

# Reordering a tree according to an order on its leaves Laurent Bulteau, Philippe Gambette, Olga Seminck

## ▶ To cite this version:

Laurent Bulteau, Philippe Gambette, Olga Seminck. Reordering a tree according to an order on its leaves. CPM 2022, Jun 2022, Prague, Czech Republic. hal-03413413v1

## HAL Id: hal-03413413 https://hal.science/hal-03413413v1

Submitted on 3 Nov 2021 (v1), last revised 15 Apr 2022 (v2)

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### <sup>2</sup> leaves

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#### <sup>10</sup> — Abstract

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

 $_{25}$  2012 ACM Subject Classification Theory of computation  $\rightarrow$  Parameterized complexity and exact  $_{26}$  algorithms

Keywords and phrases tree, clustering, order, permutation, inversions, FPT algorithm, NP-hardness,
 tree drawing, OTCM, OTDE, TTDE

29 Supplementary Material https://github.com/oseminck/tree\_order\_evaluation

<sup>30</sup> Funding *Philippe Gambette*: "Investissements d'avenir" program, reference ANR-16-IDEX-0003

31 (I-Site Future, programme "Cité des dames, créatrices dans la cité").

Olga Seminck: "Investissements d'avenir" program, reference ANR19-P3IA-0001 (PRAIRIE 3IA
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<sup>&</sup>lt;sup>2</sup> 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

#### <sup>34</sup> **1** Introduction

The problem of optimizing the consistency between a tree and a given order on its leaves 35 was first introduced in bioinformatics in the context of visualization of multiple phylogenetic 36 trees [6], under the name "one-layer STOP (stratified tree ordering problem)". The authors 37 provided an  $O(n^2)$  time algorithm to minimize, by exchanging the left and right children of 38 internal nodes, the number of inversions between the left-to-right order of the leaves of a 39 binary tree and an input order on its leaves. The problem was renamed OTCM (ONE-TREE 40 CROSSING MINIMIZATION) in [9], where an  $O(n \log^2 n)$  time algorithm is provided, as well as 41 a reduction to 3-HITTING SET of a variant of the problem where the goal is to minimize 42 the number of leaves to delete from the tree in order to be able to perfectly match the 43 input order on the remaining leaves, called OTDE (ONE-TREE DRAWING BY DELETING 44 EDGES). An  $O(n \log^2 n / \log \log n)$  time algorithm is later provided for OTCM by [1], improved 45 independently in 2010 by [10] and [21] to obtain an  $O(n \log n)$  time complexity. About OTDE, 46 the authors of [10] note that "the efficient dynamic-programming algorithm derived for the 47 related problem OTCM [...] cannot be transferred to this problem. However, we have no 48 proof for NP-hardness for OTDE nor TTDE, either". TTDE (TWO-TREE DRAWING BY 49 DELETING EDGES) is a variant of OTDE where two leaf-labeled trees are provided as input 50 and the goal is to delete the minimum number of leaves such that the remaining leaves of 51 both trees can be ordered with the same order. We give below an answer to both sentences, 52 providing a dynamic-programming algorithm solving OTDE for trees with fixed maximum 53 degree as well as an NP-hardness proof in the general case for OTDE and for TTDE. 54

Although this problem was initially introduced in the context of comparing tree embed-55 dings, one tree having its embedding (that is the left-to-right order of all children) fixed, 56 we can note that only the order on the leaves of the tree with fixed embedding is useful 57 to define both problems OTCM and OTDE. Both problems therefore consist not really in 58 comparing trees but rather in reordering the internal nodes of one tree in order to optimize 59 its consistency with an order on its leaves provided as input. A popular problem consisting 60 in finding an optimal order on the leaves of a tree is "seriation", often used for visualization 61 purposes [7], where the optimized criterion is computed on data used to build the tree. For 62 example, a classical criterion, called "optimal leaf ordering", is to maximize the similarity 63 between consecutive elements in the optimal order [3, 2, 4]. Another possibility is to minimize 64 a distance criterion, the "bilateral symmetric distance", computed on pairs of elements in 65 consecutive clusters [5]. Seriation algorithms have been implemented for example in the 66 R-packages seriation [12] and dendsort [19]. 67

