# Combining Tree Partitioning, Precedence, Incomparability, and Degree Constraints, with an Application to Phylogenetic and Ordered-Path Problems

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**Abstract.** The *tree* and *path* constraints, for digraph partitioning by vertex-disjoint trees and paths respectively, are unified within a single global constraint, including a uniform treatment of a variety of useful side constraints, such as precedence, incomparability, and degree constraints. The approach provides a sharp improvement over an existing *path* constraint, but can also efficiently handle tree problems, such as the phylogenetic supertree construction problem. The key point of the filtering is to take partially into account the strong interactions between the tree partitioning problem and all the side constraints.

## 1 Introduction

In [5], we proposed a complete polynomial characterisation of the *tree* constraint, which partitions a given digraph $\mathcal{G}$ into a set of vertex-disjoint anti-arborescences.[1] Our aim now is to extend that original tree partitioning constraint with four kinds of useful side constraints, namely:

- *Precedence constraints* that enforce a partial order on the vertices: a vertex $u$ *precedes* a vertex $v$ if $u$ and $v$ belong to the same tree and there exists a path from $u$ to $v$.
- *Incomparability constraints* that keep some vertices incomparable: two vertices $u$ and $v$ are *incomparable* if they do not belong to the same tree or if there is no path from $u$ to $v$ and no path from $v$ to $u$.
- *Degree constraints* that restrict the in-degrees of the vertices in the tree partition.

[1] A digraph $\mathcal{A}$ is an *anti-arborescence* with *anti-root* $r$ iff there exists a path from all vertices of $\mathcal{A}$ to $r$ and the undirected graph associated with $\mathcal{A}$ is a tree rooted in $r$.Throughout this article, we use for simplicity the term *tree* rather than the term anti-arborescence, and the term *forest* for a set of such trees.

- *Constraints on the number of proper trees* where a *proper tree* is defined as a tree involving at least two vertices.

Many well-known particular cases of digraph partitioning by trees can be tackled using this extended tree constraint, such as the construction of a phylogenetic supertree from given species trees [2, 6, 13, 15], possibly under degree constraints requiring the resulting speciation supertree to be binary, as well as digraph partitioning by paths [10, 17] or circuits [8],[2] which can be done with degree constraints on tree partitions. In general, note how precedence constraints (sometimes also called dominance constraints [3, 17, 20]) can be used to express the vertex ordering inherent in many tree or path problems. Similarly, incomparability constraints can be used to prevent incomparable vertices in trees from becoming comparable, or to force vertices to belong to distinct paths. Finally, degree constraints can be used to get tree partitions limited to paths (which are "unary" trees) or binary trees, for instance.

The main contribution of this article is to show that, by considering the strong interaction between all these additional constraints, one can get a drastically improved filtering algorithm. As a consequence, the corresponding extended *tree* constraint can directly handle partitioning problems such as phylogenetic supertree problems or ordered disjoint path problems, which until now were addressed by distinct approaches.

The extended *tree* constraint has the form $tree(\mathtt{NTREE}, \mathtt{NPROP}, \mathtt{VER})$, where NTREE is a domain variable[3] specifying the number of trees in the forest, NPROP is a domain variable specifying the number of proper trees (i.e., acyclic connected components with at least two vertices [11]) in the forest, and VER is the collection of $n$ vertices $\mathtt{VER}[1], \ldots, \mathtt{VER}[n]$ of the given digraph. Each vertex $v_i = \mathtt{VER}[i]$ has the following attributes, which complete the description of the digraph:

- L is a unique integer in $[1, n]$. It can be interpreted as the *label* of $v_i$.
- F is a domain variable whose domain consists of elements (vertex labels) of $[1, n]$. It can be interpreted as the *unique successor* (or *father*) of $v_i$. Notice that if $i \in dom(\mathtt{VER}[i].\mathtt{F})$ then we said that there is a self-loop on $v_i$.
- P is a possibly empty set of integers, its elements (vertex labels) being in $[1, n]$. It can be interpreted as the set of *mandatory ancestors* (or *precedences*) of $v_i$.
- I is a possibly empty set of integers, its elements (vertex labels) being in $[i + 1, n]$. It can be interpreted as the set of vertices that are *incomparable* with $v_i$.
- D is a domain variable in $[0, n - 1]$. It can be interpreted as the *in-degree* of $v_i$ (thus ignoring the possible self-loop on $v_i$).

For each $i \in [1, n]$, the terms $\mathtt{VER}[i].\mathtt{L}$, $\mathtt{VER}[i].\mathtt{F}$, $\mathtt{VER}[i].\mathtt{P}$, $\mathtt{VER}[i].\mathtt{I}$, and $\mathtt{VER}[i].\mathtt{D}$ respectively denote the L, F, P, I, and D attributes of $\mathtt{VER}[i]$. When speaking of global constraints, it is often convenient to reason about a digraph that models the constraint rather than directly about the constraint. We model the extended *tree* constraint by the digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ in which the vertices represent the elements of VER and the arcs represent the successor relation between them. Formally, $\mathcal{G}$ is defined as follows:

[2] Searching for a circuit in a digraph can be modelled as searching for an elementary path if one of the vertices of the digraph is duplicated.

[3] A *domain variable* $V$ is a variable ranging over a finite set of integers denoted by $dom(V)$; let $\min(V)$ and $\max(V)$ respectively denote the minimum and maximum possible values for $V$.

**Definition 1.** *The* associated digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ *of a* $tree(\texttt{NTREE}, \texttt{NPROP}, \texttt{VER})$ *constraint is defined by* $\mathcal{V} = \{v_i \mid i \in [1, n]\}$ *and* $\mathcal{E} = \{(v_i, v_j) \mid j \in dom(\texttt{VER}[i].\texttt{F})\}$*. Let* $m = |\mathcal{E}|$ *be the number of arcs of this associated digraph.*

A $tree(\texttt{NTREE}, \texttt{NPROP}, \texttt{VER})$ constraint specifies that its associated digraph $\mathcal{G}$ should be a forest of NTREE trees, of which NPROP trees are proper, that fulfils its precedence, incomparability, and degree constraints. Formally:

**Definition 2.** *A ground instance of a* $tree(\texttt{NTREE}, \texttt{NPROP}, \texttt{VER})$ *constraint is said to be* satisfied *if and only if:*

- $\forall i \in [1, n] : \texttt{VER}[i].\texttt{L} = i$.
- *Its associated digraph* $\mathcal{G}$ *consists of* NTREE *connected components.*
- $\mathcal{G}$ *contains* NPROP *connected components involving at least two vertices.*
- *Each connected component of* $\mathcal{G}$ *does not contain any circuit involving more than one vertex.*
- *For every vertex* $\texttt{VER}[i]$*, there exists an elementary path*[4] *in* $\mathcal{G}$ *from* $\texttt{VER}[j]$ *to* $\texttt{VER}[i]$ *for every* $j \in \texttt{VER}[i].\texttt{P}$.
- *For every vertex* $\texttt{VER}[i]$*, there is no path in* $\mathcal{G}$ *from* $\texttt{VER}[i]$ *to* $\texttt{VER}[j]$ *and no path in* $\mathcal{G}$ *from* $\texttt{VER}[j]$ *to* $\texttt{VER}[i]$ *for every* $j \in \texttt{VER}[i].\texttt{I}$.
- *For every vertex* $\texttt{VER}[i]$*, there are* $\texttt{VER}[i].\texttt{D}$ *other vertices* $\texttt{VER}[j]$ *, with* $j \neq i$*, such that* $\texttt{VER}[j]$ *is a predecessor of* $\texttt{VER}[i]$ *(i.e.,* $\texttt{VER}[j].\texttt{F} = i$*) in* $\mathcal{G}$.

Before illustrating Definition 2, let us introduce some terminology that will be used throughout this article.

**Definition 3.** *An arc* $(i, j)$ *of the associated digraph* $\mathcal{G}$ *of a* $tree$ *constraint is an* S-arc *(sure) if* $dom(\texttt{VER}[i].\texttt{F}) = \{j\}$*, otherwise* $(i, j)$ *is an* M-arc *(maybe). A vertex* $i$ *is an* S-succ *if all its out-going arcs are S-arcs, otherwise* $i$ *is an* M-succ*. Similarly, a vertex* $i$ *is an* S-pred *if all its incoming arcs are S-arcs, otherwise* $i$ *is an* M-pred*.*

**Definition 4.** *Given a* $tree(\texttt{NTREE}, \texttt{NPROP}, \texttt{VER})$ *constraint and its associated digraph* $\mathcal{G} = (\mathcal{V}, \mathcal{E})$*, the* fixed-father digraph $\mathcal{G}_{true} = (\mathcal{V}, \mathcal{E}_{true})$ *is defined by* $\mathcal{E}_{true} = \{(i, j) \mid i \neq j \wedge (i, j)$ *is an S-arc of* $\mathcal{G}\}$.

*Example 1.* Consider the constraint $tree(\texttt{NTREE}, \texttt{NPROP}, \texttt{VER})$, where $dom(\texttt{NTREE}) = \{1, 2, 3, 4\} = dom(\texttt{NPROP})$, and the attributes of the vertices are as given in Part (a) of Table 1. The digraph $\mathcal{G}$ is depicted in Figure 1(a). In Figure 1(b) and 1(c), precedence constraints are depicted in dashed arcs, while in 1(c) incomparability constraints are in bidirectional dotted arcs. Observe that the degree constraints have no impact on the number of solutions here, as the largest observed in-degree in $\mathcal{G}$ does not exceed the maximum value of any in-degree variable. Without considering the precedence, incomparability, and degree constraints, this $tree$ constraint has 220 solutions. When considering only the precedence and degree constraints, the $tree$ constraint has two solutions, depicted in Figures 1(b) and 1(c), with $\texttt{NTREE} = 1 = \texttt{NPROP}$ and $\texttt{NTREE} = 2 \wedge \texttt{NPROP} = 1$,

[4] An *elementary path* between two vertices $i$ and $j$ of a digraph $\mathcal{G}$, denoted by $\mathcal{P}_{\langle i,j \rangle}$, is a path from $i$ to $j$ such that all vertices of $\mathcal{P}_{\langle i,j \rangle}$ are distinct.

