APPENDIX
Forbidden Time Travel: Characterization of Time-Consistent Tree Reconciliation Maps

A Observable Scenarios

Lemma 1. Condition (O2) implies that $\{L_{T_{\overline{\mathcal{E}}}}(\rho_1), \dots, L_{T_{\overline{\mathcal{E}}}}(\rho_k)\}$ forms a partition of $\mathbb{G}$.

Proof. Since $L_{T_{\overline{\mathcal{E}}}}(\rho_i) \subseteq V(T)$, it suffices to show that $L_{T_{\overline{\mathcal{E}}}}(\rho_i)$ does not contain vertices of $V(T) \setminus \mathbb{G}$. Note, $x \in L_{T_{\overline{\mathcal{E}}}}(\rho_i)$ with $x \notin \mathbb{G}$ is only possible if all edges (x, y) are removed.

Let $x \in V$ with $t(x) = \triangle$ such that all edges (x, y) are removed. Thus, all such edges (x, y) are contained in $\mathcal{E}$. Therefore, every edge of the form (x, y) is a transfer edge; a contradiction to (O2). ◀

Recall that all edges labeled "0" transmit the genetic material vertically, i.e., from one species to a descendant lineage.

Lemma. Conditions (O1) – (O3) imply (Σ1).

Proof. Since (O2) is satisfied we can apply Lemma 1 and conclude that neither $\sigma(L_{T_{\overline{\mathcal{E}}}}(v)) = \emptyset$ nor $\sigma(L_{T_{\overline{\mathcal{E}}}}(w)) = \emptyset$. Let $x \in V(T)$ with $t(x) = \bullet$. By Condition (O1) x has (at least two) children. Moreover, (O3) implies that there are (at least) two children v and w in T that are contained in distinct species V and W that are incomparable in S. Note, the edges (x, v) and (x, w) remain in $T_{\overline{\mathcal{E}}}$, since only transfer edges are removed. Since no transfer is contained in $T_{\overline{\mathcal{E}}}$, the genetic material v and w of V and W, respectively, is always vertically transmitted. Therefore, for any leaf $v' \in L_{T_{\overline{\mathcal{E}}}}(v)$ we have $\sigma(v') \preceq_S V$ and for any leaf $w' \in L_{T_{\overline{\mathcal{E}}}}(w)$ we have $\sigma(w') \preceq_S W$ in S. Assume now for contradiction, that $\sigma(L_{T_{\overline{\mathcal{E}}}}(v)) \cap \sigma(L_{T_{\overline{\mathcal{E}}}}(w)) \neq \emptyset$. Let $z_1 \in L_{T_{\overline{\mathcal{E}}}}(v)$ and $z_2 \in L_{T_{\overline{\mathcal{E}}}}(w)$ with $\sigma(z_1) = \sigma(z_2) = Z$. Since $Z \preceq_S V, W$ and S is a tree, the species V and W must be comparable in S; a contradiction to (O3). ◀

Lemma. Conditions (O1) – (O3) imply (Σ2).

Proof. Since (O2) is satisfied we can apply Lemma 1 and conclude that neither $\sigma(L_{T_{\overline{\mathcal{E}}}}(v)) = \emptyset$ nor $\sigma(L_{T_{\overline{\mathcal{E}}}}(w)) = \emptyset$. Let $(v, w) \in \mathcal{E}$. By (O3) the species containing V and W are are incomparable in S. Now we can argue along the same lines as in the proof of the previous Lemma to conclude that $\sigma(L_{T_{\overline{\mathcal{E}}}}(v)) \cap \sigma(L_{T_{\overline{\mathcal{E}}}}(w)) = \emptyset$. ◀

B DTL-scenario

In case that the event-labeling of T is unknown, but the gene tree T and a species tree S are given, the authors in [21, 3] provide an axiom set, called DTL-scenario, to reconcile T with S. This reconciliation is then used to infer the event-labeling t of T. Instead of defining a DTL-scenario as octuple [21, 3], we use the notation established above:

▶ **Definition 13** (DTL-scenario)**.** For a given gene tree $(T; t, \sigma)$ on $\mathbb{G}$ and a species tree S on $\mathbb{S}$ the map $\gamma : V(T) \to V(S)$ maps the gene tree into the species tree such that

(I) For each leaf $x \in \mathbb{G}$, $\gamma(u) = \sigma(u)$.

(II) If $u \in V(T) \setminus \mathbb{G}$ with children v, w, then

(a) $\gamma(u)$ is not a proper descendant of $\gamma(v)$ or $\gamma(w)$, and
(b) at least one of $\gamma(v)$ or $\gamma(w)$ is a descendant of $\gamma(u)$.

