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1 Reordering a tree according to an order on its 2 leaves

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10 — Abstract —

11 In this article, we study two problems consisting in reordering a tree to fit with an order on its leaves
12 provided as input, which were earlier introduced in the context of phylogenetic tree comparison for
13 bioinformatics, OTCM and OTDE. The first problem consists in finding an order which minimizes
14 the number of inversions with an input order on the leaves, while the second one consists in removing
15 the minimum number of leaves from the tree to make it consistent with the input order on the
16 remaining leaves. We show that both problems are NP-complete when the maximum degree is
17 not bounded, as well as a problem on tree alignment, answering two questions opened in 2010 by
18 Henning Fernau, Michael Kaufmann and Mathias Poths. We provide a polynomial-time algorithm
19 for OTDE in the case where the maximum degree is bounded by a constant and an FPT algorithm
20 in a parameter lower than the number of leaves to delete. Our results have practical interest not
21 only for bioinformatics but also for digital humanities to evaluate, for example, the consistency of
22 the dendrogram obtained from a hierarchical clustering algorithm with a chronological ordering
23 of its leaves. We explore the possibilities of practical use of our results both on trees obtained by
24 clustering the literary works of French authors and on simulated data.²

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33 Institute)

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² The code is available in the following (anonymized) shared folder for evaluation purposes, the git repository will be made available in the final version. <https://www.dropbox.com/sh/6xkpiov9pbyrbf7/AABSjgQDSgGrvTgyDTvL6xdja?dl=0>

1 Introduction

The problem of optimizing the consistency between a tree and a given order on its leaves was first introduced in bioinformatics in the context of visualization of multiple phylogenetic trees [6], under the name “one-layer STOP (stratified tree ordering problem)”. The authors provided an $O(n^2)$ time algorithm to minimize, by exchanging the left and right children of internal nodes, the number of inversions between the left-to-right order of the leaves of a binary tree and an input order on its leaves. The problem was renamed OTCM (ONE-TREE CROSSING MINIMIZATION) in [9], where an $O(n \log^2 n)$ time algorithm is provided, as well as a reduction to 3-HITTING SET of a variant of the problem where the goal is to minimize the number of leaves to delete from the tree in order to be able to perfectly match the input order on the remaining leaves, called OTDE (ONE-TREE DRAWING BY DELETING EDGES). An $O(n \log^2 n / \log \log n)$ time algorithm is later provided for OTCM by [1], improved independently in 2010 by [10] and [21] to obtain an $O(n \log n)$ time complexity. About OTDE, the authors of [10] note that “the efficient dynamic-programming algorithm derived for the related problem OTCM [...] cannot be transferred to this problem. However, we have no proof for NP-hardness for OTDE nor TTDE, either”. TTDE (TWO-TREE DRAWING BY DELETING EDGES) is a variant of OTDE where two leaf-labeled trees are provided as input and the goal is to delete the minimum number of leaves such that the remaining leaves of both trees can be ordered with the same order. We give below an answer to both sentences, providing a dynamic-programming algorithm solving OTDE for trees with fixed maximum degree as well as an NP-hardness proof in the general case for OTDE and for TTDE.

Although this problem was initially introduced in the context of comparing tree embeddings, one tree having its embedding (that is the left-to-right order of all children) fixed, we can note that only the order on the leaves of the tree with fixed embedding is useful to define both problems OTCM and OTDE. Both problems therefore consist not really in comparing trees but rather in reordering the internal nodes of one tree in order to optimize its consistency with an order on its leaves provided as input. A popular problem consisting in finding an optimal order on the leaves of a tree is “seriation”, often used for visualization purposes [7], where the optimized criterion is computed on data used to build the tree. For example, a classical criterion, called “optimal leaf ordering”, is to maximize the similarity between consecutive elements in the optimal order [3, 2, 4]. Another possibility is to minimize a distance criterion, the “bilateral symmetric distance”, computed on pairs of elements in consecutive clusters [5]. Seriation algorithms have been implemented for example in the R-packages `seriation` [12] and `dendsort` [19].

With the OTCM and OTDE problems, our goal is not to reorder a tree using directly the data used to build it, but using external data about some expected order on its leaves. In the context where the leaves of the tree can be ordered chronologically, for example, this would help providing an answer to the question: how much is this tree consistent with the chronological order? This issue is relevant for several fields of digital humanities, when objects associated with a publication date are classified with a hierarchical clustering algorithm, for example literature analysis [14], political discourse analysis [15] or language evolution [17], as noticed in [11].

In this article, we first give useful definitions in Section 1.1. We answer two open problems from [10], proving that OTDE and TTDE are NP-complete, as well as OTCM, in Section 2. We then provide a dynamic programming algorithm solving OTDE in polynomial time for trees with fixed maximum degree in Section 3. This algorithm also works in the more general case where the order on the leaves is not strict. We then provide an FPT algorithm for the

81 OTDE problem parameterized by the deletion-degree of the solution, which is lower than
 82 the number of leaves to delete, in Section 4. We also give an example of a tree and an order
 83 built to have a distinct solution for the OTCM and OTDE problems in Section 5. Finally,
 84 we illustrate the relevance of this problem, and of our implementations of algorithms solving
 85 them, for applications in digital humanities, with experiments on trees built from literary
 86 works, as well as simulated trees, in Section 6.

87 1.1 Definitions

88 Given a set X of elements, we define an X -tree T as a rooted tree whose leaves are bijectively
 89 labeled by the elements of X . The set of leaves of T is denoted by $L(T)$ and the set of leaves
 90 below some vertex v of T is denoted by $L(T, v)$ (or simply $L(v)$ if T is clear from the context).
 91 A set of vertices of T is *independent* if no vertex of T is an ancestor of another vertex of T .

92 We say that σ is a strict order on X if it is a bijection from X to $[1..n]$ and that it
 93 is a weak order on X if it is a surjection from X to $[1..m]$, where $|X| \geq m$. Given any
 94 (strict or weak) order σ , we denote by $a \leq_\sigma b$ the fact that $\sigma(a) \leq \sigma(b)$ and by $a <_\sigma b$
 95 the fact that $\sigma(a) < \sigma(b)$. Considering the elements x_1, \dots, x_n of X such that for each
 96 $i \in [1..n-1]$, $\sigma(x_i) \leq \sigma(x_{i+1})$, we denote by $(x_1 x_2 \dots x_n)$ the (weak or strict) order σ .

