$ possibilities for choosing the $\ell+1$ long prefix of x_2. By a similar argument, there are $2^{\ell+1} - 3$ possibilities for choosing the $\ell+1$ long prefix of x_3. So, given that $x_0 = 0^n$, the number of possibilities for choosing the $\ell+1$ long prefixes of x_1, x_2, x_3 is $2 \cdot (2^\ell - 1) \cdot (2^{\ell+1} - 3) = 2^{2\ell+2} - 5 \cdot 2^{\ell+1} + 6$.

Let us now turn to the suffixes. Let $b_0 b_1 \ldots b_{k-1} b_k \in \{0,1\}^k$ denote the $k+1$ long suffix of x_2. This determines uniquely the $k+1$ long suffix of x_3, which equals $\overline{b}_0 b_1 \ldots b_{k-1} b_k \in \{0,1\}^k$. For $S_{2,3}$ to hold, both should differ from the $k+1$ long suffix of x_0, which equals 0^{k+1}. In particular, the $k+1$

long suffix of x_2 must differ from both 0^{k+1} and 10^k. This leaves $2^{k+1}-2=2(2^k-1)$ possibilities for choosing the $k+1$ long suffix of x_2, and then $2^{k+1}-3$ possibilities for choosing the $k+1$ long suffix of x_1. So, given that $x_0=0^n$, the number of possibilities for choosing the $k+1$ long suffixes of x_1, x_2, x_3 is $2\cdot(2^k-1)\cdot(2^{k+1}-3)=2^{2k+2}-5\cdot 2^{k+1}+6$.

Finally, each of x_1, x_2, x_3 has $n-\ell-k-2$ "free bits" in the middle, not overlapping neither the prefix nor the suffix. These can vary over all possibilities, independently of each other. The total number of possibilities for the free bits of the three sequences is thus $2^{3n-3\ell-3k-6}$, and the total number of possibilities for all of x_1, x_2, x_3, given that $x_0=0^n$, is

$$\begin{aligned}&2^{3n-3\ell-3k-6}\cdot\left(2^{2\ell+2}-5\cdot 2^{\ell+1}+6\right)\cdot\left(2^{2k+2}-5\cdot 2^{k+1}+6\right)\\=&2^{3n-4}\cdot\left(2^{-\ell+1}-5\cdot 2^{-2\ell}+3\cdot 2^{-3\ell}\right)\cdot\left(2^{-k+1}-5\cdot 2^{-2k}+3\cdot 2^{-3k}\right)\end{aligned}$$

Summing over ℓ and k in the relevant range, we get

$$2^{3n-4}\cdot\sum_{\ell=1}^{n-3}\left(2^{-\ell+1}-5\cdot 2^{-2\ell}+3\cdot 2^{-3\ell}\right)\cdot\sum_{k=1}^{n-\ell-2}\left(2^{-k+1}-5\cdot 2^{-2k}+3\cdot 2^{-3k}\right)\ (*).$$

Employing a symbolic algebra package (specifically, Maple) to this sum, we get

$$\frac{16}{441}\cdot 2^{3n}-n\cdot 2^{2n}+5\cdot 2^{2n}-\frac{25}{3}\cdot n\cdot 2^n+\frac{95}{9}\cdot 2^n-\frac{36}{7}\cdot n-\frac{764}{49}\ .$$

This is the number of ordered quartets with $x_0=0^n$, satisfying case (1) of $P_{0,1}\cap S_{2,3}$.

Let us turn to case (2), where $\ell+k+1=n$, which means that the ℓ bits long prefix and the k bits long suffix do not overlap, and have one "buffer bit", which separates them. For the event $S_{2,3}$ to occur and the longest common suffix of x_2, x_3 to be of length k, the k bits long suffix of x_2 must differ from the k bits long suffixes of both x_0 and x_1.

Given $P_{0,1}, x_0=0^n$, and ℓ being the length of the longest common prefix of x_0, x_1, the $\ell+1$ bits long prefix of x_1 is $0^\ell 1$. Since $\ell+k+1=n$, the last bit of the $\ell+1$ bits long prefix of x_1 is also the first bit of its $k+1$ bits long suffix. So this suffix differs from the $k+1$ bits long suffix of x_0 (which equals 0^{k+1}).

There are 2^k possible settings of the k rightmost bits of x_1. We treat separately the case (a) where these bits are 0^k, and the case (b) where they differ from 0^k. In case (a), neither 10^k nor 0^{k+1} can serve as the $k+1$ bits suffix of x_2, but any other sequence can. There are $2^{k+1}-2$ such possibilities. Given the $k+1$ bits suffix of x_2, the $k+1$ bits suffix of x_3 is completely determined (it differs from x_2 in the buffer zone bit, and agrees with it in the other k bits). The ℓ bits long prefix of x_2 and of x_3 could be any two sequences, other than 0^ℓ. So in case (a) the overall number of possibilities for x_1, x_2, x_3 is