(III) (u, v) is a transfer edge if and only if $\gamma(u)$ and $\gamma(v)$ are incomparable.

(IV) If $u \in V(T) \setminus \mathbb{G}$ with children v, w, then
(a) $t(u) = \triangle$ if and only if either (u, v) or (u, w) is a transfer-edge,
(b) If $t(u) = \bullet$, then $\gamma(u) = \mathrm{lca}_S(\gamma(v), \gamma(w))$ and $\gamma(v), \gamma(w)$ are incomparable,
(c) If $t(u) = \square$, then $\gamma(u) \succeq \mathrm{lca}_S(\gamma(v), \gamma(w))$.

DTL-scenarios are explicitly defined for fully resolved binary gene and species trees. Indeed, Fig. 1 (right) shows a valid reconciliation between a gene tree T and a species tree S that is not consistent with DTL-scenario. To see this, let us call the duplication vertex v. The vertex v and the leaf a are both children of the speciation vertex ρ_T. Condition (IVb) implies that a and v must be incomparable. However, this is not possible since $\gamma(v) \succeq_S \mathrm{lca}_S(B, C)$ (Cond. (IVc)) and $\gamma(a) = A$ (Cond. (I)) and therefore, $\gamma(v) \succeq_S \mathrm{lca}_S(B, C) = \mathrm{lca}_S(A, B, C) \succ_S \gamma(a)$.

Nevertheless, we show in the following that, in case both gene and species trees are binary, our choice of reconciliation map is equivalent to the definition of a DTL-scenario [21, 3]. To this end, we provide first the following lemmas that establishes useful properties of the reconciliation map

▶ **Lemma 14.** *Let μ be a reconciliation map from $(T; t, \sigma)$ to S and assume that T is binary. Then the following conditions are satisfied:*

1. *If $v, w \in V(T)$ are in the same connected component of $T_{\overline{\mathcal{E}}}$, then $\mu(\mathrm{lca}_{T_{\overline{\mathcal{E}}}}(v, w)) \succeq_S \mathrm{lca}_S(\mu(v), \mu(w))$.*

Let u be an arbitrary interior vertex of T with children v, w, then:

2. *$\mu(u)$ and $\mu(v)$ are incomparable in S if and only if $(u, v) \in \mathcal{E}$.*
3. *If $t(u) = \bullet$, then $\mu(v)$ and $\mu(w)$ are incomparable in S.*
4. *If $\mu(v), \mu(w)$ are comparable or $\mu(u) \succ_S \mathrm{lca}_S(\mu(v), \mu(w))$, then $t(u) = \square$.*

Proof. We prove the Items 1 - 4 separately. Recall, Lemma 1 implies that $\sigma(L_{T_{\overline{\mathcal{E}}}}(x)) \neq \emptyset$ for all $x \in V(T)$.

Proof of Item 1: Let v and w be distinct vertices of T that are in the same connected component of $T_{\overline{\mathcal{E}}}$. Consider the unique path P connecting w with v in $T_{\overline{\mathcal{E}}}$. This path P is uniquely subdivided into a path P' and a path P'' from $\mathrm{lca}_{T_{\overline{\mathcal{E}}}}(v, w)$ to v and w, respectively. Condition (M3) implies that the images of the vertices of P' and P'' under μ, resp., are ordered in S with regards to $\preceq_S$ and hence, are contained in the intervals Q' and Q'' that connect $\mu(\mathrm{lca}_{T_{\overline{\mathcal{E}}}}(v, w))$ with $\mu(v)$ and $\mu(w)$, respectively. In particular, $\mu(\mathrm{lca}_{T_{\overline{\mathcal{E}}}}(v, w))$ is the largest element (w.r.t. $\preceq_S$) in the union of $Q' \cup Q''$ which contains the unique path from $\mu(v)$ to $\mu(w)$ and hence also $\mathrm{lca}_S(\mu(v), \mu(w))$.

Proof of Item 2: If $(u, v) \in \mathcal{E}$ then, $t(u) = \triangle$ and (M2iii) implies that $\mu(u)$ and $\mu(v)$ are incomparable. To see the converse, let $\mu(u)$ and $\mu(v)$ be incomparable in S. Item (M3) implies that for any edge $(x, y) \in E(T_{\overline{\mathcal{E}}})$ we have $\mu(y) \preceq_S \mu(x)$. However, since $\mu(u)$ and $\mu(v)$ are incomparable it must hold that $(u, v) \notin E(T_{\overline{\mathcal{E}}})$. Since (u, v) is an edge in the gene tree T, $(u, v) \in \mathcal{E}$ is a transfer edge.