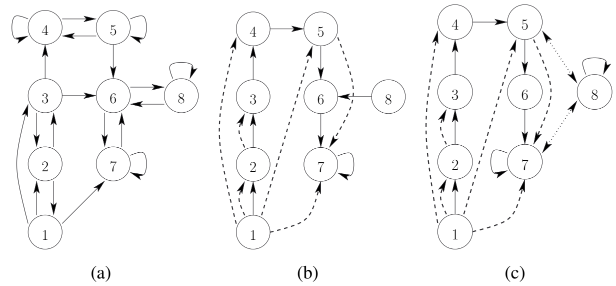


**Fig. 1.** Figure 1(a) the associated digraph $\mathcal{G}$ of the *tree* constraint given in Example 1. Figure 1(b)--1(c) the two only solutions according to the degree and precedence constraints, the latter being depicted by dashed arcs, going from $i$ to $j$ for each $j \in [1, n]$ and each $i \in \texttt{VER}[j].\texttt{P}$. Figure 1(c) the only solution according to the degree, precedence, and incomparability constraints, the latter being depicted by bidirectional dotted arcs, connecting $i$ and $j$ for each $i \in [1, n]$ and each $j \in \texttt{VER}[i].\texttt{I}$. Note that within solution 1(b) the vertices 7 and 8 are comparable.

| $i$ | $\texttt{VER}[i].\texttt{L}$ | Part (a) | | | Part (b) | | Part (c) | | |
|---|---|---|---|---|---|---|---|---|---|
| | | $\texttt{VER}[i].\texttt{F}$ | $\texttt{VER}[i].\texttt{P}$ | $\texttt{VER}[i].\texttt{D}$ | $\texttt{VER}[i].\texttt{F}$ | $\texttt{VER}[i].\texttt{D}$ | $\texttt{VER}[i].\texttt{F}$ | $\texttt{VER}[i].\texttt{I}$ | $\texttt{VER}[i].\texttt{D}$ |
| 1 | 1 | $\{2, 3, 7\}$ | $\emptyset$ | $[0, 4]$ | $\{2\}$ | $\{0\}$ | $\{2\}$ | $\emptyset$ | $\{0\}$ |
| 2 | 2 | $\{1, 3\}$ | $\{1\}$ | $[0, 4]$ | $\{3\}$ | $\{1\}$ | $\{3\}$ | $\emptyset$ | $\{1\}$ |
| 3 | 3 | $\{2, 4, 6\}$ | $\{2\}$ | $[0, 4]$ | $\{4\}$ | $\{1\}$ | $\{4\}$ | $\emptyset$ | $\{1\}$ |
| 4 | 4 | $\{4, 5\}$ | $\{1\}$ | $[0, 4]$ | $\{5\}$ | $\{1\}$ | $\{5\}$ | $\emptyset$ | $\{1\}$ |
| 5 | 5 | $\{4, 5, 6\}$ | $\{1\}$ | $[0, 4]$ | $\{6\}$ | $\{1\}$ | $\{6\}$ | $\{8\}$ | $\{1\}$ |
| 6 | 6 | $\{7, 8\}$ | $\emptyset$ | $[0, 4]$ | $\{7\}$ | $\{2\}$ | $\{7\}$ | $\emptyset$ | $\{1\}$ |
| 7 | 7 | $\{6, 7\}$ | $\{1, 5\}$ | $[0, 4]$ | $\{7\}$ | $\{1\}$ | $\{7\}$ | $\{8\}$ | $\{1\}$ |
| 8 | 8 | $\{6, 8\}$ | $\emptyset$ | $[0, 4]$ | $\{6\}$ | $\{0\}$ | $\{8\}$ | $\emptyset$ | $\{0\}$ |

**Table 1.** Part (a) provides the domains of the father and degree variables depicted by Figure 1(a), as well as the set of precedence constraints. Part (b) gives a solution for the instance depicted by Figure 1(a). Part (c) provides a solution for the instance depicted by Figure 1(a) enriched by the set of incomparability constraints.

respectively. Finally, when also considering the incomparability constraints, the *tree* constraint has a single solution, given in Figure 1(c). Note that, since in Figure 1(a) no father variables are fixed, all arcs are M-arcs and all vertices are M-succs and M-preds. As a consequence, $\mathcal{G}_{true}$ does not contain any arcs.

The rest of this article is organised as follows. First, temporarily ignoring the incomparability, degree, and number-of-proper-trees constraints, Section 2 provides necessary conditions for partitioning the associated digraph $\mathcal{G}$ of a *tree* constraint into trees according to a potential number of trees and a set of precedence constraints only. Since achieving arc-consistency for even this constraint is NP-hard, some pruning rules are derived from relaxations of these necessary conditions. Next, Section 3 completes those results by also considering the incomparability constraints. New necessary conditions are added to ensure that there exists at least one tree partitioning of $\mathcal{G}$ according to the precedence and incomparability constraints. Moreover, some pruning rules are derived to enhance the pruning proposed in the previous section. Then, Section 4 shows how to model the degree constraints by adapting the flow model of the global cardinality constraint [18] in order to ignore self-loops.[5] Next, the number-of-proper-trees constraint is considered in Section 5. To summarise the theoretical results so far, Section 6 provides a synthetic overview of all propositions of the different aspects of the *tree* constraint. It shows that many interactions between the tree partitioning, precedence, incomparability, and number-of-proper-trees constraints have been taken into account to improve the filtering. Section 7 then presents our experimental results with the extended *tree* constraint, including on the problems of constructing a supertree of given phylogenetic species trees and an ordered simple path with mandatory vertices. Finally, Section 8 reviews related work, discusses future work and concludes.

## 2 Combining the Tree Partitioning and Precedence Constraints

We show how to extend the work on the original *tree* constraint [5] in order to take into account precedence constraints. In Section 2.1, we provide a normal form for a set of precedence constraints and indicate how it can be dynamically updated whenever a new father variable becomes fixed. Then, in Section 2.2, we argue that this normal form can also be updated in the presence of information derived from the associated digraph $\mathcal{G}$ of the *tree* constraint. Next, in Section 2.3, we show how to exploit this normal form in order to get a tighter upper bound on the number NTREE of trees. In Section 2.4, we identify necessary feasibility conditions from the precedence constraints. Finally, in Section 2.5, we derive filtering rules from these necessary conditions.

### 2.1 Normalising a Set of Precedence Constraints

We first show how to handle the precedence constraints provided by the P attributes of the VER collection, and this independently of the tree partitioning constraint. Observe that the set of precedence constraints increases as father variables get fixed: the assignment $\mathtt{VER}[i].\mathtt{F} = j$ adds a new precedence constraint, namely $i \in \mathtt{VER}[j].\mathtt{P}$. Towards this, we maintain a normal form of the precedence digraph obtained from all the precedence constraints.

**Definition 5.** *The* precedence digraph $\mathcal{G}_p = (\mathcal{V}, \mathcal{E}_p)$ *of a* $tree(\mathtt{NTREE}, \mathtt{NPROP}, \mathtt{VER})$ *constraint with associated digraph* $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ *has as arc set* $\mathcal{E}_p$ *the transitive reduction of* $\{(i, j) \mid i \in \mathtt{VER}[j].\mathtt{P}\}$. *An arc* $(i, j) \in \mathcal{E}_p$ *is called a* precedence arc*, or* P-arc *for short.*

We can derive a trivial necessary condition for the feasibility of a set of precedence constraints according to a *tree* constraint:

**Proposition 1.** *If a tree constraint is feasible, then there do not exist any circuits in the precedence digraph.*

*Proof.* Trivially derived from the definition of a precedence. □

[5] Ignoring the fact that the $i$-th father variable $\mathtt{VER}[i].\mathtt{F}$ is eventually assigned value $i$.

**Algorithm 1** Adding an arc $(i, j)$ to $\mathcal{G}_p$

1. **Checking feasibility:**
   Perform a first depth-first search (DFS) from vertex $j$, using the successor links of $\mathcal{G}_p$, and mark by 1 all the reached vertices and $j$. If $i$ is reached, then generate a failure, since a circuit was detected.
2. **Checking that $(i, j)$ is not a transitive arc:**
   Perform a second DFS from $i$ to search for $j$. If $j$ is reached then exit, as the arc $(i,j)$ is transitive and $\mathcal{G}_p$ remains unchanged (i.e., $(i,j)$ is not added to $\mathcal{G}_p$). During this second DFS, we skip the vertices reached in Step 1, since $\mathcal{G}_p$ does not contain any circuits.
3. **Removing transitive arcs:**
   Perform a third DFS from $i$, using the predecessor links of $\mathcal{G}_p$, and mark by 2 all the reached vertices as well as $i$. Remove from $\mathcal{G}_p$ all arcs $(k,l)$ where $k$ is 2-marked and $l$ is 1-marked.
4. **Updating $\mathcal{G}_p$:**
   Add the arc $(i,j)$ to $\mathcal{G}_p$.

The precedence digraph of a feasible *tree* constraint is thus a Hasse digraph, that is an acyclic digraph without any transitive arcs [1]. When a *tree* constraint is posted, the precedence digraph $\mathcal{G}_p = (\mathcal{V}, \mathcal{E}_p)$ is created, using the algorithm given by [14], with a time complexity of $O(n \cdot |\mathcal{E}_p|)$. Then, each time a father variable VER$[i]$.F is fixed to some $j$ (with $j \neq i$), for instance during search, we add the arc $(i, j)$ to $\mathcal{G}_p$ by using Algorithm 1, which has a worst-case complexity of $O(n + |\mathcal{E}_p|)$ time.

*Example 2.* Consider the *tree* constraint given by Figure 2(a) and assume that the father variable for vertex 3 is instantiated to vertex 6. Figure 2(b) depicts the state of $\mathcal{G}$ and $\mathcal{G}_p$ after normalisation: the transitive arc $(3, 5)$ was removed from $\mathcal{G}_p$ when the arc $(3, 6)$, in bold, was added.

### 2.2 Deriving Precedence Constraints from $\mathcal{G}$

We saw in the previous sub-section that each time some father variable VER$[i]$.F is fixed to some $j$ (that is, each time some $(i, j)$ becomes an S-arc), a new precedence constraint is created and added to $\mathcal{G}_p$. However, there also exist some precedence constraints in $\mathcal{G}_p$ that can never be *directly* satisfied, because there exist arcs $(u, v)$ in $\mathcal{G}_p$ that are not in $\mathcal{G}$. We thus introduce some updating rules (Propositions 2 to 5 below) for the precedence digraph $\mathcal{G}_p$ that add new precedence constraints and replace some precedence constraints that can never be directly satisfied. Let us first show the intuition of these updates on an example.

*Example 3.* Consider again the *tree* constraint given by Figure 2(b). Then, Figure 2(c) depicts the precedence digraph $\mathcal{G}_p$ enriched by new precedence constraints:

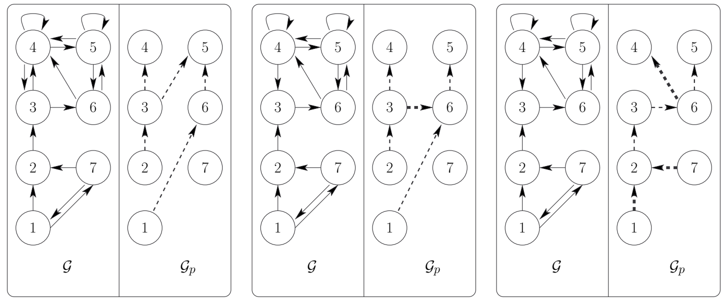



**Fig. 2.** 2(a) The digraphs $\mathcal{G}$ and $\mathcal{G}_p$ of a *tree* constraint before instantiation of the father variable for vertex 3 to vertex 6. 2(b) The digraphs $\mathcal{G}$ and $\mathcal{G}_p$ after the choice of the arc $(3, 6)$ and normalisation, where $(3, 6)$ is a new precedence (bold dashed arc). 2(c) The digraph $\mathcal{G}_p$ after adding and replacing precedence constraints, where the new precedences are the bold dashed arcs.

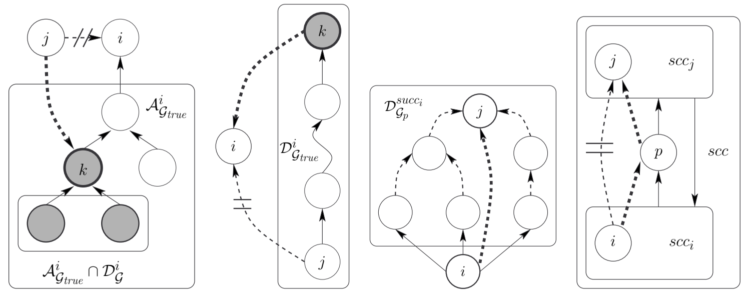
- From $\mathcal{G}_p$, the vertex $1$ precedes $6$. Moreover, observe that if $2$ is removed from $\mathcal{G}$ then there are no more paths from $1$ to $6$ in $\mathcal{G}$. As a consequence, the vertex $1$ must precede $2$ and $(1, 6)$ becomes a transitive arc of $\mathcal{G}_p$.
- As $3$ has only successor $6$ in $\mathcal{G}$, the precedence $(3, 4)$ cannot be directly satisfied. As a consequence, the precedence $(3, 4)$ is replaced by $(6, 4)$.
- Since, within $\mathcal{G}$, all paths from $7$ to a vertex having a self-loop contain the vertex $2$, the vertex $7$ precedes $2$.

