Cophenetic metrics for phylogenetic trees, after Sokal and Rohlf (Supplementary Material)

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Proofs of Propositions 1–4

Proof of Proposition 1

By Lemma 1, it is enough to prove that the minimum non-zero value of D_0 is 1, and that all pairs $T, T' \in \mathcal{UT}_n$ such that $D_0(T,T') = 1$ also satisfy that $D_p(T,T') = 1$ for every $p \geqslant 1$.

As we have seen in Example 2, if we contract a pendant arc in a tree T, we obtain a new tree T' such that $D_p(T,T') = 1$, for every $p \in \{0\} \cup [1,\infty[$, and this is of course the smallest possible non-negative value of D_p on $\mathcal{UT}_n$. It remains to prove that this is the only way we can obtain a pair of trees such that $D_0(T,T') = 1$.

So, let $T, T' \in \mathcal{UT}_n$ be such that $\varphi(T) = \varphi(T') + m \cdot e_{i,j}$ for some $m \geqslant 1$ and $1 \leqslant i,j \leqslant n$ (where $e_{i,j}$ stands for the vector of length $n(n+1)/2$ with all entries 0 except an 1 in the entry corresponding to the pair (i,j)); that is, T and T' are such that $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$, for some $m \geqslant 1$, and $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j)$. Let us prove first of all that $m = 1$. So, assume that $m \geqslant 2$ and let us reach a contradiction.

Since $\varphi_T(i,j) > 0$, there exists some taxon $k \neq i,j$ that is a descendant in T of the parent of $[i,j]_T$. In other words, such that $[i,k]_T = [j,k]_T$ is the parent of $[i,j]_T$. But then

$$\varphi_{T'}(i,k) = \varphi_T(i,k) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j) + (m-1) > \varphi_{T'}(i,j)$$
$$\varphi_{T'}(j,k) = \varphi_T(j,k) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j) + (m-1) > \varphi_{T'}(i,j)$$

which cannot hold simultaneously: if $\varphi_{T'}(i,k) > \varphi_{T'}(i,j)$, then $\varphi_{T'}(j,k) = \varphi_{T'}(i,j)$. This shows that $m = 1$, and thus $\varphi(T) = \varphi(T') + e_{i,j}$.

Let us prove now that it cannot happen that $i \neq j$. Indeed, assume that $i \neq j$. If $\varphi_{T'}(i,j) = \delta_{T'}(i)$, then

$$\varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \delta_{T'}(i) + 1 = \delta_T(i) + 1,$$

which is impossible. This implies that $\varphi_{T'}(i,j) < \delta_{T'}(i), \delta_{T'}(j)$. If, now, $\varphi_{T'}(i,j) < \delta_{T'}(i) - 1$, then there will exist some leaf k such that $[i,k]_{T'}$ is the child of $[i,j]_{T'}$ in the path from $[i,j]_{T'}$ to i. Then $\varphi_{T'}(i,k) = \varphi_{T'}(i,j) + 1$ and $\varphi_{T'}(j,k) = \varphi_{T'}(i,j)$, which entail that

$$\varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j) > \varphi_{T'}(i,j) = \varphi_{T'}(j,k) = \varphi_T(j,k),$$

which is also impossible. So, if $i \neq j$, the only possibility is that $\varphi_{T'}(i,j) = \delta_{T'}(i) - 1 = \delta_{T'}(j) - 1$, but then it would imply that $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \delta_T(i) = \delta_T(j)$ and hence that $[i,j]_T = i = j$, which is again impossible.

So, if $\varphi(T) = \varphi(T') + e_{i,j}$ then it must happen that $i = j$. In this case, moreover, i must be a leaf in T with unlabeled parent. Indeed, if i is not a leaf, then there is some leaf k such that $i = [i,k]_T$ and hence $\delta_T(i) = \varphi_T(i,k)$. Then, $\delta_{T'}(i) = \delta_T(i) - 1 = \varphi_T(i,k) - 1 = \varphi_{T'}(i,k) - 1$, which is impossible. So, i is a leaf in T. And if its parent is labeled, say with l, then $\delta_T(i) = \delta_T(l) + 1$ and $\delta_T(l) = \varphi_T(i,l)$. Thus, in T', $\delta_{T'}(i) = \delta_T(i) - 1 = \delta_T(l) = \delta_{T'}(l)$ and $\delta_{T'}(i) = \delta_T(l) = \varphi_T(i,l) = \varphi_{T'}(i,l)$, which is also impossible, since it would imply that $[i,l]_{T'} = i = l$.

So, finally, it must happen that i is a leaf in T and its parent is not labeled. Let T_0 be the phylogenetic tree obtained from T by contracting the pendant arc ending in i. Then $\varphi(T_0) = \varphi(T) - e_{i,i} = \varphi(T')$, and this implies, by Theorem 1, that $T_0 = T'$.

This finishes the proof that the only pairs $T, T' \in \mathcal{WT}_n$ such that $D_0(T,T') = 1$ are those where one of them is obtained from the other by the contraction of a pendant arc. Since these pairs of trees also satisfy that $D_p(T,T') = 1$ for every $p \geqslant 1$, this completes the proof of the proposition. □

Proof of Proposition 2

To ease the task of the reader, we split this proof into several lemmas. To begin with, notice that there are pairs of trees $T, T' \in \mathcal{T}_n$ such that $D_p(T,T') = 3$ for every $p \in \{0\} \cup [1, \infty[$: for instance, by Example 2, when T' is obtained from T by contracting an arc ending in the root of a cherry. So, the minimum non-zero value of $D_p(T,T')$ on $\mathcal{T}_n$ is at most 3.

Lemma 1. *If $T, T' \in \mathcal{T}_n$ are such that $D_0(T,T') > 0$, then there exists a pair of different taxa $i \neq j$ such that $\varphi_T(i,j) \neq \varphi_{T'}(i,j)$.*

Proof. If $\varphi_T(i,j) = \varphi_{T'}(i,j)$ for every $i \neq j$, then, by Corollary 1, $T = T'$ and therefore $D_0(T,T') = 0$. □

So, every pair of phylogenetic trees in $\mathcal{T}_n$ at non-zero D_0 distance must have a pair of different leaves with different cophenetic values.

Lemma 2. *Let $T, T' \in \mathcal{T}_n$ be such that $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$, for some $1 \leqslant i < j \leqslant n$ and some $m \geqslant 1$. Let $k \neq i,j$ be a leaf such that there exists a path from $[i,j]_{T'}$ to $[i,k]_{T'}$ of length l, for some $l \geqslant 1$. Then:*

(a) If $\varphi_T(i,k) = \varphi_{T'}(i,k)$, then $\varphi_T(j,k) \geqslant \varphi_{T'}(j,k) + \min\{m,l\}$

(b) If $\varphi_T(j,k) = \varphi_{T'}(j,k)$, then $\varphi_T(i,k) = \varphi_{T'}(i,k) - l$

Proof. From the assumptions we have that $\varphi_{T'}(i,k) = \varphi_{T'}(i,j) + l = \varphi_{T'}(j,k) + l$. Now:

(a) Assume that $\varphi_T(i,k) = \varphi_{T'}(i,k)$. Then,

$$\varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(i,j) + l = \varphi_T(i,j) - (m-l),$$

and then

- If $m > l$, then $\varphi_T(i,k) < \varphi_T(i,j)$, that is, $[i,j]_T \prec [i,k]_T$, and thus

$$\varphi_T(j,k) = \varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(j,k) + l$$

- If $m = l$, then $\varphi_T(i,k) = \varphi_T(i,j)$, that is, $[i,k]_T = [i,j]_T$, and thus

$$\varphi_T(j,k) \geqslant \varphi_T(i,j) = \varphi_{T'}(i,j) + m = \varphi_{T'}(j,k) + m$$

- If $m < l$, then $\varphi_T(i,k) > \varphi_T(i,j)$, that is, $[i,k]_T \prec [i,j]_T$, and thus

$$\varphi_T(j,k) = \varphi_T(i,j) = \varphi_{T'}(i,j) + m = \varphi_{T'}(j,k) + m$$

(b) Assume that $\varphi_T(j,k) = \varphi_{T'}(j,k)$. Then

$$\varphi_T(j,k) = \varphi_{T'}(j,k) = \varphi_{T'}(i,j) = \varphi_T(i,j) - m,$$

so that $[i,j]_T \prec [j,k]_T$, and thus

$$\varphi_T(i,k) = \varphi_T(j,k) = \varphi_{T'}(j,k) = \varphi_{T'}(i,j) = \varphi_{T'}(i,k) - l$$

□

As a direct consequence of this lemma we obtain the following result.

Corollary 1. *Let $T, T' \in \mathcal{T}_n$ be such that $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$, for some $1 \leqslant i < j \leqslant n$ and some $m \geqslant 1$. Let N be the number of leaves k such that $k \neq i,j$ and either $[i,k]_{T'} \prec [i,j]_{T'}$ or $[j,k]_{T'} \prec [i,j]_{T'}$. Then,*

$$D_0(T,T') \geqslant N + 1.$$

□

Lemma 3. *Let $T, T' \in \mathcal{T}_n$ be such that $D_0(T,T') \leqslant 3$. If $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$, for some $1 \leqslant i < j \leqslant n$ and some $m \geqslant 1$, then $m = 1$.*

Proof. If $\delta_{T'}(i) = \delta_T(i)$, then $\delta_{T'}(i) = \delta_T(i) > \varphi_T(i,j) = \varphi_{T'}(i,j) + m$ which implies that there are at least m leaves k such that $[i,k]_{T'} \prec [i,j]_{T'}$. Then, by the last corollary, $D_0(T,T') \geqslant m+1$. Now, if $\delta_{T'}(j) = \delta_T(j)$, then for the same reason there are at least m leaves k such that $[j,k]_{T'} \prec [i,j]_{T'}$ and they increase $D_0(T,T')$ to at least $2m+1$, while if $\delta_{T'}(j) \neq \delta_T(j)$, then $D_0(T,T') \geqslant m+2$. We conclude then that if $\delta_{T'}(i) = \delta_T(i)$, then $m = 1$. By symmetry, if $\delta_{T'}(j) = \delta_T(j)$, then $m = 1$, either.