Proof of Item 3: Let $t(u) = \bullet$. Since none of (u, v) and (u, w) are transfer-edges, it follows that both edges are contained in $T_{\overline{\mathcal{E}}}$. Then, since T is a binary tree, it follows that $L_{T_{\overline{\mathcal{E}}}}(u) = L_{T_{\overline{\mathcal{E}}}}(v) \cup L_{T_{\overline{\mathcal{E}}}}(w)$ and therefore, $\sigma_{T_{\overline{\mathcal{E}}}}(u) = \sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)$.

Therefore and by Item (M2i),

$$\mu(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)) = \mathrm{lca}_S(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)), \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))).$$

Assume for contradiction that $\mu(v)$ and $\mu(w)$ are comparable, say, $\mu(w) \succeq_S \mu(v)$. By Lemma 3, $\mu(w) \succeq_S \mu(v) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$ and $\mu(w) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$. Thus,

$$\mu(w) \succeq_S \mathrm{lca}_S(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)), \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))).$$

Thus, $\mu(w) \succeq_S \mu(u)$; a contradiction to (M3ii).

Proof of Item 4: Let $\mu(v), \mu(w)$ be comparable in S. Item 3 implies that $t(u) \neq \bullet$. Assume for contradiction that $t(u) = \triangle$. Since by (O2) only one of the edges (u, v) and (u, w) is a transfer edge, we have either $(u, v) \in \mathcal{E}$ or $(u, w) \in \mathcal{E}$. W.l.o.g. let $(u, v) \in \mathcal{E}$ and $(u, w) \in E(T_{\overline{\mathcal{E}}})$. By Condition (M3), $\mu(u) \succeq_S \mu(w)$. However, since $\mu(v)$ and $\mu(w)$ are comparable in S, also $\mu(u)$ and $\mu(v)$ are comparable in S; a contradiction to Item 2. Thus, $t(u) \neq \triangle$. Since each interior vertex is labeled with one event, we have $t(u) = \square$.

Assume now that $\mu(u) \succ_S \mathrm{lca}_S(\mu(v), \mu(w))$. Hence, $\mu(u)$ is comparable to both $\mu(v)$ and $\mu(w)$ and thus, (M2iii) implies that $t(u) \neq \triangle$. Lemma 3 implies $\mu(v) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$ and $\mu(w) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$.

$$\mathrm{lca}_S(\mu(v), \mu(w)) \succeq_S \mathrm{lca}_S(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)), \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)).$$

Since $T(u) \neq \triangle$ it follows that neither $(u, v) \in \mathcal{E}$ nor $(u, w) \in \mathcal{E}$ and hence, both edges are contained in $T_{\overline{\mathcal{E}}}$. By the same argumentation as in Item 3 it follows that $\sigma_{T_{\overline{\mathcal{E}}}}(u) = \sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)$ and therefore, $\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. Hence, $\mu(u) \succ_S \mathrm{lca}_S(\mu(v), \mu(w)) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. Now, (M2i) implies $t(u) \neq \bullet$. Since each interior vertex is labeled with one event, we have $t(u) = \square$. ◀

▶ **Lemma 15.** *Let μ be a reconciliation map for the gene tree $(T; t, \sigma)$ and the species tree S as in Definition 2. Moreover, assume that T and S are binary. Set for all $u \in V(T)$:*

$$\gamma(u) = \begin{cases} \mu(u) & \text{,if } \mu(u) \in V(S) \\ y & \text{,if } \mu(u) = (x, y) \in E(S) \end{cases}$$

Then $\gamma : V(T) \to V(S)$ is a map according to the DTL-scenario.

Proof. We first emphasize that, by construction, $\mu(u) \succeq_S \gamma(u)$ for all $u \in V(T)$. Moreover, $\mu(u) = \mu(v)$ implies that $\gamma(u) = \gamma(v)$, and $\gamma(u) = \gamma(v)$ implies that $\mu(u)$ and $\mu(v)$ are comparable. Furthermore, $\mu(u) \prec_S \mu(v)$ implies $\gamma(u) \preceq_S \gamma(v)$, while $\gamma(u) \prec_S \gamma(v)$ implies that $\mu(u) \prec_S \mu(v)$. Thus, $\mu(u)$ and $\mu(v)$ are comparable if and only if $\gamma(u)$ and $\gamma(v)$ are comparable.

Item (I) and (M1) are equivalent.