The first two propositions below consider a precedence constraint $(j, i)$ such that $i \notin dom(\texttt{VER}[j].\texttt{F})$ and either all predecessors of $i$ in $\mathcal{G}$ are already known (i.e., vertex $i$ is an S-pred), or the successor of $j$ is already fixed. In this context, one can try to replace the precedence $(j, i)$. We first need to introduce a terminology and notation derived from [4] for specifying the descendants and ascendants of a given digraph $G$.

**Definition 6.** *Let $u$ and $v$ be two, not necessarily distinct, vertices of a digraph $G = (V, E)$. We say that $v$ is a* descendant *of $u$ in $G$ (and $u$ is an* ascendant *of $v$ in $G$), which is denoted by $u \lhd_G^* v$, if there exists a path from $u$ to $v$ in $G$. The set of descendants of $u$ in $G$ is denoted by $\mathcal{D}_G^u = \{v \in V \mid u \lhd_G^* v\}$, and the set of ascendants of $v$ in $G$ is denoted by $\mathcal{A}_G^v = \{u \in V \mid u \lhd_G^* v\}$.*

At any given stage, consider for a vertex $i$ the set $\mathcal{A}^i_{\mathcal{G}_{true}}$ of its mandatory ancestors in $\mathcal{G}$ (i.e., the vertices $k$ such that there is a path from $k$ to $i$ in $\mathcal{G}_{true}$). Now, consider the restriction of $\mathcal{A}^i_{\mathcal{G}_{true}}$ to the vertices reachable from $j$ in $\mathcal{G}$ (i.e., $\mathcal{A}^i_{\mathcal{G}_{true}} \cap \mathcal{D}^j_{\mathcal{G}}$). Since $j$ has to precede $i$, there must be a path, in $\mathcal{G}$, from $j$ to one of the vertices of $\mathcal{A}^i_{\mathcal{G}_{true}} \cap \mathcal{D}^j_{\mathcal{G}}$. As a consequence, we get the following propositions, illustrated by Figure 3(a) and Figure 3(b).

**Proposition 2.** *A precedence $(j, i) \in \mathcal{E}_p$ is replaced by a precedence $(j, k)$ such that $k$ is the first common descendant of the vertices of $\mathcal{A}^i_{\mathcal{G}_{true}} \cap \mathcal{D}^j_{\mathcal{G}}$.*




(a) Proposition 2 (b) Proposition 3 (c) Proposition 4 (d) Proposition 5

**Fig. 3.** Plain arcs represent arcs of $\mathcal{G}$, while dashed arcs represent arcs of $\mathcal{G}_p$. Dashed and bold arcs represent new precedences found by the propositions while barred arcs represent old precedence constraints which are removed. Within graph 3(d), $scc$ represents the original strongly connected component containing the vertices $i$, $j$, and $p$, while $scc_i$ and $scc_j$ represent the two strongly connected components obtained after removing $p$.

**Proposition 3.** *A precedence $(j, i) \in \mathcal{E}_p$ is replaced by a precedence $(k, i)$ such that $k$ is the sink of $\mathcal{G}_{true}$ contained in $\mathcal{D}^j_{\mathcal{G}_{true}}$.*

The following two propositions characterise conditions on $\mathcal{G}$ and $\mathcal{G}_p$ from which new arcs can be added to $\mathcal{G}_p$ (see Figures 3(c) and 3(d)).

**Proposition 4.** *For each pair of vertices $i$, $j$ such that $j$ is the first common descendant in $\mathcal{G}_p$ of the possible successors of $i$ in $\mathcal{G}$, the arc $(i, j)$ can be added to $\mathcal{G}_p$.*

*Proof.* Consider the set $\mathcal{S}$ of possible successors of a vertex $i$ of $\mathcal{G}$. If there exists a first common descendant $j$ in $\mathcal{G}_p$ for the vertices of $\mathcal{S}$, then for every $k \in \mathcal{S}$ there exists a path from $k$ to $j$ in any solution to the $tree$ constraint. As a consequence, there also exists a path from $i$ to $j$ and the precedence $(i, j)$ can be added to $\mathcal{G}_p$. □

Before introducing the next proposition, we need to present the notion of strong articulation point.

**Definition 7.** *A* strong articulation point *of a strongly connected digraph G is a vertex such that, if we remove it, G is broken into at least two strongly connected components.*

**Proposition 5.** *Given the associated digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and the precedence digraph $\mathcal{G}_p = (\mathcal{V}, \mathcal{E}_p)$ of a $tree$(`NTREE`, `NPROP`, `VER`) constraint, consider an arc $(i, j) \in \mathcal{E}_p$ and a strong articulation point $p$ of $\mathcal{G}$. If there does not exist a path from $i$ to $j$ in $\mathcal{G} \setminus \{p\}$, then the two arcs $(i, p)$ and $(p, j)$ can be added to $\mathcal{G}_p$.*

*Proof.* If there exists an arc $(i, j)$ in $\mathcal{E}_p$, then in any solution there exists a path from $i$ to $j$. Moreover, if the withdrawal of a strong articulation point $p$ implies that $i$ cannot reach $j$, then there exists a path from $i$ to $p$ and a path from $p$ to $j$, hence $(i, p)$ and $(p, j)$ are mandatory precedence arcs. □

### 2.3 Upper Bound on the Number of Trees According to Precedence Constraints

We now provide an upper bound on the number of trees that partition the associated digraph $\mathcal{G}$ of a *tree* constraint, according to the precedence digraph $\mathcal{G}_p$. We first introduce the notion of potential roots of those trees, namely the vertices with a self-loop in $\mathcal{G}$.

**Definition 8.** *A* potential root $r$ *is a vertex such that* $r \in \texttt{VER}[r].\texttt{F}$.

A first upper bound, given in [5] and denoted by MAXTREE, is the number of potential roots of $\mathcal{G}$. Since this bound does not consider the precedence constraints, we now provide a tighter bound that considers $\mathcal{G}_p$ as well. The idea is to count among the connected components of $\mathcal{G}_p$ those that are necessarily connected to another one. For this purpose, a $\{0,1\}$-value is associated to each connected component $C_i$ of $\mathcal{G}_p$, depending on whether there is a vertex in $C_i$ whose potential father vertices are all outside $C_i$.

**Definition 9.** *For each connected component $C_i$ of the precedence digraph $\mathcal{G}_p$ of a tree constraint, let:*

$$out_i = \begin{cases} 1 & \textit{if } \exists u \in C_i : \forall v \in dom(\texttt{VER}[u].\texttt{F}) : v \notin C_i \\ 0 & \textit{otherwise} \end{cases}$$

**Proposition 6.** *Given a tree*(NTREE, NPROP, VER) *constraint and its precedence digraph $\mathcal{G}_p$, consisting of $k$ connected components, an upper bound on* NTREE *is:*

$$\texttt{MAXTREE}_{\mathcal{G}_p} = k - \sum_{i=1}^{k} out_i$$

*Proof.* From Definition 9. □

**Proposition 7.** $\texttt{MAXTREE}_{\mathcal{G}_p}$ *is tighter than* MAXTREE.

*Proof.* Let $p = \texttt{MAXTREE}$ be the number of potential roots of $\mathcal{G}$. We know that:

$$k - p \leq \sum_{i=1}^{k} out_i \leq k$$

Hence:

$$0 \leq k - \sum_{i=1}^{k} out_i \leq p$$

Thus, we showed that $0 \leq \texttt{MAXTREE}_{\mathcal{G}_p} \leq \texttt{MAXTREE}$. □

### 2.4 Feasibility of a *tree* Constraint According to the Precedence Constraints

We now give necessary conditions for the feasibility of a *tree* constraint that consider the interaction between the associated digraph $\mathcal{G}$ and the precedence digraph $\mathcal{G}_p$. We first recall the necessary and sufficient feasibility conditions (Proposition 8) for the original *tree* constraint [5], which still apply in our context but only as necessary conditions. Since these conditions ignore precedences, we then introduce new necessary conditions (in Proposition 9) for the extended *tree* constraint and show that their evaluation is NP-complete (Proposition 10). Finally, we derive from Proposition 9 a set of necessary conditions (Propositions 11 and 12) that can be evaluated in polynomial time. Before recalling in Proposition 8 the necessary feasibility conditions [5] obtained for the original *tree* constraint, we need to introduce some concepts.

**Definition 10.** *A strongly connected component of the associated digraph $\mathcal{G}$ of a tree constraint that contains at least one potential root is called a* rooted component*.*
*A strongly connected component of $\mathcal{G}$ that has no out-going arcs is called a* sink component*.*

**Proposition 8 ([5]).** *There is a solution to a $tree(\mathtt{NTREE}, \mathtt{VER})$ constraint iff the following conditions hold:*

1. *All the sink components of the associated digraph $\mathcal{G}$ are rooted components.*
2. *$dom(\mathtt{NTREE}) \cap [\mathtt{MINTREE}, \mathtt{MAXTREE}] \neq \emptyset$, where $\mathtt{MINTREE}$ is the number of sink components in $\mathcal{G}$ and $\mathtt{MAXTREE}$ is the number of potential roots in $\mathcal{G}$.*

We now provide general necessary conditions (Proposition 9) for the extended *tree* constraint that consider the precedence and tree partitioning constraints. We first need to introduce the notion of compatibility of an arc of $\mathcal{G}$ with $\mathcal{G}_p$.

**Definition 11.** *An arc $(u, v)$, with $u \neq v$, of $\mathcal{G}$ is* compatible *with $\mathcal{G}_p$ if there does not exist an elementary path from $v$ to $u$ in $\mathcal{G}_p$ and there does not exist a path of length $> 1$ from $u$ to $v$ in $\mathcal{G}_p$.*

The intuition of the next proposition is that, for each vertex $u$ of the associated digraph $\mathcal{G}$ of a *tree* constraint, there should exist an elementary path, from $u$ to a potential root, in $\mathcal{G}$ that contains all the descendants of $u$ in the precedence digraph $\mathcal{G}_p$, such that each arc of this elementary path is compatible with $\mathcal{G}_p$.

**Proposition 9.** *If a $tree$ constraint is feasible, then, for each vertex $u$ of the associated digraph $\mathcal{G}$, there exists an elementary path $\mathcal{P}_{\langle u,r\rangle}$ in $\mathcal{G}$, where $r$ is a potential root, such that:*

1. *For each vertex $v \in \mathcal{P}_{\langle u,r\rangle}$, the set $\mathcal{D}^v_{\mathcal{G}_p}$ is included in the vertices of $\mathcal{P}_{\langle v,r\rangle}$.*
2. *Each arc $(v, w)$ of $\mathcal{P}_{\langle u,r\rangle}$ is compatible with the precedence digraph $\mathcal{G}_p$.*

**Proposition 10.** *Checking Proposition 9 is NP-complete.*

*Proof.* Figure 4 shows a configuration of constraints where checking Proposition 9 is equivalent to searching for a Hamiltonian path in $\mathcal{G}$. Since the precedence digraph $\mathcal{G}_p$ consists of a single connected component with a single source and four sinks, by definition of *tree*, all sinks have to be located on an elementary path starting from the source. Thus, for this configuration, checking Proposition 9 may be reduced to the `HAM-PATH` problem [12, p. 199], which is an NP-complete problem. □

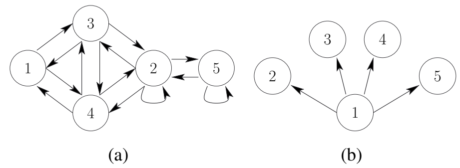



**Fig. 4.** 4(a) The associated digraph $\mathcal{G}$. 4(b) The precedence digraph $\mathcal{G}_p$. The two only solutions are the Hamiltonian paths $\langle 1, 3, 4, 2, 5\rangle$ and $\langle 1, 4, 3, 2, 5\rangle$.