Finally, if $\delta_{T'}(i) \neq \delta_T(i)$ and $\delta_{T'}(j) \neq \delta_T(j)$, and since $\varphi_T(i,j) \neq \varphi_{T'}(i,j)$, we have that $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,i),(j,j),(i,j)$. Let now $k \neq i,j$ be a taxon such that $[i,k]_T = [j,k]_T$ is the parent of $[i,j]_T$ in T. Then

$$\varphi_{T'}(i,k) = \varphi_T(i,k) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j) + (m-1)$$

and therefore, if $m \geqslant 2$, $\varphi_{T'}(i,k) > \varphi_{T'}(i,j)$ and then, by Lemma 2, either $\varphi_T(i,k) \neq \varphi_{T'}(i,k)$ or $\varphi_T(j,k) \neq \varphi_{T'}(j,k)$, which, as we have seen, is impossible. Thus, $m = 1$ in all cases. □

Lemma 4. *Let $T, T' \in \mathcal{T}_n$ be such that $D_0(T,T') \leqslant 3$. If $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, for some $1 \leqslant i < j \leqslant n$, then $(\delta_{T'}(i) - \varphi_{T'}(i,j)) + (\delta_{T'}(j) - \varphi_{T'}(i,j)) \leqslant 3$.*

Proof. Let us assume that $(\delta_{T'}(i) - \varphi_{T'}(i,j)) + (\delta_{T'}(j) - \varphi_{T'}(i,j)) \geqslant 4$ and let us reach a contradiction.

Assume first that $\delta_{T'}(i) \geqslant \varphi_{T'}(i,j) + 3$. Then, there are at least two leaves k_1, k_2 such that $[i,k_1]_{T'}, [i,k_2]_{T'} \prec [i,j]_{T'}$. Since each such leaf contributes at least 1 to $D_0(T,T') \leqslant 3$, we conclude that there must be exactly two such leaves and, moreover, $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k_1),(j,k_1),(i,k_2),(j,k_2)$. But then, on the one hand, $\delta_T(j) = \delta_{T'}(j)$ and, on the other hand, $\delta_{T'}(j) = \varphi_{T'}(i,j) + 1$ (otherwise, there would be some other leaf k such that $[j,k]_{T'} \prec [i,j]_{T'}$, which, by Lemma 2 would satisfy that $\varphi_T(i,k) \neq \varphi_{T'}(i,k)$ or $\varphi_T(j,k) \neq \varphi_{T'}(j,k)$). Combining these two equalities we obtain $\delta_T(j) = \varphi_T(i,j)$, which is impossible in a tree without nested taxa. This proves that $\delta_{T'}(i) \leqslant \varphi_{T'}(i,j) + 2$ and, by symmetry, that $\delta_{T'}(j) \leqslant \varphi_{T'}(i,j) + 2$, as we claimed.

Thus, it remains to prove that the case $\delta_{T'}(i) = \delta_{T'}(j) = \varphi_{T'}(i,j) + 2$ is impossible. So, assume this case holds, and let's reach a contradiction. By Corollary 1, if $D_0(T,T') \leqslant 3$ and $\delta_{T'}(i) = \delta_{T'}(j) = \varphi_{T'}(i,j) + 2$, then there can exist only one extra leaf k pending from the parent of i and one extra leaf l pending from the parent of j: see Fig. 1, where the grey triangle stands for the (possibly empty) subtree consisting of all other descendants of $[i,j]_{T'}$. Moreover, since $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$ and since both k and l contribute at least 1 to $D_0(T,T') \leqslant 3$, we conclude that $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k),(j,k),(i,l),(j,l)$. In particular

$$\begin{array}{l}\varphi_T(k,l) = \varphi_{T'}(k,l) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1\\ \delta_T(i) = \delta_{T'}(i) = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1\\ \delta_T(j) = \delta_T(k) = \delta_T(l) = \varphi_T(i,j) + 1 \text{ for the same reason}\end{array}$$

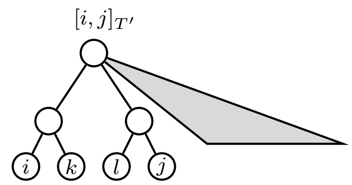


Figure 1: The subtree of T' rooted at $[i,j]_{T'}$ in the proof of Lemma 4.

Now we shall prove that, in this situation, each one of k,l contributes actually at least 2 to $D_0(T,T')$, and therefore $D_0(T,T') \geqslant 5$, which contradicts the assumption that $D_0(T,T') \leqslant 3$.

(1) Assume that $\varphi_T(i,k) = \varphi_{T'}(i,k)$. Then, by Lemmas 2.(a) and 3, $\varphi_T(j,k) = \varphi_{T'}(j,k) + 1$, and hence

$$\begin{array}{l}\varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(j,k) + 1 = \varphi_T(j,k)\\ \varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)\\ \delta_T(i) = \delta_T(j) = \delta_T(k) = \delta_T(l) = \varphi_T(i,j) + 1\\ \varphi_T(k,l) = \varphi_T(i,j) - 1\end{array}$$

Thus, the subtree of T rooted at $[k,l]_T$ contains a subtree of the form described in Fig. 2, for at least one leaf h. But then

$$\varphi_{T'}(l,h) = \varphi_T(l,h) = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \varphi_{T'}(l,j)$$

which is impossible, since it would imply that h is another descendant of $[l,j]_{T'}$. Therefore, $\varphi_T(i,k) \neq \varphi_{T'}(i,k)$ and, by symmetry, $\varphi_T(j,l) \neq \varphi_{T'}(j,l)$.

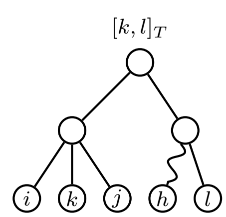


Figure 2: A subtree of the subtree of T rooted at $[k,l]_T$ in case (1) in the proof of Lemma 4.

(2) Assume now that $\varphi_T(i,l) = \varphi_{T'}(i,l)$. Then, by Lemma 2.(b), $\varphi_T(j,l) = \varphi_{T'}(j,l) - 1$, and then

$$\begin{array}{l} \varphi_T(i,l) = \varphi_{T'}(i,l) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 \\ \varphi_T(j,l) = \varphi_{T'}(j,l) - 1 = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 \\ \varphi_T(k,l) = \varphi_T(i,j) - 1 \\ \delta_T(i) = \delta_T(j) = \delta_T(k) = \delta_T(l) = \varphi_T(i,j) + 1 \end{array}$$

Therefore, the subtree of T rooted at $[k,l]_T$ contains a subtree of the form described in Fig. 3, for at least one leaf h. Moreover, $h \neq k$ because $\varphi_T(h,l) > \varphi_T(j,l) = \varphi_T(k,l)$. But then, again,

$$\varphi_{T'}(l,h) = \varphi_T(l,h) = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \varphi_{T'}(l,j)$$

which is again impossible by the same reason as in (1). Therefore, $\varphi_T(i,l) \neq \varphi_{T'}(i,l)$ and, by symmetry, $\varphi_T(j,k) \neq \varphi_{T'}(j,k)$.

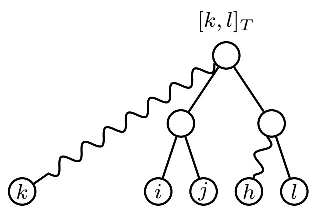


Figure 3: A subtree of the subtree of T rooted at $[k,l]_T$ in case (2) in the proof of Lemma 4.

So,

$$\varphi_T(i,k) \neq \varphi_{T'}(i,k), \varphi_T(i,l) \neq \varphi_{T'}(i,l), \varphi_T(j,k) \neq \varphi_{T'}(j,k), \varphi_T(j,l) \neq \varphi_{T'}(j,l)$$

and thus $D_0(T,T') \geqslant 5$. □

Summarizing the last lemmas, we have proved so far that if $D_0(T,T') \leqslant 3$ and $\varphi_T(i,j) \neq \varphi_{T'}(i,j)$, then, up to interchanging T and T', $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$ and either i and j are sibling in T' or one of these leaves is a sibling of the parent of the other one in T'. Next two lemmas cover these two remaining cases.

Lemma 5. *Let $T, T' \in \mathcal{T}_n$ be such that $D_0(T,T') \leqslant 3$, and assume that $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, for some $1 \leqslant i < j \leqslant n$. If i and j are sibling in T', then they are also sibling in T, they have no other sibling in T, and T' is obtained from T by contracting the arc ending in $[i,j]_T$. And then, $D_0(T,T') = 3$.*

Proof. If $\delta_{T'}(i) = \delta_{T'}(j) = \varphi_{T'}(i,j) + 1$, then it must happen that $\delta_T(i) = \delta_{T'}(i) + 1$ and $\delta_T(j) = \delta_{T'}(j) + 1$. Indeed, if $\delta_T(i) \leqslant \delta_{T'}(i)$, then $\delta_T(i) \leqslant \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$, which is impossible. Therefore, $\delta_T(i) > \delta_{T'}(i)$

and by symmetry $\delta_T(j) > \delta_{T'}(j)$. Since $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, $D_0(T,T') \leqslant 3$ implies that $\varphi_T(x,y) = \varphi_{T'}(x,y)$, for every $(x,y) \neq (i,j),(i,i),(j,j)$. Now, if, say $\delta_T(i) \geqslant \delta_{T'}(i)+2$, then

$$\delta_T(i) \geqslant \delta_{T'}(i)+2 = \varphi_{T'}(i,j)+3 = \varphi_T(i,j)+2$$

and there would exist some leaf k such that $[i,k]_T$ is a child of $[i,j]_T$. But then

$$\varphi_{T'}(i,k) = \varphi_T(i,k) = \varphi_T(i,j)+1 = \varphi_{T'}(i,j)+2 = \delta_{T'}(i)+1,$$

which is impossible. This proves that $\delta_T(i) = \delta_{T'}(i)+1$ and, by symmetry, $\delta_T(j) = \delta_{T'}(j)+1$.