With the OTCM and OTDE problems, our goal is not to reorder a tree using directly 68 the data used to build it, but using external data about some expected order on its leaves. 69 In the context where the leaves of the tree can be ordered chronologically, for example, this 70 would help providing an answer to the question: how much is this tree consistent with the 71 chronological order? This issue is relevant for several fields of digital humanities, when objects 72 associated with a publication date are classified with a hierarchical clustering algorithm, for 73 example literature analysis [14], political discourse analysis [15] or language evolution [17], 74 as noticed in [11]. 75

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

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

#### 87 1.1 Definitions

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

We say that  $\sigma$  is a strict order on X if it is a bijection from X to [1..n] and that it is a weak order on X if it is a surjection from X to [1..m], where  $|X| \ge m$ . Given any (strict or weak) order  $\sigma$ , we denote by  $a \le_{\sigma} b$  the fact that  $\sigma(a) \le \sigma(b)$  and by  $a <_{\sigma} b$ the fact that  $\sigma(a) < \sigma(b)$ . Considering the elements  $x_1, \ldots, x_n$  of X such that for each  $i \in [1..n-1], \sigma(x_i) \le \sigma(x_{i+1})$ , we denote by  $(x_1x_2\ldots x_n)$  the (weak or strict) order  $\sigma$ .

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

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

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

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

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

**Input:** An X-tree T, an order  $\sigma$  on X and an integer k.

**Output:** Yes if there exists an order  $\sigma'$  on X suitable on T such that the number of inversions for  $\sigma'$  and  $\sigma$  is at most k, no otherwise.

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

123 **Input**: An X-tree T, an order  $\sigma$  on X and an integer k.

**Output:** Yes if there exists a subset X' of X of size at least |X| - k such that  $\sigma[X']$  is suitable on T[X'], no otherwise.

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

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- **Output:** Yes if there exists a subset X' of X of size at least |X| k and an order  $\sigma'$  on X' that is suitable on  $T_1[X']$  and on  $T_2[X']$ , no otherwise.

#### <sup>131</sup> 2 NP-hardness

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

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

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

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

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

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

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

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

<sup>159</sup> 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 <sup>160</sup> 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  $v_j$ <sup>161</sup> in S);

162 for each vertex  $v_i$  not in S we remove  $v'_i$ .

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

<sup>167</sup>  $\Leftarrow$ : Suppose that there exists a set L of at most m + n - k leaves such that  $\sigma(G)[X - L]$ <sup>168</sup> 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 <sup>169</sup> 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  $S = \{v1, v4\}$  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 on the remaining leaves suitable for the order. (2) Reduction from an OTDE instance  $(T, \sigma)$  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  $\sigma$ , and  $T_2$  according to the input tree T.

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 the set L of leaves to be deleted.

We now consider the trees  $T_{e_i}$  for each  $i \in [1..m]$ : by construction of  $\sigma(G)$ , as both leaves 172 of each such tree are separated by some  $B_{i'}$ , therefore by  $n^2 > m + n - k$  leaves, one of these 173 two leaves has to be removed, so it has to belong to L. We call L' the set of such leaves of L. 174 therefore there exists a set L - L' of at most n - k other leaves to delete. So there exists a 175 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 176 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 177  $v_i$  and  $v'_i$  are not in L and all  $e^j_i$  are in L'. We claim that the vertices of G corresponding 178 to  $S_L$  are an independent set of G. Suppose by contradiction that it is not the case, then 179 there exists an edge  $e = e_i^{i'} = e_j^{j'}$  between two vertices  $v_i$  and  $v_j$  of G. By construction of 180 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': 181

182 contradiction.