We now present polynomial-time necessary conditions involving precedences and show that they are derived from the general necessary conditions of Proposition 9. Beyond checking whether each arc of a ground instance of a *tree* constraint is compatible with the precedence digraph, the following proposition ensures that all the precedence constraints will be effectively represented in a ground instance of a *tree* constraint. It is derived from a relaxation of Condition 1 of Proposition 9.

**Proposition 11.** *If a tree constraint is feasible, then, for each vertex $u$ of the associated digraph $\mathcal{G}$, we have $\mathcal{D}^u_{\mathcal{G}_p} \subseteq \mathcal{D}^u_{\mathcal{G}}$, where $\mathcal{G}_p$ is the precedence digraph.*

*Proof.* Assume that there exists a vertex $w \in \mathcal{D}^u_{\mathcal{G}_p}$ such that $w \notin \mathcal{D}^u_{\mathcal{G}}$. Then, for each vertex $v \in \mathcal{D}^w_{\mathcal{G}_p}$, the precedence constraint $(v, w)$ cannot be respected in $\mathcal{G}$. □

The next proposition, derived from Proposition 9, shows how to check whether there exists a feasible potential root in each sink component of $\mathcal{G}$.

**Proposition 12.** *If a tree constraint is feasible, then, in each sink component of the associated digraph $\mathcal{G}$, there exists a potential root $r$ that is a sink in the precedence digraph $\mathcal{G}_p$.*

*Proof.* The potential root $r$ mentioned in Proposition 9 has to be a sink in $\mathcal{G}_p$, otherwise Condition 1 of Proposition 9, namely $\mathcal{D}^u_{\mathcal{G}_p} \subseteq \mathcal{P}_{\langle v,r\rangle}$, cannot hold. □

The overall time complexity for checking the feasibility of an extended *tree* constraint mentioning precedences is $O(n \cdot m)$, since:

- Proposition 8 (with `MAXTREE` replaced by $\texttt{MAXTREE}_{\mathcal{G}_p}$) can be checked in $O(n+m)$ time, as shown in [5].
- Proposition 11 can be checked by the lines 2-8 of Algorithm 2 in $O(n \cdot m)$ time.
- Proposition 12 can be checked by the lines 9-10 of Algorithm 2 in $O(n \cdot m)$ time.

### 2.5 Filtering Related to the Precedence Constraints

In the previous sub-section, Proposition 9 was used to derive necessary conditions that can be evaluated in polynomial time. We now show how to further exploit Proposition 9 for pruning the arcs of $\mathcal{G}$ according to the precedence constraints.

**Algorithm 2** Checking feasibility according to Propositions 11 – 12

1. **For each** sink component $\mathcal{S}_i$ of $\mathcal{G}$ **do** $s_i \leftarrow \mathit{false}$;
2. **For each** vertex $u$ of $\mathcal{G}$ **do**
3. Mark the descendants of $u$ in $\mathcal{G}_p$ with a first DFS;
4. Make a second DFS from $u$ in $\mathcal{G}$ in the following way:
5. **For each** arc $(v, w)$ encountered **do**
6. **If** vertex $w$ is a descendant of vertex $u$ in $\mathcal{G}_p$ **then**
7. $w$ is marked as reached;

// *Proposition 11*

8. **If** not all the descendants of $u$ in $\mathcal{G}_p$ have been reached by this second DFS **then** `fail`;
9. **If** $u$ is a potential root contained in a sink component $\mathcal{S}_i$ **and** $u$ is a sink in $\mathcal{G}_p$ **then** $s_i \leftarrow \mathit{true}$;

// *Proposition 12*

10. **If** there exists a sink component $\mathcal{S}_i$ with $s_i = \mathit{false}$ **then** `fail`;

**Proposition 13.** *For each pair of vertices $u, v \in \mathcal{V}$ such that $(u, v)$ is not compatible with the precedence digraph $\mathcal{G}_p$, the arc $(u, v)$ is infeasible.*

**Proposition 14.** *All the arcs $(u, v)$ of $\mathcal{G}$, such that $\mathcal{D}^u_{\mathcal{G}_p} \nsubseteq \mathcal{D}^v_{\mathcal{G}}$, are infeasible.*

*Proof.* Let us suppose that there exists $u' \in \mathcal{D}^u_{\mathcal{G}_p}$, such that $u' \notin \mathcal{D}^v_{\mathcal{G}}$, then the precedence constraint $(u, u')$ is violated if the arc $(u, v)$ is enforced in $\mathcal{G}$, thus $(u, v)$ is infeasible. □

**Proposition 15.** *For each potential root $r$ of $\mathcal{V}$ that is not a sink in $\mathcal{G}_p$, the arc $(r, r)$ is infeasible.*

Similarly to the definition of compatible arc of $\mathcal{G}$ with $\mathcal{G}_p$ (see Definition 11), we now introduce the definition of compatible arc of the reduced digraph of $\mathcal{G}$ with $\mathcal{G}_p$. The *reduced digraph* $\mathcal{G}_r$ is derived from $\mathcal{G}$ in the following way: to each strongly connected component of $\mathcal{G}$ we associate a vertex of $\mathcal{G}_r$; to each arc of $\mathcal{G}$ that connects different strongly connected components corresponds an arc in $\mathcal{G}_r$ (multiple arcs from a given strongly connected component to another strongly connected component are merged).

**Definition 12.** *A transitive arc $(u_r, v_r)$ of $\mathcal{G}_r$ is* compatible *with $\mathcal{G}_p$ if there does not exist any $w_r$ belonging to an elementary path $\mathcal{P}_{\langle u_r, v_r \rangle}$ (with $w_r \notin \{u_r, v_r\}$), such that there exist $u \in u_r$ and $w \in \mathcal{D}^u_{\mathcal{G}_p}$ (with $w \in w_r$).*

**Proposition 16.** *For each pair of vertices $u_r, v_r$ of $\mathcal{G}_r$ such that the arc $(u_r, v_r)$ is not compatible with the precedence digraph $\mathcal{G}_p$, all the arcs $(u, v)$ in $\mathcal{G}$, such that $u \in u_r$ and $v \in v_r$, are infeasible.*

*Proof.* Since $w \in \mathcal{D}^u_{\mathcal{G}_p}$, there must exist a path from $u$ to $w$ in $\mathcal{G}$ (see Figure 5). If an arc $(u', v')$ ($u' \in u_r$ and $v' \in v_r$) is enforced in $\mathcal{G}$ then there does not exist anymore paths from $u$ to $w$ since $w$ cannot be reached anymore from $v'$ (i.e., $\mathcal{G}_r$ does not contain any circuit). □

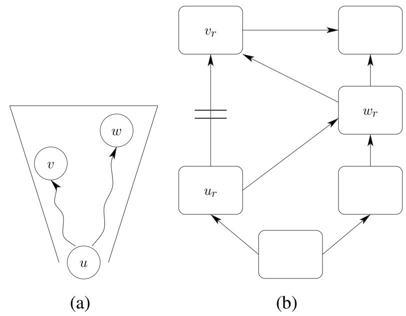



**Fig. 5.** 5(a) The set of descendants of $u$ in $\mathcal{G}_p$. 5(b) $\mathcal{G}_r$ such that each vertex (subscripted by $r$) represents a strongly connected component of $\mathcal{G}_p$.

Algorithm 3 removes the infeasible arcs detected by Propositions 13, 14, 15, and 16 in $O(n \cdot m)$ time. Indeed, the time complexity is dominated by the complexity of computing the transitive closures (lines 1-2) inherent to the precedence digraph $\mathcal{G}_p$ and the digraph $\mathcal{G}$.

## 3 Taking into Account the Incomparability Constraints

We now show how to extend the results of Section 2 in order to take into account the incomparability constraints. In Section 3.1, we characterise hidden incomparability constraints, in order to improve the detection of infeasible arcs in $\mathcal{G}$. Finally, in Section 3.3, we derive filtering rules from these necessary conditions.

### 3.1 Deriving Incomparability Constraints from $\mathcal{G}_p$

Section 2 has shown that new precedence constraints can be added as the father variables get progressively fixed. Similarly, the next proposition shows that the precedence digraph $\mathcal{G}_p$ implicitly contains more and more incomparability constraints as new precedences are dynamically added. As a consequence, detecting the structural incomparability constraints hidden in $\mathcal{G}_p$ leads to improving the filtering dedicated to incomparability constraints.

**Proposition 17.** *For each pair of incomparable vertices $u, v$, all the ancestors of $u$ in $\mathcal{G}_p$ are incomparable with all the ancestors of $v$ in $\mathcal{G}_p$ (see Figure 6).*

*Proof.* First, suppose that a path from $w_u \in \mathcal{A}^u_{\mathcal{G}_p}$ to $w_v \in \mathcal{A}^v_{\mathcal{G}_p}$ is enforced in $\mathcal{G}$. Then in all solutions there must exist a path from $w_u$ to $u$ as well as a path from $w_v$ to $v$ (in order to respect precedence constraints). But such a path starts from $w_u$ and reaches $w_v$, $u$, and $v$, which is impossible because of the precedence constraints $(w_u, u)$ and $(w_v, v)$. So there does not exist any path from $w_u$ to $w_v$ in $\mathcal{G}$. Similarly, there does not exist any path from $w_v$ to $w_u$ in $\mathcal{G}$. $\square$

**Algorithm 3** Filtering according to Propositions 13-16

1. Compute the transitive closure $\mathcal{T}(\mathcal{G}_p)$ of $\mathcal{G}_p$;
2. Compute the transitive closure $\mathcal{T}(\mathcal{G})$ of $\mathcal{G}$;
   *// Proposition 13*
3. **For each** arc $(u,v) \in \mathcal{G}$ such that $(u,v) \in \mathcal{T}(\mathcal{G}_p)$ **and** $(u,v) \notin \mathcal{G}_p$ **do**
4.   Remove $(u,v)$ from $\mathcal{G}$;
5. **For each** arc $(u,v) \in \mathcal{G}$ such that $(v,u) \in \mathcal{T}(\mathcal{G}_p)$ **do**
6.   Remove $(u,v)$ from $\mathcal{G}$;
   *// Proposition 14*
7. **For each** arc $(u,v) \in \mathcal{G}$ such that $\exists (u,w) \in \mathcal{T}(\mathcal{G}_p)$ **and** $(v,w) \notin \mathcal{T}(\mathcal{G})$ **do**
8.   Remove $(u,v)$ from $\mathcal{G}$;
   *// Proposition 15*
9. **For each** vertex $u$ of $\mathcal{G}$ **do**
10.   **If** $u$ is a potential root in a sink component of $\mathcal{G}$
      **and** $u$ is not a sink in $\mathcal{G}_p$ **then**
11.     Remove the self-loop $(u,u)$ from $\mathcal{G}$;
    *// Proposition 16*
12. Given $i_r$ a vertex of $\mathcal{G}_r$, compute $\texttt{Source}_{i_r}$ the set of source vertices of $\mathcal{G}_p$ such that $i_r$ contains at least one vertex which is a descendant of a source vertex of $\mathcal{G}_p$;
13. **For each** $i_r$ of $\mathcal{G}_r$ containing at least one source of $\mathcal{G}_p$ **do**
14.   Perform a DFS, $\texttt{DFS}^{i_r}_{\mathcal{G}_r}$ in $\mathcal{G}_r$, starting from $i_r$ and exploring first the vertices $j_r$ such that $\texttt{Source}_{i_r} \cap \texttt{Source}_{j_r} \neq \emptyset$;
15.   **For each** arc $(u_r, v_r)$ of $\mathcal{G}_r$ which is transitive in $\texttt{DFS}^{i_r}_{\mathcal{G}_r}$ **do**
16.     **If** there exists $w_r$ between $u_r$ and $v_r$ in $\texttt{DFS}^{i_r}_{\mathcal{G}_r}$ **and** $\texttt{Source}_{w_r} \cap \texttt{Source}_{i_r} \neq \emptyset$ **then** Remove $(u_r, v_r)$ from $\mathcal{G}_r$;

Let us notice that a side effect of the previous proposition is that incomparable vertices do not have a common ancestor in $\mathcal{G}_p$ otherwise the constraint is infeasible.