For Item (II) let $u \in V(T) \setminus \mathbb{G}$ be an interior vertex with children v, w. If $(u, w) \notin \mathcal{E}$, then $w \prec_{T_{\overline{\mathcal{E}}}} u$. Applying Condition (M3) yields $\mu(w) \preceq_S \mu(u)$ and thus, by construction, $\gamma(w) \preceq_S \gamma(u)$. Therefore, $\gamma(u)$ is not a proper descendant of $\gamma(w)$ and $\gamma(w)$ is a descendant of $\gamma(u)$. If one of the edges, say (u, v), is a transfer edge, then $t(u) = \triangle$ and by Condition (M2iii) $\mu(u)$ and $\mu(v)$ are incomparable. Hence, $\gamma(u)$ and $\gamma(v)$ are incomparable. Therefore, $\gamma(u)$ is no proper descendant of $\gamma(v)$. Note that (O2) implies that for each vertex $u \in V(T) \setminus \mathbb{G}$ at least one of its outgoing edges must be a non-transfer edge, which implies that $\gamma(w) \preceq_S \gamma(u)$ or $\gamma(v) \preceq_S \gamma(u)$ as shown before. Hence, Item (IIa) and (IIb) are satisfied.

For Item (III) assume first that $(u, v) \in \mathcal{E}$ and therefore $t(u) = \triangle$. Then, (M2iii) implies that $\mu(u)$ and $\mu(v)$ are incomparable and thus, $\gamma(u)$ and $\gamma(v)$ are incomparable. Now assume that (u, v) is an edge in the gene tree T and $\gamma(u)$ and $\gamma(v)$ are incomparable. Therefore, $\mu(u)$ and $\mu(v)$ are incomparable. Now, apply Lemma 14(2).

Item (IVa) is clear by the event-labeling t of T and since (O2). Now assume for (IVb) that $t(u) = \bullet$. Lemma 14(3) implies that $\mu(v)$ and $\mu(w)$ are incomparable and thus, $\gamma(v)$ and $\gamma(w)$ must be incomparable as well. Furthermore, Condition (M2i) implies that $\mu(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. Lemma 3 implies that $\mu(v) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$ and $\mu(w) \succeq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$. The latter together with the incomparability of $\mu(v)$ and $\mu(u)$ implies that

$$\begin{aligned}\mathrm{lca}_S(\mu(v), \mu(w)) &= \mathrm{lca}_S(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)), \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))) \\ &= \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v) \cup \sigma_{T_{\overline{\mathcal{E}}}}(w)) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) = \mu(u).\end{aligned}$$

If $\mu(v)$ is mapped on the edge (x, y) in T, then $\gamma(v) = y$. By definition of lca for edges, $\mathrm{lca}_S(\mu(v), \gamma(w)) = \mathrm{lca}_S(y, \gamma(w)) = \mathrm{lca}_S(\gamma(v), \gamma(w))$. The same argument applies if $\mu(w)$ is mapped on an edge. Since for all $z \in V(T)$ either $\mu(z) \succ_S \gamma(z)$ (if $\mu(z)$ is mapped on an edge) or $\mu(z) = \gamma(z)$, we always have

$$\mathrm{lca}_S(\gamma(v), \gamma(w)) = \mathrm{lca}_S(\mu(v), \mu(w)) = \mu(u).$$

Since $t(u) = \bullet$, (M2i) implies that $\mu(u) \in V(S)$ and therefore, by construction of γ it holds that $\mu(u) = \gamma(u)$. Thus, $\gamma(u) = \mathrm{lca}_S(\gamma(v), \gamma(w))$. For (IVc) assume that $t(u) = \square$. Condition (M3) implies that $\mu(u) \succeq_S \mu(v), \mu(w)$ and therefore, $\gamma(u) \succeq_S \gamma(v), \gamma(w)$. If $\gamma(v)$ and $\gamma(w)$ are incomparable, then $\gamma(u) \succeq_S \gamma(v), \gamma(w)$ implies that $\gamma(u) \succeq_S \mathrm{lca}_S(\gamma(v), \gamma(w))$. If $\gamma(v)$ and $\gamma(w)$ are comparable, say $\gamma(v) \succeq_S \gamma(w)$, then $\gamma(u) \succeq_S \gamma(v) = \mathrm{lca}_S(\gamma(v), \gamma(w))$. Hence, Statement (IVc) is satisfied. ◀

▶ **Lemma 16.** *Let $\gamma : V(T) \to V(S)$ be a map according to the DTL-scenario for the binary the gene tree $(T; t, \sigma)$ and the binary species tree S.*

Set for all $u \in V(T)$:

$$\mu(u) = \begin{cases} \gamma(u) & \text{,if } t(u) \in \{\bullet, \odot\} \\ (x, \gamma(u)) \in E(S) & \text{,if } t(u) \in \{\triangle, \square\} \end{cases}$$

Then $\mu : V(T) \to V(S) \cup E(S)$ is a reconciliation map according to Definition 2.