$$1\cdot(2^{k+1}-2)\cdot(2^\ell-1)^2=2\cdot(2^k-1)\cdot(2^\ell-1)^2\ .$$

In case (b), there are 2^k-1 possibilities for the k bits long suffix of x_1. The k rightmost bits of x_2 must differ from both the k rightmost bits of x_1, and from 0^k. Thus, there are 2^k-2 possibilities for the k bits long suffix of x_2, and 2 possibilities for the buffer zone bit of x_2. Overall, this leaves $2\cdot(2^k-2)$ possibilities for the $k+1$ bits suffix of x_2, which completely determine the $k+1$ bits suffix of x_3. Like case (a), the ℓ bits long prefix of x_2 and of x_3 have $2^\ell - 1$ possibilities each. So in case (b) the overall number of possibilities for x_1, x_2, x_3, for a given value of k and ℓ, is

$$2 \cdot (2^k - 1) \cdot (2^k - 2) \cdot (2^\ell - 1)^2 .$$

Summing the numbers in cases (a) and (b), we get

$$\begin{aligned} & 2 \cdot (2^k - 1) \cdot (2^\ell - 1)^2 + 2 \cdot (2^k - 1) \cdot (2^k - 2) \cdot (2^\ell - 1)^2 \\ = {} & (2^k - 1) \cdot (2^\ell - 1)^2 \cdot \big(2 + 2 \cdot (2^k - 2)\big) \\ = {} & 2 \cdot (2^k - 1)^2 \cdot (2^\ell - 1)^2 . \end{aligned}$$

In case (2) $\ell + k + 1 = n$, so $\ell = n - k - 1$. Furthermore, $k, \ell \geq 1$, so k is in the range $1 \leq k \leq n - 2$. Summing over all values of k, we get that the number of ordered quartets with $x_0 = 0^n$, satisfying case (2) of $P_{0,1} \cap S_{2,3}$, equals

$$\begin{aligned} & \sum_{k=1}^{n-2} 2 \cdot \left(2^k - 1\right)^2 \cdot \left(2^{n-k-1} - 1\right)^2 \\ = {} & \frac{1}{2} \cdot n \cdot 2^{2n} - \frac{8}{3} \cdot 2^{2n} + 4 \cdot n \cdot 2^n - 4 \cdot 2^n + 2 \cdot n + \frac{20}{3} . \end{aligned}$$

We will now turn to case (3), where $n \leq \ell + k$, so there is no buffer bit between the ℓ bits long prefix and the k bits long suffix, and if $n < \ell + k$, they even overlap. Again, we assume that $x_0 = 0^n$, thus the $\ell + 1$ leftmost bits of x_1 are $0^\ell 1$. We then have $2^{n-\ell-1}$ ways to choose x_1's suffix. Since $n - \ell - 1 < k$, it is guaranteed that even if x_0 and x_1 shared $n - \ell - 1$ suffix bits, their common suffix won't be longer than k.

Now, given x_0 and x_1, we want to determine the number of possibilities for x_2 and x_3. Note that the $n - k - 1$ bit of x_2 and x_3 must differ (otherwise the length of the common suffix would be greater than k.

Consider the $(k + \ell) - n$ bits of x_2, x_3, where the ℓ long prefix and k long suffix overlap (if $k + \ell = n$, this overlap is empty). These bits are part of the k long suffix, shared by x_2 and x_3. Let us consider the 2 following sub cases:

(i) The $(k + \ell) - n$ bits of x_2, x_3 equal $0^{k+\ell-n}$.

In this case, the $n - \ell$ rightmost bits of of x_2, x_3 must differ from the $n - \ell$ rightmost bits of x_0 (which are all 0) and of x_1 (which are not all 0). The number of possibilities is thus $2^{n-\ell} - 2$. Suppose, without loss of generality, that the $n - k - 1$ bit of x_2 equals 0. The $n - k - 1$ long prefix of x_2 must differ from 0^{n-k-1} (otherwise it would share an ℓ long prefix with both x_0 and x_1). There are $2^{n-k-1} - 1$ possibilities for this prefix. There is no such restrictions on the $n - k - 1$ bit long prefix of x_3, so there are 2^{n-k-1} possibilities for it. Overall, the number of possible sequences in case (i) is $2 \cdot 2^{n-\ell-1} \cdot (2^{n-\ell} - 2) \cdot (2^{n-k-1} - 1) \cdot 2^{n-k-1}$, where the leading 2 accounts for the cases where either the $n - k - 1$ bit of x_2 or that bit of x_3 equals 0.

(ii) The $(k + \ell) - n$ bits of x_2, x_3 differ from $0^{k+\ell-n}$.

There are $2^{(k+\ell)-n} - 1$ ways to determine these $(k + \ell) - n$ bits of x_2, x_3. And there are $2^{n-\ell}$ ways to determine the $n - \ell$ bit long suffix of x_2, x_3. Suppose, without loss of generality, that the $n-k-1$ bit of x_2 equals 0. There are no additional restrictions on the $n-k-1$ long prefix of x_2, so there are 2^{n-k-1} possibilities for this prefix. There are exactly that many possibilities for the $n-k-1$ long prefix of x_3. Overall, the number of possible sequences in case (ii) is $2 \cdot (2^{(k+\ell)-n} - 1) \cdot 2^{n-\ell-1} \cdot 2^{n-\ell} \cdot 2^{n-k-1} \cdot 2^{n-k-1}$, where the leading 2 accounts for the cases where either the $n-k-1$ bit of x_2 or that bit of x_3 equals 0.