### 3.2 Feasibility of a *tree* Constraint According to Incomparability Constraints

We now give two necessary conditions for the feasibility of an extended *tree* constraint that consider the interaction between the set of incomparability constraints and the associated digraph $\mathcal{G}$ (Figure 7(a)) as well as the precedence digraph $\mathcal{G}_p$ (Figure 7(b)).

**Proposition 18.** *If a tree constraint is feasible then, for each connected component $C_i$ of $\mathcal{G}_{true}$ rooted in $r_i$, there exists at least one successor $s$ of $r_i$ in $\mathcal{G}$ such that, for every vertex $u \in C_i$, there does not exist a vertex $v \in \mathcal{D}^s_{\mathcal{G}_{true}}$ that is incomparable with $u$.*

*Proof.* If there exists an incomparability constraint between a vertex $u \in C_i$ and a vertex $v$ of $\mathcal{D}^s_{\mathcal{G}_{true}}$, then the arc $(r_i, s)$ cannot be added to $\mathcal{G}_{true}$. □

**Proposition 19.** *If a tree constraint is feasible then, for every incomparability constraint between two vertices $u$ and $v$ of $\mathcal{G}$, we must have neither $u \lhd^*_{\mathcal{G}_p} v$ nor $v \lhd^*_{\mathcal{G}_p} u$.*

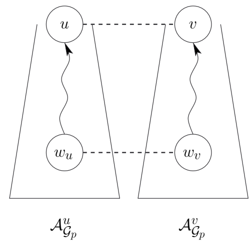
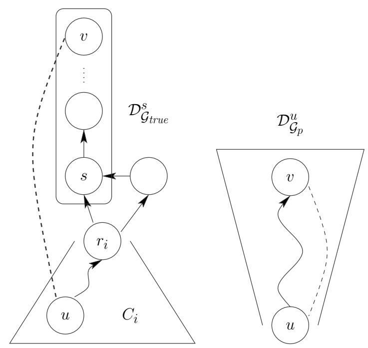



**Fig. 6.** If $u$ and $v$ are two incomparable vertices of $\mathcal{G}$ (dashed edge $(u, v)$), then all the ancestors of $u$ in $\mathcal{G}_p$ become incomparable with all the ancestors of $v$ in $\mathcal{G}_p$ (dashed edge $(w_u, w_v)$).




(a) Propositions 18 (b) Propositions 19

**Fig. 7.** Two fail cases for Propositions 18 and 19.

*Proof.* We cannot maintain both a precedence and an incomparability constraint between two vertices of $\mathcal{G}$. □

Algorithm 4 checks the feasibility of the incomparability constraints in $O(n \cdot m)$ time. Indeed, Lines 1-6 (i.e., Proposition 18) are checked in $O(n \cdot m)$ time and Lines 7-9 (i.e., Proposition 19) are checked in $O(n^2)$ time because $\mathcal{D}^u_{\mathcal{G}_p}$ and $\mathcal{D}^v_{\mathcal{G}_p}$ are incrementally maintained.

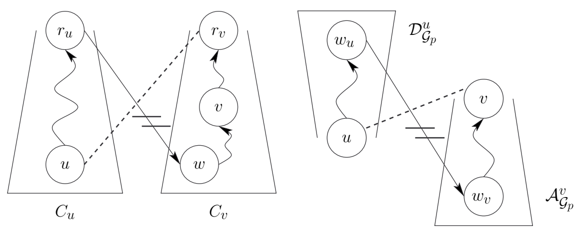
### 3.3 Filtering Related to the Incomparability Constraints

Given a *tree* constraint and one of its incomparability constraints, we now show how to filter the father variables according to the associated digraph $\mathcal{G}$ (Figure 8(a)), the precedence digraph $\mathcal{G}_p$ (Figure 8(b)), and the number NTREE of trees (when NTREE $= 1$).

**Proposition 20.** *Given a tree constraint and its associated digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, consider two incomparable vertices $u$ and $v$ that belong to two distinct connected components of the fixed-father digraph $\mathcal{G}_{true}$ that have $r_u$ and $r_v$ as roots. All the arcs $(r_u, w) \in \mathcal{E}$ (resp. $(r_v, w) \in \mathcal{E}$) such that $w \lhd^*_{\mathcal{G}_{true}} v$ (resp. $w \lhd^*_{\mathcal{G}_{true}} u$) are infeasible.*

**Algorithm 4** Checking feasibility according to Propositions 18-19

*// Proposition 18*
**For each** connected component $C_i$ of $\mathcal{G}_{true}$ **do**
  *incompatible* $\leftarrow 0$;
  Let $\mathcal{S}$ be the set of successors in $\mathcal{G}$ of the root $r_i$ of $C_i$;
  **For each** vertex $s \in \mathcal{S}$ **do**
    **If** there exists $u \in C_i$ and $v \in \mathcal{D}^s_{\mathcal{G}_{true}}$ with $v \in \mathtt{VER}[u].\mathtt{I}$ **or** $u \in \mathtt{VER}[v].\mathtt{I}$ **then** *incompatible* $\leftarrow$ *incompatible* $+ 1$;
    **If** $|\mathcal{S}| = incompatible$ **then** `fail`;
*// Proposition 19*
**For each** vertex $u$ of $\mathcal{G}$ **do**
  **For each** $v \in \mathtt{VER}[u].\mathtt{I}$ **do**
    **If** $v \in \mathcal{D}^u_{\mathcal{G}_p} \vee u \in \mathcal{D}^v_{\mathcal{G}_p}$ **then** `fail`;




(a) Proposition 20 (b) Proposition 21

**Fig. 8.** Illustrations of filtering rules given by Propositions 20 and 21.

*Proof.* If there exists an arc $(r_u, w) \in \mathcal{E}$ such that $w \lhd^*_{\mathcal{G}_{true}} v$, then $r_u \lhd^*_{\mathcal{G}} v$ and we infer that $u \lhd^*_{\mathcal{G}} v$, hence an incomparability constraint is violated. The proof is similar for an arc $(r_v, w) \in \mathcal{E}$. □

**Proposition 21.** *Given a tree constraint, its associated digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, and its precedence digraph $\mathcal{G}_p$, consider two incomparable vertices $u$ and $v$. All the arcs $(w_u, w_v) \in \mathcal{E}$ such that $u \lhd^*_{\mathcal{G}_p} w_u$ and $w_v \lhd^*_{\mathcal{G}_p} v$ are infeasible.*

*Proof.* If there exists an arc $(w_u, w_v) \in \mathcal{E}$ such that $u \lhd^*_{\mathcal{G}_p} w_u$ (resp. $v \lhd^*_{\mathcal{G}_p} w_u$) and $w_v \lhd^*_{\mathcal{G}_p} v$, then $u \lhd^*_{\mathcal{G}} v$ and the incomparability constraint involving $u$ and $v$ is violated. □

**Proposition 22.** *Given a* $tree(1, \mathtt{NPROP}, \mathtt{VER})$ *constraint and its associated digraph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, all self-loops $(v, v)$ of $\mathcal{E}$ such that the vertex $v$ belongs to an incomparability constraint are infeasible.*

*Proof.* If a self-loop on $v$ is enforced then $v$ is comparable with all the other vertices of $\mathcal{G}$ and then an incomparability constraint is violated. □

Algorithm 5 remove all infeasible arcs of $\mathcal{G}$ detected by Propositions 20 to 22. Lines 1–3 filter according to Proposition 20 and lines 4–5 filter according to Propo-

**Algorithm 5** Filtering according to Propositions 20-22

// *Proposition 20*
1. **For each** connected component $C_u$ of $\mathcal{G}_{true}$ with root $r_u$ **do**
2. **For each** successor $w$ of $r_u$ in $\mathcal{G}$ **do**
3. **If** there exist $u \in C_u$ and $v \in \mathcal{D}^{w}_{\mathcal{G}_{true}}$ such that $u$ and $v$ are incomparable **then** Remove $(r_u, w)$;

// *Proposition 21*
4. **For each** vertex $u$ of $\mathcal{G}_p$ such that there exists a vertex $v$ incomparable with $u$ **do**
5. **If** there exists $w_u \in \mathcal{D}^{u}_{\mathcal{G}_p}$ and $w_v \in \mathcal{A}^{v}_{\mathcal{G}_p}$ such that $(w_u, w_v) \in \mathcal{G}$ **then** Remove $(w_u, w_v)$;

// *Proposition 22*
6. **If** NTREE $= 1$ **then**
7. **For each** vertex $u$ such that $u$ belong to an incomparability constraint **do** Remove $(u, u)$;

sition 21 in $O(n \cdot m)$ time, while lines 6–7 filter according to Proposition 22 in $O(n)$ time.

## 4 Taking into Account the In-Degree Constraints

Constraints on the number of children are quite common in the phylogenetic supertree problem [6] (see Section 7.1) for instance. They also allow the modelling of path partitioning problems without creating any specific path constraint. We now show how to handle such in-degree constraints on the number of children of each vertex. We provide a flow model of this constraint based on the flow model of the *global cardinality* constraint [18].

To each vertex $v_i$ of the associated digraph $\mathcal{G}$ of a $tree$(NTREE, NPROP, VER) constraint, the domain variable VER$[i]$.D, with domain $[d^i_{min}, d^i_{max}]$, denotes the number of *proper* predecessors of $v_i$ (i.e., any self-loop on $v_i$ is ignored).

Observe that the in-degree constraint is very similar to the global cardinality constraint, except that the potential roots have to be handled differently. Figure 9 depicts the modified flow model where an extra value node $\ell$, corresponding to potential roots, is added. Formally, the corresponding flow digraph is defined as follows.

**Definition 13.** *The* flow digraph $\mathcal{F} = (\mathcal{V}_{\mathcal{F}}, \mathcal{E}_{\mathcal{F}})$ *of the associated digraph* $\mathcal{G}$ *of a* $tree$(NTREE, NPROP, VER) *constraint is defined by:*

- $\mathcal{V}_{\mathcal{F}}$ *is the union of the following three sets of vertices:*
  - $\mathcal{V}_{left} = \{$VER$[i]$.F $\mid i \in [1, n]\}$*, each such vertex being labelled by* $v_i$.
  - $\mathcal{V}_{right} = \{$VER$[i]$.L $\mid i \in [1, n]\}$*, each such vertex being labelled by* $i$.
  - $\{s, t, \ell\}$*, which are respectively called the* source*,* sink*, and* loop *vertices.*
- $\mathcal{E}_{\mathcal{F}}$ *is the set of the following capacitated arcs:*
  - *There is an arc from the source* $s$ *to each vertex* $v_i \in \mathcal{V}_{left}$*, with a capacity of* $[1, 1]$.

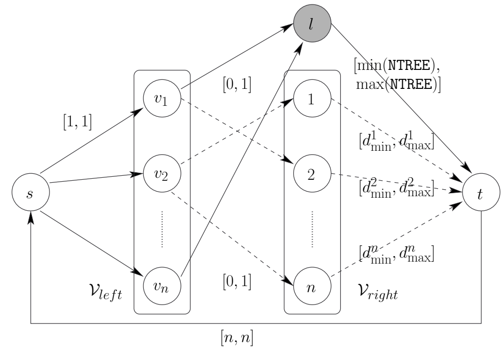



**Fig. 9.** Flow digraph of the associated digraph $\mathcal{G}$. Each left vertex $v_i$ represents a father variable, while each right vertex $i \neq \ell$ represents a vertex of $\mathcal{G}$. The vertex $\ell$ depicts a potential roots (i.e., there is an arc from $v_i$ to $\ell$ iff $i \in dom(\texttt{VER}[i].\texttt{F})$).