Proof. Let $\gamma : V(T) \to V(S)$ be a map a DTL-scenario for the binary the gene tree $(T; t, \sigma)$ and the species tree S.

Condition (M1) is equivalent to (I).

For (M3) assume that $v \preceq_{T_{\overline{\mathcal{E}}}} w$. The path P from v to w in $T_{\overline{\mathcal{E}}}$ does not contain transfer edges. Thus, by (III) all vertices along P are comparable. Moreover, by (IIa) we have that $\gamma(w)$ is not a proper descendant of the image of its child in S, and therefore, by repeating these arguments along the vertices x in P_{wv}, we obtain $\gamma(v) \preceq_S \gamma(x) \preceq_S \gamma(w)$.

If $\gamma(v) \prec_S \gamma(w)$, then by construction of μ, it follows that $\mu(v) \prec_S \mu(w)$. Thus, (M3) is satisfied, whenever $\gamma(v) \prec_S \gamma(w)$. Assume now that $\gamma(v) = \gamma(w)$. If $t(v), t(w) \in \{\square, \triangle\}$ then $\mu(v) = (x, \gamma(v)) = (x, \gamma(w)) = \mu(w)$ and thus (M3i) is satisfied. If $t(v) = \bullet$ and $t(w) \neq \bullet$ then since $\mu(v) = \gamma(v)$ and $\mu(w) = (x, \gamma(w))$. Thus $\mu(v) \prec_S \mu(w)$. Now assume that $\gamma(v) = \gamma(w)$ and w is a speciation vertex. Since $t(w) = \bullet$, for its two children w' and w'' the images $\gamma(w')$ and $\gamma(w'')$ must be incomparable due to (IVb). W.l.o.g. assume that w' is a vertex of P_{wv}. Since $\gamma(v) \preceq_S \gamma(x) \preceq_S \gamma(w)$ for any vertex x along P_{wv} and $\gamma(v) = \gamma(w)$, we obtain $\gamma(w') = \gamma(w)$. However, since $\gamma(w'') \preceq_S \gamma(w)$, the vertices $\gamma(w')$ and $\gamma(w'')$ are comparable in S; contradicting (IVb). Thus, whenever w is a speciation vertex, $\gamma(w') = \gamma(w)$ is not possible. Therefore, $\gamma(v) \preceq_S \gamma(w') \prec_S \gamma(w)$ and, by construction of μ, $\mu(v) \prec_S \mu(w)$. Thus, (M3ii) is satisfied.

Finally, we show that (M2) is satisfied. To this end, observe first that (M2ii) is fulfilled by construction of μ and (M2iii) is an immediate consequence of (III). Thus, it remains to show that (M2i) is satisfied. Thus, for a given speciation vertex u we need to show that $\mu(u) = \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. By construction, $\mu(u) = \gamma(u)$. Note, $T_{\overline{\mathcal{E}}}$ does not contain transfer edges. Applying (III) implies that for all edges (x, y) in $T_{\overline{\mathcal{E}}}$ the images $\gamma(x)$ and $\gamma(y)$ must be comparable. The latter and (IIa) implies that for all edges (x, y) in $T_{\overline{\mathcal{E}}}$ we have $\gamma(y) \preceq_S \gamma(x)$. Take the latter together, $\sigma(z) = \gamma(z) \preceq_S \gamma(u)$ for any leaf $z \in L_{T_{\overline{\mathcal{E}}}}(u)$. Therefore $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S \gamma(u) = \mu(u)$. Assume for contradiction that $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \prec_S \gamma(u) = \mu(u)$. Consider the two children u' and u'' of u in $T_{\overline{\mathcal{E}}}$. Since neither $(u, u') \in \mathcal{E}$ nor $(u, u'') \in \mathcal{E}$ and T is a binary tree, it follows that $L_{T_{\overline{\mathcal{E}}}}(u) = L_{T_{\overline{\mathcal{E}}}}(u') \cup L_{T_{\overline{\mathcal{E}}}}(u'')$ and we obtain that $\sigma_{T_{\overline{\mathcal{E}}}}(u) = \sigma_{T_{\overline{\mathcal{E}}}}(u') \cup \sigma_{T_{\overline{\mathcal{E}}}}(u'')$. Moreover, re-using the arguments above, $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u')) \preceq_S \gamma(u')$ and $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u'')) \preceq_S \gamma(u'')$. By the arguments we used in the proof for (M3), we have $\gamma(u') \prec_S \gamma(u)$ and $\gamma(u'') \prec_S \gamma(u)$. In particular, $\gamma(u')$ and $\gamma(u'')$ must be contained in the subtree of S that is rooted in the child a of $\gamma(u)$ in S with $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S a$, as otherwise, $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u')) \not\preceq_S \gamma(u')$ or $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u'')) \not\preceq_S \gamma(u'')$. Moreover, neither $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u'))$ nor $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u''))$ is possible since then $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u')) \preceq_S \gamma(u')$ and $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u'')) \preceq_S \gamma(u'')$ implies that $\gamma(u')$ and $\gamma(u'')$ would be comparable; contradicting (IVb). Hence, there remains only one way to locate $\gamma(u')$ and $\gamma(u'')$, that is, they must be located in the subtree of S that is rooted in $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. But then we have $\text{lca}_S(\gamma(u'), \gamma(u'')) \preceq_S \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \prec_S \gamma(u)$; a contradiction to (IVb) $\gamma(u) = \text{lca}_S(\gamma(u'), \gamma(u''))$. Therefore, $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) = \gamma(u) = \mu(u)$ and (M2i) is satisfied. ◀

