Visualizing Multispecies Coalescent Trees: Drawing Gene Trees Inside Species Trees

Jonathan Klawitter\textsuperscript{1,2}, Felix Klesen\textsuperscript{1}, Moritz Niederer\textsuperscript{3}, and Alexander Wolff\textsuperscript{1}

\textsuperscript{1} Universität Würzburg, Germany
\textsuperscript{2} University of Auckland, New Zealand
\textsuperscript{3} HTW Saar, Germany

Abstract. We consider the problem of drawing multiple gene trees inside a single species tree in order to visualize multispecies coalescent trees. Specifically, the drawing of the species tree fills a rectangle in which each of its edges is represented by a smaller rectangle, and the gene trees are drawn as rectangular cladograms (that is, orthogonally and downward, with one bend per edge) inside the drawing of the species tree. As an alternative, we also consider a style where the widths of the edges of the species tree are proportional to given effective population sizes.

In order to obtain readable visualizations, our aim is to minimize the number of crossings between edges of the gene trees in such drawings. We show that planar instances can be recognized in linear time and that the general problem is NP-hard. Therefore, we introduce two heuristics and give an integer linear programming (ILP) formulation that provides us with exact solutions in exponential time. We use the ILP to measure the quality of the heuristics on real-world instances. The heuristics yield surprisingly good solutions, and the ILP runs surprisingly fast.

1 Introduction

Visualizations of trees to present information have been used for centuries \cite{24} and the study of producing readable, compact representations of trees has a long tradition \cite{31,33}. Trees and their drawings are also an ubiquitous and fundamental tool in the field of phylogenetics. In particular, a phylogenetic tree is used to model the evolutionary history and relationships of a set \(X\) of taxa such as species, genes, or languages \cite{34}. There exist many different models, but most commonly a \textit{phylogenetic tree} on \(X\) is a tree \(T\) whose leaves are bijectively labeled with \(X\); see Fig. 1. In a \textit{rooted} phylogenetic tree, each internal vertex represents a branching event (such as species divergence); time (or genetic distance) is represented by the edge lengths from the root towards the leaves. In most applications, the

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1}
\caption{A rectangular cladogram drawing of a rooted binary phylogenetic tree on seven taxa.}
\end{figure}
tree is binary, that is, each internal vertex has indegree one, outdegree two, and thus represents a bifurcation event. An unrooted phylogenetic tree, on the other hand, models only the relatedness of the taxa. A phylogenetic tree where the taxa are species is called a species tree. If the taxa are biological sequences, such as particular genes or protein sequences, the tree is called a gene tree.

Multispecies coalescent models. One of the main tasks in phylogenetics is the inference of a phylogenetic tree for some given data and model. When inferring a species tree based on sequencing data, one might be inclined to set the species tree as that of an inferred gene tree. However, gene trees can differ from the species tree in the presence of so-called incomplete lineage sorting\(^4\) or when divergence times are small\(^5\), which can lead to inaccurate edge lengths or even to an incorrectly inferred species tree [1,25,28,32]. To address these issues, multispecies coalescent (MSC) models have been developed. An MSC model provides a framework for inferring species trees while accounting for conflicts between gene trees and species trees [15,18,30]. Roughly speaking, by using multiple samples (genes) per species, the model coestimates multiple gene trees that are constrained within their shared species tree. In doing so, the model can infer not only divergence times for inner vertices but also the effective population size for each edge (branch) in the species tree. There exist several models for population sizes [38], two of which we define here. In the continuous linear model, for each branch, the population size between the top and the bottom is linearly interpolated, and for a branch not incident to a leaf, the population size at the bottom equals the sum of the population sizes at the top of its two child branches; see Fig. 2a. In the piecewise constant model, the population size of each branch is constant from the top to the bottom of the branch and there are no restrictions between adjacent branches [12]; see Fig. 2b.

For a phylogenetic tree \(T\), let \(V(T)\) be the vertex set of \(T\), let \(E(T)\) be the edge set of \(T\), and let \(L(T)\) be the leaf set of \(T\). We define an MSC tree as a triple \((S,T,\varphi)\) consisting of a species tree \(S\), a gene tree \(T\), and a mapping \(\varphi: L(T) \to L(S)\) with the following properties. Both \(S\) and \(T\) are rooted binary phylogenetic trees where all vertices have an associated height \(h\) that are strictly decreasing from root to leaf. We consider only the case where \(h(\ell)\) is zero for each leaf \(\ell\) in \(L(S)\) and \(L(T)\). For gene trees, we use the terms leaf, vertex, and edge; whereas we use the terms species, node, and branch if we want to stress that we talk about species trees. Each branch in \(E(S)\) is associated with an upper and a lower population size. The mapping \(\varphi\) describes which leaves of \(T\) belong to which species in \(S\). Next, consider two leaves \(\ell\) and \(\ell'\) of \(T\) with \(\varphi(\ell) \neq \varphi(\ell')\). Let \(v\) be the lowest common ancestor of \(\ell\) and \(\ell'\). In the MSC model we have that a divergence event of \(v\) occurred before the divergence event

\(^4\) We speak of incomplete lineage sorting if (i) in a population of an ancestral species two (or more) variants of a gene were present, say red and blue, and (ii) when the species diverged, this did not result in one child species having the red variant and the other having the blue variant, but, e.g., one child species having both variants [32].

\(^5\) A small divergence time corresponds to a short edge in the phylogenetic tree, which can be hard to infer correctly.
at a node \(s\) of \(S\) that ultimately split \(\varphi(\ell)\) and \(\varphi(\ell')\). Hence, \(h(v) > h(s)\) and we can extrapolate \(\varphi\) to a mapping of each inner vertex \(v\) of \(T\) to a branch of \(S\).

Lastly, we assume that the input consists of a single gene tree; otherwise we merge multiple given gene trees by connecting all their roots to a super root.

A

B

C

D
effective population size
time

(a) Continuous linear model.

A

B

C

D
effective population size
time

(b) Piecewise constant model.

Fig. 2: Multispecies coalescent of a species tree on four species \(A, B, C, D\) and a gene tree on eleven taxa under two different models.

Visualizing MSC trees. Visualizations of an MSC tree usually show the species and gene tree together. This allows the user to detect any discordance between them such as whether they have different topologies and where incomplete lineage sorting occurs. It is also interesting to see where these events occur with respect to the inferred population sizes. Furthermore, these drawings are used to diagnose whether the parameters of the model are set up well. E.g., if all inner vertices of the gene tree occur directly above nodes of the species tree or if all occur near the root of the species tree, parameters may have been chosen poorly.

Wilson et al. [38] suggested a tree-in-tree style for an MSC tree \(\langle S, T, \varphi \rangle\) under continuous models similar to the one shown in Fig. 2a. There, the species tree \(S\) is drawn in a space-filling fashion such that the branch widths of \(S\) reflect the associated population sizes and the gene tree \(T\) is then drawn into \(S\) as a classic node-link diagram. Without these constraints on the branch widths, \(T\) could be drawn as a classic rectangular cladogram as in Fig. 1. As noted above, the MSC model ensures that \(T\) can be drawn inside \(S\) without edges of \(T\) crossing edges of \(S\) since, for each edge \(uv\) of \(T\), we have that, if \(u\) and \(v\) lie inside the branches \(e_u\) and \(e_v\) of \(S\), respectively, then either \(e_u\) precedes \(e_v\) or \(e_u = e_v\).

Douglas [12] developed the tool UglyTrees that generates tree-in-tree drawings for MSC trees under the piecewise constant model; Fig. 2b resembles such a drawing. He points out that the results are in many cases visually unpleasing (as reflected in his choice for the tool’s name), in particular if the difference in width between parent and child is large. This is amplified in practice by the inverse relationship between the number of gene tree vertices and population sizes, which results in clusters of vertices in the narrowest branches [12].
Fig. 3: Representation of co-phylogenetic trees with the host tree as background shape and the parasite tree drawn with a node-link diagram (after Calamoneri et al. [9]).

Related work. There exist several applications where multiple phylogenetic trees are displayed together. In a tanglegram, two phylogenetic trees on the same set of taxa are drawn opposite each other and the corresponding leaves are connected by line segments for easy comparison [8,14]. The tool DensiTree [7] allows the user to compare many trees simultaneously by drawing them on top of each other. A co-phylogenetic tree consists of two rooted phylogenetic trees, namely, a host tree $H$ and a parasite tree $P$, together with a mapping (reconciliation) of the vertices of $P$ to vertices of $H$. Other than in an MSC tree, the vertices of $P$ commonly do not have heights but are mapped to nodes of $H$, the host branches do not have associated population sizes, and the edges of $P$ can go from one subtree of $H$ to another, representing so-called host switches. Several tools visualize the reconciliation of co-phylogenetic trees [10,11,26,35]. Commonly, the branches of $H$ are drawn with thick lines such that $P$ can be embedded into $H$; see Fig. 3. Recently, Calamoneri et al. [9] suggested a tree-in-tree style for reconciliation similar to the one for MSC trees above. They draw $H$ in a space-filling way and embed $P$ into $H$ as an orthogonal node-link diagram.