97 Given an X -tree T and a (weak or strict) order σ on X , we say that an independent
 98 pair $\{u, v\}$ of vertices of T is a *conflict wrt.* σ if there exist leaves $a, c \in L(u)$ and $b \in L(v)$
 99 such that $a <_\sigma b <_\sigma c$. Conversely, if $\{u, v\}$ is not a conflict, then either $a \leq_\sigma b$ for all
 100 $a \in L(u), b \in L(v)$, or $b \leq_\sigma a$; we then write respectively $u \preceq_\sigma v$ or $v \preceq_\sigma u$. We say that σ is
 101 *suitable* on T if T has no conflict with respect to σ .

102 Given two (strict or weak) orders σ_1 and σ_2 on X and two elements $a \neq b$ of X , we say
 103 that $\{a, b\}$ is an *inversion* for σ_1 and σ_2 if $a \leq_{\sigma_1} b$ and $b <_{\sigma_2} a$, or $b \leq_{\sigma_1} a$ and $a <_{\sigma_2} b$.

104 Given an X -tree T , a subset X' of X and an order σ on X , we denote by $\sigma[X']$ the order
 105 σ restricted to X' , and by $T[X']$ the tree T restricted to X' , that is the X' -tree obtained
 106 from T by removing leaves labeled by $X \setminus X'$ and contracting any arc to a non-labeled leaf,
 107 from a degree-2 vertex or from the root if the root has degree 1. We define the *deletion-degree*
 108 of X' as the maximum degree of the tree induced by the deleted leaves, i.e. $T[X \setminus X']$.
 109 Intuitively, the deletion-degree measures how deletions in different branches converge on a
 110 few nodes or if they merge progressively. Note that by definition, the deletion-degree of X'
 111 is upper-bounded both by the maximum degree of T and by the size of $X \setminus X'$.

112 We now define the two main problems addressed in this paper. As explained in the
 113 introduction, we differ from previous definitions which considered two trees, one with a fixed
 114 order on the leaves, as input, as only the leaf order of the second tree is useful to define the
 115 problem and not the tree itself.

116 We therefore define the OTCM (ONE-TREE CROSSING MINIMIZATION) problem as
 117 follows:

- 118 ■ **Input:** An X -tree T , an order σ on X and an integer k .
- 119 ■ **Output:** Yes if there exists an order σ' on X suitable on T such that the number of
 120 inversions for σ' and σ is at most k , no otherwise.

121 We also define the OTDE (ONE-TREE DRAWING BY DELETING EDGES) problem as
 122 follows:

- 123 ■ **Input:** An X -tree T , an order σ on X and an integer k .
- 124 ■ **Output:** Yes if there exists a subset X' of X of size at least $|X| - k$ such that $\sigma[X']$ is
 125 suitable on $T[X']$, no otherwise.

126 We finally define the TTDE (TWO-TREE DRAWING BY DELETING EDGES) problem in
127 the following way:

- 128 ■ **Input:** Two X -trees T_1 and T_2 and an integer k .
- 129 ■ **Output:** Yes if there exists a subset X' of X of size at least $|X| - k$ and an order σ' on
130 X' that is suitable on $T_1[X']$ and on $T_2[X']$, no otherwise.

131 2 NP-hardness

132 2.1 OTDE and TTDE are NP-complete for trees with unbounded 133 degree

134 ► **Theorem 1.** *The OTDE problem is NP-complete for strict orders and a fortiori for weak
135 orders.*

136 **Proof.** First note that OTDE is in NP, since, given an X -tree T , an order σ and a set L
137 of leaves to remove, we can check in linear time, by a recursive search of the tree, saving
138 on each node the minimum and the maximum leaf in $\sigma[X - L]$ appearing below, whether
139 $\sigma[X - L]$ is suitable on $T[X - L]$. Regarding NP-hardness, we now give a reduction from
140 INDEPENDENT SET, which is NP-hard on cubic graphs [16], to OTDE when the input trees
141 have unbounded degree.

142 We consider an instance of the INDEPENDENT SET problem, that is a cubic graph
143 $G = (V = \{v_1, \dots, v_n\}, E)$ such that $|E| = m = 3n/2$ and an integer k . For each vertex v_i ,
144 we write e_i^1, e_i^2 and e_i^3 for the three edges incident with v_i .

145 We now define an instance of the OTDE problem. The set of leaf labels consists of *vertex*
146 *labels* denoted v_i and v'_i for each $i \in [1..n]$, one *edge labels* for each edge e (also denoted e),
147 and a set of n^2 *separating labels* $B_i = \{b_i^1, b_i^2, \dots, b_i^{n^2}\}$ for each $i \in [1..n - 1]$.

148 First, we define the strict order $\sigma(G) = (v_1 e_1^1 e_1^2 e_1^3 v'_1 b_1^1 b_1^2 \dots b_1^{n^2} v_2 e_2^1 e_2^2 e_2^3 v'_2 b_2^1 b_2^2 \dots b_2^{n^2} v_n e_n^1$
149 $e_n^2 e_n^3 v'_n)$. Then, let T_{v_i} be the tree with leaves v_i and v'_i attached below the root, T_e be the tree
150 with leaves $e_i^{j'}$ and $e_j^{j'}$ attached below the root for each edge $e = \{v_i, v_j\}$ of G (with $i', j' \in$
151 $[1..3]$), and T_{B_i} be the tree with leaves $b_i^1, \dots, b_i^{n^2}$ attached below the root for each $i \in [1, n - 1]$.
152 We finally define $T(G)$ as the tree such that $T_{v_1}, T_{v_2}, \dots, T_{v_n}, T_{e_1}, T_{e_2}, \dots, T_{e_m}, T_{B_1}, T_{B_2}, \dots$
153 and $T_{B_{n-1}}$ are attached below the root.