Lemma 15 and 16 imply

▶ **Theorem 17.** *For a binary gene tree $(T; t, \sigma)$ and a binary species tree S there is DTL-scenario if and only if there is a reconciliation μ for $(T; t, \sigma)$ and S*

C Proof of Theorem 7

Proof. In the following, x and u denote vertices in S and T, respectively.

($\Longrightarrow$) Assume that there is a time-consistent reconciliation map μ from $(T; t, \sigma)$ to S, and thus two time-maps τ_S and τ_T for S and T, respectively, that satisfy (C1) and (C2).

To see (D1), observe that if $\mu(u) = x \in V(S)$, then (M1) and (M2) imply that $t(u) \in \{\bullet, \odot\}$. Now apply (C1).

To show (D2), assume that $t(u) \in \{\square, \triangle\}$ and $x \preceq_S lca_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. By Condition (M2) it holds that $\mu(u) = (y, z) \in E(S)$. Together with Lemma 3 we obtain that $x \preceq_S \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S z \prec_S \mu(u)$. By the properties of τ_S we have

$$\tau_S(x) \geq \tau_S(\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \geq \tau_S(z) \overset{(C2)}{>} \tau_T(u).$$

To see (D3), assume that $(u, v) \in \mathcal{E}$ and $z := \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S x$. Since $t(u) = \triangle$ and by (M2ii), we have $\mu(u) = (y, y') \in E(S)$. Thus, $\mu(u) \prec_S y$. By (M2iii) $\mu(u)$ and $\mu(v)$ are incomparable and therefore, we have either $\mu(v) \prec_S y$ or $\mu(v)$ and y are incomparable. In either case we see that $y \preceq_S z$, since Lemma 3 implies that $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S \mu(u)$ and $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S \mu(v)$. In summary, $\mu(u) \prec_S y \preceq_S z \preceq_S x$. Therefore,

$$\tau_T(u) \overset{(C2)}{>} \tau_S(y) \geq \tau_S(z) \geq \tau_S(x).$$

Hence, conditions (D1)-(D3) are satisfied.

($\Longleftarrow$) To prove the converse, assume that there exists a reconciliation map μ that satisfies (D1)-(D3) for some time-maps τ_T and τ_S. In the following we will make use of τ_S and τ_T to construct a time-consistent reconciliation map μ'.

First we define "anchor points" by $\mu'(v) = \mu(v)$ for all $v \in V(T)$ with $t(v) \in \{\bullet, \odot\}$. Condition (D1) implies $\tau_T(v) = \tau_S(\mu(v))$ for these vertices, and therefore μ' satisfies (C1).

The next step will be to show that for each vertex $u \in V(T)$ with $t(u) \in \{\square, \triangle\}$ there is a unique edge (x, y) along the path from $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ to ρ_S with $\tau_S(x) < \tau_T(u) < \tau_S(y)$. We set $\mu'(u) = (x, y)$ for these points. In the final step we will show that μ' is a valid reconciliation map.