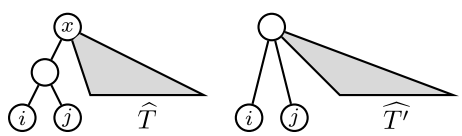
So, in summary, $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, $\delta_T(i) = \delta_{T'}(i)+1$, $\delta_T(j) = \delta_{T'}(j)+1$ and $\varphi_T(x,y) = \varphi_{T'}(x,y)$, for every $(x,y) \neq (i,j),(i,i),(j,j)$, and in particular $d_{\varphi,p}(T,T') = 3$.

Now, $\delta_T(i) = \delta_{T'}(i)+1 = \varphi_{T'}(i,j)+2 = \varphi_T(i,j)+1$, and by symmetry, $\delta_T(j) = \varphi_T(i,j)+1$, either. Therefore, i and j are sibling in T. Let us see that they have no other sibling in this tree. Indeed, if k is a sibling of i and j in T, then

$$\varphi_{T'}(i,k) = \varphi_T(i,k) = \varphi_T(i,j) = \varphi_{T'}(i,j)+1 = \delta_{T'}(i)$$

which is impossible.

Let x be the parent of $[i,j]_T$, and assume that the subtree T_0 of T rooted at x is as described in Fig. 4.(a), for some (possibly empty) subtree $\widehat{T}$. Moreover, let T_0' be the subtree of T' rooted at $[i,j]_{T'}$, which is as described in Fig. 4.(b) for some subtree $\widehat{T'}$. We shall prove that $\widehat{T} = \widehat{T'}$.



(a) T_0 (b) T_0'

Figure 4: (a) The subtree T_0 of T rooted at the parent of $[i,j]_T$ in the proof of Lemma 5. (b) The subtree T_0' of T' rooted at $[i,j]_{T'}$ in the proof of the same Lemma.

For every $k \in L(\widehat{T})$,

$$\varphi_{T'}(i,k) = \varphi_T(i,k) = \varphi_T(i,j)-1 = \varphi_{T'}(i,j),$$

which entails that $k \in L(\widehat{T'})$. Conversely, if $k \in L(\widehat{T'})$, then

$$\varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(i,j) = \varphi_T(i,j)-1,$$

which entails that $k \in L(\widehat{T})$. Thus, $L(\widehat{T}) = L(\widehat{T'})$. And finally, for every (not necessarily different) $k, l \in L(\widehat{T})$,

$$\varphi_{\widehat{T}}(k,l) = \varphi_T(k,l) - \delta_T(x) = \varphi_T(k,l) - \varphi_T(i,j) + 1 = \varphi_{T'}(k,l) - \varphi_{T'}(i,j) = \varphi_{\widehat{T'}}(k,l),$$

which implies by Theorem 1 that $\widehat{T} = \widehat{T'}$ (notice that $\widehat{T}$ and $\widehat{T'}$ can have elementary roots).

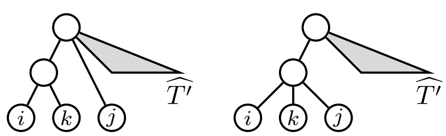
Finally, let us prove now that T and T' are exactly the same except for T_0 and T_0'. More specifically, let T_1 and T_1' be obtained by replacing in T and T' the subtrees T_0 and T_0' by a single leaf x. Since for every $p, q \notin L(T_0) = L(T_0')$,

$$\begin{array}{l} \varphi_{T_1'}(p,q) = \varphi_{T'}(p,q) = \varphi_T(p,q) = \varphi_{T_1}(p,q), \\ \varphi_{T_1'}(x,p) = \varphi_{T'}(i,p) = \varphi_T(i,p) = \varphi_{T_1}(p,x), \end{array}$$

we deduce, again by Theorem 1, that $T_1 = T_1'$.

This completes the proof that T' is obtained from T by replacing in it the subtree T_0 rooted at the parent x of $[i,j]_T$ by the subtree T_0' obtained from T_0 by contracting the arc $(x, [i,j]_T)$. □

Lemma 6. *Let $T, T' \in \mathcal{T}_n$ be such that $D_0(T,T') \leqslant 3$. Assume that $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, for some $1 \leqslant i < j \leqslant n$, and that j is a sibling of the parent of i in T'. Then, the subtree of T' rooted at $[i,j]_{T'}$ is the tree T_0' depicted in Fig. 5.(a), for some taxon $k \neq i,j$ and some (possibly empty) subtree $\widehat{T'}$, and T is obtained from T' by replacing T_0' by the tree T_0 depicted in Fig. 5.(b). And then, $D_0(T,T') = 3$.*



(a) T_0' (b) T_0

Figure 5: (a) The subtree T_0' of T' rooted at $[i,j]_{T'}$ in the statement of Lemma 6. (b) The subtree T_0 which replaces T_0' in T in the same statement.

Proof. We assume that $\delta_{T'}(i) = \varphi_{T'}(i,j) + 2$ and $\delta_{T'}(j) = \varphi_{T'}(i,j) + 1$. This implies that there exists at least one leaf k such that $[i,k]_{T'} \prec [i,j]_{T'}$. Since $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, $|\varphi_T(i,k) - \varphi_{T'}(i,k)| + |\varphi_T(j,k) - \varphi_{T'}(j,k)| \geqslant 1$ and $\delta_T(j) > \delta_{T'}(j)$ (because, otherwise, $\delta_T(j) \leqslant \delta_{T'}(j) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$, which is impossible), $D_0(T,T') \leqslant 3$ entails that $\varphi_T(i,k) = \varphi_{T'}(i,k)$ or $\varphi_T(j,k) = \varphi_T(j,k)$, and that $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j), (i,k), (j,k), (j,j)$ (and, in particular, k is the only leaf different from i such that $[i,k]_{T'} \prec [i,j]_{T'}$). Moreover, we have that $D_0(T,T') = 3$.

Let us see now that $\delta_T(j) = \delta_{T'}(j) + 1$. Indeed, if $\delta_T(j) \geqslant \delta_{T'}(j) + 2$, then

$$\delta_T(j) \geqslant \delta_{T'}(j) + 2 = \varphi_{T'}(i,j) + 3 = \varphi_T(i,j) + 2$$

and there would exist some leaf l such that $[j,l]_T$ is a child of $[i,j]_T$. But then

$$\varphi_{T'}(j,l) = \varphi_T(j,l) = \varphi_T(i,j) + 1 = \varphi_{T'}(i,j) + 2 = \delta_{T'}(j) + 1$$

and we reach a contradiction.

So, in summary, the subtree T'_0 of T' rooted a $[i,j]_{T'}$ is as described in Fig. 5.(a), and $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, $\delta_T(j) = \delta_{T'}(j) + 1$, $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j), (i,k), (j,k), (j,j)$, and either $\varphi_T(i,k) = \varphi_{T'}(i,k)$ or $\varphi_T(j,k) = \varphi_T(j,k)$. Now, we discuss these two possibilities.

(a) If $\varphi_T(j,k) = \varphi_{T'}(j,k)$, then $\varphi_T(i,k) = \varphi_{T'}(i,k) - 1$ by Lemma 2.(b). In this case

$$\begin{array}{l}
\varphi_T(i,k) = \varphi_{T'}(i,k) - 1 = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 \\
\varphi_T(j,k) = \varphi_{T'}(j,k) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 \\
\delta_T(i) = \delta_{T'}(i) = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1 \\
\delta_T(j) = \delta_{T'}(j) + 1 = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1 \\
\delta_T(k) = \delta_{T'}(k) = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1
\end{array}$$

This means that the subtree of T rooted at $[i,k]_T = [j,k]_T$ contains a subtree of the form described in Fig. 6, for at least some new leaf h. But then

$$\varphi_{T'}(k,h) = \varphi_T(k,h) = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \varphi_{T'}(i,k)$$

which is impossible in T', because i and k are the only descendants of $[i,k]_{T'}$ in T'. So, this case is impossible.

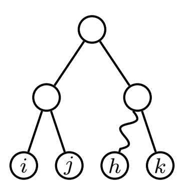


Figure 6: A subtree contained in the subtree of T rooted at $[i,j]_T$ in case (a) in the proof of Lemma 6.

(b) If $\varphi_T(i,k) = \varphi_{T'}(i,k)$, then $\varphi_T(j,k) = \varphi_{T'}(j,k) + 1$ Lemmas 2.(a) and 3. In this case

$$\begin{array}{l}
\varphi_T(i,k) = \varphi_{T'}(i,k) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j) \\
\varphi_T(j,k) = \varphi_{T'}(j,k) + 1 = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j) \\
\delta_T(i) = \delta_T(j) = \delta_T(k) = \varphi_T(i,j) + 1 \text{ as in (a)}
\end{array}$$

This implies that i, j, k are sibling in T. If l is any other sibling of them in T, then

$$\varphi_{T'}(i,l) = \varphi_T(i,l) = \varphi_T(i,k) = \varphi_{T'}(i,k)$$

which entails that l is another descendant of $[i,k]_{T'}$ in T', which is impossible. Therefore, the subtree T_0 of T rooted at the parent of $[i,j]_T$ has the form depicted in Fig. 7, for some subtree $\widehat{T}$.

Finally, the same argument as in the last part of the proof of the last lemma shows that $\widehat{T} = \widehat{T'}$, and that if T_1 and T_1' are obtained by replacing in T and T' the subtrees T_0 and T_0' by a single leaf x, then $T_1 = T_1'$. We leave the details to the reader.