Summing up cases (i, ii), we get that the number of possibilities for x_1, x_2, x_3 equals

$$\begin{aligned} &2 \cdot 2^{n-\ell-1} \cdot (2^{n-\ell} - 2) \cdot (2^{n-k-1} - 1) \cdot 2^{n-k-1} \\ &+2 \cdot (2^{(k+\ell)-n} - 1) \cdot 2^{n-\ell-1} \cdot 2^{n-\ell} \cdot 2^{n-k-1} \cdot 2^{n-k-1} \end{aligned}$$

Summing over values of k and ℓ, satisfying $n \leq k + \ell$, we get

$$\begin{aligned} &\sum_{\ell=1}^{n-1} \sum_{k=n-\ell}^{n-1} \big(2 \cdot 2^{n-\ell-1} \cdot (2^{n-\ell} - 2) \cdot (2^{n-k-1} - 1) \cdot 2^{n-k-1} \\ &\qquad + 2 \cdot (2^{(k+\ell)-n} - 1) \cdot 2^{n-\ell-1} \cdot 2^{n-\ell} \cdot 2^{n-k-1} \cdot 2^{n-k-1}\big) \\ &= \frac{1}{2} \cdot n \cdot 2^{2n} - \frac{7}{3} \cdot 2^{2n} + 2 \cdot n \cdot 2^n + 2^n + \frac{4}{3} \ . \end{aligned}$$

Summing the contributions from cases (1), (2), and (3), we conclude that the number of ordered quartets with $x_0 = 0^n$ in $P_{0,1} \cap S_{2,3}$ equals

$$\frac{16}{441} \cdot 2^{3n} - \frac{7}{3} \cdot n \cdot 2^n + \frac{68}{9} \cdot 2^n - \frac{22}{7} \cdot n - \frac{372}{49} \ .$$

Note that the $\theta(n \cdot 2^{2n})$, $\theta(2^{2n})$ terms were cancelled.

3.2 $P_{0,1} \cap S_{0,1}$

We denote the length of the longest common prefix of x_0, x_1 by ℓ ($\ell \leq n-1$), and the length of the longest common suffix of x_0, x_1 by k ($k \leq n - \ell - 1$). For $P_{0,1}$, $\ell \geq 1$ should hold, and for $S_{0,1}$, $k \geq 1$ should hold. Note that in this case, the locations of the longest common suffix and the longest common prefix cannot intersect . We treat separately the following two cases:

(1) $\ell + k + 2 \leq n$ (the ℓ long prefix plus one bit buffer zone, and the k long suffix plus one bit buffer zone, do not overlap). Since $1 \leq k$, ℓ is bounded by $\ell \leq n-3$.

(2) $\ell + k + 1 = n$.

Note that $\ell + k < n$ must hold, for otherwise we would have $x_0 = x_1$. Given that x_0 is 0^n, it is then clear that x_1's $\ell + 1$ long prefix is $0^\ell 1$ and its $k+1$ long suffix is 10^k.

In case (1), $\ell + k + 1 < n$, and x_1 has the form $x_1 = 0^\ell 1 x 1 0^k$ where $x \in \{0,1\}^{n-k-\ell-2}$. x can be chosen with no constrains from $\{0,1\}^{n-k-\ell-2}$, so there are $2^{n-k-\ell-2}$ ways to choose x. There are $2^{\ell+1} - 2$ ways to choose the $\ell + 1$ long prefix of x_2 (it must differ from the $\ell + 1$ long prefix of x_0 and

x_1), and $2^{\ell+1}-3$ ways to choose the $\ell+1$ long prefix of x_3 (it must differ from the $\ell+1$ long prefixes of x_0, x_1, and x_2). In a similar manner, there are $2^{k+1}-2$ ways to choose the $k+1$ long suffix of x_2, and $2^{k+1}-3$ ways to choose the $k+1$ long suffix of x_3. Finally, the remaining $n-k-\ell-2$ bits of the buffer zone in each of x_2, x_3 can be chosen freely. All by all, the number of possibilities of case (1) for given values of ℓ and k is

$$2^{3(n-k-\ell-2)} \cdot (2^{\ell+1}-2) \cdot (2^{\ell+1}-3) \cdot (2^{k+1}-2) \cdot (2^{k+1}-3) \ .$$

We remark that this expression is the same as the one derived for case (1) of $P_{0,1} \cap S_{2,3}$.