More generally, visualizations have been studied for various models in phylogenetics, such as rooted phylogenetic trees [2,6,31], in conjunction with a geographic map [27,29], unrooted phylogenetic trees, and split networks [13,23,36]. In recent years, research has been extended from drawings of trees to drawings of phylogenetic networks [19–22,37], which are more general.

All these applications share the main combinatorial objective of finding drawings where the number of crossings between edges is minimized. To this end, good embeddings of the trees (or networks) have to be found, which are mostly fully defined by the order of the leaves. For example, Calamoneri et al. [9] investigated the problem of minimizing the number of crossings of the parasite tree in their drawings. They showed that this problem is in general NP-hard, though planar instances can be identified efficiently, and they suggested two heuristics.

Contribution. Motivated by the drawing styles of Wilson et al. [38] and by the recently proposed space-filling drawing style for reconciliation [9] and phylogenetic networks [37], we formally define tree-in-tree drawing styles for MSC trees (Section 2). In our base, rectangular style, we draw the species tree such that it completely fills a rectangle; the branch widths are based on the number of leaves
in the respective gene subtree. Additionally, population sizes can be represented, e.g., by a background color gradient. This avoids visual overload and can be used for any population size model. Nonetheless, based on this, we also define a style where the branch widths are proportional to the associated population sizes.

We then study the problem of minimizing the number of crossings between edges of the gene tree both for the case when the embedding of the species tree is already fixed and when it is left variable. We show that the crossing minimization problem is NP-hard in both cases (Section 3). On the positive side, we show that crossing-free instances can be identified in linear time (Section 4) and we introduce two heuristics and an integer linear program (ILP) formulation for the non-planar cases (Section 5). We measure the performance of the heuristics on real-world instances by comparing them to optimal solutions obtained via the ILP, which we have tuned to solve medium-size instances in reasonable time.

Complete proofs to some of our claims and detailed descriptions of our algorithms can be found in Section 5. Implementations of our algorithm are shared upon request.

2 Drawing Style

In this section, we define styles for tree-in-tree drawings of an MSC tree \( \langle S, T, \varphi \rangle \). A drawing is defined for particular leaf orders \( \pi(S) \) and \( \pi(T) \) of \( S \) and \( T \), respectively, and we assume that they satisfy the following requirements. (i) At least one leaf is mapped to each species. (ii) The leaf order \( \pi(T) \) is consistent with \( \varphi \) and \( \pi(S) \), that is, the sets of leaves of \( T \) mapped by \( \varphi \) to a species \( s \) are consecutive in \( \pi(T) \) and succeed all leaves mapped to the species that precede \( s \) in \( \pi(S) \). (iii) If all the leaves of a subtree \( T' \) of \( T \) are mapped to the same species \( s \), then these leaves must be consecutive in \( \pi(T) \), and \( T' \) must admit a plane drawing above the leaves. We first describe the rectangular style where branch widths are proportional to the number of leaves in subtrees, and then the proportional style where branch widths are proportional to the population sizes. Finally, we define the crossing minimization problem for tree-in-tree drawings.

Rectangular style. Our drawing area is an axis-aligned rectangle \( R \). The width of \( R \) is twice the number of leaves of \( T \). We assume that the roots of \( S \) and \( T \) have out-degree 1. We scale \( h \) such that the heights of the roots equal the height of \( R \). The given heights of vertices and nodes thus correspond to heights in \( R \).

The species tree \( S \) is drawn as follows; see Fig. 4. For a species \( s \in L(S) \), we define \( n(s) = |\varphi^{-1}(s)| \), that is, the number of leaves of \( T \) mapped to \( s \) by \( \varphi \). The branches of \( S \) are represented by internally disjoint rectangles whose union covers \( R \). Of each such rectangle we only draw the left and the right border – the delimiters. Their \( y \)-coordinates are defined by the heights of their start and target nodes. The \( x \)-coordinates are defined recursively: A branch incident to a species \( s \) has width \( 2n(s) \) and an internal branch has width equal to the width of its two child branches; see Fig. 4b. Note that the branch incident to the root has a width equal to the width of \( R \).
Fig. 4: In the rectangular drawing style for an MSC tree, the branch widths are proportional to the number of leaves in the contained subtree.

The gene tree $T$ is drawn in a classical orthogonal cladogram style: The leaves of $T$ are evenly distributed at the base of $R$ by placing them on odd coordinates and ordered by $\pi(T)$. Since $\pi(T)$ is consistent with $\varphi$ and $\pi(S)$, for each species $s$, the leaves $\varphi^{-1}(s)$ are thus placed at the baseline of the branch incident to $s$. Each inner vertex of $T$ is centered horizontally between its two children and placed at its respective height.

Note that two or more vertical line segments can end up with the same x-coordinate. Suppose that this is the case for two vertical line segments $e_u$ and $e_v$ that also overlap vertically and that have end vertices $u$ and $v$, respectively; see Fig. 4b for an example. Further suppose that $e_u$ ends below $e_v$. We then shift $u$ slightly in the direction of its parent and $v$ into the opposite direction. Overlaps of horizontal line segments could be handled analogously, though one would have to point out that the given heights are then misrepresented.

In this style, the population sizes are not represented by the branch widths. Instead, one could set the background color of each branch to a corresponding intensity. We advocate the rectangular tree-in-tree style (with or without coloring) since it yields a clear representation for MSC trees. This is helpful for model diagnosis and for finding incomplete lineage sorting events.

**Proportional style.** The proportional style conceptually follows the rectangular style, though here the population sizes of each branch are represented by its width in the drawing; see Fig. 2a for an example. We require that the shape of $S$ is symmetric with respect to the central vertical axis. Therefore, each branch $e$ is represented by a sequence of trapezoids whose widths are derived from the population sizes associated with $e$. Embedding $T$ into $S$ may force the non-horizontal line segments of $T$ to take various different slopes, “following” the trapezoids. The combinatorial properties of a drawing in the rectangular style and a drawing in the proportional style may thus differ.

A proportional-style drawing can be computed as follows. First, we draw $S$ bottom to top by adding one row of trapezoids for each inner node $u$ of $S$ encountered. More precisely, at the height of $u$, we calculate the width of each “active”
branch and the total width of \( S \). We can then extend the delimiters between the branches. Second, the width of each species \( s \) is subdivided into \( 2|\varphi^{-1}(s)| \) pieces at the baseline, such that each gene leaf can be placed at an odd position and according to \( \pi(T) \). The rest of the gene tree can then be computed bottom-up. For each inner vertex \( v \) of \( T \), a sequence of line segments is drawn from each of its two children up to the height of \( v \). The two ends are connected with a horizontal line segment on which \( v \) is placed centrally. The slope of a non-horizontal line segment \( f \) is set such that \( f \) splits the top edge and the bottom edge of the trapezoid containing \( f \) in the same ratio.

Crossing minimization problems. In the drawing styles above, by our assumptions for \( S, T \), and \( \varphi \), no edge of \( T \) crosses a segment that represents \( S \). However, edges of \( T \) may cross each other. Such crossings are determined by \( \pi(S) \) and \( \pi(T) \). We do not know \( \pi(T) \), and we consider two subproblems: in one \( \pi(S) \) is given, in the other \( \pi(S) \) is not given. Our objective is to find a leaf order of \( \pi(T) \) and possibly of \( \pi(S) \) such that the number of crossings among edges of \( T \) is minimized.

We define this problem formally for both drawing styles. In the VARIABLE TREE-IN-TREE DRAWING CROSSING MINIMIZATION (VTT) problem, we are given an MSC tree \( \langle S, T, \varphi \rangle \) and an integer \( k \), and the task is to find a tree-in-tree drawing (in rectangular or proportional style) such that \( T \) has at most \( k \) crossings; a solution is specified by leaf orders \( \pi(S) \) and \( \pi(T) \). In the FIXED TREE-IN-TREE DRAWING CROSSING MINIMIZATION (FTT) problem, we have the same task, but we are additionally given a leaf order \( \pi(S) \); a solution is specified by a leaf order \( \pi(T) \).