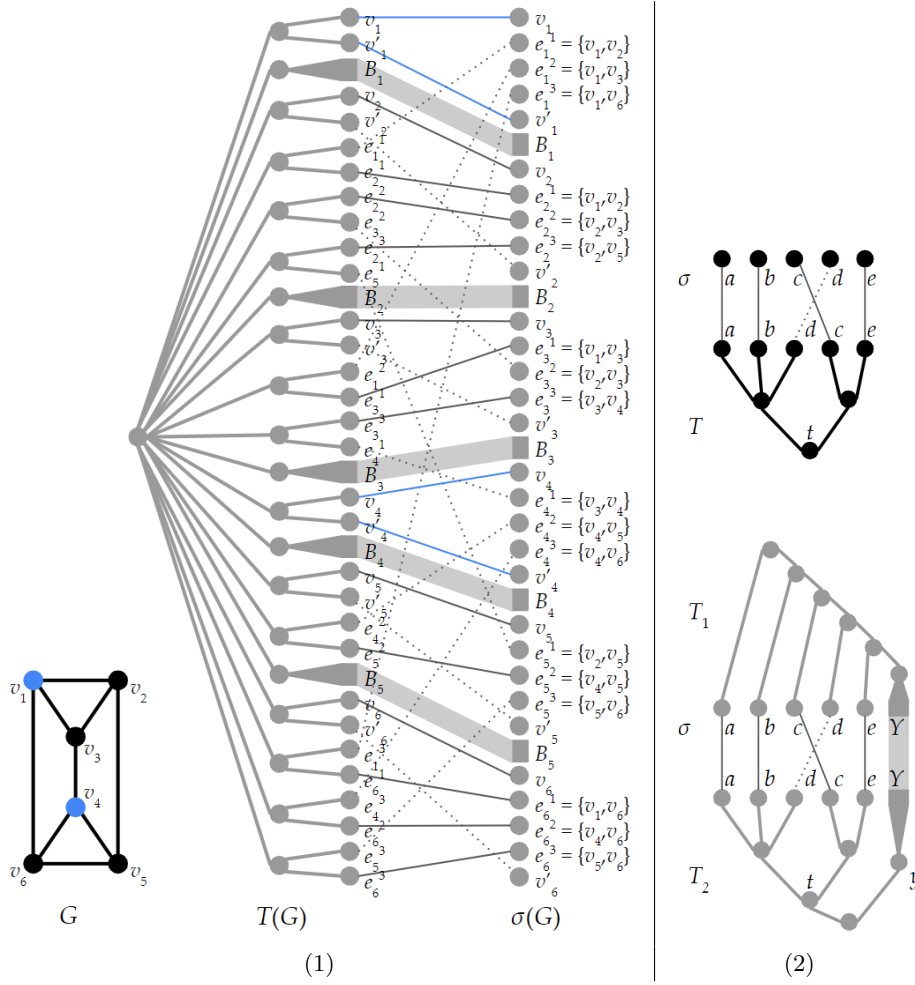
154 We claim that G has an independent set of size at least $k \Leftrightarrow$ the instance $(T(G), \sigma(G))$
155 of the OTDE problem has a solution with a set L of at most $m + n - k$ leaves to remove.

156 \Rightarrow : Suppose that there exists a size- k independent set $S = \{s_1, \dots, s_k\}$ of G . We then
157 remove the following leaves (also contracting along the way the edge from their parent to the
158 root of $T(G)$) in order to get a new tree T' :

- 159 ■ for each edge $\{v_i, v_j\} = e_i^{i'} = e_j^{j'}$, we remove $e_i^{i'}$ if $v_i \in S$ or if neither v_i nor v_j belong to
160 S and we remove $e_j^{j'}$ if $v_j \in S$ (as S is an independent set we cannot have both v_i and v_j
161 in S);
- 162 ■ for each vertex v_i not in S we remove v'_i .

163 By ordering the children of the root of $T(G)$ such as in Figure 1(1), that is by putting, for each
164 v_i with $i \in [1, n]$, T_{v_i} , then $T_{e_1^1}, T_{e_1^2}$ and $T_{e_1^3}$ for each of the $e_i^{i'}$ which were not removed and
165 then T_{B_i} (except for $i = n$), the order $\sigma(G)$ restricted to the remaining $m + n + k + n^2(n - 1)$
166 leaves is suitable on T' .

167 \Leftarrow : Suppose that there exists a set L of at most $m + n - k$ leaves such that $\sigma(G)[X - L]$
168 is suitable on $T(G)[X - L]$. For each parent p_{B_i} of the leaves of B_i and any other vertex v of
169 T such that $\{p_{B_i}, v\}$ is a conflict wrt. $\sigma(G)$, we can delete this conflict either by deleting no



■ **Figure 1** Illustration of the reductions of INDEPENDENT SET to OTDE and of OTDE to TTDE. (1) a graph G with independent set $S = \{v_1, v_4\}$ of size 2 and the corresponding tree $T(G)$ as well as the order $\sigma(G)$ such that only the leaves connected with a dotted line to be deleted to make $T(G)$ restricted to the remaining leaves suitable for the order. (2) Reduction from an OTDE instance (T, σ) to a TTDE instance (T_1, T_2) . A large set of leaves labelled Y can be seen as a fixed-point, around which T_1 must be ordered according to σ , and T_2 according to the input tree T .

170 leaf of B_i or all leaves of B_i . As each B_i has size $n^2 > m + n - k$, its leaves cannot belong to
 171 the set L of leaves to be deleted.

172 We now consider the trees T_{e_i} for each $i \in [1..m]$: by construction of $\sigma(G)$, as both leaves
 173 of each such tree are separated by some $B_{i'}$, therefore by $n^2 > m + n - k$ leaves, one of these
 174 two leaves has to be removed, so it has to belong to L . We call L' the set of such leaves of L ,
 175 therefore there exists a set $L - L'$ of at most $n - k$ other leaves to delete. So there exists a
 176 subset S_L of $[1..n]$ of size at least k such that for any element $i \in S_L$, neither v_i , nor v'_i , nor
 177 any of the leaves e_i^j for $j \in \{1, 2, 3\}$ belong to $L - L'$. Note that for such $i \in S_L$, all vertices
 178 v_i and v'_i are not in L and all e_i^j are in L' . We claim that the vertices of G corresponding
 179 to S_L are an independent set of G . Suppose by contradiction that it is not the case, then
 180 there exists an edge $e = e_i^{i'} = e_j^{j'}$ between two vertices v_i and v_j of G . By construction of
 181 L' , exactly one of the leaves labeled by $e_i^{i'}$ and $e_j^{j'}$ is in L' so the second one is in $L - L'$:

182 contradiction. ◀

183 ▶ **Corollary 2.** *The TTDE problem is NP-complete.*

184 **Proof.** TTDE is clearly in NP. We prove hardness by reduction from OTDE (see Figure 1(2)
185 for an illustration). Consider an instance (T, σ) of OTDE with σ a strict order on n labels
186 X . Introduce a set Y of n new labels. Build T_1 as a caterpillar with $2n$ leaves (ordered from
187 the leaf attached to the root to the leaf farthest from the root), where the first n leaves are
188 labelled with X according to σ (in the same order), and the last n leaves are labelled with
189 Y (in any order). Build T_2 as a tree, where the root has two children y, t , where y has n
190 children which are leaves labelled with Y , and t is the root of a subtree equal to T .

191 We now show our main claim: given $0 \leq k < n$, OTDE(T, σ) admits a solution with at
192 most k deletions \Leftrightarrow TTDE(T_1, T_2) admits a solution with at most k deletions.