In case (2), $\ell+k+1=n$, and x_1 has the form $x_1 = 0^\ell 10^k$, so it is completely determined. Unlike case (1), the $\ell+1$ long prefix and $k+1$ long suffix overlap, which makes the treatment slightly more involved. We therefore partition case (2) into two subcases: (i) x_2 and x_3's common suffix length is shorter than k, and (ii) x_2 and x_3's common suffix length is exactly k. For case (i) we can still choose x_2 and x_3's prefixes as we have done in (1), namely there are $(2^{\ell+1}-2)\cdot(2^{\ell+1}-3)$ ways to choose them. Given the $\ell+1$ long suffixes, both x_2 and x_3 still got $n-\ell-1=k$ bits that are not yet determined. Since the length of their shared suffix is shorter than k, the two choices must be different from each other, and from 0^k. So there are $(2^k-1)\cdot(2^k-2)$ ways to choose the remaining k bits. All by all, the number of possibilities in subcase (i) is $(2^{\ell+1}-2)\cdot(2^{\ell+1}-3)\cdot(2^k-1)\cdot(2^k-2)$ possibilities.

For subcase (ii), x_2 and x_3's k long suffixes are the same, but the $(k+1)$th bits (from the right) are different. The $k+1$ long suffixes must be different from both 0^{k+1} and 10^k. This leaves $2^{k+1}-2$ choices for x_2's $k+1$ long suffix, and determines x_3's $k+1$ long suffix. Now the ℓ long prefixes of both can be chosen freely, as long as they both are not 0^ℓ. So there are $(2^\ell-1)^2$ ways to choose the prefixes for x_2 and x_3. In subcase (2)(ii) there are $(2^\ell-1)^2\cdot(2^{k+1}-2)$ possibilities. All by all, the number of possibilities in case (2) for given values of ℓ and k is

$$(2^{\ell+1}-2)\cdot(2^{\ell+1}-3)\cdot(2^k-1)\cdot(2^k-2)+(2^\ell-1)^2\cdot(2^{k+1}-2) \ .$$

Substituting $k=n-\ell-1$, we get

$$(2^{\ell+1}-2)\cdot(2^{\ell+1}-3)\cdot(2^{n-\ell-1}-1)\cdot(2^{n-\ell-1}-2)+(2^\ell-1)^2\cdot(2^{n-\ell}-2) \ .$$

We now sum over the relevant values of ℓ and k. For case (1), we have

$$\sum_{\ell=1}^{n-3}\sum_{k=1}^{n-\ell-2}(2^{\ell+1}-2)\cdot(2^{\ell+1}-3)\cdot(2^{k+1}-2)\cdot(2^{k+1}-3)\cdot 2^{3(n-\ell-k-2)})$$
$$= 5\cdot 2^{2n} - \frac{764}{49} + \frac{95}{9}\cdot 2^n - \frac{25}{3}\cdot n\cdot 2^n - n\cdot 2^{2n} - \frac{36}{7}\cdot n + \frac{16}{441}\cdot 2^{3n} \ .$$

While in case (2), the number of quartets is

$$\sum_{\ell=1}^{n-2}\Big((2^{\ell+1}-2)\cdot(2^{\ell+1}-3)\cdot(2^{n-\ell-1}-1)\cdot(2^{n-\ell-1}-2)+\big(2^\ell-1\big)^2\cdot(2^{n-\ell}-2)\Big)$$
$$= 28 + 10\cdot n - 22\cdot 2^n - 6\cdot 2^{2n} + n\cdot 2^{2n} + 13\cdot n\cdot 2^n \ .$$

Summing up the expressions for (1) and (2), the number of ordered quartets with $x_0 = 0^n$ in $P_{0,1}\cap S_{0,1}$ is

$$\frac{16}{441}\cdot 2^{3n} - 2^{2n} + \frac{14}{3}\cdot n\cdot 2^n - \frac{103}{9}\cdot 2^n + \frac{34}{7}\cdot n + \frac{608}{49} \ .$$

Note that the $\theta(n\cdot 2^{2n})$ terms were again cancelled.

3.3 $P_{0,1} \cap P_{2,3} \cap S_{0,1}$

We denote the length of the longest common prefix of x_0, x_1 by ℓ ($\ell \leq n-1$), and the length of the longest common suffix of x_0, x_1 by k ($k \leq n-1$). For $P_{0,1}$, $\ell \geq 1$ should hold, and for $S_{0,1}$, $k \geq 1$ should hold. Note that in this case, the locations of the longest common suffix and the longest common prefix cannot intersect . We treat separately the following two cases:

(1) $\ell + k + 2 \leq n$ (the ℓ long prefix plus one bit buffer zone, and the k long suffixes plus one bit buffer zone, do not overlap). Since $1 \leq k$, ℓ is bounded by $\ell \leq n-3$.

(2) $\ell + k + 1 = n$.