- *There is an arc from the sink $t$ to the source $s$, with a capacity of* $[n, n]$.
- *There is an arc from vertex $v_i \in \mathcal{V}_{left}$ to vertex $j \in \mathcal{V}_{right}$, with a capacity of* $[0, 1]$*, if* $j \in dom(\texttt{VER}[i].\texttt{F})$ *and* $j \neq i$.
- *There is an arc from vertex $v_i \in \mathcal{V}_{left}$ to the loop vertex $\ell$, with a capacity of* $[0, 1]$*, if* $i \in dom(\texttt{VER}[i].\texttt{F})$.
- *There is an arc from vertex $i \in \mathcal{V}_{right}$ to the sink $t$, with a capacity of* $dom(\texttt{VER}[i].\texttt{D}) = [d^i_{min}, d^i_{max}]$.
- *There is an arc from the loop vertex $\ell$ to the sink $t$, with a capacity of* $[\min(\texttt{NTREE}), \max(\texttt{NTREE})]$.

Notice that, for each $i \in \mathcal{V}_{right}$, if $i \neq \ell$ then $d^i_{min}$ and $d^i_{max}$ respectively denote the minimum and maximum values of the in-degree of the vertex $v_i$ of $\mathcal{G}$. The number of trees to build is integrated within the flow model as the capacity $[\min(\texttt{NTREE}), \max(\texttt{NTREE})]$ on the out-going arc of $\ell$. We use the classical flow-based filtering algorithm described in [18] to prune every arc of $\mathcal{G}$ that is incompatible with the in-degree constraints.

## 5 Taking into Account the Number-of-Proper-Trees Constraint

In many practical partitioning problems, we do not have to cover all the vertices of the associated digraph $\mathcal{G}$ [17]. In this context, the set of vertices that are not covered will be modelled as a set of self-loops. Consequently, we want to distinguish proper trees (i.e., trees involving at least two vertices) from isolated self-loops. Beside the basic inequality $\texttt{NTREE} \geq \texttt{NPROP}$, we now show how to propagate according to the variable `NPROP` corresponding to the number of proper trees.

**Proposition 23.** *The minimum number of* proper *trees, denoted by* `MINPROP`*, that can be used to partition $\mathcal{G}$ is the number of connected components of $\mathcal{G}_{true}$ involving at least two vertices, including a vertex $r$ such that* $dom(\texttt{VER}[r].\texttt{F}) = \{r\}$.

**Proposition 24.** *The maximum number of* proper *trees, denoted by* MAXPROP*, that can be used to cover* $\mathcal{G}$ *is the number of potential roots in* $\mathcal{G}$ *minus the number of vertices* $v$ *such that* $dom(\texttt{VER}[v].\texttt{F}) = \{v\}$ *and* $\forall u \neq v$*,* $v \notin dom(\texttt{VER}[u].\texttt{F})$.

The next two propositions filter the arcs of $\mathcal{G}$ when one of the two previous bounds on NPROP is reached.

**Proposition 25.** *If* $\texttt{NPROP} = \texttt{MINPROP}$*, then, for each potential root* $u$ *that cannot reach a connected component of* $\mathcal{G}_{true}$ *containing at least two vertices including a vertex* $r$ *such that* $dom(\texttt{VER}[r].\texttt{F}) = \{r\}$*, the self-loop on* $u$ *is enforced and any other arc* $(v, u)$*,* $v \neq u$*, is removed.*

**Proposition 26.** *If* $\texttt{NPROP} = \texttt{MAXPROP}$*, then for each vertex* $v$ *such that* $v \in dom(\texttt{VER}[v].\texttt{F})$*, the self-loop on* $v$ *is enforced.*

## 6 Synthetic Overview of the *tree* Constraint

Table 2 summarises the theoretical results of this article. It is divided into five horizontal parts. The first part shows that the upper bound on NTREE has been improved over [5] without any overhead. The second part provides upper and lower bounds on the number of proper trees. The third part recalls that evaluating the feasibility of an extended *tree* constraint is NP-hard and points out some necessary conditions that can be evaluated in polynomial time. The fourth part provides polynomial-time filtering rules derived from the previous necessary conditions. The last part recalls how each instantiation of a father variable leads to updating the precedence digraph $\mathcal{G}_p$ as well as the set of incomparability constraints (here denoted by $\mathcal{I}$). For each set of propositions and algorithms an upper bound on the time complexity is provided, where $n$ and $m$ respectively denote the numbers of vertices and arcs in the associated digraph $\mathcal{G}$.

## 7 Experimental Results

We now report on several experiments we have conducted to evaluate the extended *tree* constraint. First, in Section 7.1, we discuss our experiments on the molecular biology problem of constructing phylogenetic supertrees, both in its pure form and with side constraints. Then, in Section 7.2, we present our results on the routing problem of constructing ordered simple paths with mandatory vertices. Finally, after reporting the performance on random instances of the extended *tree* constraint in Section 7.3, we make a quantitative and qualitative analysis of its efficiency in Section 7.4.

Unless otherwise posted, all experiments were performed with the Choco constraint programming system (which is a Java library) on an Intel Pentium 4 CPU with 3GHz and a 1GB RAM, but with only 32MB allocated to the Java Virtual Machine.

### 7.1 The Phylogenetic Supertree Problem

The objective of phylogeny is to construct the genealogy of the species, called the *tree of life* (assuming that evolution happens only by mutations, as with recombinations

| | *Interaction* | *Effects* | *Related Propositions and Algorithms* | *Time Complexity* |
|---|---|---|---|---|
| *Bounds on* NTREE | $\mathcal{G}$ | $\min(\texttt{NTREE})$ | MINTREE, [5], Prop.1 | $O(n+m)$ |
| | $\mathcal{G}$ | $\max(\texttt{NTREE})$ | MAXTREE, [5], Prop.2 | $O(n)$ |
| | $\mathcal{G}$ & $\mathcal{G}_p$ | $\max(\texttt{NTREE})$ | $\texttt{MAXTREE}_{\mathcal{G}_p}$, Prop. 6 | $O(n+m)$ |
| *Bounds on* NPROP | $\mathcal{G}$ | $\min(\texttt{NPROP})$ | MINPROP, Prop. 23 | $O(n+m)$ |
| | $\mathcal{G}$ | $\max(\texttt{NPROP})$ | MAXPROP, Prop. 24 | $O(n)$ |
| *Feasibility* | $\mathcal{G}$ | $fail$ | Prop. 8 (Prop.3 of [5]) | $O(n+m)$ |
| | $\mathcal{G}_p$ | | Prop. 1 | $O(n+m)$ |
| | $\mathcal{G}$ & $\mathcal{G}_p$ | | Prop. 9 | *NP*-hard |
| | $\mathcal{G}$ & $\mathcal{G}_p$ | | Prop. 11, 12 | $O(n \cdot m)$ |
| | $\mathcal{G}$ & $\mathcal{I}$ | | Prop. 18 | $O(n \cdot m)$ |
| | $\mathcal{G}_p$ & $\mathcal{I}$ | | Prop. 19 | $O(n \cdot m)$ |
| *Direct Filtering* | $\mathcal{G}$ | $\mathcal{G}$ | [5], Prop. 5, 6, 7 | $O(n \cdot m)$ |
| | $\mathcal{G}$ | | Section 4, [18] | $O(n^2 \cdot m)$ |
| | $\mathcal{G}$ | | Prop. 25, 26 | $O(n+m)$ |
| | $\mathcal{G}$ & $\mathcal{G}_p$ | | Prop. 13, 14, 15 (12), 16 | $O(n \cdot m)$ |
| | $\mathcal{G}$ & $\mathcal{I}$ | | Prop. 20 (18), 22 | $O(n \cdot m)$ |
| | $\mathcal{G}_p$ & $\mathcal{I}$ | | Prop. 21 (19) | $O(n \cdot m)$ |
| *Internal Deductions* | $\mathcal{G}$ & $\mathcal{G}_p$ | $\mathcal{G}_p$ | Algo. 1, Prop. 2, 3, 4, 5 | $O(n^2 \cdot m)$ |
| | $\mathcal{G}_p$ | $\mathcal{I}$ | Prop. 17 | $O(n \cdot m)$ |

**Table 2.** Summary of the *tree* constraint. In the fourth column, "Prop. $i$ ($j$)" means that Proposition $i$ was derived from Proposition $j$.

one actually obtains a network), whose leaves represent the contemporary species and whose internal vertices are not necessarily named.

An important constraint satisfaction problem in phylogeny is the construction of a supertree [6] that is compatible with several given trees $\mathcal{T}_1, \ldots, \mathcal{T}_k$ (of which any two share at least one species). The given trees and the supertree are not necessarily binary: we speak of *polytomy* when an internal vertex has more than two subtrees; polytomies can be *hard* (the mutation was not binary) or *soft* (information for further structure in the tree is lacking). A first supertree algorithm was given in [2], with an application for database management systems; it takes $O(n^2)$ time, where $n$ is the number of leaves in the given trees. Many derived algorithms for the supertree problem have emerged from the phylogeny field, for instance [15]. The algorithm in [7] from computational linguistics has supertree construction as a particular case. The first constraint program was proposed in [13], using standard (non-global) constraints.

Nowadays, many side constraints to the pure supertree problem are emerging from the demands of biologists. For instance, *relative ancestral divergence dates* [9] can be used to order speciation events; this gives rise to numerical side constraints of the form $mrca(a, b) < mrca(c, d)$, where $mrca(x, y)$ denotes the rank of the most recent common ancestor of the leaf species $x$ and $y$, the rank of the root being zero. Addressing this is future work, but trivial for the constraint model of [13]. Another side constraint concerns *nested species* [19], where the internal vertices of the trees can be named, possibly by names of leaf species of other trees, so that a side constraint emerges for preserving ancestries. Interestingly, our *tree* constraint is powerful enough to model this side constraint, and it is also simple to adapt the constraint model of [13]. Hence no new algorithms have to be designed for dealing with such side constraints, nor for enumerating all solutions. This is not the case in classical phylogeny research, where new deterministic algorithms have to be designed, and then integrated and made non-deterministic, for each new side constraint.

Let us denote the set of vertices of a tree $\mathcal{T}$ by $\mathcal{N}(\mathcal{T})$. The supertree problem can be modelled by a $tree(1, 1, \texttt{VER})$ constraint, such that the associated digraph $\mathcal{G}$ is the complete digraph with vertex set $\mathcal{V} = \mathcal{N}(\mathcal{T}_1) \cup \cdots \cup \mathcal{N}(\mathcal{T}_k)$ and edge set $\mathcal{E} = \{(u, v) \mid u, v \in \mathcal{V}\}$, the precedence digraph $\mathcal{G}_p = (\mathcal{V}, \mathcal{E}_p)$ is dictated by $\mathcal{T}_1, \ldots, \mathcal{T}_k$, and the incomparability constraints are generated from the incomparable vertices of each tree $\mathcal{T}_1, \ldots, \mathcal{T}_k$. All the leaves of $\mathcal{T}_1, \ldots, \mathcal{T}_k$ that are not internal vertices of any tree $\mathcal{T}_i$ must remain leaves and thus have an in-degree of zero: $\texttt{VER}[i].\texttt{D} = 0$. All the other vertices of $\mathcal{V}$ have the degree constraint $\texttt{VER}[i].\texttt{D} \in [1, 2]$ if a binary supertree is requested, and $\texttt{VER}[i].\texttt{D} \in [1, n-1]$ otherwise, where $n = |\mathcal{V}|$. A smallest-domain heuristic is used to select a father variable at each waking up of the *tree* constraint, and the value selection heuristic favours, for a selected vertex $v_i$, a father $v_j$ such that there exists a minimum-length path from $v_i$ to $v_j$ or vice-versa in the precedence digraph $\mathcal{G}_p$.