193 \Rightarrow Let X' be a size- $(n - k)$ subset of X such that $\sigma[X']$ is suitable on $T[X]$. Then let γ
194 be any order on Y : the concatenation $\sigma[X']\gamma$ is suitable both on $T_1[X' \cup Y]$ and $T_2[X' \cup Y]$,
195 so it is a valid solution for TTDE(T_1, T_2) of size $2n - k$, i.e. with k deletions.

196 \Leftarrow Let X', Y' be subsets of X, Y respectively and σ' be an order on $X' \cup Y'$ such that
197 σ' is suitable on both $T_1[X' \cup Y']$ and $T_2[X' \cup Y']$, and such that $|X' \cup Y'| \geq 2n - k > n$
198 (in particular, Y' contains at least one element denoted y , and $|X'| \geq n - k$). From T_2 , it
199 follows that σ' is the concatenation (in any order) of an order σ_x of X' suitable for $T[X']$
200 and an order σ_y of Y' . Assume first that σ_x appears before σ_y . Then for each internal node
201 of the caterpillar T_1 with a child in X' , this child must be ordered before the other subtree
202 (which contains y). Thus, the nodes in X' are ordered according to $\sigma[X']$, and $\sigma_x = \sigma[X']$,
203 and $T[X']$ is suitable with $\sigma[X']$. For the other case, where σ_y is ordered before σ_x , then for
204 each node of the caterpillar with a child in X' , this child must be after the subtree containing
205 y , and the nodes in X' are ordered according to the reverse of $\sigma[X']$ (i.e. $\sigma_x = \overline{\sigma[X']}$). Thus,
206 the reverse of $\sigma[X']$ is suitable for $T[X']$, and $\sigma[X']$ as well (this is obtained by reversing
207 the permutation of all children of internal nodes of T). In both cases, X' is a solution for
208 OTDE(T, σ) with $|X'| \geq n - k$. ◀

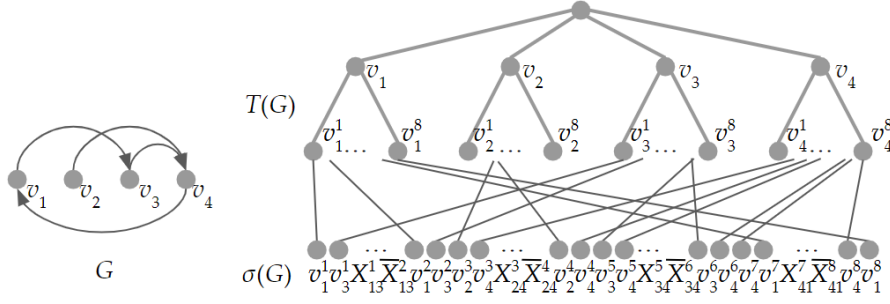
209 2.2 OTCM is NP-complete for trees with unbounded degree

210 ▶ **Theorem 3.** *The OTCM problem is NP-complete for strict orders and a fortiori for weak
211 orders.*

212 **Proof.** First note that OTCM is in NP, since, given an X -tree T with its leaves ordered
213 according to an order σ' on X suitable on T , an order σ and a set L of leaves to remove, the
214 number of inversions between σ' and σ can be counted in $O(|L|^2)$. Regarding NP-hardness,
215 we now give a reduction from FEEDBACK ARC SET, which is NP-hard [13], to OTCM.

216 We consider an instance of the FEEDBACK ARC SET problem, that is a directed graph
217 $G = (V = \{v_1, \dots, v_n\}, A)$ such that $|A| = m$ and an integer f .

218 We now define an instance of the OTCM problem, illustrated in Figure 2. The set X
219 of leaf labels is $\bigcup_{i \in [1..n], j \in [1..m]} \{v_i^j\}$. We define the order $\sigma(G)$ in the following way. For
220 each arc (v_i, v_j) of G where $i < j$, taken in the lexicographic order, we add to $\sigma(G)$ a k^{th}
221 supplementary ordered sequence (which we will later call a “block” corresponding to this arc)
222 $v_i^{2k-1} v_j^{2k-1} X_{i,j}^{2k-1} \overline{X}_{i,j}^{2k} v_i^{2k} v_j^{2k}$, where $X_{i,j}^{k'}$ is the ordered sequence of $v_{i'}^{k'}$ where i' ranges from
223 1 to n , excluding i and j , and $\overline{X}_{i,j}^{k'}$ is the reverse of $X_{i,j}^{k'}$ (i.e. the ordered sequence of $v_{i'}^{k'}$
224 where i' ranges from n down to 1, excluding i and j). The tree $T(G)$ is made of a root with
225 n children v_1 to v_n , each v_i having $2m$ children, the leaves labeled by $v_i^{k'}$ for $k' \in [1..2m]$.



■ **Figure 2** Illustration of the reduction of FEEDBACK ARC SET to OTCM: a graph G with feedback arc set $S = \{(v_4, v_1)\}$ of size 1 and the corresponding tree $T(G)$ as well as the order $\sigma(G)$.

226 Given an ordering σ' suitable for T , and an inversion $(v_i^k, v_{i'}^{k'})$ forming an inversion
 227 between $\sigma(G)$ and σ' , we say that this pair is *short-ranged* if $k = k'$, and *long-ranged*
 228 otherwise. Furthermore, we say that σ' is *vertex-consistent* if, for every i and $k < k'$, we have
 229 $\sigma'(v_i^k) < \sigma(v_{i'}^{k'})$. Finally, given σ' , we write σ'' for the permutation of the $[1..n]$ corresponding
 230 to the children of the root.

231 We first claim that for any σ' suitable for T , there are at least $2 \binom{n}{2} \binom{2m}{2}$ long-range
 232 inversions between σ' and $\sigma(G)$, and this bound is reached if σ' is vertex-consistent. Indeed,
 233 pick any pair $(v_i^k, v_{i'}^{k'})$ with $i \neq i'$ and $k \neq k'$. Then $v_i^k <_{\sigma(G)} v_{i'}^{k'}$ iff $k < k'$ (since they are
 234 respectively in blocks k and k' of $\sigma(G)$), and $v_i^k <_{\sigma'} v_{i'}^{k'}$ iff $\sigma''(i) < \sigma''(i')$ (since they are
 235 respectively in $L(T, v_i)$ and $L(T, v_{i'})$). Overall, among $4 \binom{n}{2} \binom{2m}{2}$ such pairs of elements, there
 236 are $2 \binom{n}{2} \binom{2m}{2}$ pairs creating an inversion (which is long-range by definition). For the case
 237 $i = i'$, note that pairs $(v_i^k, v_i^{k'})$ do not create any inversion iff σ' is vertex-consistent, which
 238 completes the proof of the claim.