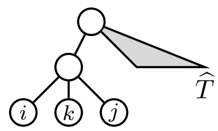


Figure 7: The subtree T_0 rooted at the parent of $[i,j]_T$ in case (b) in the proof of Lemma 6.

This completes the proof that T and T' are as described in the statement. $\square$

We have proved so far that the minimum value of D_0 on $\mathcal{T}_n$ is 3, and we have characterized those pairs of trees $T, T' \in \mathcal{T}_n$ such that $D_0(T,T') = 3$. To extend this result to every D_p, $p \geqslant 1$, it is enough to check that every pair of trees in $\mathcal{T}_n$ such that $D_0(T,T') = 3$ also satisfies that $D_p(T,T') = 3$ for every $p \geqslant 1$, which is straightforward. This completes the proof of Proposition 2.

Proof of Proposition 3

As in Proposition 2, we also split this proof into several lemmas. First of all, notice that there are pairs of trees $T, T' \in \mathcal{BT}_n$ such that $D_p(T,T') = 4$ for every $p \in \{0\} \cup [1, \infty[$: see, for instance, Fig. 8. Therefore, the minimum value of D_p on $\mathcal{BT}_n$ is at most 4.

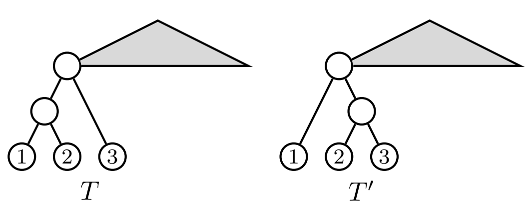


Figure 8: A pair of binary trees such that $D_p(T,T') = 4$. The grey triangles represent the same tree.

Notice also that Lemma 1 also applies in $\mathcal{BT}_n$, and therefore, if $T, T' \in \mathcal{BT}_n$ are such that $D_0(T,T') > 0$, then there exist two taxa $i \neq j$ such that $\varphi_T(i,j) \neq \varphi_{T'}(i,j)$. And, of course, Lemma 2 also applies in $\mathcal{BT}_n$.

Lemma 7. *Let $T, T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$, for some $1 \leqslant i < j \leqslant n$ and some $m \geqslant 1$, then $m = 1$.*

Proof. Assume that $\varphi_T(i,j) = \varphi_{T'}(i,j) + m$ with $m \geqslant 2$, and let us reach a contradiction.

If $\delta_{T'}(i) = \delta_T(i)$, then $\delta_{T'}(i) > \varphi_T(i,j) = \varphi_{T'}(i,j) + m$, and therefore there exist leaves $x_1, \ldots, x_m$ such that $\varphi_T(i,x_l) = \varphi_{T'}(i,j) + l$, for $l = 1, \ldots, m$. By Lemma 2, each such leaf x_l adds at least 1 to $D_0(T,T')$. Therefore $D_0(T,T') \geqslant 1 + m$. Now, if moreover $\delta_{T'}(j) = \delta_T(j)$, then there also exist leaves $y_1, \ldots, y_m$ such that $\varphi_T(j,y_l) = \varphi_{T'}(i,j) + l$, for $l = 1, \ldots, m$, and each such leaf y_l also adds at least 1 to $D_0(T,T')$, which entails $D_0(T,T') \geqslant 1 + 2m \geqslant 5$. So, if $D_0(T,T') \leqslant 4$, it must happen that $\delta_{T'}(i) \neq \delta_T(i)$ or $\delta_{T'}(j) \neq \delta_T(j)$ (or both). Let assume that $\delta_{T'}(j) \neq \delta_T(j)$.

Now, $\varphi_T(i,j) = \varphi_{T'}(i,j) + m \geqslant m$, and therefore there exist leaves $z_1, \ldots, z_m$ such that $\varphi_T(i,z_l) = \varphi_T(j,z_l) = \varphi_T(i,j) - l$, for $l = 1, \ldots, m$. If $\varphi_T(i,k_l) = \varphi_{T'}(i,k_l)$, then

$$\varphi_{T'}(i,k_l) = \varphi_T(i,k_l) = \varphi_T(i,j) - l = \varphi_{T'}(i,j) + (m - l) \geqslant \varphi_{T'}(i,j)$$

and therefore, by Lemma 2, $\varphi_{T'}(j,k_l) \neq \varphi_T(j,k_l)$, and thus, each such leaf z_l adds at least 1 to $D_0(T,T')$, which entails $D_0(T,T') \geqslant 2 + m$. Therefore, if $D_0(T,T') \leqslant 4$ and $m \geqslant 2$, it must happen $m = 2$ and, moreover, $\varphi_T(a,b) = \varphi_{T'}(a,b)$ for every $(a,b) \neq (i,j), (j,j), (i,z_1), (i,z_2), (j,z_1), (j,z_2)$.

In particular, $\delta_T(i) = \delta_{T'}(i)$, which as we have seen implies that there are at least two leaves x_1, x_2 such that $i \prec [i,x_2]_{T'} \prec [i,x_1]_{T'} \prec [i,j]_{T'}$. Since

$$\varphi_{T'}(z_1,z_2) = \varphi_T(z_1,z_2) = \varphi_T(i,j) - 2 = \varphi_{T'}(i,j)$$

implies that (up to interchanging z_1 and z_2) $i \prec [i,z_1]_{T'} \prec [i,j]_{T'}$ and $j \prec [j,z_2]_{T'} \prec [i,j]_{T'}$, we conclude that $\{x_1, x_2, z_1, z_2\}$ are at least 3 different leaves and hence they contribute at least 3 to $D_0(T,T')$, making $D_0(T,T') \geqslant 5$. □

Lemma 8. *Let $T, T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, for some $1 \leqslant i < j \leqslant n$, then $\delta_{T'}(i), \delta_{T'}(j) \leqslant \varphi_{T'}(i,j) + 2$.*

Proof. Let us assume that $\delta_{T'}(i) \geqslant \varphi_{T'}(i,j) + 3$, and let us reach a contradiction. The case when $\delta_{T'}(j) \geqslant \varphi_{T'}(i,j) + 3$ is symmetrical.

Since $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1 > 0$, there exists some taxon k_0 such that $[i,k_0]_T$ is the parent of $[i,j]_T$. Let us distinguish several cases.

(a) Assume that $\varphi_T(i,k_0) = \varphi_{T'}(i,k_0)$. Then, $\varphi_{T'}(i,k_0) = \varphi_T(i,k_0) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j)$ implies that $[j,k_0]_{T'} \prec [i,j]_{T'}$ and thus $\varphi_{T'}(j,k_0) > \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 = \varphi_T(j,k_0)$ and in particular, by the previous lemma $\varphi_{T'}(j,k_0) = \varphi_T(j,k_0) + 1 = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1$. Now, since $D_0(T,T') \leqslant 4$, by Lemma 3 the number of leaves $a \neq i,j,k_0$ such that $a \prec [i,j]_{T'}$ is at most 2.

If $\delta_{T'}(i) \geqslant \varphi_{T'}(i,j) + 3$, then there exist leaves k_1,k_2 such that $\varphi_{T'}(i,k_1) = \varphi_{T'}(i,j) - 1$ and $\varphi_{T'}(i,k_2) = \varphi_{T'}(i,j) - 2$ and then $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k_0),(j,k_0),(k_1,i),(k_1,j),(k_2,i),(k_2,j)$. In particular, no leaf other than i,j,k_0,k_1,k_2 descends from $[i,j]_{T'}$. But then

$$\begin{array}{ll} \varphi_T(k_1,k_0) = \varphi_{T'}(k_1,k_0) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1, & \varphi_T(k_2,k_0) = \varphi_T(i,j) - 1 \\ \varphi_T(k_1,k_2) = \varphi_{T'}(k_1,k_2) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j) & \end{array}$$

imply that, up to interchanging k_1 and k_2, $i \prec [i,k_1]_T \prec [i,j]_T$ and $j \prec [j,k_2]_T \prec [i,j]_T$, and then

$$\delta_{T'}(j) = \delta_T(j) > \varphi_T(i,j) + 1 = \varphi_{T'}(i,j) + 2$$

implies the existence of at least another leaf h such that $j \prec [j,h]_{T'} \prec [j,k_0]_{T'} \prec [i,j]_{T'}$, which, as we have mentioned, is impossible. So, this case cannot happen.

(b) Assume now that $\varphi_T(j,k_0) = \varphi_{T'}(j,k_0)$. By symmetry with the previous case, this implies that $\varphi_{T'}(i,k_0) = \varphi_{T'}(i,j) + 1$, $\varphi_{T'}(i,k_0) = \varphi_T(i,k_0) + 1$ and that the number of leaves $a \neq i,j,k_0$ such that $a \prec [i,j]_{T'}$ is at most 2. Now we have three new subcases to discuss.

(b.1) If $\delta_{T'}(i) = \varphi_{T'}(i,j) + 4$, so that there exist leaves $k_1,k_2 \neq i$ such that $\varphi_{T'}(i,k_0), \varphi_{T'}(i,k_1), \varphi_{T'}(i,k_2) > \varphi_{T'}(i,j)$, and no leaf other that i,j,k_0,k_1,k_2 descends from $[i,j]_{T'}$. Then $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k_0),(j,k_0),(k_1,i),(k_1,j),(k_2,i),(k_2,j)$. But in this case it must happen that $\delta_T(j) = \delta_{T'}(j) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$, which is impossible. So, this case cannot happen.

(b.2) If $\delta_{T'}(i) = \varphi_{T'}(i,j) + 3$ and $\delta_{T'}(j) = \varphi_{T'}(i,j) + 2$, so that there exist leaves k_1,k_2 such that $\varphi_{T'}(j,k_1) = \varphi_{T'}(i,j) + 1$, $\varphi_{T'}(i,k_2) = \varphi_{T'}(i,j) + 2$ and, recall, $\varphi_{T'}(i,k_0) = \varphi_{T'}(i,j) + 1$, then $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k_0),(j,k_0),(k_1,i),(k_1,j),(k_2,i),(k_2,j)$. But then

$$\varphi_T(k_1,k_0) = \varphi_{T'}(k_1,k_0) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1$$

implies that $k_1 \prec [i,j]_T$, and then

$$\begin{array}{l}\delta_T(j) = \delta_{T'}(j) = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1, \\ \delta_T(k_1) = \delta_{T'}(k_1) = \varphi_{T'}(i,j) + 2 = \varphi_T(i,j) + 1\end{array}$$

imply that j and k_1 are the only children of $[i,j]_T$, which is, of course, impossible. So, this case cannot happen, either.