Note that $\ell + k < n$ must hold, for otherwise we would have $x_0 = x_1$. For case (1), by following an argument very similar to case (1) of $P_{0,1} \cap S_{0,1}$, we get that the number of ordered quartets is

$$2^{3(n-k-\ell-2)} \cdot (2^{\ell+1} - 2) \cdot (2^{k+1} - 2) \cdot (2^{k+1} - 3) \ .$$

Summing over all values of ℓ and k, we get

$$\sum_{\ell=1}^{n-3} \sum_{k=1}^{n-l-2} (2^{\ell+1} - 2) \cdot (2^{k+1} - 2) \cdot (2^{k+1} - 3) \cdot 2^{3(n-\ell-k-2)})$$
$$= \frac{4}{441} 2^{3n} - \frac{1}{3} 2^{2n} + \frac{5}{3} n2^n - \frac{37}{9} 2^n + \frac{12}{7} n + \frac{652}{147}$$

For case (2), given that x_0 is 0^n, we have $x_1 = 0^\ell 1 0^k$. The $\ell+1$ prefix of x_2 must differ from $0^{\ell+1}$ and from $0^\ell 1$, thus there are $2^{\ell+1} - 2$ possibilities. Since the longest common prefix of x_2, x_3 is also of length ℓ, the $\ell+1$ long prefix of x_2 determines the $\ell+1$ long prefix of x_3. The k long suffix of x_2 and of x_3 must differ from 0^k. There are no further constraints, and in particular these two suffixes can be the same, as the next bit of x_2 already differs from that of x_3. The number of possibilities for the k long suffix of x_2 and of x_3 is thus $(2^k - 1)^2$. Substituting $k = n - \ell - 1$, the number of ordered quartets in case (2) is

$$(2^{\ell+1} - 2) \cdot (2^k - 1)^2 = (2^{\ell+1} - 2) \cdot (2^{n-\ell-1} - 1)^2 \ .$$

Summing over all values of ℓ, we get

$$\sum_{\ell=1}^{n-2} (2^{\ell+1} - 2) \cdot (2^{n-\ell-1} - 1)^2$$
$$= \frac{1}{3} 2^{2n} - 2 \cdot n2^n + 5 \cdot 2^n - 2 \cdot n - \frac{16}{3} \ .$$

Adding the two expressions together, we conclude that number of ordered quartets with $x_0 = 0^n$ in $P_{0,1} \cap P_{2,3} \cap S_{0,1}$ equals

$$\frac{4}{441} \cdot 2^{3n} - \frac{1}{3} \cdot n2^n + \frac{8}{9} \cdot 2^n - \frac{2}{7} \cdot n - \frac{44}{49} \ .$$

3.4 $P_{0,1} \cap P_{2,3} \cap S_{0,1} \cap S_{2,3}$

We denote the length of the longest common prefix of x_0, x_1 by ℓ ($\ell \leq n-1$), and the length of the longest common suffix of x_0, x_1 by k ($k \leq n-1$). Like before, $k, \ell \geq 1$, and we treat separately the following two cases:

(1) $\ell + k + 2 \leq n$ (the ℓ long prefix plus one bit buffer zone, and the k long suffix plus one bit buffer zone, do not overlap). Since $1 \leq k$, ℓ is bounded by $\ell \leq n-3$.

(2) $\ell + k + 1 = n$.

In case (1), it is (now) easy to see that the number of ordered quartets is

$$2^{3(n-k-\ell-2)} \cdot (2^{\ell+1} - 2) \cdot (2^{k+1} - 2) \ .$$

Summing over all values of ℓ and k, we get

$$\begin{aligned} & \sum_{\ell=1}^{n-3} \sum_{k=1}^{n-l-2} (2^{\ell+1} - 2) \cdot (2^{k+1} - 2) \cdot 2^{3(n-\ell-k-2)}) \\ = & \frac{1}{441}\, 2^{3n} - \frac{1}{3}\, n2^n + \frac{11}{9}\, 2^n - \frac{4}{7}\, n - \frac{60}{49} \end{aligned}$$

While in case (2), the number of possibilities is

$$(2^{\ell+1} - 2) \cdot (2^k - 1) = (2^{\ell+1} - 2) \cdot (2^{n-\ell-1} - 1) \ .$$

Summing over all values of ℓ, we get

$$\sum_{\ell=1}^{n-2} (2^{\ell+1} - 2) \cdot (2^{n-\ell-1} - 1) = \ n2^n - 4 \cdot 2^n + 2 \cdot n + 4 \ .$$

Summing the expressions for case (1) and case (2), we conclude that overall, the number of ordered quartets with $x_0 = 0^n$ satisfying $P_{0,1} \cap P_{2,3} \cap S_{0,1} \cap S_{2,3}$ is

$$\frac{1}{441}\, 2^{3n} + \frac{2}{3} \cdot n2^n - \frac{25}{9} \cdot 2^n + \frac{10}{7} \cdot n + \frac{136}{49} \ .$$

4 Putting Everything Together

Consider the event

$$A = (P_{0,1} \cup P_{2,3}) \cap (S_{0,1} \cup S_{2,3}) \ ,$$

A simple manipulation yields

$$\begin{aligned} A = & \quad (P_{0,1} \cup P_{2,3}) \cap (S_{0,1} \cup S_{2,3}) \\ = & \quad (P_{0,1} \cap S_{0,1}) \cup (P_{0,1} \cap S_{2,3}) \cup (P_{2,3} \cap S_{0,1}) \cup (P_{2,3} \cap S_{2,3}) \end{aligned}$$