3 NP-Hardness

In this section, we show that VTT and FTT are NP-complete. For showing hardness, we reduce from MAX-CUT, which is NP-hard [16]. Recall that in an instance of MAX-CUT, we are given a graph \( G \) and a positive integer \( c \). The task is to decide whether there exists a bipartition \( \{A,B\} \) of the vertex set \( V(G) \) of \( G \) such that at least \( c \) edges have one endpoint in \( A \) and one endpoint in \( B \).

In the proofs below, we use the rectangular style. Since the branch widths of the rectangles can also be seen as population sizes, the proofs also hold for the proportional style. We make use of the following construction where we replace a single leaf with a particular subtree. Let \( \ell \) be a leaf of \( T \) with its parent \( p \) at height \( h(p) \). Suppose that we replace \( \ell \) with a full binary subtree \( T_\ell \) that has a specific number of leaves, say \( n_\ell \) many. (Recall that a binary tree is \textit{full} if every vertex has either 0 or 2 children.) Now we have two options to influence the shape of \( T_\ell \) in the solution drawing. In option 1, we set the height of the lowest inner vertex of \( T_\ell \) to at least \( h(p) - \varepsilon \) for some appropriately small \( \varepsilon > 0 \). Now if the vertical line segment incident to \( \ell \) is initially crossed by at least one horizontal segment, then any drawing of \( T_\ell \) will contain at least \( n_\ell \) many crossings. In this case, we call \( T_\ell \) a \textit{thick expanded leaf}. In option 2, we set the height of the root
of $T_i$ to $\varepsilon'$, for some appropriately small $\varepsilon' > 0$. Then a drawing of $T_i$ will require $n_t$ horizontal space. In this case, we call $T_i$ a wide expanded leaf.

**Theorem 1.** The VTT problem is NP-complete.

**Proof.** The problem is in NP since, given an MCS tree $\langle S, T, \varphi \rangle$, an integer $k$, and leaf orders $\pi(S)$ and $\pi(T)$, we can check in polynomial time whether the resulting drawing has at most $k$ crossings. To prove NP-hardness, we reduce from MAX-CUT as follows.

For a MAX-CUT instance $(G, c)$, we construct an instance $\langle \langle S, T, \varphi \rangle, k \rangle$ of the VTT problem with a species tree $S$, a gene tree $T$, a leaf mapping $\varphi$, and a positive integer $k$; see Fig. 5. Let $V(G) = \{v_1, \ldots, v_n\}$ ($n \geq 3$), let $m = |E(G)|$, and let $\{A, B\}$ be some partition of $V(G)$. Let $S$ be a caterpillar tree on $2n+1$ species labeled $0, 1, 1', \ldots, n, n'$ with decreasing depth, that is, $S$ contains phylogenetic subtrees on species sets $\{0, 1\}, \{0, 1, 1'\}, \ldots, \{0, 1, 1', \ldots, n, n'\}$. For each $i \in \{1, \ldots, n\}$, we add to $T$ a vertex gadget (described below) to enforce that species $i$ and $i'$ are on opposite sites of 0. Then species $i$ being to the left of 0 corresponds to $v_i$ being in $A$, whereas $i$ being to the right of 0 corresponds to $v_i$ being in $B$. Furthermore, for each edge $\{v_i, v_j\} \in E(G)$ with $i < j$, we add to $T$ an edge gadget that consists of a cherry (i.e., a subtree on two leaves) from $i$ to $j'$ and that induces $n^3$ crossings if and only if $i$ and $j$ are both to the left or both to the right of 0. By construction, all pairs of vertex gadgets will induce at most $n^2$ crossings, all pairs of edge gadgets will induce at most $n^4$ crossings, and all pairs of vertex and edge gadgets will induce at most $2n^3$ crossings. In total, these gadgets induce at most $2n^4$ crossings (using $n \geq 3$). Hence, by setting $k = (m - c)n^5 + 2n^4$, we get that a tree-in-tree drawing of $\langle S, T, \varphi \rangle$ with less than $k$ crossings exists if and only if $G$ admits a cut containing at least $c$ edges.

A vertex gadget consists of two cherries; see Fig. 6. The first cherry has one leaf each in species 0 and $i'$ and their parent $p$ gets some height $h(p)$. The second cherry has one leaf each in species 0 and $i$ and their parent gets height $h(p) + 1$. We replace the leaf in $i$ with a thick expanded leaf on $n^8$ many leaves. Note that if $i$ and $i'$ are on the same side of 0, then $i$ lies between $i'$ and 0. Hence, in this case, $i$ and $i'$ induce no more than $n^3$ crossings (using $n \geq 3$).
Fig. 6: The vertex gadget for $v_i$ forces the species $i$ and $i'$ on opposite sites of species 0.

(a) If $i$ and $i'$ are on different sides of 0, the gadget induces no crossings.
(b) If $i$ and $i'$ are on the same side of 0, the gadget induces $n^8$ many crossings.

case, the horizontal line segment through $p$ crosses the thick expanded leaf and causes $n^8$ crossings. Since $n^8 > k$, the vertex gadgets work as intended.

We set the heights of the roots of the edge gadget cherries above those of all vertex gadgets. Furthermore, we add a thick expanded leaf on $n^8$ leaves in species 0 with the lowest inner vertex higher than any edge gadget. Hence, the horizontal line segment of an edge gadget crosses $n^8$ vertical segments if and only if $i$ and $j$ are both in $A$ or both in $B$.

To tie everything together in $T$, we introduce a path from the thick expanded leaf in 0 to the root. To this path, going upwards, we first connect the cherries of the vertex gadgets, whose leaves are in $1, 1', \ldots, n, n'$, in this order. Above those, we then connect the cherries of the edge gadgets to the path. ☐

A full proof of the following statement can be found in Appendix A.

**Theorem 2.** The FTT problem is NP-complete.

**Proof (sketch).** To prove NP-hardness, we again reduce from MAX-CUT. For a MAX-CUT instance $(G, c)$, we construct an instance $\langle \langle S, T, \varphi \rangle, \pi(S), k \rangle$ of FTT. Let $V(G) = \{v_1, \ldots, v_n\}$, and let $\{A, B\}$ be some partition of $V(G)$. Our construction consists of three parts and uses several different gadgets; see Fig. 7. On the left side, we have a vertex gadget for each vertex $v_i$. For each edge $v_iv_j$, we have an edge gadget that connects the vertex gadgets of $v_i$ and $v_j$. The gadget has a further leaf at the far right. We simulate $v_i$ being in either partition by having a thick expanded leaf always being either left or right of all attached edge gadgets; otherwise it would cause too many crossings. Using spacer gadgets, the leaves of edge gadgets to the far right are horizontally placed such that the root of each edge gadget lies exactly where we place a cut gadget. The cut gadget will induce $n^4$ crossings with the incoming edge of the root of each edge gadget only if the respective vertices are in the same partition. While some parts of our construction induce a fixed number of crossings, others cause in total at most $n^3$ crossings. Hence, as in the proof of Theorem 1, we can set $k$ with respect to $c$ such that the instance admits a tree-in-tree drawing with at most $k$ crossings if and only if $G$ admits a cut with at least $c$ edges. ☐
4 Planar Instances

In this section, we show that we can decide in linear time whether an FTT or VTT instance admits a planar drawing.

**Theorem 3.** Both when the embedding of $S$ is fixed or variable, we can decide, in linear time, whether an MSC tree $(S, T, \varphi)$ admits a planar rectangular tree-in-tree drawing. If yes, such a drawing can be constructed within the same time bound.

**Proof.** Bertolazzi et al. [5] devised a constructive linear-time algorithm for upward planarity testing of a single-source (or single-sink) digraph, that is, whether the given digraph can be drawn with each edge $uv$ drawn as a monotonic upward curve from $u$ to $v$. For both the VTT and FTT problem, we can extend $T$ to a single-source digraph $\tilde{T}$ that admits an upward planar embedding if and only if $(T, \varphi)$ admits a planar tree-in-tree drawing (respecting any given leaf order for $S$). We can thus apply Bertolazzi et al.’s algorithm to $\tilde{T}$.

First, suppose the embedding of $S$ is variable. Let $L_1, L_2, \ldots, L_m$ be the subsets of $L(T)$ corresponding to the $m$ species of $S$. For $i \in \{1, \ldots, m\}$, we merge all vertices in $L_i$ into a single vertex $v_i$. We then connect the vertices $v_1, \ldots, v_m$ to a new vertex $t$; see Fig. 8b. We use the resulting single-source digraph as $T$, which clearly has the desired properties.

**Fig. 7:** Sketch of the reduction of the graph from Fig. 5a to a rectangular tree-in-tree drawing with fixed species tree embedding. Each edge gadget is drawn in the color of the respective edge in Fig. 5a. The gadget for the edge $v_1v_3$ (orange) has $n^4$ crossings more than the other edge gadgets; namely with the cut gadget (purple).