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

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

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

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

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

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

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

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

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

We now define an instance of the OTCM problem, illustrated in Figure 2. The set X218 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 219 each arc  $(v_i, v_j)$  of G where i < j, taken in the lexicographic order, we add to  $\sigma(G)$  a  $k^{\text{th}}$ 220 supplementary ordered sequence (which we will later call a "block" corresponding to this arc) 221  $v_i^{2k-1}v_j^{2k-1}X_{i,j}^{2k-1}\overline{X}_{i,j}^{2k}v_i^{2k}v_j^{2k}$ , where  $X_{i,j}^{k'}$  is the ordered sequence of  $v_{i'}^{k'}$  where i' ranges from 222 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  $v_{i'}^{k'}$ 223 where i' ranges from n down to 1, excluding i and j). The tree T(G) is made of a root with 224 *n* children  $v_1$  to  $v_n$ , each  $v_i$  having 2m children, the leaves labeled by  $v_i^{k'}$  for  $k' \in [1..2m]$ . 225



**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  $\sigma(G)$ .

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

We first claim that for any  $\sigma'$  suitable for T, there are at least  $2\binom{n}{2}\binom{2m}{2}$  long-range inversions between  $\sigma'$  and  $\sigma(G)$ , and this bound is reached if  $\sigma'$  is vertex-consistent. Indeed, 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 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 respectively in  $L(T, v_i)$  and  $L(T, v_j)$ ). Overall, among  $4\binom{n}{2}\binom{2m}{2}$  such pairs of elements, there are  $2\binom{n}{2}\binom{2m}{2}$  pairs creating an inversion (which is long-range by definition). For the case i = i', note that pairs  $(v_i^k, v_i^{k'})$  do not create any inversion iff  $\sigma'$  is vertex-consistent, which completes the proof of the claim.

Towards counting the number of short-ranged inversions, we say that an arc  $(v_i, v_j)$  of G 239 is satisfied by  $\sigma''$  if  $\sigma''(i) < \sigma''(j)$ . Consider two pairs  $(v_i^{2k-1}, v_i^{2k-1})$  and  $(v_i^{2k}, v_i^{2k})$ . Then 240 these two pairs are necessarily in the same order in  $\sigma'$ . If the  $k^{th}$  arc of G is  $(v_i, v_j)$ , then 241 these two pairs are also in the same order in  $\sigma$ . Note that they (both) form an inversion 242 iff  $(v_i, v_j)$  is not satisfied by  $\sigma''$ . If the k<sup>th</sup> arc of G is any other arc, then exactly one of 243  $(v_i^{2k-1}, v_j^{2k-1}), (v_i^{2k}, v_j^{2k})$  forms an inversion. Overall a pair i, j such that one of  $(v_i, v_j), (v_j, v_i)$ 244 is a satisfied arc yields m-1 short-range inversions, a pair i, j such that one of  $(v_i, v_j), (v_i, v_i)$ 245 is an unsatisfied arc yields m + 1 short-range inversions, and any other pair  $\{i, j\}$  with  $i \neq j$ 246 yields m inversions. Overall, if there are f unsatisfied arcs,  $\sigma'$  yields  $\binom{m}{2} - m + 2f$  inversions. 247 We can now complete the proof with our main claim: G has a feedback arc set of size at 248 most  $f \Leftrightarrow$  the OTCM problem has a solution with at most  $\binom{n}{2}\binom{2m}{2} + \binom{m}{2} - m + 2f$  inversions. 249  $\Rightarrow$ : If G has a feedback arc set F of size f, as G[A-F] is acyclic, we consider an order  $\sigma''$ 250 over n such that for all arcs  $(v_i, v_j)$  in A - F,  $\sigma''(i) < \sigma''(j)$  (i.e.  $\sigma''$  is the topological order 251 of the vertices in G[A-F]). We now order the children  $v_i$  of the root of T(G) according to 252 this order  $\sigma''$  and call  $\sigma'$  the induced order on the leaves of T(G) (also sorting all leaves  $v_i^j$ 253 below each  $v_i$  by increasing values of j). Note that  $\sigma'$  is vertex-consistent, and that an arc 254  $(v_i, v_j)$  is satisfied by  $\sigma''$  iff  $(v_i, v_j) \notin F$ . Thus,  $\sigma'$  yields  $\binom{n}{2}\binom{2m}{2} + \binom{m}{2} - m + 2f$  inversions. 255  $\Leftarrow$ : Consider an order  $\sigma'$  suitable for T with at most  $\binom{n}{2}\binom{2m}{2} + \binom{m}{2} - m + 2f$  inversions. Let 256  $\sigma''$  be the corresponding order on the leaves of the root, and let F be the set of arcs unsatisfied 257 by  $\sigma''$ . Since  $\sigma'$  has at least  $\binom{n}{2}\binom{2m}{2}$  long-range inversions, it has at most  $\binom{m}{2} - m + 2f$ 258 short-range inversions, and  $|F| \leq f$ . Finally, since all arcs in A - F are satisfied by  $\sigma''$ , 259 G[A-F] is acyclic and F is a feedback arc set. 260