(b.3) If $\delta_{T'}(i) = \varphi_{T'}(i,j)+3$ and $\delta_{T'}(j) = \varphi_{T'}(i,j)+1$, then on the one hand there exists a leaf k_1 such that $\varphi_{T'}(i,k_1) = \varphi_{T'}(j,k_0) - 1 = \varphi_{T'}(i,j) - 2$ and, on the other hand, as we have seen in (b.1), $\delta_T(j) > \delta_{T'}(j)$. Then, $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(j,j),(i,k_0),(j,k_0),(k_1,i),(k_1,j)$, and in particular no leaf other than i,j,k_0,k_1 descends from $[i,j]_{T'}$.

Now,

$$\varphi_T(k_1,k_0) = \varphi_{T'}(k_1,k_0) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$$

implies that $k_1 \not\prec [i,j]_T$, and

$$\delta_T(i) = \delta_{T'}(i) = \varphi_{T'}(i,j) + 3 = \varphi_T(i,j) + 2$$

implies that there exists a leaf $h \neq k_0, k_1$ such that $i \prec [i,h]_T \prec [i,j]_T$ and hence

$$\varphi_{T'}(i,h) = \varphi_T(i,h) > \varphi_T(i,j) + 1 = \varphi_{T'}(i,j)$$

would entail that $h \prec [i,j]_{T'}$, which is impossible. Thus, this case cannot happen, either.

(c) Assume finally that $\varphi_T(i,k_0) \neq \varphi_{T'}(i,k_0)$ and $\varphi_T(j,k_0) \neq \varphi_{T'}(j,k_0)$. The contribution to D_0 of the pairs $(i,j),(i,k_0),(j,k_0)$ is at least 3, and therefore there can only exist at most one other pair of leaves with different cophenetic value in T and in T'. Since every $x \neq i,j$ such that $x \prec [i,j]_{T'}$ defines at least one such pair, we conclude that if $\delta_{T'}(i) \geqslant \varphi_{T'}(i,j) + 3$, then, it must happen that $[i,k_0]_{T'} \prec [i,j]_{T'}$ and that there can only exist one leaf $k_1 \neq k_0, i$ such that $[i,k_1]_{T'} \prec [i,j]_{T'}$, and then, moreover $[i,k_0]_{T'} \neq [i,k_1]_{T'}$. In this case, $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every $(x,y) \neq (i,j),(i,k_0),(j,k_0),(k_1,i),(k_1,j)$. But then, in particular, $\delta_{T'}(j) = \varphi_{T'}(i,j) + 1$ and $\delta_T(j) = \delta_{T'}(j)$, which implies $\delta_T(i) = \varphi_T(i,j)$, which is impossible

This finishes the proof that, if $D_0(T,T') \leqslant 4$, then $\delta_{T'}(i) \leqslant \varphi_{T'}(i,j) + 2$ and $\delta_{T'}(j) \leqslant \varphi_{T'}(i,j) + 2$. □

Lemma 9. *Let $T,T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$, for some $1 \leqslant i < j \leqslant n$, then i,j are sibling in T.*

Proof. Let k_0 be any leaf such that $[i,k_0]_T = [j,k_0]_T$ is the parent of $[i,j]_T$ in T. If $\varphi_T(i,k_0) = \varphi_{T'}(i,k_0)$, then $\varphi_{T'}(i,k_0) = \varphi_T(i,k_0) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j)$ implies that $[j,k_0]_{T'} \prec [i,j]_{T'}$ and thus $\varphi_{T'}(j,k_0) > \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 = \varphi_T(j,k_0)$. Therefore, $|\varphi_T(i,k_0) - \varphi_{T'}(i,k_0)| + |\varphi_T(j,k_0) - \varphi_{T'}(j,k_0)| \geqslant 1$.

Assume now that i,j are not sibling in T, and let h be a leaf such that $[i,h]_T$ is a child of $[i,j]_T$. If $\varphi_T(i,h) \leqslant \varphi_{T'}(i,h)$, then

$$\delta_{T'}(i) \geqslant \varphi_{T'}(i,h) + 1 \geqslant \varphi_T(i,h) + 1 = \varphi_T(i,j) + 2 = \varphi_{T'}(i,j) + 3$$

which is impossible by the previous lemma. Therefore, $\varphi_T(i,h) > \varphi_{T'}(i,h)$, and by Lemma 7, $\varphi_T(i,h) = \varphi_{T'}(i,h) + 1$.

In a similar way, if $\delta_T(i) = \delta_{T'}(i)$, then

$$\delta_{T'}(i) = \delta_T(i) \geqslant \varphi_T(i,h) + 1 = \varphi_T(i,j) + 2 = \varphi_{T'}(i,j) + 3$$

which is again impossible by the previous lemma. Therefore, $\delta_T(i) \neq \delta_{T'}(i)$, too. So, (i,j), (i,k_0), (j,k_0), (i,i), and (i,h) contribute at least 4 to $D_0(T,T') \leqslant 4$, which implies that $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every other pair of leaves (x,y). But then,

$$\begin{array}{l} \varphi_{T'}(j,h) = \varphi_T(j,h) = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 \\ \varphi_{T'}(i,h) = \varphi_T(i,h) - 1 = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 \end{array}$$

which is impossible. Therefore, i and j are sibling in T. ☐

Lemma 10. *Let $T, T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, for some $1 \leqslant i < j \leqslant n$, then i,j are not sibling in T'.*

Proof. Assume that i,j are sibling in T', and recall that we already know that they are sibling in T. Let k_0 be any leaf such that $[i,k_0]_T = [j,k_0]_T$ is the parent of $[i,j]_T$ in T. If $\varphi_T(i,k_0) = \varphi_{T'}(i,k_0)$, then

$$\varphi_{T'}(i,k_0) = \varphi_T(i,k_0) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j)$$

which is impossible if i,j are sibling in T'. Thus, $\varphi_T(i,k_0) \neq \varphi_{T'}(i,k_0)$ and, by symmetry, $\varphi_T(j,k_0) \neq \varphi_{T'}(j,k_0)$. On the other hand, if $\delta_T(i) = \delta_{T'}(i)$, then

$$\delta_T(i) = \delta_{T'}(i) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$$

which is also impossible. Therefore, $\delta_T(i) \neq \delta_{T'}(i)$ and, by symmetry, $\delta_T(j) \neq \delta_{T'}(j)$. But, then, $D_0(T,T') \geqslant 5$. ☐

Summarizing what we know so far, we have proved that if $D_0(T,T') \leqslant 4$ and $\varphi_T(i,j) \neq \varphi_{T'}(i,j)$, then, up to interchanging T and T', $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, i,j are sibling in T, and then the subtree of T' rooted at $[i,j]_{T'}$ is a triplet or a totally balanced quartet; cf. Fig. 9. Next two lemmas cover these two possibilities.

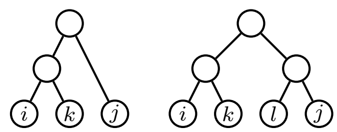


Figure 9: The only possibilities for the subtree of T' rooted at $[i,j]_{T'}$ if $D_0(T,T') \leqslant 4$ and $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$.

Lemma 11. *Let $T,T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, for some $1 \leqslant i < j \leqslant n$, and the subtree of T' rooted at $[i,j]_{T'}$ is the triplet depicted in the left hand side of Fig. 9, then T is obtained from T' by interchanging j and k: cf. Fig. 10. And, then $D_0(T,T') = 4$.*

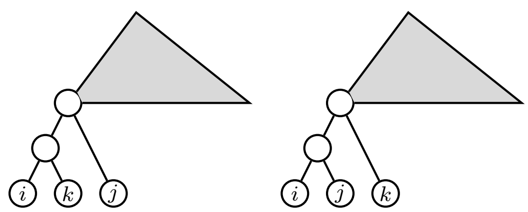


Figure 10: The only pairs of trees T,T' such that $D_0(T,T') \leqslant 4$ and $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, when the subtree of T' rooted at $[i,j]_{T'}$ is a triplet.

Proof. Assume that the subtree of T' rooted at $[i,j]_{T'}$ has the form depicted in the left hand side of Fig. 9, and that $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$. Then, since i and j are sibling in T,

$$\delta_T(j) = \varphi_T(i,j)+1 = \varphi_{T'}(i,j)+2 = \delta_{T'}(j)+1.$$

Now, if $\varphi_T(i,k) \geqslant \varphi_{T'}(i,k)$, then

$$\varphi_T(i,k) \geqslant \varphi_{T'}(i,k) = \varphi_{T'}(i,j)+1 = \varphi_T(i,j)$$

which is impossible, because i and j are sibling in T. Therefore, $\varphi_T(i,k) < \varphi_{T'}(i,k)$ and, by Lemma 7, $\varphi_T(i,k) = \varphi_{T'}(i,k)-1$, and in particular $\varphi_T(i,k) = \varphi_T(j,k) = \varphi_T(i,j)-1$. Therefore, $[i,k]_T$ is the parent of $[i,j]_T$ in T.