239 Towards counting the number of short-ranged inversions, we say that an arc (v_i, v_j) of G
 240 is *satisfied* by σ'' if $\sigma''(i) < \sigma''(j)$. Consider two pairs (v_i^{2k-1}, v_j^{2k-1}) and (v_i^{2k}, v_j^{2k}) . Then
 241 these two pairs are necessarily in the same order in σ' . If the k^{th} arc of G is (v_i, v_j) , then
 242 these two pairs are also in the same order in σ . Note that they (both) form an inversion
 243 iff (v_i, v_j) is not satisfied by σ'' . If the k^{th} arc of G is any other arc, then exactly one of
 244 (v_i^{2k-1}, v_j^{2k-1}) , (v_i^{2k}, v_j^{2k}) forms an inversion. Overall a pair i, j such that one of (v_i, v_j) , (v_j, v_i)
 245 is a satisfied arc yields $m - 1$ short-range inversions, a pair i, j such that one of (v_i, v_j) , (v_j, v_i)
 246 is an unsatisfied arc yields $m + 1$ short-range inversions, and any other pair $\{i, j\}$ with $i \neq j$
 247 yields m inversions. Overall, if there are f unsatisfied arcs, σ' yields $\binom{m}{2} - m + 2f$ inversions.

248 We can now complete the proof with our main claim: G has a feedback arc set of size at
 249 most $f \Leftrightarrow$ the OTCM problem has a solution with at most $\binom{n}{2} \binom{2m}{2} + \binom{m}{2} - m + 2f$ inversions.

250 \Rightarrow : If G has a feedback arc set F of size f , as $G[A - F]$ is acyclic, we consider an order σ''
 251 over n such that for all arcs (v_i, v_j) in $A - F$, $\sigma''(i) < \sigma''(j)$ (i.e. σ'' is the topological order
 252 of the vertices in $G[A - F]$). We now order the children v_i of the root of $T(G)$ according to
 253 this order σ'' and call σ' the induced order on the leaves of $T(G)$ (also sorting all leaves v_i^j
 254 below each v_i by increasing values of j). Note that σ' is vertex-consistent, and that an arc
 255 (v_i, v_j) is satisfied by σ'' iff $(v_i, v_j) \notin F$. Thus, σ' yields $\binom{n}{2} \binom{2m}{2} + \binom{m}{2} - m + 2f$ inversions.

256 \Leftarrow : Consider an order σ' suitable for T with at most $\binom{n}{2} \binom{2m}{2} + \binom{m}{2} - m + 2f$ inversions. Let
 257 σ'' be the corresponding order on the leaves of the root, and let F be the set of arcs unsatisfied
 258 by σ'' . Since σ' has at least $\binom{n}{2} \binom{2m}{2}$ long-range inversions, it has at most $\binom{m}{2} - m + 2f$
 259 short-range inversions, and $|F| \leq f$. Finally, since all arcs in $A - F$ are satisfied by σ'' ,
 260 $G[A - F]$ is acyclic and F is a feedback arc set. ◀

3 A polynomial-time algorithm for fixed-degree trees

We start by providing a dynamic programming algorithm for fixed-degree trees, which is easy to implement and leads to an algorithm in $O(n^4)$ time for binary trees. The FPT algorithm presented in the next section has a better complexity but is more complex and reuses the dynamic programming machinery presented in this section, which explains why we start with this simpler algorithm.

► **Theorem 4.** *The OTDE problem can be solved in time $O(d!n^{d+2})$ for trees with fixed maximum degree d and for strict or weak orders.*

Proof. Given a vertex v of a rooted tree T , a (strict or weak) order $\sigma : L(T) \rightarrow [1..m]$ and two integers $l \leq r \in [1..m]$. We denote by $\mathcal{X}(v, l, r)$ a subset of $L(T, v)$ of maximum size such that $\sigma[\mathcal{X}(v, l, r)]$ is suitable with $T[\mathcal{X}(v, l, r)]$ and $\forall \ell \in \mathcal{X}(v, l, r), \sigma(\ell) \in [l, r]$. Note that $\mathcal{X}(v, l, r)$ also depends on T and σ but we simplify the notation by not mentioning them as they can clearly be identified from the context.

Denoting by c_1, \dots, c_k the children of v in T , we claim that the following formula allows to recursively compute $\mathcal{X}(v, l, r)$ in polynomial time:

$$\begin{aligned} \blacksquare \quad |\mathcal{X}(v, l, r)| &= \max_{\substack{\text{permutation } \pi \text{ of } [1..k] \\ x_1=l \leq x_2 \leq \dots \leq x_k \leq x_{k+1}=r}} \sum_{i=1}^k |\mathcal{X}(c_{\pi(i)}, x_i, x_{i+1})| \text{ if } v \text{ is an internal node of } T; \\ \blacksquare \quad &\text{for any leaf } \ell \text{ of } T, |\mathcal{X}(\ell, l, r)| = 1 \text{ if } \sigma(\ell) \in [l, r], 0 \text{ otherwise.} \end{aligned}$$

Correctness: We prove by induction on the size of $L(v)$ that $\mathcal{X}(v, l, r)$ is indeed a subset of $L(T, v)$ of maximum size such that $\sigma[\mathcal{X}(v, l, r)]$ is suitable with $T[\mathcal{X}(v, l, r)]$ and $\forall \ell \in \mathcal{X}(v, l, r), \sigma(\ell) \in [l, r]$.

This is obvious for any leaf, so let us consider a vertex v of T with a set $\{c_1, \dots, c_k\}$ of children. Suppose by contradiction that there exists a set of integers $l \leq r$ and a subset X' of $L(v)$ of size strictly greater than $\mathcal{X}(v, l, r)$ such that $\sigma[X']$ is suitable with $T[X']$ and $\forall \ell \in X', \sigma(\ell) \in [l, r]$. We then denote by X'_1, \dots, X'_k the sets of leaves $L(c_1) \cap X', \dots, L(c_k) \cap X'$ respectively. Without loss of generality we consider that the children c_i of v are labeled such that $\max_{\ell \in X'_i} \{\sigma(\ell)\} \leq \min_{\ell \in X'_{i+1}} \{\sigma(\ell)\}$. For all $i \in [2..k]$, we define $m_i = \min_{\ell \in X'_i} \{\sigma(\ell)\}$, $m_1 = l$ and $m_{k+1} = r$. Using the induction hypothesis we know that for each $i \in [1..k]$, $|X'_i| \leq |\mathcal{X}(v, \min_{\ell \in X'_i} \{\sigma(\ell)\}, \max_{\ell \in X'_i} \{\sigma(\ell)\})|$, so $|X'_i| \leq |\mathcal{X}(v, m_i, m_{i+1})|$ because $[\min_{\ell \in X'_i} \{\sigma(\ell)\}, \max_{\ell \in X'_i} \{\sigma(\ell)\}] \subseteq [m_i, m_{i+1}]$. Therefore, $|X'| = \sum_{i=1}^k |X'_i| \leq \sum_{i=1}^k |\mathcal{X}(v, m_i, m_{i+1})|$ so by definition of $\sigma[\mathcal{X}(v, l, r)]$, $|X'| \leq \sigma[\mathcal{X}(v, l, r)]$: contradiction!