Consider the unique path $\mathcal{P}_u$ from $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ to ρ_S. By construction, $\tau_S(\rho_S) < \tau_T(\rho_T) \leq \tau_T(u)$ and by Condition (D2) it we have $\tau_T(u) < \tau_S(\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)))$. Since τ_S is a time map for S, every edge $(x, y) \in E(S)$ satisfies $\tau_S(x) < \tau_S(y)$. Therefore, there is a unique edge $(x_u, y_u) \in E(S)$ along $\mathcal{P}_u$ such that either $\tau_S(x_u) < \tau_T(u) < \tau_S(y_u)$, $\tau_S(x_u) = \tau_T(u) < \tau_S(y_u)$, or $\tau_S(x_u) < \tau_T(u) = \tau_S(y_u)$. The addition of a sufficiently small perturbation ϵ_u to $\tau_T(u)$ does not violate the conditions for τ_T being a time-map for T. Clearly ϵ_u can be chosen to break the equalities in the latter two cases in such a way that $\tau_S(x_u) < \tau_T(u) < \tau_S(y_u)$ for each vertex $u \in V(T)$ with $t(u) \in \{\square, \triangle\}$. We then continue with the perturbed version of τ_T and set $\mu'(u) = (x_u, y_u)$. By construction, μ' satisfies (C2).

It remains to show that μ' is a valid reconciliation map from $(T; t, \sigma_{T_{\overline{\mathcal{E}}}})$ to S. Again, let $\mathcal{P}_u$ denote the unique path from $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ to ρ_S for any $u \in V(T)$.

By construction, Conditions (M1), (M2i), (M2ii) are satisfied. To check condition (M2iii), assume $(u, v) \in \mathcal{E}$. The original map μ is a valid reconciliation map, and thus, Lemma 3 implies that $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \prec_S \mu(u)$ and $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S \mu(v)$. Since $\mu(u)$ and $\mu(v)$ are incomparable in S and $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v))$ lies on both paths $\mathcal{P}_u$ and $\mathcal{P}_v$ we have $\mu(u), \mu(v) \preceq_S \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) =: x$. In particular, $x \neq \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ and $x \neq \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$.

Conditions (D1) and (D2) imply that $\tau_S(x) < \tau_T(u) < \tau_S(\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)))$ and $\tau_S(x) < \tau_T(v) \leq \tau_S(\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)))$. By construction of μ', the vertex u is mapped to a unique edge $e_u = (x_u, y_u)$ and v is mapped either to $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) \neq x$ or to the unique edge $e_v = (x_v, y_v)$, respectively. In particular, $\mu'(u)$ lies on the path $\mathcal{P}'$ from x to $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ and $\mu'(v)$ lies one the path $\mathcal{P}''$ from x to $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$. The paths $\mathcal{P}'$ and $\mathcal{P}''$ are edge-disjoint and have x as their only common vertex. Hence, $\mu'(u)$ and $\mu'(v)$ are incomparable in S, and (M2iii) is satisfied.

In order to show (M3), assume that $u \prec_{T_{\overline{\mathcal{E}}}} v$. Since $u \prec_{T_{\overline{\mathcal{E}}}} v$, we have $\sigma_{T_{\overline{\mathcal{E}}}}(u) \subseteq \sigma_{T_{\overline{\mathcal{E}}}}(v)$. Hence, $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq \text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S \rho_S$. In other words, $\text{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$ lies on the path $\mathcal{P}_u$ and thus, $\mathcal{P}_v$ is a subpath of $\mathcal{P}_u$. By construction of μ', both $\mu'(u)$ and $\mu'(v)$ are comparable in S. Moreover, since $\tau_T(u) > \tau_T(v)$ and by construction of μ', it immediately follows that $\mu'(u) \preceq_S \mu'(v)$.

Its now an easy task to verify that (M3) is fulfilled by considering the distinct event-labels in (M3i) and (M3ii), which we leave to the reader. ◀

D Theorem 18

▶ **Theorem 18.** *Let μ be a reconciliation map from $(T; t, \sigma)$ to S. There is a time-consistent reconciliation map $(T; t, \sigma)$ to S if and only if there is a time map τ_T such that for all $u, v, w \in V(T)$:*

(T1) *If $t(u) = t(v) \in \{\bullet, \odot\}$ then*

(a) If $\mu(u) = \mu(v)$, then $\tau_T(u) = \tau_T(v)$.

(b) If $\mu(u) \prec_S \mu(v)$, then $\tau_T(u) > \tau_T(v)$.