**Fig. 8:** We can test efficiently whether a tree-in-tree instance $(S, T, \varphi)$ admits a planar drawing with a single-source upward planarity test on an extended gene tree.
Second, if the embedding of $S$ is fixed, we extend $\bar{T}$ from above further to ensure that the subsets $L_1, \ldots, L_m$ end up in correct order. Let the species of $S$ be $s_1, \ldots, s_m$ from left to right. For $i \in \{1, \ldots, m-1\}$, we add a vertex $u_i$ and edges $v_i u_i$, $v_{i+1} u_i$, and $u_i t$; see Fig. 8c. The resulting graph is our new $\bar{T}$, which works again as intended.

In both cases, $\bar{T}$ has a linear size and can be constructed in linear time. □

5 Algorithms

For non-planar instances of the FTT and the VTT problem, we propose a heuristic as well as an ILP. We describe the main ideas of the algorithms here; more details can be found in Appendix B. The ILP, which models a drawing in a straightforward fashion, is described in Appendix C. Overlaps of vertical segments in an ILP solution are resolved in a post-processing step. We focus here on the rectangular tree-in-tree style, though the heuristics can also be set up analogously for the proportional style. However, since the computation for the proportional style is more involved, as alternative, one can simply use leaf orders computed for the rectangular style.

**Heuristic for FTT.** Let $\langle S, T, \varphi \rangle$ be an MSC tree and $\pi(S)$ a leaf order for $S$. The idea of the heuristic is to greedily sort the leaves in each species from the left and from the right towards the centre. To this end, the algorithm (i) goes through the inner vertices in order of increasing height and (ii) when the subtree $T(v)$ of an inner vertex $v$ has leaves in more than one species, then any unplaced leaves of $T(v)$ are put on a left stack or a right stack of their respective species; see Fig. 9. In doing so, we aim at a placement that minimizes the horizontal dimension of a drawing of $T(v)$. In particular, $T(v)$ initially has unplaced leaves in at most two species. Therefore, we place the leaves in the left species $s$ on the right stack of $s$ and the leaves in the right species $s'$ on the left stack of $s'$; see Fig. 9b. When leaves are pushed on a stack, it is ensured that any subtree with all leaves in one species admits a planar drawing. This can be done in linear time.

**Heuristic for VTT.** We extend the heuristic for FTT to also compute a leaf order for $S$ as follows. The main idea is to set the rotation of inner nodes of $S$ such that subtrees of $T$ horizontally span over few species. Therefore, when we handle an inner vertex $v$ with children $x$ and $y$ and we try to move the roots of $T(x)$ and $T(y)$ close together. Suppose $x$ lies in the branch ending at node $x'$ of $S$. Let $S(x')$ be the minimal phylogenetic subtree of $S$ on all species that contain a leaf of $T(x)$; define $S(y')$ analogously. If $S(x')$ and $S(y')$ are disjoint, then we set the rotation of each unfixed vertex on the path from the root of $S(x)$ to the root of $S(y)$ such that the species of $S(x)$ and $S(y)$ get as close together as possible; see Fig. 10. Only then is $v$ processed with the FTT heuristic. There are a few other cases to consider, which can be handled along the same line (see Appendix B for details). Overall, handling an inner vertex of $T$ can be done in linear time and so the overall running time is quadratic.
The heuristic sorts the leaves in each species from the sides towards the centre by using a left stack and a right stack for each species (plus a central bucket of unplaced (orange) leaves), here on the example from Figs. 2 and 4.

The heuristic for the VTT problem rotates inner nodes of $S$ to bring the leaves of the currently handled gene subtree closer together. Here, for the second inner vertex $v$ of $T$, two nodes would be rotated to bring the species $A$ and $E$ together.

Note if an instance admits a planar solution, then the heuristics find one. That is, because any rotation of a node of $S$ or an assignment to stacks keeps the leaves of a subtree of $T$ consecutively whenever possible.

**Experimental evaluation.** We tested the heuristic and the ILP on three different real world data sets Gopher ($S$ on 8 species, $T$ on 26 gene taxa, 1083 instances, i.e., different topologies and heights for pairs of $S$ and $T$) [4], Barrow (21 species, 88 gene taxa, 312 instances), and Hamilton (36 species, 83 gene taxa, 99 instances) [17]. On a laptop with 4 cores, 8 GB of RAM, Ubuntu 20.04, and CPLEX 12.10 we tested each heuristic and the ILP on each instance once with the default (start) embedding of $S$ from the input file and 10 times with a random (start) embedding for $S$. A proper experimental evaluation is out of scope for this paper, but we observed the following:

- The VTT heuristic got a better result than the FTT heuristic for 60–75% of the instances, the same result for 6–27%, and a worse result for 13–20%. For the Barrow instances, they improved the average number of 24.5 crossings of the default embeddings to 10.3 (FTT) and 7.2 (VTT) or even to 6.6 and 5.7 using random starting embeddings of $S$.
- Concerning FTT, the optimal solutions found by the ILP show that the FTT heuristic also found the optimal solution for about 50–55% of the instances;
e.g., for the Barrow instances, the FTT heuristic had on average only 1.3 crossings more than the optimal. Concerning VTT, the heuristics also got within zero to few crossings to the best ILP solution for Gopher instances.

- Both heuristics are sensitive to the initial embedding of $S$ as the lowest number of crossings was achieved with a random start embedding for 70–90% and for 44–75% of the instances for FTT and for VTT, respectively. The results between start embeddings vary more for VTT than for FTT.
- The FTT and the VTT heuristic run in a fraction of a second per instance, while the ILP for the FTT problem takes about 1–4s for most instances. The ILP for the VTT problem only found solutions for the Gopher instance within reasonable time for some instances.

Since the heuristics are so fast, our recommendation is to run both heuristics for several different start embeddings of $S$ and then take the best found solution.

To the best of our knowledge, this is the first software to visualize MSC trees for the continuous linear model and so we hope that this will help researchers in the emerging field of MSC to visualize their results.

Acknowledgments

We thank the reviewers for their comments and J. Douglas for providing us with the test data and his helpful explanations concerning MSC.

References

1. B. S. Arbogast, S. V. Edwards, J. Wakeley, P. Beerli, and J. B. Slowinski. Estimating divergence times from molecular data on phylogenetic and population genetic timescales. *Ann. Rev. Ecol. Syst.*, 33:707–740, 2002. doi:10.2307/3069277.
2. C. Bachmaier, U. Brandes, and B. Schlieper. Drawing phylogenetic trees. In X. Deng and D.-Z. Du, editors, *Int. Symp. Algorithms & Computation (ISAAC)*, volume 3827 of *LNCS*, pages 1110–1121. Springer, 2005. doi:10.1007/11602613_110.
3. L. N. Barrow, H. F. Ralicki, S. A. Emme, and E. M. Lemmon. Species tree estimation of North American chorus frogs (Hylidae: Pseudacris) with parallel tagged amplicon sequencing. *Mol. Phyl. Evol.*, 75:78–90, 2014. doi:10.1016/j.ympev.2014.02.007.
4. N. M. Belfiore, L. Liu, and C. Moritz. Multilocus phylogenetics of a rapid radiation in the genus Thomomys (Rodentia: Geomyidae). *Syst. Biol.*, 57(2):294–310, 2008. doi:10.1080/10635150802044011.
5. P. Bertolazzi, G. Di Battista, C. Mannino, and R. Tamassia. Optimal upward planarity testing of single-source digraphs. *SIAM J. Comput.*, 27(1):132–169, 1998. doi:10.1137/S0097539794279626.
6. J. J. Besa, M. T. Goodrich, T. Johnson, and M. C. Osegueda. Minimum-width drawings of phylogenetic trees. In Y. Li, M. Cardei, and Y. Huang, editors, *Int. Conf. Combin. Optim. Appl. (COCOA)*, volume 11949 of *LNCS*, pages 39–55, 2019. doi:10.1007/978-3-030-36412-0_4.
7. R. R. Bouckaert. DensiTree: Making sense of sets of phylogenetic trees. *Bioinf.*, 26(10):1372–1373, 2010. doi:10.1093/bioinformatics/btq110.

8. K. Buchin, M. Buchin, J. Byrka, M. Nöllenburg, Y. Okamoto, R. I. Silveira, and A. Wolff. Drawing (complete) binary tanglegrams – hardness, approximation, fixed-parameter tractability. *Algorithmica*, 62(1–2):309–332, 2012. doi: 10.1007/s00453-010-9456-3.