We therefore obtain a correct solution of $OTDE(T, \sigma)$ by computing $\mathcal{X}(\text{root}(T), 0, m)$.

Running-time: For each v , we compute the table of the $O(n^2)$ values of $\mathcal{X}(v, l, r)$ for all intervals $[l, r]$. Each of these values can be computed by generating the $k!$ permutations of children of v to consider any possible order among the children and splitting the interval $[l, r]$ into any possible configurations of d consecutive intervals with integer bounds partitioning $[l, r]$, which can be done in time $O(n^{d-1})$. So the computation of each $\mathcal{X}(v, l, r)$ is done in time $O(d!n^{d-1})$, therefore the total computation of all $\mathcal{X}(v, l, r)$ is done in time $O(n \times n^2 \times d!n^{d-1})$, that is in $O(d!n^{d+2})$. ◀

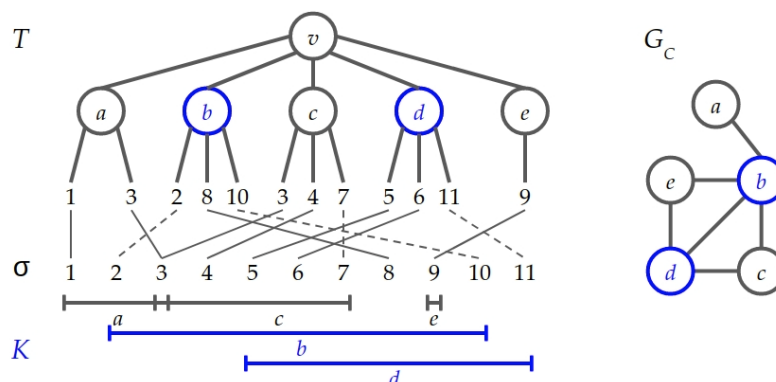


Figure 3 An instance (T, σ) of OTDE (top-left), with a vertex v having children set $C = \{a, b, c, d, e\}$. The conflict graph G_C of C (right) has a size-2 vertex cover $K = \{b, d\}$. Based on the span of each vertex (bottom-right), the dynamic programming algorithm tests permutations of C such that (a, c, e) appear in this order, interleaved in any possible way with b and d . In particular, the final solution corresponds to the permutation $(a c d b e)$ of C . Note that since σ may be a weak order (two leaves are labelled 3 in the example), the conflict graph does not correspond exactly to the intersection graph of the span intervals, e.g. vertices a and c are *not* in conflict, even though their spans overlap.

299 **4** An FPT algorithm for the *deletion-degree* parameter for OTDE

300 We recall that with a reduction of OTDE to 3-HITTING SET [10], using the best algorithm
 301 known so far to solve this problem³, we can obtain an $O^*(2.08^k)$ [22] algorithm to solve
 302 OTDE, where k is the number of leaves to delete. In this section we obtain an FPT algorithm
 303 in time $O(n^4 d \partial^{2\partial})$, where d is the maximum degree of the tree and ∂ is the deletion-degree
 304 of the solution.

305 **► Theorem 5.** *The OTDE problem parameterized by the deletion-degree ∂ of the solution is*
 306 *FPT and can be solved in time $O(n^4 d \partial^{2\partial})$ for strict or weak orders.*

307 We adapt the dynamic programming algorithm from Theorem 4, using a vertex cover
 308 subroutine to have a good estimation of the permutation of the children of each node.

309 We first introduce some definitions (see Figure 3 for a illustration of these definitions
 310 and the algorithm in general). Given any vertex v of T , let C_v be the (independent) set of
 311 children of v , and let G_v be the *conflict graph* with vertex set C_v and with one edge per
 312 conflict. Let K be a vertex cover of C_v . Then the vertices of $C_v \setminus K$ have a *canonical order*
 313 $(w_1, \dots, w_{k'})$, with $k' = |C_v \setminus K|$ and $w_i \preceq_\sigma w_j$ for all $i \leq j$ (ties may happen when two
 314 children contain a single leaf each which are equal, such ties are broken arbitrarily). We say
 315 that $P \subseteq C_v$ is a *prefix of C_v wrt. K* if $P \setminus K$ is a prefix of this order (i.e. for some $i \leq k'$,
 316 $P \setminus K = \{w_1, \dots, w_i\}$). In other words, ignoring all subtrees below vertices of K , all leaves
 317 below vertices of a prefix P are necessarily ordered before leaves below vertices outside of P .

318 **► Lemma 6.** *If X' is a solution of OTDE with deletion-degree ∂ , then for any vertex v of*
 319 *T , the conflict graph G_v admits a vertex cover of size at most ∂ .*

320 **Proof.** Given a subset X' of X , we say that a node v of T has a *deletion* if some $L(v) \not\subseteq X'$,
 321 i.e. if v has a leaf in $X \setminus X'$. Let $\{u, v\}$ be any conflict (edge) of the conflict graph G_v , then

³ <http://fpt.wikidot.com/fpt-races>

322 at least one of u, v has a deletion for X' (indeed, the conflict involves three leaves a, b, c , of
 323 which at least one must be deleted). Thus, the vertices with a deletion in G_v form a vertex
 324 cover of this graph. The lemma follows from the fact that at most ∂ vertices have a deletion
 325 in each conflict graph. ◀

326 The first step of our algorithm consists in computing, for each node v of the graph, the
 327 set C of children of v , its conflict graph G_v , and a minimum vertex cover K_v of G_C . Since
 328 each K_v has size at most ∂ (by Lemma 6), K_v can be computed in time $O(1.3^\partial + \partial n)$ [5],
 329 and overall this first step takes $O(1.3^\partial n + \partial n^2)$.

330 We proceed with the dynamic programming part of our algorithm. To this end, we
 331 generalize the table \mathcal{X} to sets of nodes (instead of only v) as follows: $\mathcal{X}(P, l, r)$ corresponds
 332 to the largest set X of leaves in $\bigcup_{u \in P} L(u)$ such that σ_X is suitable for $T[X]$. Note that for
 333 a node v with children set C , $\mathcal{X}(v, l, r) = \mathcal{X}(\{v\}, l, r) = \mathcal{X}(C, l, r)$.