Finally, if $\delta_T(k) \geqslant \varphi_T(i,j)+1$, then there exists at least some other leaf $l \prec [i,k]_T = [j,k]_T$. But then $\varphi_T(i,l) \neq \varphi_{T'}(i,l)$, because otherwise

$$\varphi_{T'}(i,l) = \varphi_T(i,l) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j),$$

which is impossible because the only leaves descending from $[i,j]_{T'}$ are i,j,k. And, by symmetry $\varphi_T(j,l) \neq \varphi_{T'}(j,l)$, and we reach $D_0(T,T') \geqslant 5$. Therefore,

$$\delta_T(k) = \varphi_T(i,j) = \varphi_{T'}(i,j) + 1 = \delta_{T'}(k) - 1.$$

So, in summary, $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, $\delta_T(j) = \delta_{T'}(j)+1$, $\varphi_T(i,k) = \varphi_{T'}(i,k)-1$, and $\delta_T(k) = \delta_{T'}(k)-1$, and $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every (x,y) other than $(i,j),(j,j),(i,k),(k,k)$. Moreover, in T, k is the other child of the parent of $[i,j]_T$.

So, the subtree T_0 of T rooted at the parent of $[i,j]_T$ is obtained by interchanging j and k in the subtree T_0' of T' rooted at $[i,j]_{T'}$. Finally, let us prove now that T and T' are exactly the same except for T_0 and T_0'. More specifically, let T_1 and T_1' be obtained by replacing in T and T' the subtrees T_0 and T_0' by a single leaf x. Since for every $p,q \notin \{i,j,k\}$,

$$\begin{aligned}\varphi_{T_1'}(p,q) = \varphi_{T'}(p,q) = \varphi_T(p,q) = \varphi_{T_1}(p,q),\\ \varphi_{T_1'}(x,p) = \varphi_{T'}(i,p) = \varphi_T(i,p) = \varphi_{T_1}(x,p),\end{aligned}$$

we deduce, by Theorem 1, that $T_1 = T_1'$.

This completes the proof that T is obtained from T' by interchanging the leaf j and its nephew k. □

Lemma 12. *Let $T,T' \in \mathcal{BT}_n$ be such that $D_0(T,T') \leqslant 4$. If $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, for some $1 \leqslant i < j \leqslant n$, and the subtree of T' rooted at $[i,j]_{T'}$ is the quartet depicted in the right hand side of Fig. 9, then T is obtained from T' by interchanging j and k: cf. Fig. 11. And, then $D_0(T,T') = 4$.*

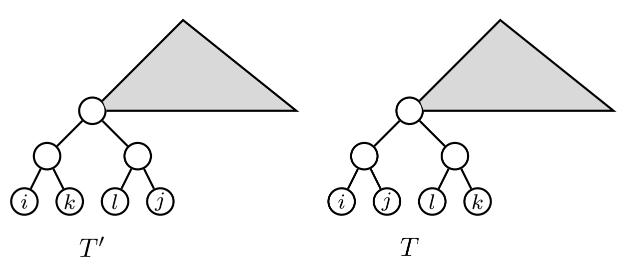


Figure 11: The only pairs of trees T,T' such that $D_0(T,T') \leqslant 4$ and $\varphi_T(i,j) = \varphi_{T'}(i,j)+1$, when the subtree of T' rooted at $[i,j]_{T'}$ is a quartet.

Proof. Assume that the subtree of T' rooted at $[i,j]_{T'}$ has the form depicted in the right hand side of Fig. 9, and that $\varphi_T(i,j) = \varphi_{T'}(i,j) + 1$.

If $\varphi_T(i,k) \geqslant \varphi_{T'}(i,k)$, then

$$\varphi_T(i,k) \geqslant \varphi_{T'}(i,k) = \varphi_{T'}(i,j) + 1 = \varphi_T(i,j)$$

which is impossible if i,j are sibling in T. Therefore, $\varphi_T(i,k) < \varphi_{T'}(i,k)$ and, by Lemma 7, $\varphi_T(i,k) = \varphi_{T'}(i,k) - 1$, and in particular $\varphi_T(i,k) = \varphi_T(i,j) - 1$. By symmetry, $\varphi_T(j,l) = \varphi_{T'}(j,l) - 1$ and hence $\varphi_T(j,l) = \varphi_T(i,j) - 1$, too. Therefore, both k and l are descendants of the parent of $[i,j]_T$. But then,

$$\varphi_{T'}(k,l) = \varphi_{T'}(i,j) = \varphi_T(i,j) - 1 < \varphi_T(k,l)$$

and therefore, by Lemma 7, $\varphi_T(k,l) = \varphi_{T'}(k,l) + 1 = \varphi_T(i,j)$.

At this point, $D_0(T,T') \leqslant 4$ entails that $\varphi_T(x,y) = \varphi_{T'}(x,y)$ for every (x,y) other than $(i,j),(i,k),(j,l),(k,l)$. Moreover, i,k,j,l are the only descendant leaves of the parent of $[i,j]_T$ in T. Indeed, if h is another descendant leaf of the parent of $[i,j]_{T'}$, then

$$\varphi_{T'}(i,h) = \varphi_T(i,h) = \varphi_T(i,j) - 1 = \varphi_{T'}(i,j)$$

and therefore h would be another descendant of $[i,j]_{T'}$. And, as we have seen, the subtree T_0 of T rooted at this node is obtained from the subtree T_0' of T' rooted at $[i,j]_{T'}$ by interchanging j and k. Finally, arguing as in the last part of the proof of the previous lemma, we deduce that T and T' are exactly the same except for T_0 and T_0'. □

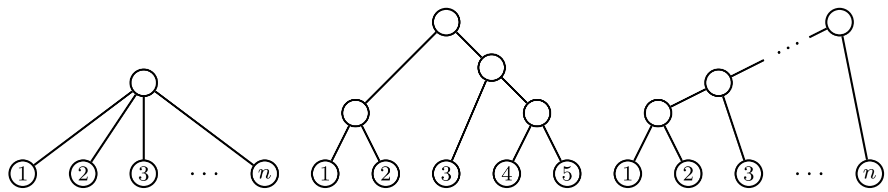
We have proved so far that the minimum value of D_0 on $\mathcal{BT}_n$ is 4, and we have characterized the pairs of trees $T,T' \in \mathcal{BT}_n$ such that $D_0(T,T') = 4$. To extend this result to every D_p, $p \geqslant 1$, it is enough to check that every pair of binary trees such that $D_0(T,T') = 4$ also satisfies that $D_p(T,T') = 4$ for every $p \geqslant 1$, which is straightforward. This completes the proof of Proposition 3.

Proof of Proposition 4

Let X_n denote any space $\mathcal{UT}_n$, $\mathcal{T}_n$ or $\mathcal{BT}_n$, and let $\Delta_p(X_n)$, $p \in \{0\} \cup [1,\infty[$, denote the diameter of $d_{\varphi,p}$ on X_n.

We consider first the case $p = 1$, which will be used later to prove the case $p > 1$. For every $T \in \mathcal{UT}_n$, let

$$S(T) = \sum_{i=1}^{n} \delta_T(i), \qquad \Phi(T) = \sum_{1\leqslant i<j\leqslant n} \varphi_T(i,j).$$



(a) (b) (c)

Figure 12: (a) The rooted star with n leaves. (b) The only maximally balanced tree with 5 leaves, up to relabelings. (c) A rooted caterpillar with n leaves.

S and Φ are the extensions to $\mathcal{UT}_n$ of the *Sackin index* [3] and the *total cophenetic index* [1] for phylogenetic trees without nested taxa, respectively. Notice that $\|\varphi(T)\|_1 = S(T) + \Phi(T)$. We have the following results on these indices:

- It is straightforward to check that the minimum values of $S(T)$ and $\Phi(T)$ on $\mathcal{T}_n$ are both reached at the *rooted star tree* with n leaves (the phylogenetic tree with all its leaves of depth 1; see Fig. 12.(a)), and these minimum values are, respectively,

$$\min S(\mathcal{T}_n) = n, \quad \min \Phi(\mathcal{T}_n) = 0.$$

- It is also straightforward to check that the minimum values of $S(T)$ and $\Phi(T)$ on $\mathcal{UT}_n$ are both reached at the rooted star tree with $n-1$ leaves and with the root labeled with n, and these minimum values are, respectively,

$$\min S(\mathcal{UT}_n) = n-1, \quad \min \Phi(\mathcal{UT}_n) = 0.$$

- The minimum values of $S(T)$ and $\Phi(T)$ on $\mathcal{BT}_n$ are both reached at the *maximally balanced trees* with n leaves (those binary trees such that, for every internal node, the numbers of descendant leaves of its two children differ at most in 1; see, for instance, Fig. 12.(b)). And then, these minimum values are, respectively,

$$\min S(\mathcal{BT}_n) = n\lfloor \log_2(4n) \rfloor - 2^{\lfloor \log_2(2n) \rfloor}$$
$$\min \Phi(\mathcal{BT}_n) = \sum_{k=0}^{n-1} a(k), \text{ where } a(k) \text{ is the highest power of 2 that divides } n!$$

For the proofs, see [4] combined with [2] for S, and [1] for Φ. From the first formula it is clear that $\min S(\mathcal{BT}_n)$ is in $\Theta(n \log(n))$. As far as $\min \Phi(\mathcal{BT}_n)$ goes, it is shown in [1] that it satisfies the recurrence

$$\min \Phi(\mathcal{BT}_n) = \min \Phi(\mathcal{BT}_{\lceil n/2 \rceil}) + \min \Phi(\mathcal{BT}_{\lfloor n/2 \rfloor}) + \binom{\lceil n/2 \rceil}{2} + \binom{\lfloor n/2 \rfloor}{2}, \quad \text{for } n \geqslant 3$$

from where it is obvious that its order is in $\Theta(n^2)$.

- The maximum values of $S(T)$ and $\Phi(T)$ on both $\mathcal{T}_n$ and $\mathcal{BT}_n$ are reached at the *rooted caterpillar trees* with n leaves (binary phylogenetic trees such that all their internal nodes have a leaf child; see Fig. 12.(c)). And then, these maximum values are, respectively,

$$\max S(\mathcal{T}_n) = \max S(\mathcal{BT}_n) = \binom{n+1}{2} - 1, \quad \max \Phi(\mathcal{T}_n) = \max \Phi(\mathcal{BT}_n) = \binom{n}{3},$$

  which are thus in $\Theta(n^2)$ and $\Theta(n^3)$, respectively. For the proofs, see again [4] for S and [1] for Φ.