By the inclusion exclusion principle

$$
\begin{aligned}
|A| =& |(P_{0,1}\cap S_{0,1})\cup(P_{0,1}\cap S_{2,3})\cup(P_{2,3}\cap S_{0,1})\cup(P_{2,3}\cap S_{2,3})| \\
=& |P_{0,1}\cap S_{0,1}| + |P_{0,1}\cap S_{2,3}| + |P_{2,3}\cap S_{0,1}| + |P_{2,3}\cap S_{2,3}| \\
& - |P_{0,1}\cap S_{0,1}\cap S_{2,3}| - |P_{0,1}\cap S_{0,1}\cap P_{2,3}| \\
& - 2\,|P_{0,1}\cap S_{0,1}\cap P_{2,3}\cap S_{2,3}| - |P_{0,1}\cap S_{2,3}\cap P_{2,3}| \\
& - |P_{2,3}\cap S_{0,1}\cap S_{2,3}| + 4\,|P_{0,1}\cap S_{0,1}\cap P_{2,3}\cap S_{2,3}| \\
& - |P_{0,1}\cap S_{0,1}\cap P_{2,3}\cap S_{2,3}| \\
=& |P_{0,1}\cap S_{0,1}| + |P_{0,1}\cap S_{2,3}| + |P_{2,3}\cap S_{0,1}| + |P_{2,3}\cap S_{2,3}| \\
& - |P_{0,1}\cap S_{0,1}\cap S_{2,3}| - |P_{0,1}\cap S_{0,1}\cap P_{2,3}| \\
& - |P_{0,1}\cap S_{2,3}\cap P_{2,3}| - |P_{2,3}\cap S_{0,1}\cap S_{2,3}| \\
& + |P_{0,1}\cap S_{0,1}\cap P_{2,3}\cap S_{2,3}| \\
=& 2\,|P_{0,1}\cap S_{0,1}| + 2\,|P_{0,1}\cap S_{2,3}| - 4\,|P_{2,3}\cap S_{0,1}\cap S_{2,3}| + |P_{0,1}\cap S_{0,1}\cap P_{2,3}\cap S_{2,3}|
\end{aligned}
$$

Substituting the expressions we derived for the various subsets, we conclude that the number of ordered quartets with $x_0 = 0^n$ in A equals

$$\frac{1}{9}\,2^{3n} - 2\cdot 2^{2n} + \frac{20}{3}\,n2^n - \frac{127}{9}\,2^n + 6\,n + 16\ .$$

Removing the $x_0 = 0^n$ restriction, the number of ordered quartets in A equals

$$\frac{1}{9}\,2^{4n} - 2\cdot 2^{3n} + \frac{20}{3}\,n2^{2n} - \frac{127}{9}\,2^{2n} + 6\,n2^n + 16\cdot 2^n\ .$$

We now introduce two related sets, B and C:

$$B = (P_{0,2}\cup P_{1,3})\cap(S_{0,2}\cup S_{1,3})\ \ , C = (P_{0,3}\cup P_{1,2})\cap(S_{0,3}\cup S_{1,2})\ \ .$$

Clearly A, B, C are mutually exclusive and A, B, C have the same number of ordered quartets. Therefore

$$|A\cup B\cup C| = \frac{1}{3}\,2^{4n} - 6\cdot 2^{3n} + 20\cdot n2^{2n} - \frac{127}{3}\,2^{2n} + 18\cdot n2^n + 48\cdot 2^n\ .$$

We observe that the union $A\cup B\cup C$ contains exactly those ordered quartets on x_0, x_1, x_2, x_3 that agree in both prefix and suffix trees.

5 Unordered Quartet and the Quartet Distance

So far, we counted ordered quartets. In the quartet distance problem, we are interested in *unordered* quartets and not in ordered ones. There are $4! = 24$ permutations over a set of 4 distinct elements, $\{x_0, x_1, x_2, x_3\}$. We will show that for any set $\{x_0, x_1, x_2, x_3\}$, either the suffix and the prefix tree agree for all the ordered 4-tuples corresponding to these 24 permutations, (namely the ordered event $A\cup B\cup C$, is satisfied), or there is no agreement for any of the permutations. This statement implies that the number of unordered quartets where the two trees agree is exactly this number for the ordered case, divided by 24.

We will show that A is invariant under exactly 8 permutations of ordered 4-tuples. A different set of 8 permutations maps ordered 4-tuples that satisfy A to different orders where the 4-tuple satisfies B, and yet another 8 permutations map ordered 4-tuples that satisfy A to different orders satisfying C.

Suppose the ordered pair (x_0, x_1, x_2, x_3) satisfies A, namely

$$(P_{0,1}(x_0, x_1, x_2, x_3) \cup P_{2,3}(x_0, x_1, x_2, x_3)) \ \cap \ (S_{0,1}(x_0, x_1, x_2, x_3) \cup S_{2,3}(x_0, x_1, x_2, x_3)) \ .$$

Membership in A is invariant under each of the following 3 permutations and their compositions: Transposing x_0, x_1; transposing x_2, x_3; replacing x_0, x_1 by x_2, x_3. These 3 permutations generate a subgroup of size 8.