334 We first compute $\mathcal{X}(\{v\}, l, r)$ for each leaf v : clearly $\mathcal{X}(\{v\}, l, r) = \{u\}$ if $l \leq \sigma(v) \leq r$,
 335 and $\mathcal{X}(\{v\}, l, r) = \emptyset$ otherwise. For each internal vertex v (visiting the tree bottom-up), we
 336 obtain $\mathcal{X}(\{v\}, l, r)$ by first computing $\mathcal{X}(P, l, r)$ for each prefix P of C_v by increasing order
 337 of size, using the following formulas:

$$\begin{aligned}
 338 \quad |\mathcal{X}(P, l, r)| &= \emptyset \text{ if } P = \emptyset \\
 339 \quad &= \max_{\substack{x \in [l..r], u \in P \\ P \setminus \{u\} \text{ prefix of } C_v}} |\mathcal{X}(P \setminus \{u\}, l, x)| + |\mathcal{X}(\{u\}, x, r)| \\
 340 \quad |\mathcal{X}(\{v\}, l, r)| &= |\mathcal{X}(C_v, l, r)| \\
 341
 \end{aligned}$$

342 Each vertex v has at most $d2^\partial$ prefixes, so the dynamic programming table \mathcal{X} has at
 343 most $n^3 d2^\partial$ cells to fill. For each prefix P , there exist at most $\partial + 1$ vertices $u \in P$ such that
 344 $P \setminus \{u\}$ is a prefix (u can be any vertex in $P \cap K_v$, or the maximum vertex for \preceq_σ in $P \setminus K_v$).
 345 Overall, the *max* is taken over $O(n\partial)$ elements, and \mathcal{X} can be filled in time $O(n^4 d \partial 2^\partial)$.

346 Before proving the correctness of the above formula, we need a final definition: given
 347 a set of leaves $X' \subseteq X$ and a vertex v of T , we write $\text{span}_{X'}(v)$ for the smallest interval
 348 containing $\sigma(u)$ for each leaf $u \in L(u) \cap X'$ (note that $\text{span}_{X'}(v)$ may be empty, if all its
 349 leaves are deleted in X').

350 ► **Lemma 7.** *Let X' be a solution of $OTDE(T, \sigma)$, $v \in T$ and $1 \leq l \leq r \leq m$ such that*
 351 *$\text{span}_{X'}(v) \subseteq [l, r]$. Then there exists a permutation $(c_1 \dots c_k)$ of the children of v and*
 352 *integers $x_0 = l \leq x_1 \leq \dots \leq x_k = r$ such that, for each $i \leq k$,*

- 353 (a) $\text{span}_{X'}(c_i) \subseteq [x_{i-1}, x_i]$, and
 354 (b) $P_i = \{c_1, \dots, c_i\}$ is a prefix of the children of v wrt. σ .

355 **Proof.** Recall that we write C_v and K_v respectively for the set of children of v and the
 356 vertex cover in the conflict graph induced by these children. For each element c of C_v with a
 357 non-empty span, let $x(c) = \max(\text{span}(c))$. For each element w_i of $C_v \setminus K_v$ with an empty
 358 span (taking i for the rank according to the canonical order), let $x(w_i) = x(w_{i-1})$ (and
 359 $x(w_1) = l$ for $i = 1$). For the remaining vertices (in K_v with an empty span), set $x(c) = l$.
 360 Finally, order vertices c_1, \dots, c_k by increasing values of $x(c_i)$ (breaking ties according to the
 361 canonical order when applicable, or arbitrarily otherwise), and set $x_i = x(c_i)$.

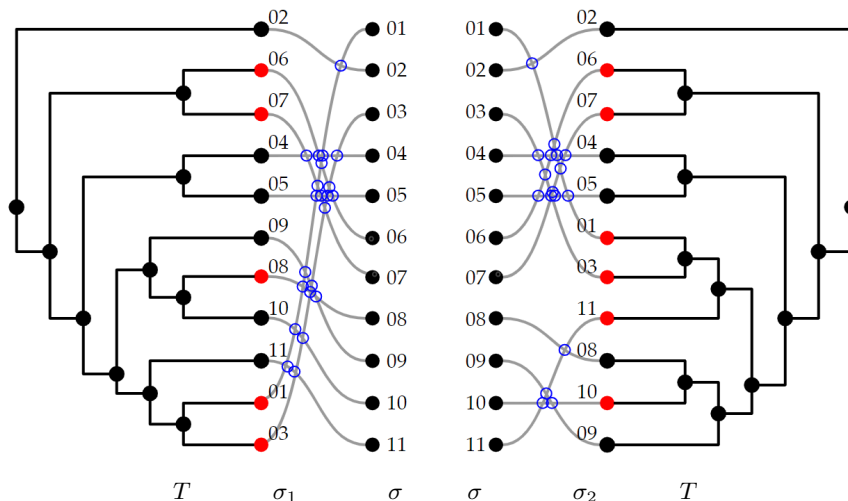
362 Condition (a) follows from the fact that X' is a solution for $OTDE(T, \sigma)$, so that the
 363 span covered by the leaves under siblings do not overlap. For condition (b) we refer to the
 364 definition of prefix: each $P_i \setminus K_c$ is indeed a prefix in the canonical ordering of $C_v \setminus K_v$. ◀

365 The dynamic programming formula follows from the above remark: one can build the
 366 solution by incrementing prefixes one vertex at a time (rather than trying all possible
 367 permutations of children, as in Theorem 4).

368 5 Optimizing OTCM and OTDE are two different things

369 In order to ensure that OTCM and OTDE are actually optimizing different criteria, we
 370 provide in Figure 4 an example of X -tree and an order of its leaves where the order reaching
 371 the best k for a positive answer of the OTCM problem does not provide the optimal value
 372 for the number of leaves to delete in a positive answer of OTDE and where the best k for a
 373 positive answer of the OTDE problem does not provide an optimal value for the number of
 374 inversions for a positive answer of the OTCM problem.

375 We checked the optimality for both criteria by implementing the “naive” dynamic
 376 programming $O(n^2)$ algorithm described in Section 2.1 of [10] to solve the OTCM problem
 377 and the $O(n^4)$ algorithm described in Section 3 to solve the OTDE problem on binary trees.
 378 Both implementations are available in Python, under the GPLv3 licence, at https://github.com/oseminck/tree_order_evaluation, as well as the file `inputCounterExample1.txt`
 379 containing the Newick encoding for the tree of Figure 4.
 380



■ **Figure 4** Two planar embeddings of a rooted tree T : the one on the left is optimal for the OTDE problem (deleting the 5 red leaves makes the order σ suitable on T restricted to the remaining leaves, but the order σ_1 suitable on T has 22 inversions, shown with blue circles, with σ); the other one is optimal for the OTCM problem with the order σ_2 suitable on T having 17 inversions with σ but not for the OTDE problem (6 leaves, for example the 6 red ones, need to be deleted to make the order σ suitable on T restricted to the remaining leaves).