Table 3 compares the performance of this constraint program with the one of [13] (which has been improved since then[6]), until the first solution is found or the absence of solutions is established. For the latter model, we have run a re-implementation in OPL 3.7 (which is commonly believed to be 3 to 4 times faster than Choco) on a similar computer, namely an Intel Pentium 4 CPU with 2.53GHz, a 1GB RAM, and a 512 KB cache. There are 17 leaf species in the two spider trees of [19], which were taken from study S1x6x97c14c42c30 in TreeBASE (`http://www.treebase.org/`); they feature nested species and one of them is not binary, hence there is no binary supertree. There are 23 leaf species in the two cat trees of [19], which were taken from biology journals; one of them is not binary, hence there is no binary supertree. There are 34 leaf species in the two sea-bird trees of [13], which were taken from an ornithology journal; both are binary. As these real-life instances are not small, the numbers of solutions are huge (which is denoted by $\ggg$) on the pure version of the problem (cats and sea birds), but small in the presence of side constraints (spiders). Our model generates symmetric solutions (in the sense that some internal vertices are fathers of only one other vertex, which is also internal, so that their roles can be inverted unless they are named), whereas the one of [13] generates unique solutions modulo all symmetries. On the other hand, our model has only $\Theta(\ell)$ domain variables, where $\ell$ is the number of leaf species in the given trees,[7] whereas the model of [13] has $\Theta(\ell^2)$ domain variables. In order to compare the scalability of the two models, six larger instances (given in Appendix A) were randomly generated, such that the two generated trees contain 60 leaves in total and share 6 leaves. For these larger instances, the extended *tree* constraint always

[6] Personal communication by Patrick Prosser.

[7] In a binary phylogenetic tree, only the leaves have empty subtrees, so if there are $\ell$ leaves, then there are $2\ell - 1$ vertices and it does not matter asymptotically whether we count leaves or vertices.

| Supertree instances | degree | #trees | extended *tree* | | | Gent *et al.* [13] | |
|---|---|---|---|---|---|---|---|
| | | | wake-ups | failures | time | failures | time |
| spiders [19] | any | 13 | 13 | 0 | 72ms | 82 | 80ms |
| | binary | 0 | 1 | 0 | 20ms | 3 | 60ms |
| cats [19] | any | $\ggg$ | 22 | 0 | 300ms | 67 | 220ms |
| | binary | 0 | 1 | 0 | 20ms | 21249 | 74020ms |
| sea birds [13] | any | $\ggg$ | 10 | 0 | 520ms | 126 | 620ms |
| | binary | $\ggg$ | 9 | 0 | 486ms | 3 | 700ms |
| inst60-10-01 | any | $\ggg$ | 63 | 5 | 7738ms | 2149 | 4420ms |
| | binary | $\ggg$ | 46 | 5 | 5631ms | 1 | 4620ms |
| inst60-10-02 | any | $\ggg$ | 23 | 0 | 8919ms | 1702 | 3740ms |
| | binary | $\ggg$ | 22 | 0 | 11053ms | 2 | 4500ms |
| inst60-10-03 | any | $\ggg$ | 56 | 0 | 12972ms | 1208 | 3790ms |
| | binary | $\ggg$ | 39 | 0 | 10385ms | 0 | 4340ms |
| inst60-10-04 | any | $\ggg$ | 16 | 0 | 5253ms | 1232 | 4340ms |
| | binary | $\ggg$ | 16 | 0 | 5245ms | 0 | 3840ms |
| inst60-10-05 | any | $\ggg$ | 9 | 0 | 3801ms | 548 | 3490ms |
| | binary | $\ggg$ | 10 | 0 | 6374ms | 0 | 3710ms |
| inst60-10-06 | any | $\ggg$ | 32 | 0 | 7142ms | 1294 | 3820ms |
| | binary | $\ggg$ | 32 | 0 | 7045ms | 0 | 4360ms |

**Table 3.** Results for some phylogenetic supertree construction instances

backtracks rarely (namely at most $5$ times), while the model of [13] backtracks significantly more often (namely from $548$ to $2149$ times) in the non-binary case. However, this robustness of the extended $tree$ constraint on the number of backtracks penalises significantly its run time performance (after adjusting for the difference between Choco and OPL, it is not significantly faster than the model of [13]).

The supertree problem becomes a constraint optimisation problem if some of the given trees are inconsistent. The so-called 'modified min-cut' objective function [16] preserves a maximum of sub-trees of each given tree that are not inconsistent with the other given trees. Addressing this is future work.

### 7.2 The Ordered Simple Path Problem with Mandatory Nodes

The *ordered disjoint path problem* (ODP) consists in partitioning a given (di)graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ into $k$ mutually vertex-disjoint paths [12, p.217] subject to precedence constraints between some vertices. We here consider a restriction of this problem, called the *ordered simple path problem with mandatory nodes* (OSPMN) and described in [17], which consists in finding a simple path containing a set of mandatory vertices in a given order.

The OSPMN problem can be modelled by a $tree$ constraint such that the associated digraph $\mathcal{G}$ is the digraph to be covered, but enriched by a loop on each vertex, while the set of mandatory vertices is contained in a connected component of the precedence digraph $\mathcal{G}_p$ such that each mandatory vertex succeeds the first vertex of the path and

| OSPMN instances | extended *tree* | | | Quesada *et al.* [17] | |
|---|---|---|---|---|---|
| | wake-ups | failures | time | failures | time |
| SPMN_22 | 7 | 0 | 0.071sec | 13 | 4.45sec |
| SPMN_22Full | 3 | 0 | 0.036sec | 0 | 1.22sec |
| SPMN_52b | 20 | 0 | 1.685sec | 100 | 402sec |
| SPMN_52Full | 6 | 0 | 0.692sec | 3 | 45.03sec |
| SPMN_52Order_a | 16 | 0 | 0.892sec | 16 | 57.07sec |
| SPMN_52Order_b | 1 | 0 | 0.020sec | 41 | 117sec |

**Table 4.** Results for the OSPMN instances in [17]

precedes the final vertex of the path, and if there exist precedence constraints between two mandatory vertices, then an arc is added between them. All the other vertices represent connected components of size 1 in $\mathcal{G}_p$. An ordered-path heuristic is used to select a father variable at each waking up of the $tree$ constraint. This heuristic forces an incremental building of the path by selecting as new variable to instantiate the value chosen at the previous step: when an arc $(v_i, v_j)$ is enforced at a given step, then an arc starting from $v_j$ is selected at the next step.

Table 4 shows that this model based on the extended $tree$ constraint compares favourably, both in time and the number of failures, with the results reported in [17] (which have been improved since then[8]) for an equivalent hardware, until the first solution is found or the absence of solutions is established. Within [17] three constraints (namely *domReachability*, *noCycle*, and *All Different*) are used to model the OSPMN problem, and multiple views of the graph $\mathcal{G}$ are explicitely represented as graph variables.

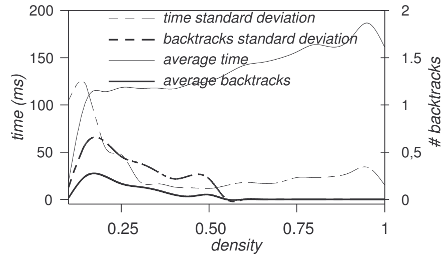
### 7.3 Random Instances for the Hamiltonian Path Problem

Two models for the Hamiltonian path problem can be proposed using the extended $tree$ constraint. First, the Hamiltonian path problem is a $tree$ constraint for which each vertex of the given digraph $\mathcal{G}$ has an in-degree of exactly one, excepted the origin vertex of the path which have a in-degree of zero. Second, it is possible to add a set of precedences in the instance such that the origin of the path precedes all the other vertices of $\mathcal{G}$ and all these vertices precede the final vertex of the path.

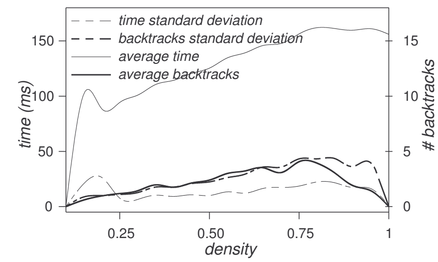
For each density[9] in $[0.10, 1]$, with a step of $0.05$, a total of $100$ random connected digraphs $\mathcal{G}$ of sizes $25$, $50$, $75$, $100$, and $150$ were considered. For any size of $\mathcal{G}$ among $\{25, 50, 75, 100, 150\}$, notice that adding precedences to the instance improves significantly the results on the number of backtracks and does not increase the average time complexity. Moreover, the standard deviation of the number of backtracks when precedences are added is significantly lower than without adding the precedence constraints. Thus, adding dynamically precedence constraints provides a strong robustness on the number of backtracks and the standard deviation. Notice that for the instances of size

[8] Personal communication by Luis Quesada.

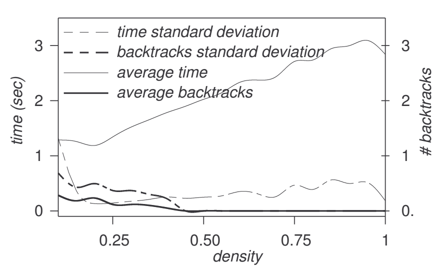
[9] The *density* of a digraph $G$ of size $n$ is $\frac{m}{n^2}$, where $m$ is the number of arcs of $G$.



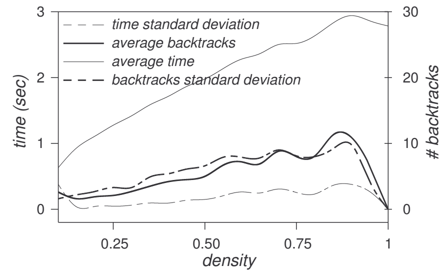

(a) Instances of size 25 with precedences



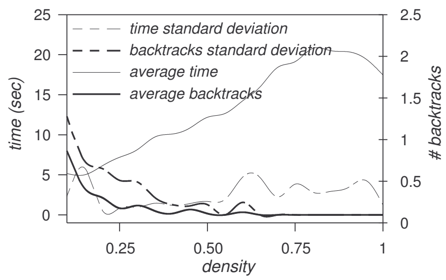

(b) Instances of size 25 without precedences



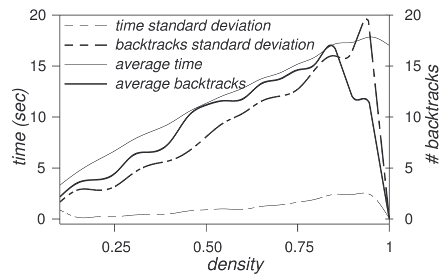

(c) Instances of size 50 with precedences




(d) Instances of size 50 without precedences




(e) Instances of size 75 with precedences



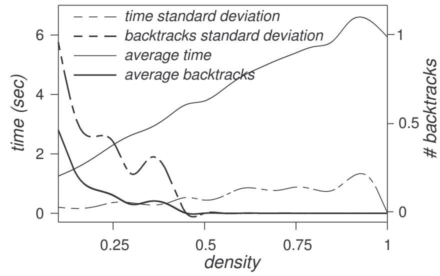

(f) Instances of size 75 without precedences

150, the deviation between the case for which precedences are dynamically added and the case without any precedences is poor. Obviously, there exists pathological graphs, such as Tutte's graph [21],[10] for which we still need 179 backtracks to prove that there do not exist any Hamiltonian circuits.

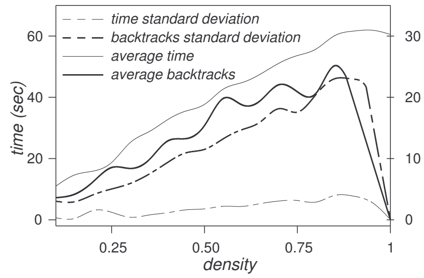
### 7.4 Quantitative and Qualitative Evaluation

**Phylogenetic Supertree Problems:** the sea-bird phylogenetic instance has a complete associated digraph $\mathcal{G}$ of size 66 (i.e., 66 vertices and $66^2 = 4356$ arcs). The precedence digraph $\mathcal{G}_p$ is built from the two given trees. The set $\mathcal{I}$ of incomparability constraints is computed from the incomparable vertices of the given trees. Table 3 shows that, in the unrestricted case, the $tree$ constraint solves this instance in 10 search vertices, 0 backtracks, and 520ms.