Starting with an ordered quartet (x_0, x_1, x_2, x_3) in A, and transposing x_1 with x_2, the new ordered quartet (x_0, x_2, x_1, x_3) is now in B. By first applying one of the 8 permutations keeping (x_0, x_1, x_2, x_3) in A, and then this transposition, we conclude that there is a coset of 8 permutations, moving an ordered quartet from A to B. A similar argument holds regarding moving from A to C, employing the transposition of x_1 with x_3. Clearly, the same argument is applicable if we start with an ordered quartet that satisfies B or C.

We conclude that if the prefix and suffix trees agree on one ordered quartet, then they will agree on all 24 permutations of it. Dividing the number of ordered permutations on n-bit strings where this event occurs by 24, we conclude that the number of *unordered* permutations that agree equals

$$\left(\frac{1}{3}\, 2^{4n} - 6 \cdot 2^{3n} + 20 \cdot n2^{2n} - \frac{127}{3}\, 2^{2n} + 18 \cdot n2^n + 48 \cdot 2^n\right) /24 \ .$$

The number of unordered quartets equals

$$\frac{2^n \cdot (2^n - 1) \cdot (2^n - 2) \cdot (2^n - 3)}{24} = \frac{2^{4n} - 6 \cdot 2^{3n} + 11 \cdot 2^{2n} - 6 \cdot 2^n}{24} \ .$$

Thus the quartet distance between the two trees equals

$$\frac{2^{4n} - 6 \cdot 2^{3n} + 11 \cdot 2^{2n} - 6 \cdot 2^n - \left(\frac{1}{3}\, 2^{4n} - 6 \cdot 2^{3n} + 20 \cdot n2^{2n} - \frac{127}{3}\, 2^{2n} + 18 \cdot n2^n + 48 \cdot 2^n\right)}{24}$$

$$= \frac{\frac{2}{3} \cdot 2^{4n} - 20 \cdot n2^{2n} + \frac{160}{3} \cdot 2^{2n} - 18 \cdot n2^n - 54 \cdot 2^n}{24} \ .$$

The ratio, or *normalized* quartet distance for the suffix and prefix trees on $N = 2^n$ leaves equals

$$\frac{\frac{2}{3} \cdot 2^{4n} - 20 \cdot n2^{2n} + \frac{160}{3} \cdot 2^{2n} - 18 \cdot n2^n - 54 \cdot 2^n}{2^{4n} - 6 \cdot 2^{3n} + 11 \cdot 2^{2n} - 6 \cdot 2^n} \ .$$

It is easy to see that this ratio indeed converges to $2/3$ as $n \to \infty$. What is not so obvious is that this ratio is a monotonically decreasing function of n. For small values of n we get the following distances and ratios. For these values (and many others we tested numerically) the ratio indeed decreases monotonically with growing values of n.

n	3	4	5	6	7	8	9	10
distance	60	1452	26944	454224	7396416	119011264	1907486208	30535571712
ratio	0.857	0.797	0.749	0.714	0.693	0.680	0.674	0.670

To prove the above mentioned monotonicity, we show that the ratio for $N = 2^n$ is larger than the ratio for $N_1 = 2^{n+1}$. The proof involves somewhat tedious yet elementary arithmetic manipulations.

Let $R(n)$ denote the ratio (number of disagreeing unordered quartets, divided by the total number of unordered quartets) for the prefix and suffix trees with $N = 2^n$ leaves. Then

$$R(n) = \frac{\frac{2}{3} \cdot 2^{4n} - 20 \cdot n2^{2n} + \frac{160}{3} \cdot 2^{2n} - 18 \cdot n2^n - 54 \cdot 2^n}{2^{4n} - 6 \cdot 2^{3n} + 11 \cdot 2^{2n} - 6 \cdot 2^n}$$

$$R(n+1) = \frac{\frac{2}{3} \cdot 2^{4(n+1)} - 20 \cdot (n+1)2^{2(n+1)} + \frac{160}{3} \cdot 2^{2(n+1)} - 18 \cdot (n+1)2^{n+1} - 54 \cdot 2^{n+1}}{2^{4(n+1)} - 6 \cdot 2^{3(n+1)} + 11 \cdot 2^{2(n+1)} - 6 \cdot 2^{n+1}} .$$

To show that $R(n) > R(n+1)$, we first compute

$$\text{numerator}(R(n)) \cdot \text{denominator}(R(n+1)) - \text{numerator}(R(n+1)) \cdot \text{denominator}(R(n)) ,$$

and then take the derivative of this expression with respect to the (real) variable n. The result (obtained using Maple) equals

$$\begin{aligned}
&-3792 \cdot 2^{4n} \ln(2) + 1440 \cdot 2^{4n} \cdot n \cdot \ln(2) + 360 \cdot 2^{4n} - 240 \cdot \ln(2)\, 2^{5n} \\
&-342 \cdot 2^{3n} - 1026 \cdot 2^{3n} \cdot n \cdot \ln(2) + 10908 \cdot 2^{3n} \ln(2) \\
&-1944 \cdot 2^{2n} \cdot n \cdot \ln(2) - 972 \cdot 2^{2n} - 7824 \cdot 2^{2n} \ln(2) \\
&+954 \cdot 2^{n} \cdot n \cdot \ln(2) + 954 \cdot 2^{n} + 948 \cdot 2^{n} \ln(2)
\end{aligned}$$