- Given any tree in $\mathcal{UT}_n$ with a nested taxon, if we replace this nested taxon by a new leaf labeled with it pending from the node previously labeled with it (cf. Fig. 13), we obtain a new tree in $\mathcal{UT}_n$ with strictly larger value of S and the same value of Φ. This shows that the maximum values of $S(T)$ and $\Phi(T)$ on $\mathcal{UT}_n$ are reached at trees in $\mathcal{T}_n$, and hence at the rooted caterpillar trees with n leaves. Therefore, they are also in $\Theta(n^2)$ and $\Theta(n^3)$, respectively.

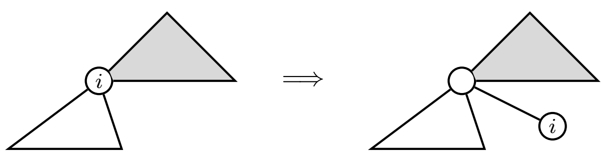


Figure 13: This operation increases the value of S and does not modify the value of Φ.

From these properties we deduce the following result.

Lemma 13. *The minimum value of $\|\varphi(T)\|_1$ on $\mathcal{UT}_n$ and $\mathcal{T}_n$ is in $\Theta(n)$. The minimum value of $\|\varphi(T)\|_1$ on $\mathcal{BT}_n$ is at most in $\Theta(n^2)$. The maximum value of $\|\varphi(T)\|_1$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ and $\mathcal{BT}_n$ is in $\Theta(n^3)$.* □

Now, we can apply this lemma to find the order of the diameter of $d_{\varphi,1}$ on the spaces X_n of unweighted phylogenetic trees.

Lemma 14. *The diameter of $d_{\varphi,1}$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ and $\mathcal{BT}_n$ is in $\Theta(n^3)$.*

Proof. Let $T_1, T_2 \in X_n$. Then, on the one hand,

$$d_{\varphi,1}(T_1, T_2) = \|\varphi(T_1) - \varphi(T_2)\|_1 \leqslant \|\varphi(T_1)\|_1 + \|\varphi(T_2)\|_1 \leqslant 2 \cdot \max \|\varphi(X_n)\|_1 = \Theta(n^3)$$

which shows that $\Delta_1(X_n) \leqslant O(n^3)$. On the other hand, if $\|\varphi(T_1)\|_1 \geqslant \|\varphi(T_2)\|_1$, then

$$d_{\varphi,1}(T_1, T_2) = \|\varphi(T_1) - \varphi(T_2)\|_1 \geqslant \|\varphi(T_1)\|_1 - \|\varphi(T_2)\|_1$$

and therefore $\Delta_1(X_n) \geqslant \max \|\varphi(X_n)\|_1 - \min \|\varphi(X_n)\|_1$, which is again in $O(n^3)$. This shows that $\Delta_1(X_n)$ is in $\Theta(n^3)$, as we claimed. □

Let us consider now the case $p > 1$. Since, for every $x \in \mathbb{R}^m$, $\|x\|_1 \leqslant m^{1-\frac{1}{p}}\|x\|_p$, we have that, for every pair of trees $T_1, T_2 \in X_n$,

$$d_{\varphi,1}(T_1, T_2) \leqslant \binom{n+1}{2}^{1-\frac{1}{p}} d_{\varphi,p}(T_1, T_2).$$

and therefore

$$\Delta_1(X_n) \leqslant \binom{n+1}{2}^{1-\frac{1}{p}} \Delta_p(X_n),$$

from where we deduce that

$$\Delta_p(X_n) \geqslant \Delta_1(X_n) \cdot \binom{n+1}{2}^{-1+\frac{1}{p}} = O(n^{(p+2)/p}).$$

To prove the converse inequality, let

$$\varphi^{(p)}(T) = \sum_{1 \leqslant i \leqslant j \leqslant n} \varphi_T(i,j)^p.$$

We have that, for every $T_1, T_2 \in X_n$,

$$\begin{aligned} d_{\varphi,p}(T_1, T_2) &= \|\varphi(T_1) - \varphi(T_2)\|_p \leqslant \|\varphi(T_1)\|_p + \|\varphi(T_2)\|_p = \sqrt[p]{\varphi^{(p)}(T_1)} + \sqrt[p]{\varphi^{(p)}(T_2)} \\ &\leqslant 2\sqrt[p]{\max \varphi^{(p)}(X_n)}, \end{aligned}$$

which implies that $\Delta_p(X_n) \leqslant 2\sqrt[p]{\max \varphi^{(p)}(X_n)}$. Therefore, to prove that the diameter of $d_{\varphi,p}$ on each X_n is bounded from above by $O(n^{(p+2)/p})$, it is enough to prove that $\max \varphi^{(p)}(X_n) \leqslant O(n^{p+2})$. We do it in the next lemma.

Lemma 15. *The maximum value of $\varphi^{(p)}(T)$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ or $\mathcal{BT}_n$ is reached at the rooted caterpillars, and its value is in $\Theta(n^{p+2})$.*

Proof. Arguing as in the case $p = 1$, we have that the maximum value of $\varphi^{(p)}(T)$ on $\mathcal{UT}_n$ is reached on trees in $\mathcal{T}_n$, because if we replace each nested taxon in a tree by a new leaf labeled with the same taxon as in Fig. 13, the value of $\varphi^{(p)}$ increases. On the other hand, if a tree $T \in \mathcal{T}_n$ contains a node with $k \geqslant 3$ children, as in the left hand side of Fig. 14, and we replace its subtree rooted at this node as described in the right hand side of Fig. 14, we obtain a new tree $T' \in \mathcal{T}_n$ with larger $\varphi^{(p)}$ value: the values of $\varphi(i,j)^p$ for $i, j \in L(T_1) \cup \cdots \cup L(T_{k-1})$ increase, and the other values of $\varphi(i,j)^p$ do not change. This implies that for every non-binary phylogenetic tree $T \in \mathcal{T}_n$, there always exists a binary phylogenetic tree $T' \in \mathcal{BT}_n$ such that $\varphi^{(p)}(T') > \varphi^{(p)}(T)$ and in particular that the maximum value of $\varphi^{(p)}(T)$ on $\mathcal{UT}_n$ is actually reached on $\mathcal{BT}_n$.

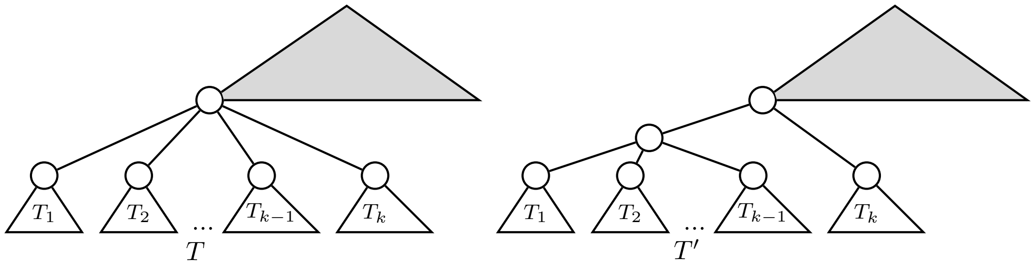


Figure 14: $\varphi^{(p)}(T') > \varphi^{(p)}(T)$.

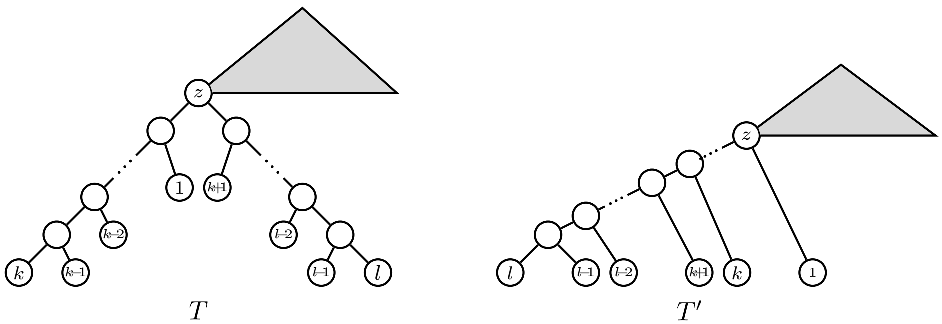


Figure 15: $\varphi^{(p)}(T') > \varphi^{(p)}(T)$.