9. T. Calamoneri, V. Di Donato, D. Mariottini, and M. Patrignani. Visualizing cophylogenetic reconciliations. *Theoret. Comput. Sci.*, 815:228–245, 2020. doi: 10.1016/j.tcs.2019.12.024.

10. F. Chevenet, J. Doyon, C. Scornavacca, E. Jacox, E. Jousselin, and V. Berry. SylvX: A viewer for phylogenetic tree reconciliations. *Bioinf.*, 32(4):608–610, 2016. doi:10.1093/bioinformatics/btv625.

11. C. Conow, D. Fielder, Y. Ovadia, and R. Libeskind-Hadas. Jane: A new tool for the cophylogeny reconstruction problem. *Algorithms Mol. Biol.*, 5(1):1–10, 2010. doi:10.1186/1748-7188-5-16.

12. J. Douglas. UglyTrees: A browser-based multispecies coalescent tree visualizer. *Bioinf.*, 07 2020. doi:10.1093/bioinformatics/btaa679.

13. A. W. M. Dress and D. H. Huson. Constructing splits graphs. *Trans. Comput. Biol. Bioinf.*, 1(3):109–115, 2004. doi:10.1145/1041503.1041506.

14. H. Fernau, M. Kaufmann, and M. Poths. Comparing trees via crossing minimization. *J. Comput. Syst. Sci.*, 76(7):593–608, 2010. doi:10.1016/j.jcss.2009.10.014.

15. T. Flouri, X. Jiao, B. Rannala, and Z. Yang. Species tree inference with BPP using genomic sequences and the multispecies coalescent. *Mol. Biol. Evol.*, 35(10):2585–2593, 2018. doi:10.1093/molbev/msy147.

16. M. R. Garey and D. S. Johnson. *Computers and Intractability: A Guide to the Theory of NP-Completeness*. W. H. Freeman & Co., San Francisco, 1979.

17. C. A. Hamilton, A. R. Lemmon, E. M. Lemmon, and J. E. Bond. Expanding anchored hybrid enrichment to resolve both deep and shallow relationships within the spider tree of life. *BMC Evol. Biol.*, 16(1):1–20, 2016. doi:10.1186/s12862-016-0769-y.

18. J. Heled and A. J. Drummond. Bayesian inference of species trees from multilocus data. *Mol. Biol. Evol.*, 27(3):570–580, 2009. doi:10.1093/molbev/msp274.

19. D. H. Huson. Drawing rooted phylogenetic networks. *IEEE/ACM Trans. Comput. Biol. Bioinf.*, 6(1):103–109, 2009. doi:10.1109/TCBB.2008.58.

20. D. H. Huson, R. Rupp, and C. Scornavacca. *Phylogenetic Networks: Concepts, Algorithms and Applications*. Cambridge Univ. Press, 2010.

21. J. Klawitter and T. Mchedlidze. Upward planar drawings with two slopes. *J. Graph Algorithms Appl.*, 26(1):171–198, 2022. doi:10.7155/jgaa.00587.

22. J. Klawitter and P. Stumpf. Drawing tree-based phylogenetic networks with minimum number of crossings. In D. Auber and P. Valtr, editors, *Graph Drawing and Network Visualization (GD)*, volume 12590 of *LNCS*, pages 173–180. Springer, 2020. doi:10.1007/978-3-030-68766-3_14.

23. T. H. Kloepfer and D. H. Huson. Drawing explicit phylogenetic networks and their integration into splitstree. *BMC Evol. Biol.*, 8(1):22, 2008. doi:10.1186/1471-2148-8-22.

24. M. Lima. *The Book of Trees: Visualizing Branches of Knowledge*. Princeton Architectural Press, 2014.

25. F. K. Mendes and M. W. Hahn. Gene tree discordance causes apparent substitution rate variation. *Syst. Biol.*, 65(4):711–721, 2016. doi:10.1093/sysbio/syw018.
26. D. Merkle and M. Middendorf. Reconstruction of the cophylogenetic history of related phylogenetic trees with divergence timing information. *Theory in Biosciences*, 123(4):277–299, 2005. doi:10.1016/j.tibio.2005.01.003.

27. R. Page. Visualising geophylogenies in web maps using geojson. *PLOS Currents*, 7, 2015. URL: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4481111.

28. P. Pamilo and M. Nei. Relationships between gene trees and species trees. *Mol. Biol. Evol.*, 5(5):568–583, 1988. doi:10.1093/oxfordjournals.molbev.a040517.

29. D. H. Parks, T. Mankowski, S. Zangoocoi, M. S. Porter, D. G. Armanini, D. J. Baird, M. G. I. Langille, and R. G. Beiko. Gengis 2: Geospatial analysis of traditional and genetic biodiversity, with new gradient algorithms and an extensible plugin framework. *PLoS ONE*, 8(7):1–10, 2013. doi:10.1371/journal.pone.0069885.

30. B. Rannala, S. V. Edwards, A. Leaché, and Z. Yang. The multi-species coalescent model and species tree inference. In C. Scornavacca, F. Delsuc, and N. Galtier, editors, *Phylogenetics in the Genomic Era*, chapter 3.3, pages 3.3:1–3.3:21. HAL, 2020. URL: https://hal.archives-ouvertes.fr/hal-02535070v3.

31. A. Rusu. Tree drawing algorithms. In R. Tamassia, editor, *Handbook on Graph Drawing and Visualization*, chapter 3, pages 155–192. Chapman and Hall/CRC, 2013.

32. D. Schrempf and G. Szöllősi. The sources of phylogenetic conflicts. In C. Scornavacca, F. Delsuc, and N. Galtier, editors, *Phylogenetics in the Genomic Era*, chapter 3.1, pages 3.1:1–3.1:23. HAL, 2020. URL: https://hal.archives-ouvertes.fr/hal-02535070v3.

33. H. Schulz. Treevis.net: A tree visualization reference. *IEEE Comput. Graphics Appl.*, 31(6):11–15, 2011. doi:10.1109/CGG.2011.103.

34. C. Semple and M. A. Steel. *Phylogenetics*, volume 24 of *Oxford Lect. Ser. Math. & Its Appl.* Oxford Univ. Press, 2003.

35. B. Sennblad, E. Schreil, A.-C. B. Sonnhammer, J. Lagergren, and L. Arvestad. primetv: A viewer for reconciled trees. *BMC Bioinf.*, 8(148), 2007. doi:10.1186/1471-2105-8-148.

36. A. Spillner, B. T. Nguyen, and V. Moulton. Constructing and drawing regular planar split networks. *IEEE/ACM Trans. Comput. Biol. Bioinf.*, 9(2):395–407, 2012. doi:10.1109/TCBB.2011.115.

37. I. G. Tollis and K. G. Kakoulis. Algorithms for visualizing phylogenetic networks. *Theoret. Comput. Sci.*, 835:31–43, 2020. doi:10.1016/j.tcs.2020.05.047.

38. I. J. Wilson, M. E. Weale, and D. J. Balding. Inferences from DNA data: Population histories, evolutionary processes and forensic match probabilities. *J. Royal Stat. Soc. Ser. A*, 166(2):155–188, 2003. doi:10.1111/1467-985X.00264.
Appendix

A Full Proof of Theorem 2

Theorem 2. The FTT problem is NP-complete.

Proof. As with the VTT problem, it is easy to see that the FTT problem is in NP. Given an instance \((S, T, \varphi), \pi(S), k\) as well as a leaf order \(\pi(T)\), we can check in polynomial time whether this yields a drawing with at most \(k\) crossings.

To prove NP-hardness, we use a reduction from Max-Cut.

For a Max-Cut instance \(G, c\), we construct an instance \((S, T, \varphi), \pi(S), k\) of the FTT problem by devising a species tree \(S\) with leaf order \(\pi(S)\), a gene tree \(T\), a leaf mapping \(\varphi\), and a positive integer \(k\). Let \(V(G) = \{v_1, \ldots, v_n\}\) and let \(\{A, B\}\) be some partition of \(V(G)\). Our construction consists of three parts and uses several different gadgets, which are described in detail below. Figure 11 shows our constructions for the Max-Cut instance from Fig. 5a. On the left side, we have a vertex gadget for each vertex \(v_i\) where we simulate \(v_i\) being in either partition. To these vertex gadgets, we connect an edge gadget for each edge that also has a leaf on the right side. Using spacer gadgets, the third leaf of an edge gadget is horizontally placed such that the root of the edge gadget lies in the centre, where we place a cut gadget. The cut gadget will induce \(n^4\) crossings with the incoming edge of the root of each edge gadget only if the respective vertices are in the same partition. While some parts of our construction induce a fixed number of crossings, others cause in total at most \(n^3\) crossings. Hence, as in the proof of Theorem 1, we can set \(k\) with respect to \(c\) such that the instance admits a drawing with at most \(k\) crossings if and only if \(G\) admits a cut with at least \(c\) edges.