381 6 Experiments and discussion

382 In this section, we investigate the potential for use of OTCM and OTDE in applications
 383 where clustering algorithms are used on distance data which is supposed to reflect some
 384 intrinsic order on the elements, for example the chronological order. We both test the running
 385 time of OTCM and OTDE on real data, and the performance of OTDE on simulated data
 386 to detect possibly misplaced leaves in the order.

tree	# leaves	OTCM time	# inversions	OTDE time	# deleted leaves
Ségur	22	1	40	200	9
Féval	23	2	47	268	8
Aimard	24	1	35	401	8
Lesueur	31	1	48	676	13
Zévaco	29	1	42	727	11
Zola	35	2	60	1203	9
Gréville	36	2	105	2211	18
Ponson	42	3	167	3447	18
Balzac	59	4	248	8292	34
Verne	58	3	183	13446	27
Sand	62	4	283	17557	39

■ **Table 1** Results of our implementations for problems OTCM and OTDE on binary trees generated from corpora of French novels of the 19th century. Time durations are given in milliseconds.

387 The first experiment deals with text data: the CIDRE corpus [20] that contains the works
388 of 11 French 19th century fiction writers dated by year (every file contains a book that is
389 annotated with its year of writing). We apply apply hierarchical clustering on the different
390 corpora using the `AgglomerativeClustering` class from the package `sklearn` [18]. Distance
391 matrices on which the clustering is based are obtained by using the relative frequencies
392 of the 500 most frequent tokens⁴ in each corpus. Distance matrices were generated using
393 the R package `stylo` [8], with the *canberra* distance metric. We obtain the results given in
394 Table 1, which provide the running time in milliseconds of the algorithms we implemented
395 to solve OTCM and OTDE. They show that both algorithms on binary trees are quick
396 enough to handle typical instances of the OTCM and the OTDE problems relevant for digital
397 humanities, a few milliseconds for the first one and a few seconds for the second one, for
398 instances of about 50 elements in the tree and in the order.

399 Our second experiment involves simulated data, to check whether, in the case the tree is
400 built to be consistent with the input order, our algorithm finding the minimum of leaves in
401 the tree to remove inconsistencies with the order is able to detect errors that we intentionally
402 add to the order. We produced 100 instances of the OTDE problem, for each chosen value of
403 n , the number of leaves, and $e < n$, the number of errors, in the following manner:

- 404 1. we randomly pick n distinct integers from the interval $[0, 999]$, which will be our set X of
405 leaves;
- 406 2. we build a distance matrix in which the distance between two elements from X is simply
407 the absolute difference between both; we add some noise to this matrix by adding or
408 subtracting in each cell a random quantity equal to at most 10% of the cell value, obtaining
409 a noisy matrix, from which we build an X-tree T using the `AgglomerativeClustering`
410 class from the package `sklearn`;
- 411 3. we randomly pick a set L_e of e leaves in X and replace their value by another integer,
412 randomly chosen from the interval $[0, 999]$, distinct from other leaf labels; σ is the set of
413 leaves ordered by increasing value taking into account these new values;

⁴ A token is (a part of) a word form or a punctuation marker. The last sentence would yield the following tokens: [“A”, “token”, “is”, “(”, “a”, “part”, “of”, “)””, “a”, “word”, “form”, “text”, “or”, “a”, “punctuation”, “marker”, “.”] Deliberately, we do not use the term “word”, because the word can be seen as a linguistic unit of form and meaning, and henceforward “punctuation marker” would be one word and the period in the end of the sentence would not be one.

$n = \# \text{ leaves}$	$e = \# \text{ errors}$	proportion of cases when $L = L_e$	when $ L - L_e = 1$
20	1	0.79	1
20	2	0.62	0.96
20	3	0.39	0.88
20	4	0.33	0.77
20	5	0.27	0.67
50	1	0.93	1
50	2	0.83	0.99
50	3	0.70	0.98
50	4	0.59	0.91
50	5	0.56	0.90

■ **Table 2** Results of the attempts to perfectly detect the set L_e of randomly relabeled leaves in simulated trees (when $L = L_e$); the situation when $|L - L_e| = 1$ corresponds to finding only $e - 1$ leaves among the e randomly relabeled leaves).

414 4. by solving the OTDE problem on T and σ , we compute the minimum set L of leaves to
 415 remove to make $\sigma[X - L]$ suitable on $T[X - L]$, and check whether $L = L_e$.
 416 This experiment simulates the situation where we would have dating errors on the elements
 417 we clustered in a tree. Note that like in the case of dating errors, the error in our simulation
 418 may not change the overall order on the leaves. Table 2 provides, for each chosen values of
 419 n and e , the proportion of simulated instances of *OTDE* where $L = L_e$, that is when our
 420 algorithm removed exactly the e leaves whose label had been randomly modified. We can
 421 observe that this happens in a majority of cases only when the number of modified leaves is
 422 small compared with the total number of leaves (up to 2 for 20 leaves, up to 4 for 50 leaves).
 423 Solving OTDE still allows to identify $e - 1$ among the e modified leaves in a majority of
 424 cases in all our experiments.

425 7 Conclusion and perspectives

426 In this article, we addressed two problems initially introduced with motivations from bioin-
 427 formatics, OTCM and OTDE. We stated them in a more simple framework with a tree
 428 and an order as input, instead of two trees as was the case when they were introduced,
 429 opening perspectives for new practical uses in digital humanities and proving that they are
 430 not equivalent. We proved that both problems, as well as a problem on two trees, TTDE,
 431 are NP-complete in the general case. We gave a polynomial-time algorithm for OTDE on
 432 trees with fixed maximum degree and an FPT algorithm in a parameter possibly smaller
 433 than the size of the solution for arbitrary trees.

434 We also investigated their potential for practical use, checking that the algorithms we
 435 implemented with open source code in Python to solve them are well suited for applications
 436 in digital humanities in terms of running time. We also observed on simulated data that it is
 437 possible to identify a small number of leaves for which there would be an ordering error if
 438 the tree is built from distance data derived from an order on its leaves. Perspectives include
 439 the search for FPT algorithms, with relevant parameters, for OTCM and TTDE.

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