Let now $T \in \mathcal{BT}_n$ and assume that it is not a caterpillar. Therefore, it has an internal node z of largest depth without any leaf child; in particular, all internal descendant nodes of z have some leaf child. Thus, and up to a relabeling of its leaves, T has the form represented in the left hand side of Fig. 15, for some $k \geqslant 2$ and some $l \geqslant k+2$. Consider then the tree T' depicted in right hand side of Fig. 15, where the grey triangle represents the same tree in both sides. It turns out that $\varphi^{(p)}(T') - \varphi^{(p)}(T) > 0$. Indeed, if q denotes the depth of the node z in both trees, then

$$\varphi_{T'}(i,j)^p - \varphi_T(i,j)^p = \begin{cases} (q+i)^p - (q+i+1)^p & \text{if } 1 \leqslant i = j \leqslant k-1 \\ 0 & \text{if } i = j = k \\ (q+i)^p - (q+i-k+1)^p & \text{if } k+1 \leqslant i = j \leqslant l-1 \\ (q+l-1)^p - (q+l-k)^p & \text{if } i = j = l \\ (q+i-1)^p - (q+i)^p & \text{if } 1 \leqslant i < j \leqslant k \\ (q+i-1)^p - (q+i-k)^p & \text{if } k+1 \leqslant i < j \leqslant l \\ (q+i-1)^p - q^p & \text{if } 1 \leqslant i \leqslant k < j \leqslant l \\ 0 & \text{otherwise} \end{cases}$$

Therefore,

$$\begin{aligned}
\varphi^{(p)}(T') - \varphi^{(p)}(T) &= \sum_{i=1}^{k-1} \big((q+i)^p - (q+i+1)^p\big) + \sum_{i=k+1}^{l-1} \big((q+i)^p - (q+i-k+1)^p\big) \\
&\quad + (q+l-1)^p - (q+l-k)^p + \sum_{i=1}^{k-1} (k-i)\big((q+i-1)^p - (q+i)^p\big) \\
&\quad + \sum_{i=k+1}^{l-1} (l-i)\big((q+i-1)^p - (q+i-k)^p\big) + \sum_{i=1}^{k} (l-k)\big((q+i-1)^p - q^p\big) \\
&= (q+1)^p - (q+k)^p + \sum_{i=1}^{l-k-1} \big((q+k+i)^p - (q+1+i)^p\big) \\
&\quad + (q+l-1)^p - (q+l-k)^p + \sum_{i=1}^{k-1} (k-i)\big((q+i-1)^p - (q+i)^p\big) \\
&\quad + \sum_{i=1}^{l-k-1} (l-k-i)\big((q+k+i-1)^p - (q+i)^p\big) + \sum_{i=1}^{k} (l-k)\big((q+i-1)^p - q^p\big)
\end{aligned}$$

To prove that this sum is non-negative, let us write it as

$$\varphi^{(p)}(T') - \varphi^{(p)}(T) = S_1 + S_2 + S_3,$$

where

$$\begin{aligned}
S_1 &= \sum_{i=1}^{k-1} (k-i)\big((q+i-1)^p - (q+i)^p\big) + \sum_{i=1}^{k} (l-k)\big((q+i-1)^p - q^p\big) \\
S_2 &= \sum_{i=1}^{l-k-1} \big((q+k+i)^p - (q+1+i)^p\big) + \sum_{i=1}^{l-k-1} (l-k-i)\big((q+k+i-1)^p - (q+i)^p\big) \\
S_3 &= (q+1)^p - (q+k)^p + (q+l-1)^p - (q+l-k)^p
\end{aligned}$$

Then

$$\begin{aligned}
S_1 &= \sum_{i=1}^{k-1}(k-i)\big((q+i-1)^p-(q+i)^p\big)+\sum_{i=1}^{k}(l-k)\big((q+i-1)^p-q^p\big),\\
&= \sum_{i=1}^{k-1}(k-i)(q+i-1)^p-\sum_{i=1}^{k-1}(k-i)(q+i)^p+\sum_{i=1}^{k}(l-k)\big((q+i-1)^p-q^p\big),\\
&= \sum_{i=1}^{k-1}(k-i)(q+i-1)^p-\sum_{i=2}^{k}(k-i+1)(q+i-1)^p+(l-k)\sum_{i=1}^{k}(q+i-1)^p-k(l-k)q^p,\\
&= \sum_{i=1}^{k-1}(l-k-1)(q+i-1)^p+kq^p-(q+k-1)^p+(l-k)(q+k-1)^p-k(l-k)q^p,\\
&= (l-k-1)\sum_{i=1}^{k}\big((q+i-1)^p-q^p\big)>0\\
S_2 &= \sum_{i=1}^{l-k-1}\big((q+k+i)^p-(q+1+i)^p\big)+\sum_{i=1}^{l-k-1}(l-k-i)\big((q+k+i-1)^p-(q+i)^p\big)\\
&= \sum_{i=1}^{l-k-1}\big((q+k+i)^p-(q+1+i)^p\big)+\sum_{i=0}^{l-k-1}(l-k-i-1)\big((q+k+i)^p-(q+i+1)^p\big)\\
&= \sum_{i=1}^{l-k-1}(l-k-i)\big((q+k+i)^p-(q+1+i)^p\big)+(l-k-1)\big((q+k)^p-(q+1)^p\big)\\
&> (l-k-1)\big((q+k)^p-(q+1)^p\big).
\end{aligned}$$

and therefore

$$\begin{aligned}
\varphi^{(p)}(T')-\varphi^{(p)}(T) &= S_1+S_2+S_3\\
&> (l-k-1)\big((q+k)^p-(q+1)^p\big)+(q+1)^p-(q+k)^p+(q+l-1)^p-(q+l-k)^p\\
&= (l-k-2)\big((q+k)^p-(q+1)^p\big)+(q+l-1)^p-(q+l-k)^p>0.
\end{aligned}$$

This implies that no tree other than a rooted caterpillar can have the largest $\varphi^{(p)}$ value in $\mathcal{BT}_n$, and hence also in $\mathcal{T}_n$ and $\mathcal{UT}_n$.

Finally, if K_n denotes the rooted caterpillar with n leaves in Fig. 12.(c),

$$\varphi_{K_n}(i,j)^p=\begin{cases}(n-1)^p & \text{if } i=j=1\\ (n-i+1)^p & \text{if } 2\leqslant i=j\leqslant n\\ (n-j)^p & \text{if } 1\leqslant i<j\leqslant n\end{cases}$$

and thus

$$\begin{aligned}
\varphi^{(p)}(K_n) &= (n-2)\cdot 1^p+(n-3)\cdot 2^p+\cdots+2\cdot(n-3)^p+1\cdot(n-2)^p\\
&\qquad +1^p+2^p+\cdots+(n-2)^p+(n-1)^p+(n-1)^p\\
&= (n-1)\cdot 1^p+(n-2)\cdot 2^p+\cdots+3\cdot(n-3)^p+2\cdot(n-2)^p+(n-1)^p+(n-1)^p\\
&= \sum_{k=1}^{n-1}(n-k)\cdot k^p+(n-1)^p
\end{aligned}$$

Now, it turns out that

$$\sum_{k=1}^{n-1}k^m=\frac{1}{m+1}n^{m+1}+O(n^m). \tag{1}$$

This property is well known for natural numbers $m \in \mathbb{N}$ [5]. For arbitrary real numbers $m > 0$, it derives from the fact that

$$\int_1^{n-1} (x-1)^m dx \leqslant \sum_{k=1}^{n-1} k^m \leqslant \int_1^{n-1} x^m dx,$$

and then

$$\int_1^{n-1} (x-1)^m dx = \frac{1}{m+1}(n-2)^{m+1} = \frac{1}{m+1} n^{m+1} + O(n^m)$$
$$\int_1^{n-1} x^m dx = \frac{1}{m+1}(n-1)^{m+1} = \frac{1}{m+1} n^{m+1} + O(n^m)$$

So, by identity (1), we have that

$$\sum_{k=1}^{n-1} (n-k) \cdot k^p + (n-1)^p = n \sum_{k=1}^{n-1} k^p - \sum_{k=1}^{n-1} k^{p+1} + O(n^p) = \Big(\frac{1}{p+1} - \frac{1}{p+2}\Big) n^{p+2} + O(n^{p+1})$$

and hence $\varphi^{(p)}(K_n)$ is in $\Theta(n^{p+2})$. □

Therefore, $O(n^{(p+2)/p}) \leqslant \Delta_p(X_n) \leqslant O(n^{(p+2)/p})$, which shows that the diameter of $d_{\varphi,p}$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ and $\mathcal{BT}_n$ is indeed in $\Theta(n^{(p+2)/p})$.

We finally prove the case $p = 0$, which needs a completely different argument.

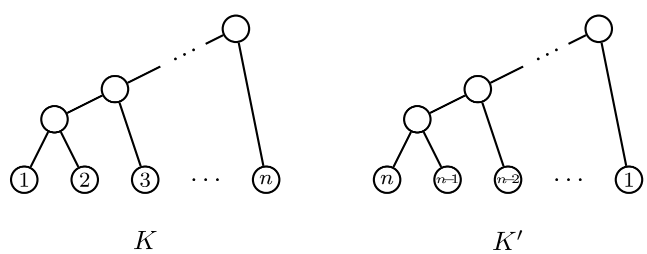


Figure 16: The caterpillars used in the proof of Lemma 16.

Lemma 16. *The diameter of $d_{\varphi,0}$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ and $\mathcal{BT}_n$ is in $\Theta(n^2)$.*

Proof. Since the cophenetic vector of a tree $T \in \mathcal{UT}_n$ lies in $\mathbb{R}^{n(n+1)/2}$, it is clear that $d_{\varphi,0}(T_1, T_2) \leqslant n(n+1)/2$, for every $T_1, T_2 \in \mathcal{UT}_n$. Now, consider the pair of rooted caterpillars with n leaves depicted in Fig. 16. We have that

$$\begin{array}{lll} \varphi_K(i,j) = n-j & \varphi_{K'}(i,j) = i-1 & \text{for every } 1 \leqslant i < j \leqslant n \\ \varphi_K(i,i) = n-i+1 & \varphi_{K'}(i,i) = i & \text{for every } 2 \leqslant i \leqslant n-1 \\ \varphi_K(1,1) = n-1 & \varphi_{K'}(1,1) = 1 & \\ \varphi_K(n,n) = 1 & \varphi_{K'}(n,n) = n-1 & \end{array}$$

This shows that the number of pairs (i,j), $1 \leqslant i \leqslant j \leqslant n$, such that $\varphi_K(i,j) = \varphi_{K'}(i,j)$ is at most $(n+1)/2$, and therefore that $d_{\varphi,0}(K, K')$ is at least $(n^2-1)/2$. So, the diameter of $d_{\varphi,0}$ on $\mathcal{UT}_n$ is bounded from above by $O(n^2)$, and its diameter on $\mathcal{BT}_n$ is bounded from below by $O(n^2)$, which implies that the diameter of $d_{\varphi,0}$ on $\mathcal{UT}_n$, $\mathcal{T}_n$ and $\mathcal{BT}_n$ is in $\Theta(n^2)$. $\square$

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