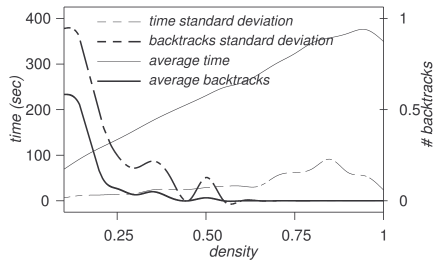
[10] *Tutte's graph* is a non-Hamiltonian 3-connected cubic graph of size 46.



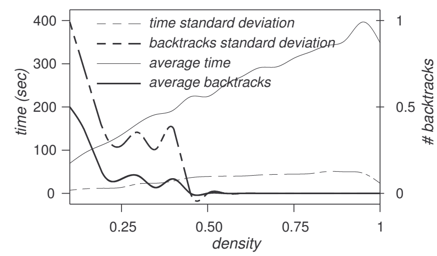

(g) Instances of size 100 with precedences




(h) Instances of size 100 without precedences




(i) Instances of size 150 with precedences



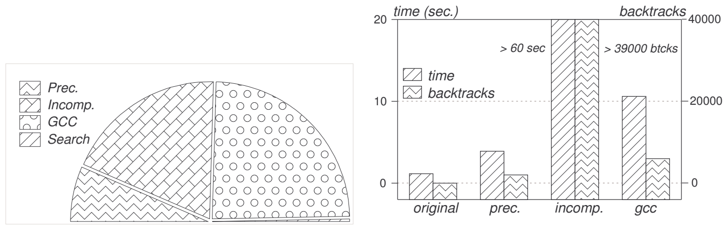

(j) Instances of size 150 without precedences

Figure 10 shows that not all parts of the *tree* constraint are necessary to construct a phylogenetic supertree. Figure 10(k) gives the pruning importance of each part of the *tree* constraint that is actually used to solve the instance. Note that the precedence, incomparability, and degree (GCC) constraints are sufficient to solve this instance efficiently, i.e., even the tree partitioning constraint does not improve the results. Moreover, Figure 10(l) highlights that the incomparability constraints are a very important aspect of the phylogenetic supertree problem. Indeed, if we inhibit the pruning related to the incomparability constraints (Prop.s 20 to 22), then the run time and the number of backtracks during the search increase vary significantly.

Figure 11 shows the dynamic aspects of the precedence and incomparability constraints. Figure 11(a) shows that inhibiting the internal derivations (which dynamically add new precedence and incomparability constraints, Prop.s 2 to 5 and Prop. 17) significantly modifies the pruning importance of each part of the *tree* constraint: the part of the pruning due to the search increases, while the part due to the incomparability constraints decreases. Moreover, Figure 11(b) illustrates that dynamically adding new precedence constraints significantly improves the run time and the number of backtracks. Note that adding incomparability constraints does not improve the performance, because all the potential pruning is carried out during the initial propagation step.

The same pattern is followed by the spider and cat phylogenetic instances.

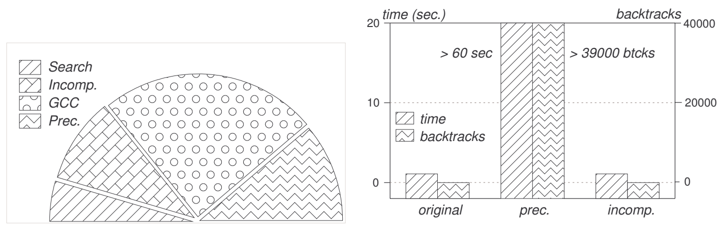
**Ordered Simple Path Problem With Mandatory Nodes Problems:** the SPMN_52Order_a OSPMN instance has an incomplete associated digraph $\mathcal{G}$ of size $52$ (namely $52$ vertices and $216$ arcs). The precedence digraph $\mathcal{G}_p$ is composed of one connected component of size $7$, and $45$ connected components of a single vertex each, and




(k) Pruning distribution

(l) Run time and backtracks when some parts of the $tree$ constraint are inhibited

**Fig. 10.** Pruning effectiveness on the sea-bird phylogenetic instance




(a) Pruning distribution without any internal derivations

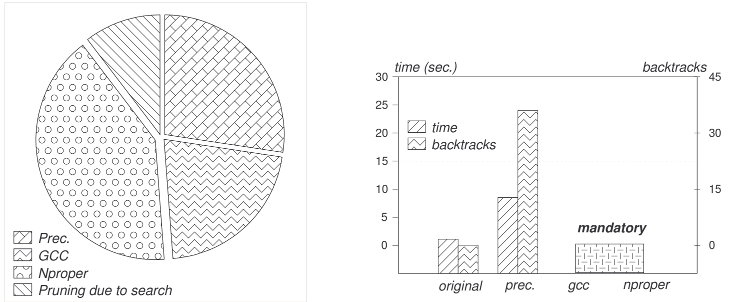
(b) Run time and backtracks when some internal derivations are inhibited

**Fig. 11.** Effectiveness of the internal derivations on the sea-bird phylogenetic instance

there are no incomparability constraints. Table 4 shows that the $tree$ constraint solves this instance in $16$ search vertices, $0$ backtracks, and $0.892$ seconds.

Figure 12 shows that, as for the phylogenetic supertree problem, not all parts of the $tree$ constraint are necessary to construct an OSPMN. Figure 12(a) gives the pruning importance of each part of the $tree$ constraint that is actually used to solve the instance. Note that the precedence, degree (GCC), and number-of-proper-trees constraints are sufficient to solve this instance efficiently, i.e., even the tree partitioning constraint does not improve the results and the incomparability constraints are not used. Figure 12(b) shows that the pruning of the degree and number-of-proper-trees constraints cannot be inhibited, as otherwise the constraint would not build or enforce a path partitioning of $\mathcal{G}$. As a consequence, only the pruning related to the precedence constraints can be inhibited and the figure shows that inhibiting this pruning increases the number of backtracks from $0$ to $34$, and the run time from $0.892$ to $8.60$ seconds.

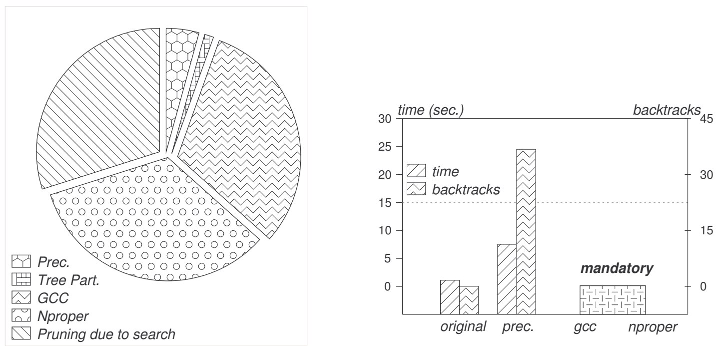
Figure 13 shows the dynamics aspect of the precedence and incomparability constraints. Figure 13(a) shows that inhibiting the internal derivations significantly modifies the pruning importance of each part of the $tree$ constraint: the part of the pruning due to the precedence constraints is divided by $6.4$, the part of the pruning due to the search increases of a factor $3$, and the pruning rules related to the original $tree$ partitioning constraint, which are not used when the internal derivations are applied, now detect infeasible arcs. Moreover, Figure 13(b) illustrates that dynamically adding new precedence constraints significantly improves the number of backtracks, as well as the




(a) Pruning distribution

(b) Run time and backtracks when some parts of the $tree$ constraint are inhibited

**Fig. 12.** Pruning effectiveness on the SPMN_52Order_a instance




(a) Pruning distribution without any internal derivations

(b) Run time and backtracks when some internal derivations are inhibited

**Fig. 13.** Effectiveness of the internal derivations on the SPMN_52Order_a instance

run time which falls from $7.30$ seconds to $0.892$ seconds. Note that adding incomparability constraints does not improve the performance, because each new incomparability constraint is already respected in the digraph $\mathcal{G}$.

The same pattern is followed by the other considered OSPMN instances.

# 8 Conclusion

The $tree$ and $path$ constraints have been unified within a single global constraint. Moreover, we have shown how to handle in a uniform way a variety of useful side constraints, such as precedence, incomparability, and degree constraints, which occur often in the context of path and tree problems. Our approach outperforms an existing $path$ constraint, but can also handle the phylogenetic supertree problem, for instance. As shown by our qualitative evaluation, the key point of the filtering is to derive dynamically new precedence and incomparability constraints. Our experiments, particularly on dense graphs, point to an important topic for future research: finding efficient filters that avoid triggering heavy algorithms when there is obviously nothing to prune.

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# Appendix

## A Random Instances for the Phylogenetic Problems

### A.1 inst60-10-01

**first tree :** `(((59,(58,57)),((55,54),56)),(53,(((51,50),(((48,47),49),(46,(45,(44,(((42,43),(41,(40,39))),(38,(((37,36),(34,35)),((33,32),(((30,29),31),((27,26),28)))))))))))),52));`

**second tree :** `((25,24),((((21,(20,19)),((18,(17,(((15,(((13,((11,((((8,7),9),10),6)),12)),14),31)),16),(29,30)))),((27,26),28))),22),23));`

### A.2 inst60-10-02

**first tree :** `((58,59),(57,(((55,54),((53,52),(((((48,47),49),50),51),((45,(((43,(42,41)),((((40,(((((36,35),37),38),39),(34,((33,(32,31)),(30,29))))),(28,(27,26))),25),24)),44)),46)))),56)));`

**second tree :** `(23,(22,((20,(19,(18,(17,(16,(((13,(12,(11,(10,((((((7,(6,29)),((27,26),28)),8),9),25),24))))),14),15)))))),21)));`

### A.3 inst60-10-03

**first tree :** `((59,(57,58)),((55,(54,((52,(51,((50,(49,((47,46),48))),(((((43,42),44),45),41),((39,(((37,((35,34),36)),((32,(31,(30,(29,(28,27))))),33)),38)),40))))),53))),56));`

**second tree :** `((26,25),(((24,23),(22,21)),((((18,(17,(((14,15),16),13))),19),((((9,((((6,32),((((27,28),29),30),31)),7),8)),10),11),12)),20)));`

### A.4 inst60-10-04

**first tree :** `((59,58),((((55,54),((53,((((51,50),(49,48)),52),(47,46))),((44,(43,(42,(41,((39,(38,(37,(36,(34,35))))),40)))))),45))),56),57));`

**second tree :** `(33,(32,(31,((30,29),((((26,25),27),(24,(((21,(20,(19,((((15,(14,((12,13),(11,(10,((8,(7,(6,(((37,((35,34),36)),38),39)))),9)))))),16),17),18)))),22),23))),28)))));`

### A.5 inst60-10-05

**first tree :** `((58,59),((((55,((54,53),((52,51),(((50,49),48), ((((((42,41),43),44),45),46),47))))),56),((40,39),((38,(37, 36)),((34,33),35))))),57));`

**second tree :** `(((31,30),32),(29,(((26,((24,(23,(22,((20,(19, (((16,(15,(14,((12,(11,(10,((((7,(6,((37,36),38))),8), ((33,34),35)),9))))),13))))),17),18))),21))))),25)),27),28)));`

### A.6 inst60-10-06

**first tree :** `((59,58),(((56,(55,((53,52),54))),((50,((49,(48, (47,46))),((44,(43,((42,41),((((((38,37),(36,((34,(33,((31, (30,(29,28))),32))),35))),39),40),27),26)))),45))),51)),57));`

**second tree :** `((25,((23,22),24)),((20,(19,((18,17),((16,15), ((((12,(11,10)),13),14),(((9,8),7),(6,((((30,(29,28)),31), 27),26)))))))),21));`