A spacer gadget consists of one species containing a wide expanded leaf of desired width. The gene tree parts of all spacer gadgets are tied together with a tree that has all internal vertices above all other gadgets, which in turn is connected to the rest of \(T\) close to the root. Hence, the spacer gadgets induce a fixed number of crossings.

A vertex gadget for a vertex \(v_i\) consists of seven species, namely, \(s_i^j\) with \(j \in \{-3, -2, -1, 0, 1, 2, 3\}\); see Fig. 12. For each edge incident to \(v_i\), there is one wide expanded leaf of width \(n^7\) of the respective edge gadget in \(s_i^0\). Moreover, \(s_i^0\)

\[\begin{align*}
\text{Fig. 11: Sketch of the reduction of the graph from Fig. 5a to a rectangular tree-in-tree drawing with fixed species tree embedding. Each edge gadget is drawn in the respective color; the one for } v_1v_3 \text{ has } n^4 \text{ more crossings with the cut gadget.}
\end{align*}\]
(a) A partitioner to the left corresponds to \( v_0 \) being in \( B \) of the partition \( \{ A, B \} \).

(b) A central partitioner would induce additional \( n^7 \) crossings.

Fig. 12: The vertex gadget for \( v_0 \) with its seven species has two edge gadgets attached.

contains a partitioner tree that consists of a thick expanded leaf of width \( n^7 \) and a wide expanded leaf of width \( n^{10} \). There are two cherries with leaves in \( s_i^{-1} \) and \( s_i^1 \) as well as in \( s_i^{-1} \) and \( s_i^3 \). The cherries are connected with a vertex \( p_i \). By setting the heights appropriately and with one spacer gadget each in \( s_i^{-2} \) and in \( s_i^2 \), we enforce that the partitioner cuts always through the horizontal line segments of both cherries (causing always \( 2n^7 \) crossings). Furthermore, only if the partitioner is all the way to the left or all the way to the right in \( s_i^0 \), then its thick expanded leaf does not cross with the horizontal line segment through \( p_i \); see again Fig. 12. Otherwise, there are another \( n^7 \) crossings which is always more than \( c \) and would thus obstruct any solution. Hence, the partitioner being at the left or at the right corresponds to \( v_i \) being in \( A \) or \( B \), respectively. The wide expanded leaf of the partitioner, which always lies next to the thick expanded leaf and below the horizontal line segment of \( p_i \), has the effect that the horizontal shift for the attached tree gadgets is substantial enough between the two configurations.

We assume that the edges are lexicographically ordered based on the indices of their vertices. The edge gadget for an edge \( v_iv_j \) contains a cherry on the expanded wide leaves in \( s^0_i \) and \( s^0_j \) and has the root \( p_{ij} \) that connects the cherry with another leaf in a species \( s_{ij} \). The height of \( p_{ij} \) is set below some value \( y^* \).

With spacer gadgets between these species (such as \( s_{ij} \)) on the right, we can enforce that \( p_{ij} \) lies in the central gap of the cut gadget only if (i) the expanded leaves of edge gadgets in \( s^0_i \) and \( s^0_j \) are lexicographic ordered from left to right and (ii) \( v_i \) and \( v_j \) are in different partitions. However, if the order is different or \( v_i \) and \( v_j \) are in the same partition, then \( p_{ij} \) lies inside a tower of the cut gadget. The gene tree parts of the edge gadgets merge into a tree above the cut gadget.
The cut gadget consists of two towers with a spacer gadget of $O(1)$ width between them; see again Fig. 7. Each tower spans $2n^4 + 1$ species, where the central one contains a spacer gadget of width $n^{10}$. It further contains $n^4$ cherries where the two leaves of each cherry are the only leaf in their respective species and that are $n^4 + 1$ species apart. The root of each such cherry gets a height between $y^*$ and $y^* + \varepsilon$ for some appropriate small $\varepsilon$. The cherries of each tower and then the two towers are connected into a single tree, which gets connected to the rest of $T$ somewhere close to the root. Now, if $p_{ij}$ lies above the central species of the cut gadget, then the vertical segment incident to $p_{ij}$ does not cut through the tower. If however $v_i$ and $v_j$ are, say, both in $A$, then $p_{ij}$ is placed further to the left (the partitioner causes a shift of $(n^{10} + n^7)/4$). In particular, even if the edge gadgets in $s_{0i}$ and $s_{0j}$ have a different order, $p_{ij}$ is placed inside the tower. Hence, in this case, the vertical segment incident to $p_{ij}$ cuts through the $n^4$ cherries of the left tower. In other words, $v_iv_j$ not being in the cut corresponds to an additional $n^4$ crossings.

\section*{B Heuristics}

In this section, we describe the heuristics that try to minimize the number of crossings in a tree-in-tree drawing of an MSC tree $(S, T, \varphi)$ in more detail. We consider first the rectangular style for both the case when a leaf order $\pi(S)$ is given (FTT problem) and when it is not (VTT problem). Afterwards we explain what changes have to be made to the heuristics when using them for the proportional style.

\subsection*{B.1 Heuristic for the FTT Problem}

Let $(S, T, \varphi)$ be an MSC tree and let $\pi(S)$ be a leaf order of $S$. Based on $\pi(S)$ the drawing of $S$ can already be computed. The heuristic then draws $T$ within $S$ in the rectangular tree-in-tree style. Recall that to this end, the heuristic (i) goes through the inner vertices in order of increasing height and (ii) when the subtree $T(v)$ of an inner vertex $v$ has leaves in more than one species, then any unplaced leaves are put on a left stack or a right stack of their respective species. More precisely, for each species $s$, the leaves in $s$ are sorted from the left towards the centre with a left stack and from the right towards the centre with a right stack. Initially no leaves of $T$ are on any left or right stack. We thus say that a leaf is unfixed and that it lies in the central bucket of its respective species; see Fig. 9. On the other hand, a leaf is called fixed if it is put on the left or right stack of its respective species. An inner vertex $v$ is called fixed if all leaves in $T(v)$ are fixed. In this case, the full drawing of $T(v)$ has been computed. At the end all leaves are fixed and the drawing of $T$ is completed. The order of the leaves in a species has emerged as the concatenation of its two stacks. Furthermore, it is ensured that any subtree $T'$ fully contained within a species the leaves of $T'$ are sorted such that $T'$ is drawn planar.
During the executing of the heuristic, we maintain for each vertex whether it is fixed or unfixed. Note that an inner vertex \( v' \) can only be unfixed if all leaves in \( T(v') \) lie in the same species \( s \). In this case, we also store the species \( s \) for \( v' \).

We now describe the different cases when handling an inner vertex \( v \). Let \( x \) and \( y \) be the two children of \( v \).

Case F1: Suppose that all leaves of \( T(v) \) lie in the same species \( s \). Then \( x \) \( y \), and \( v \) remain unfixed and the leaves of \( T(v) \) remain in the central bucket of \( s \). Using the information stored for \( x \) and \( y \), this case can be handled in \( \mathcal{O}(1) \) time.

Case F2: Suppose that \( x \) and \( y \) are unfixed and that the leaves of \( T(x) \) and \( T(y) \) lie in distinct species \( s_x \) and \( s_y \) respectively. Without loss of generality, assume that \( s_x \) lies left of \( s_y \). Then the leaves in \( T(x) \) are put on the right stack of \( s_x \) in an order such that \( T(x) \) can be drawn planar. The drawing of \( T(x) \) is then computed; see again Fig. 13. \( T(y) \) is handled analogously using the left stack of \( s_y \). This takes \( \mathcal{O}(|L(T(v))|) \) time.

Case F3: Suppose that \( x \) is unfixed and \( y \) is fixed. Let \( s_x \) be the species containing the leaves of \( T(x) \). If \( y \) lies to the left (right) or above the left (resp. right) stack of \( s_x \), then we place the leaves of \( T(x) \) on the left (resp. right) stack of \( s_x \). If \( y \) lies between the left and right stack of \( s_x \), then we place the leaves of \( T(x) \) on, say, the left stack of \( s_x \). As before, the leaves are added to a stack such that a planar drawing of \( T(x) \) can be computed. This case takes \( \mathcal{O}(L(T(x))) \) time.

Case F4: If both \( x \) and \( y \) are already fixed, then so is \( v \). The drawing of \( T(v) \) is completed by drawing \( v \) and the edges \( vx \) and \( vy \) in \( \mathcal{O}(1) \) time.

Note that the number of fixed and drawn vertices correlates linearly with the running time. Hence, the heuristic runs in \( \mathcal{O}(n) \) time.