#### <sup>261</sup> **3** A polynomial-time algorithm for fixed-degree trees

We start by providing a dynamic providing 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  $\sigma : L(T) \to [1..m]$  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  $\forall l \in \mathcal{X}(v, l, r), \sigma(l) \in [l, r]$ . Note that  $\mathcal{X}(v, l, r)$  also depends on T and  $\sigma$  but we simplify the notation by not mentioning them as they can clearly be identified from the context.

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

$${}_{276} = |\mathcal{X}(v,l,r)| = \max_{\substack{\text{permutation } \pi \text{ of } [1..k] \\ x_1 = l \le x_2 \le \ldots \le x_k \le x_{k+1} = r}} \sum_{i=1}^k |\mathcal{X}(c_{\pi(i)}, x_i, x_{i+1})| \text{ if } v \text{ is an internal node of } T; }$$

for any leaf  $\ell$  of T,  $|\mathcal{X}(\ell, l, r)| = 1$  if  $\sigma(\ell) \in [l, r]$ , 0 otherwise.

**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  $\{c_1, \ldots, c_k\}$  of 281 children. Suppose by contradiction that there exists a set of integers  $l \leq r$  and a subset 282 X' of L(v) of size strictly greater than  $\mathcal{X}(v, l, r)$  such that  $\sigma[X']$  is suitable with T[X'] and 283  $\forall \ell \in X', \sigma(\ell) \in [l, r]$ . We then denote by  $X'_1, \ldots$  and  $X'_k$  the sets of leaves  $L(c_1) \cap X', \ldots$ 284 and  $L(c_k) \cap X'$  respectively. Without loss of generality we consider that the children  $c_i$ 285 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 286 287 for each  $i \in [1..k], |X'_i| \le |\mathcal{X}(v, \min_{\ell \in X'_i} \{\sigma(\ell)\}, \max_{\ell \in X'_i} \{\sigma(\ell)\})|$ , so  $|X'_i| \le |\mathcal{X}(v, m_i, m_{i+1})|$ 288 because  $\left[\min_{\ell \in X'_i} \{\sigma(\ell)\}, \max_{\ell \in X'_i} \{\sigma(\ell)\}\right] \subseteq [m_i, m_{i+1}]$ . Therefore,  $|X'| = \sum_{i=1}^k |X'_i| \leq 1$ 289  $\sum_{i=1}^{k} |\mathcal{X}(v, m_i, m_{i+1})| \text{ so by definition of } \sigma[\mathcal{X}(v, l, r)], |X'| \leq \sigma[\mathcal{X}(v, l, r)]: \text{ contradiction!}$ 290 We therefore obtain a correct solution of  $OTDE(T, \sigma)$  by computing  $\mathcal{X}(\operatorname{root}(T), 0, m)$ . 291

**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  $(T, \sigma)$  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  $\sigma$  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.

#### <sup>299</sup> **4** An FPT algorithm for the *deletion-degree* parameter for OTDE

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

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

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

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

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

Proof. Given a subset X' of X, we say that a node v of T has a deletion if some  $L(v) \not\subseteq X'$ , 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

<sup>&</sup>lt;sup>3</sup> http://fpt.wikidot.com/fpt-races

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

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

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

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

$$|\mathcal{X}(P,l,r)| = \emptyset \text{ if } P$$

339

$$= \max_{\substack{x \in [l..r], u \in P \\ P \setminus \{u\} \text{ prefix of } C_v}} |\mathcal{X}(P \setminus \{u\}, l, x)| + |\mathcal{X}(\{u\}, x, r)|$$