It is easy to see that for $n \geq 11$, the derivative is negative, as following: The first term in the first line, $-3792 \cdot 2^{4n} \ln(2)$, dominates the third term in the same line. The difference $1440 \cdot 2^{4n} \cdot n \cdot \ln(2) - 240 \cdot \ln(2)\, 2^{5n}$ is negative for all $n \geq 5$. For $n \geq 11$, the second term in the second line, $-1026 \cdot 2^{3n} \cdot n \cdot \ln(2)$, dominates the third term in the same line, $+10908 \cdot 2^{3n} \ln(2)$. Each of the three terms containing 2^n (fourth line) is dominated by a term containing 2^{2n} (third line) with a minus sign. Finally, for (integer) values of n in the range $3 \leq n \leq 11$, direct computation verifies that $R(n) - R(n+1) > 0$.

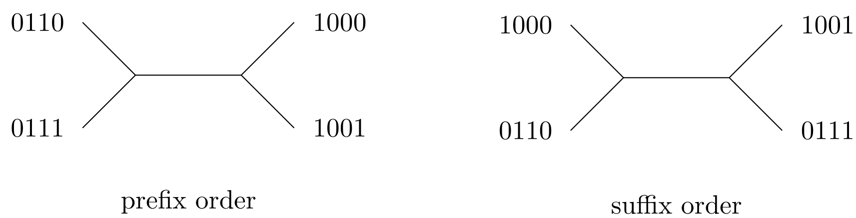
6 Concluding Remarks and Open Problems

There is more than a single notion of what an "explicit construction" means. Possibly the most popular one is that an explicit construction is (1) deterministic, and (2) it runs in polynomial time (polynomial in the size of the object being constructed). Under this definition, by de-randomizing a randomized labeling of the leaves, we would get an explicit construction with quartet distance being asymptotically $\frac{2}{3}\binom{N}{4}$. It may require some additional work to determine by how much the exact bound resulting from this approach exceeds $\frac{2}{3}\binom{N}{4}$ for concrete values of N. This construction is deterministic, and its running time is polynomial in the size of the resulting trees, $N = 2^n$. Thus, this is an explicit construction by the definition above. Furthermore, it is applicable to any two trees (not just complete, balanced binary trees), and any size N (not just a power of 2). On the other hand, it is hard to argue that (for complete, balanced binary trees) our construction is much simpler, and arguably elegant, than what the de-randomization yields.

A "strongly explicit construction" enables one to determine, given the specification of an entry in the object, the contents of this entry, in time that is polynomial in the length of the description of the entry (as opposed to the size of the complete object). This is applicable to a variety of objects, *e.g.* graphs, matrices, and codes [8]. In our context, a strongly explicit construction should be able to determine, in time polynomial in n (and *not* in 2^n) the label of a leaf, given the description of this leaf. Furthermore, given the labels of four leaves, we should be able to determine the induced quartets topologies for the two trees.

The standard de-randomized construction is *not* strongly explicit. Essentially, it mimics the randomized construction, where one first assigns labels to all leaves, and only then can determine the labels of specific leaves or the topologies of specific quartets. By way of contrast, our prefix–suffix construction is strongly explicit. Assuming we use the standard labeling of the complete, balanced binary trees by the prefix order, then the labeling of, say, `0111` in the prefix tree will be, well, `0111`, which is the rightmost leaf on the major left subtree. In the suffix tree it will be placed on the one left to the rightmost leaf, the one labeled by `1110` in prefix order (we simply reverse the binary string to move from prefix to suffix order). So determining the location is done in linear time, using a trivially simple algorithm.

Turning to quartets given four labels, in the prefix order the two labels with longest common prefix will be together, and dually for the suffix order. So determining prefix and suffix quartets topologies is also done, given the four labels, by a trivial linear time algorithm. See the following figure, for labels of length $n = 4$.



As noted above, our construction and proof are applicable only to complete, balanced binary trees on $N = 2^n$ leaves. It will be interesting to extend these results to other tree topologies, and also values of N that are not exact power of 2. We note that the tree topology may have a substantial impact on the feasibility of a proof. For example, Alon, Naves, and Sudakov [1] have shown a $(0.69 + o(1)) \cdot \binom{N}{4}$ upper bound on the normalized quartet distance of general binary trees (for large enough N), but a better $(2/3 + o(1)) \cdot \binom{N}{4}$ upper bound for caterpillar trees. Finally, it will be interesting to prove or refute the conjecture that for large enough n, the largest quartet distance on trees with $N = 2^n$ leaves is obtained by the suffix and prefix trees.

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