![configuration after four inner vertices](image1.png)

![configuration after six inner vertices](image2.png)

**Fig. 13:** The heuristic sorts the leaves in each species from the sides towards the centre by using a left stack and a right stack for each species (plus a central bucket of unplaced (orange) leaves), here on the example from Figs. 2 and 4.
B.2 Heuristic for the VTT Problem

For the VTT problem, our heuristic computes for a given an MSC tree \( \langle S, T, \varphi \rangle \) a leaf order \( \pi(S) \) given by the rotation of each inner node of \( S \) alongside a leaf order \( \pi(T) \). In order to use the heuristic for the FTT problem to compute \( \pi(T) \), when handling an inner vertex \( v \) of \( T \), the order of the species that contain leaves of \( T(v) \) is set first. We say a node of \( S \) is set if its rotation has been set; otherwise we say it is unset. Here the idea to minimize crossings is to set the rotations of the inner nodes of \( S \) such that subtrees of \( T \) horizontally span over few species.

Suppose that we handle an inner vertex \( v \) with children \( x \) and \( y \). We would then like \( x \) and \( y \) to be close together. Suppose \( x \) lies in the branch ending at node \( x' \) of \( S \) and \( y \) lies in the branch ending at node \( y' \) of \( S \). Let \( S(x') \) be the minimal rooted phylogenetic subtree of \( S \) on all species that contain a leaf of \( T(x) \); define \( S(y') \) analogously. Note that \( S(x') \) and \( S(y') \) are rooted phylogenetic subtrees of \( S \) and hence contain no nodes of degree two. Furthermore, they may contain species that do not contain a leaf of \( T(x) \) or \( T(y) \), respectively. We distinguish the following cases.

Case V1: Suppose that \( S(x') \) and \( S(y') \) are disjoint. Let \( w \) be the lowest common ancestor of \( x' \) and \( y' \) in \( S \). Without loss of generality, assume that \( x' \) lies in the left subtree of \( w \). Then set the rotation of each unset node on the path from \( x' \) to \( w \) (excluding \( w \)) such that \( x' \) lies in its right subtree. Analogously, set the rotation of each unset node on the path from \( y' \) to \( w \) (excluding \( w \)) such that \( y' \) lies in its left subtree. An example is shown in Fig. 14a.

Case V2: Suppose that \( S(y') \) is a subtree of \( S(x') \) and that no leaf of \( T(x) \) lies in a species of \( S(y) \). On the path from \( y' \) to \( x' \), let \( w \) be the first node with a species in its subtree that contains a leaf of \( T(x) \). Without loss of generality, assume that \( y' \) lies in the right subtree of \( w \). Then set the rotation of each unset node on the path from \( y' \) to \( w \) (excluding \( w \)) such that \( y' \) lies in its left subtree; see Fig. 14b. The case where \( S(x') \) and \( S(y') \) have reversed roles is handled analogously.

Case V3: Suppose that neither of the two previous cases applies. Note that then \( y' \) lies on the path from a species containing a leaf of \( T(x) \) to \( x' \) or this occurs with \( x' \) and \( y' \) in reversed roles. Since all nodes on such a path are already set, the species of \( S(x') \) and \( S(y') \) that contain leaves of \( T(x) \) and \( T(y) \) cannot be moved closer together; this might not even be clearly defined. Hence, in this case, no node of \( S \) gets set.

Note that after the respective case has been applied, the relative order of the species containing leaves of \( T(v) \) is fixed. The heuristic can thus proceed with \( T(v) \) as described in Appendix B.1. However, the whole subtree of \( S \) containing \( T(v) \) can later change its horizontal position and be horizontally mirrored. Therefore, the \( x \)-coordinate of a handled vertex \( v \) is stored relative to its parent or relative to \( S(v') \) if its parent has not been handled yet.

To determine which case applies and then to execute its respective procedure, the heuristic has to determine \( S(x') \) and \( S(y') \) as well as walk along paths in \( S \).
This requires a constant number of traversals of $S$ and $T$ and therefore for each inner vertex of $T$ can be handled in $O(n)$ time. This yields an overall running time in $O(n^2)$.

(a) For the second inner vertex of $T$, Case 1 applies since the subtrees $S(x)$ and $S(y)$ are disjoint; two nodes of $S$ are rotated.

(b) For the third inner vertex of $T$, Case 2 applies since the subtree $S(y)$ is a proper subtree of $S(y)$ and no leaf of $T(x)$ lies in species $D$; one node of $S$ is rotated.

(c) For the root of $T$, Case 3 applies. The embedding of $S$ is also already fixed.

**Fig. 14:** The heuristic for the VTT problem rotates inner nodes of the species tree to bring the leaves of the currently handled gene subtree closer together. The stacks and central bucket are not shown.

### B.3 Heuristics for the Proportional Style

The FTT heuristic works the same for the proportional style as it does for the rectangular style. The only noteworthy difference is that first computing the drawing of $S$ and then computing the drawings of subtrees of $T$ is a bit more involved.

Using the VTT heuristic for the proportional style requires that the computed drawings of subtrees of $T$ are stored differently if one wants to have a quadratic running time. This is the case because when a node $u$ of $S$ gets rotated, the drawings of a subtree of $T$ in the subtree $S(u)$ before and after the rotation might have different slopes for every edge. Therefore, instead of storing the x-coordinate or x-offset of a vertex $v$, we can store the position of $v$ relative to the total width of the branch $v$ lies in. For example, if $v$ initially lies at 20% of the width from the left delimiter, then it will lie 20% of the width from the right delimiter after the rotation. Once the heuristic has reached the root of $T$, the drawing of $T$ and in particular of the edges of $T$ can be completed using these relative positions.

### C ILP Formulation

In this section, we describe an ILP formulation for the VTT problem. We are thus given an MSC tree $\langle S, T, \varphi \rangle$ and want to compute leaf orders $\pi(S)$ and $\pi(T)$.
for \( S \) and \( T \), respectively, such that a rectangular tree-in-tree drawing of \( \langle S, T, \varphi \rangle \) with \( \pi(S) \) and \( \pi(T) \) has the minimum number of crossing among all rectangular tree-in-tree drawings of \( \langle S, T, \varphi \rangle \). We can obtain a formulation for the FTT problem by turning certain variables into constants according to the given input as described at the end of this section.

We first describe the variables and constraints to model the input \( S \), \( T \), and \( \varphi \). Next, we show how we model \( \pi(S) \), \( \pi(T) \) and coordinates to describe a rectangular tree-in-tree drawing. We can then explain how crossings are recognized and how the number of crossings can thus be minimized.

**Model of input.** Recall that \( T \) and \( S \) have vertex sets \( V(S) \) and \( V(T) \) and leaf sets \( L(S) \) and \( L(T) \), respectively. We let \( \rho_S \) and \( \rho_T \) denote the roots of \( S \) and \( T \), respectively. The input is then described as follows. First, the constants that model \( S \):

\[
\begin{align*}
\ n_S &= |L(S)| \\
\alpha(s) &\in V(S) \text{ is the first child of } s \quad \text{for } s \in V(S) \setminus L(S) \\
\beta(s) &\in V(S) \text{ is the second child of } s \quad \text{for } s \in V(S) \setminus L(S) \\
\gamma(s) &\in V(S) \text{ is the parent of } s \quad \text{for } s \in V(S) \setminus \{\rho_S\}
\end{align*}
\]

Next, \( T \) is modelled analogously. However, here we also need the heights (y-coordinates) of the vertices as well as the subset of leaves of a subtree \( T(v) \), that is, the clade \( L(v) \) of \( v \).

\[
\begin{align*}
\ n_T &= |L(T)| \\
\alpha(v) &\in V(T) \text{ is the first child of } v \quad \text{for } v \in V(T) \setminus L(T) \\
\beta(v) &\in V(T) \text{ is the second child of } v \quad \text{for } v \in V(T) \setminus L(T) \\
\gamma(v) &\in V(T) \text{ is the parent of } v \quad \text{for } v \in V(T) \setminus \{\rho_T\} \\
y(v) &\in \mathbb{Q}^+ \text{ is the y-coordinate of } v \quad \text{for } v \in V(T) \\
L(v) &\subseteq L(T) \text{ is the clade of } v \quad \text{for } v \in V(T)
\end{align*}
\]

To model \( \varphi \), we use the following constants:

\[
\begin{align*}
\varphi(v) &\in V(S) \text{ is the root of } S(v') \text{ (details below)} \quad \text{for } v \in V(T) \\
\varphi^{-1}(s) &\subseteq V(T) \text{ is the set of leaves mapped to } s \quad \text{for } s \in V(S)
\end{align*}
\]