 $= \emptyset$ 

 $|\mathcal{X}(\{v\}, l, r)| = |\mathcal{X}(C_v, l, r)|$ 

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

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

▶ Lemma 7. Let X' be a solution of  $OTDE(T, \sigma)$ ,  $v \in T$  and  $1 \leq l \leq r \leq m$  such that span<sub>X'</sub>(v)  $\subseteq [l, r]$ . Then there exists a permutation (c<sub>1</sub> ... c<sub>k</sub>) of the children of v and integers x<sub>0</sub> =  $l \leq x_1 \leq ... \leq x_k = r$  such that, for each  $i \leq k$ ,

 $_{353}(a) \operatorname{span}_{X'}(c_i) \subseteq [x_{i-1}, x_i], and$ 

354 (b)  $P_i = \{c_1, \ldots, c_i\}$  is a prefix of the children of v wrt.  $\sigma$ .

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

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

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

#### **5** Optimizing OTCM and OTDE are two different things

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

We checked the optimality for both criteria by implementing the "naive" dynamic programming  $O(n^2)$  algorithm described in Section 2.1 of [10] to solve the OTCM problem and the  $O(n^4)$  algorithm described in Section 3 to solve the OTDE problem on binary trees. 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 containing the Newick encoding for the tree of Figure 4.



**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  $\sigma$  suitable on T restricted to the remaining leaves, but the order  $\sigma_1$  suitable on T has 22 inversions, shown with blue circles, with  $\sigma$ ); the other one is optimal for the OTCM problem with the order  $\sigma_2$  suitable on T having 17 inversions with  $\sigma$  but not for the OTDE problem (6 leaves, for example the 6 red ones, need to be deleted to make the order  $\sigma$  suitable on T restricted to the remaining leaves).

#### **6** Experiments and discussion

In this section, we investigate the potential for use of OTCM and OTDE in applications where clustering algorithms are used on distance data which is supposed to reflect some intrinsic order on the elements, for example the chronological order. We both test the running time of OTCM and OTDE on real data, and the performance of OTDE on simulated data 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 19<sup>th</sup> century. Time durations are given in milliseconds.

The first experiment deals with text data: the CIDRE corpus [20] that contains the works 387 of 11 French 19<sup>th</sup> century fiction writers dated by year (every file contains a book that is 388 annotated with its year of writing). We apply apply hierarchical clustering on the different 389 corpora using the AgglomerativeClustering class from the package sklearn [18]. Distance 390 matrices on which the clustering is based are obtained by using the relative frequencies 391 of the 500 most frequent tokens<sup>4</sup> in each corpus. Distance matrices were generated using 392 the R package style [8], with the *canberra* distance metric. We obtain the results given in 393 Table 1, which provide the running time in milliseconds of the algorithms we implemented 394 to solve OTCM and OTDE. They show that both algorithms on binary trees are quick 395 enough to handle typical instances of the OTCM and the OTDE problems relevant for digital 396 humanities, a few milliseconds for the first one and a few seconds for the second one, for 397 instances of about 50 elements in the tree and in the order. 398

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

1. we randomly pick n distinct integers from the interval [0, 999], which will be our set X of leaves;

2. we build a distance matrix in which the distance between two elements from X is simply the absolute difference between both; we add some noise to this matrix by adding or subtracting in each cell a random quantity equal to at most 10% of the cell value, obtaining a noisy matrix, from which we build an X-tree T using the AgglomerativeClustering class from the package sklearn;

<sup>411</sup> **3.** we randomly pick a set  $L_e$  of e leaves in X and replace their value by another integer, <sup>412</sup> randomly chosen from the interval [0, 999], distinct from other leaf labels;  $\sigma$  is the set of <sup>413</sup> leaves ordered by increasing value taking into account these new values;

<sup>&</sup>lt;sup>4</sup> 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", "."] Deliberatly, 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.

$\mathbf{n}=\#$ leaves	e = # 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  $\sigma$ , we compute the minimum set L of leaves to 415 remove to make  $\sigma[X - L]$  suitable on T[X - L], and check whether  $L = L_e$ .

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

#### 425 **7** Conclusion and perspectives

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

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

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