Note that we extended \( \varphi \) to inner vertices of \( T \). More precisely, for an inner vertex \( v \) of \( T \) that lies in the branching ending at node \( v' \) of \( S \), we have that \( \varphi(v) \) is the root of \( S(v') \) with, as we recall from above, \( S(v') \) defined as the minimal phylogenetic subtree of \( S \) that contains the clade of \( v \). If the clade of \( v \) is completely mapped to a species, (i.e. \( \varphi(v) \in L(S) \)), we will enforce that the clade \( L(v) \) forms an interval among the leaves in \( L(T) \).
Note that a crossing can only occur between a horizontal line segment \( f_u \) and a vertical line segment \( g_v \). Suppose \( f_u \) goes through a vertex \( u \) of \( T \). The y-coordinate of \( f_u \) is thus given by the y-coordinate of \( u \) and the x-coordinates of \( f_u \) are given by the x-coordinates of the two children \( \alpha(u) \) and \( \beta(u) \) of \( u \). Suppose \( g_v \) ends at a vertex \( v \). The x-coordinate of \( g_v \) is thus given by the x-coordinate of \( v \) and the y-coordinates are given by the y-coordinates of \( v \) and the parent \( \gamma(v) \) of \( v \). To decide whether \( f_u \) and \( g_v \) cross, we have to determine whether they overlap both vertically and horizontally. Since a vertical overlap is fully determined by the input, we can precompute this and pass it to ILP as \( a(u, v) \):

\[
a(u, v) \in \{0, 1\} \text{ whether } f_u \text{ and } g_v \text{ overlap vertically for } u \in V(T) \setminus L(T) \text{ and } v \in V(T) \setminus \{\rho_T\}
\]

Model of drawing. The main variables to model a drawing are the variables for the x-coordinates of the vertices. In fact, only the variables for x-coordinates of the leaves are actually decision variables, while all other variables will be auxiliary variables required to check feasibility or to count crossings. In the following description of the variables, \( f_u \) is the horizontal line segment passing through \( u \) and \( g_v \) is a vertical line segment ending at \( v \) as defined above.

The x-coordinates of the vertices of \( T \):

\[
x_v \in \{1, \ldots, n_T\} \quad \text{for } v \in L(T) \\
x_v \in \mathbb{Q} \quad \text{for } v \in V(T) \setminus L(T)
\]

The intended meaning of \( \bar{l}_{u,v} = 0 \) (\( \bar{r}_{u,v} = 0 \)) is that \( g_v \) is left (resp. right) of \( f_u \):

\[
\bar{l}_{u,v} \in \{0, 1\} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\} \\
\bar{r}_{u,v} \in \{0, 1\} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]

The intended meaning of \( z_{u,v} = 1 \) is that \( f_u \) horizontally overlaps with \( g_v \):

\[
z_{u,v} \in \{0, 1\} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]

The intended meaning of \( I^L_v = 42 \) (\( J^L_s = 42 \)) is that the leftmost leaf (resp. species) in the clade of \( v \) (resp. \( s \)) has position 42 in the permutation of \( L(T) \) (resp. \( L(S) \)).

\[
I^L_v \in \{1, \ldots, n_T\} \quad \text{for } v \in V(T) \\
I^L_v \in \{1, \ldots, n_T\} \quad \text{for } v \in V(T) \\
J^L_s \in \{1, \ldots, n_T\} \quad \text{for } s \in V(S) \\
J^L_s \in \{1, \ldots, n_T\} \quad \text{for } s \in V(S)
\]

Note that we use the notation \( x_v \) for the x-coordinate of \( v \) but \( y(v) \) for the y-coordinate of \( v \), since \( x_v \) is a variable whereas \( y(v) \) is a given constant.
For a permutation to represent a feasible solution we need to check whether the leaves mapped to each species form a consecutive partial permutation. This can be achieved by propagating interval bounds from the leaves towards the root of $S$. The equivalent property must be checked for inner vertices of $T$ whose clade is contained within a single species.

Concerning the overlap of $f_u$ and $g_v$, note that they overlap horizontally only if $x_v \in [x_{\alpha(u)}..x_{\beta(u)}]$. This can be check with the equation $((x_{\beta(u)} - x_v) \cdot (x_v - x_{\alpha(u)})) \geq 0$. In order to linearize these constraints we have an intermediate step and the auxiliary variables $\bar{L}$ and $\bar{R}$. These check whether $x_v$ is completely left or right of the interval, respectively. In accordance with constraints below, the solver may then set $\bar{L}_{u,v}$ or $\bar{R}_{u,v}$ to 0, respectively, in order to minimize the objective function. If on the other hand neither is true, $x_v$ lies in $[x_{\alpha(u)}..x_{\beta(u)}]$ and a horizontal overlap occurs.

We use the following set of constraints to enforce the desired behavior for all the variables.

Place leaves into the interval of the species they belong to:

\[
x_v \geq J_{\phi(v)}^l \quad \text{for } v \in L(T)
\]
\[
x_v \leq J_{\phi(v)}^r \quad \text{for } v \in L(T)
\]

Distinct leaves get distinct x-coordinates:

\[
x_u \neq x_v \quad \text{for } u, v \in L(T), u \neq v
\]

Compute x-coordinates of inner vertices of $T$:

\[
x_v = \frac{(x_{\alpha(v)} + x_{\beta(v)})}{2} \quad \text{for } v \in V(T) \setminus L(T)
\]

Examine horizontal precedences:

\[
\bar{L}_{u,v} \geq \frac{x_v - x_{\alpha(u)}}{n_T} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]
\[
\bar{L}_{u,v} \geq \frac{x_v - x_{\beta(u)}}{n_T} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]
\[
\bar{R}_{u,v} \geq \frac{x_{\alpha(u)} - x_v}{n_T} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]
\[
\bar{R}_{u,v} \geq \frac{x_{\beta(u)} - x_v}{n_T} \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]

Calculate whether $g_v$ horizontally overlaps with $f_u$:

\[
z_{u,v} \geq \bar{L}_{u,v} + \bar{R}_{u,v} - 1 \quad \text{for } u \in V(T) \setminus L(T), v \in V(T) \setminus \{\rho_T\}
\]

Propagate interval limits bottom-up through $T$:

\[
I_{v}^l \leq I_{\alpha(v)}^l \quad \text{for } v \in V(T) \setminus L(T)
\]
\[
I_{v}^l \leq I_{\beta(v)}^l \quad \text{for } v \in V(T) \setminus L(T)
\]
\[
I_{v}^r \geq I_{\alpha(v)}^r \quad \text{for } v \in V(T) \setminus L(T)
\]
\[
I_{v}^r \geq I_{\beta(v)}^r \quad \text{for } v \in V(T) \setminus L(T)
\]
Propagate interval limits bottom-up through $S$:

$$J^l_s \leq J^l_{\alpha(s)} \quad \text{for } s \in V(S) \setminus L(S)$$
$$J^l_s \leq J^l_{\beta(s)} \quad \text{for } s \in V(S) \setminus L(S)$$
$$J^r_s \geq J^r_{\alpha(s)} \quad \text{for } s \in V(S) \setminus L(S)$$
$$J^r_s \geq J^r_{\beta(s)} \quad \text{for } s \in V(S) \setminus L(S)$$

Check interval limits where appropriate:

$$I^l_v = x_v \quad \text{for } v \in L(T)$$
$$I^r_v = x_v \quad \text{for } v \in L(T)$$
$$I^r_v - I^l_v + 1 = |L(v)| \quad \text{for } v \in V(T) \setminus L(T), \varphi(v) \in L(S)$$
$$J^r_s - J^l_s + 1 = |\varphi^{-1}(s)| \quad \text{for } s \in V(S)$$

*Counting crossings.* Since a crossing happens if and only if the two line segments overlap both horizontally and vertically, the objective function simply needs to count how often these two properties coincide. Note that $a(u, v)$ is part of the input and hence the objective function is linear:

$$\text{minimize} \quad \sum_{u \in V(T) \setminus L(T), \atop v \in V(T) \setminus \{\rho_T\}, \atop y(u) > y(v)} a(u, v) \cdot z_{u,v}$$

*Fixed species tree.* The ILP formulation can also be used for the FTT problem where an order of the species is part of the input. In terms of the variables and constraints above, this means that for all $s \in L(S)$ the variables $J^l_s$ and $J^r_s$ become constants.

**D Example Drawings**

We give drawings for one instance of each of the three data sets used in our experiments.
Fig. 15: Drawings of a Gopher instance.
Fig. 16: Drawings of a Barrow instance.
Fig. 17: Drawings of a Hamilton instance.