(T2) *If $t(u) \in \{\bullet, \odot\}$, $t(v) \in \{\square, \triangle\}$ and $\mu(u) \preceq_S \operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$, then $\tau_T(u) > \tau_T(v)$.*

(T3) *If $(u, v) \in \mathcal{E}$ and $\operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S \operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$ for some $w \in V(T)$, then $\tau_T(u) > \tau_T(w)$*

Proof. Suppose that μ is a time-consistent reconciliation map from $(T; t, \sigma)$ to S. By Definition 5 and Theorem 7, there are two time maps τ_T and τ_S that satisfy (D1)-(D3). We first show that τ_T also satisfies (T1)-(T3), for all $u, v \in V(T)$. Condition (T1a) is trivially implied by (D1). Let $t(u), t(v) \in \{\bullet, \odot\}$, and $\mu(u) \prec_S \mu(v)$. Since τ_T and τ_S are time maps, we may conclude that

$$\tau_T(u) \overset{(D1)}{=} \tau_S(\mu(u)) < \tau_S(\mu(v)) \overset{(D1)}{=} \tau_T(v).$$

Hence, (T1b) is satisfied.

Now, assume that $t(u) \in \{\bullet, \odot\}$, $t(v) \in \{\square, \triangle\}$ and $\mu(u) \preceq_S \operatorname{lca}(\sigma_{T_{\overline{\mathcal{E}}}}(v))$. By the properties of τ_S, we have:

$$\tau_T(u) \overset{(D1)}{=} \tau_S(\mu(u)) \overset{(D2)}{>} \tau_T(v).$$

Hence (T2) is fulfilled.

Finally, assume that $(u, v) \in \mathcal{E}$, and $x := \operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S \operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$ for some $w \in V(T)$. Lemma 3 implies that $\operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w)) \preceq_S \mu(w)$ and we obtain

$$\tau_T(w) \overset{(D2)}{<} \tau_S(x) \leq \tau_S(\operatorname{lca}(\sigma_{T_{\overline{\mathcal{E}}}}(w))) \overset{(D3)}{<} \tau_T(u).$$

Hence, (T3) is fulfilled.

To see the converse, assume that there exists a reconciliation map μ that satisfies (T1)-(T3) for some time map τ_T. In the following we construct a time map τ_S for S that satisfies (D1)-(D3). To this end, we first set

$$\tau_S(x) = \begin{cases} -1 & \text{if } x = \rho_S \\ \tau_T(v) & \text{else if } v \in \mu^{-1}(x) \\ * & \text{else, i.e., } \mu^{-1}(x) = \emptyset \text{ and } x \neq \rho_S. \end{cases}$$

We use the symbol $*$ to denote the fact that so far no value has been assigned to $\tau_S(x)$. Note, by (M2i) and (T1a) the value $\tau_S(x)$ is uniquely determined and thus, by construction, (D1) is satisfied. Moreover, if $x, y \in V(S)$ have non-empty preimages w.r.t. μ and $x \prec_S y$, then we can use the fact that τ_T is a time map for T together with condition (T1) to conclude that $\tau_S(x) > \tau_S(y)$.

If $x \in V(S)$ with $a \in \mu^{-1}(x)$, then (T2) implies (D2) (by (D1) and setting $u = a$ in (T2)) and (T3) implies (D3) (by (D1) and setting $w = a$ in (T3)). Thus, (D2) and (D3) is satisfied for all $x \in V(S)$ with $\mu^{-1}(x) \neq \emptyset$.

Using our choices $\tau_S(\rho_T) = 0$ and $\tau_S(\rho_S) = -1$ for the augmented root of S, we must have $\mu^{-1}(\rho_S) = \emptyset$. Thus, $\rho_S \succ_S \operatorname{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v))$ for any $v \in V(T)$. Hence, (D2) is trivially satisfied for ρ_S. Moreover, $\tau_T(\rho_T) = 0$ implies $\tau_T(u) > \tau_S(\rho_S)$ for any $u \in V(T)$. Hence, (D3) is always satisfied for ρ_S.

In summary, Conditions (D1)-(D3) are met for any vertex $x \in V(S)$ that up to this point has been assigned a value, i.e., $\tau_S(x) \neq *$.

We will now assign to all vertices $x \in V(S)$ with $\mu^{-1}(x) = \emptyset$ a value $\tau_S(x)$ in a stepwise manner. To this end, we give upper and lower bounds for the possible values that can be assigned to $\tau_S(x)$. Let $x \in V(S)$ with $\tau_S(x) = *$. Set

$$\begin{aligned} \mathsf{LO}(x) &= \{\tau_S(y) \mid x \prec_S y, y \in V(S) \text{ and } \tau_S(y) \neq *\} \\ \mathsf{UP}(x) &= \{\tau_S(y) \mid x \succ_S y, y \in V(S) \text{ and } \tau_S(y) \neq *\}. \end{aligned}$$

We note that $\mathsf{LO}(x) \neq \emptyset$ and $\mathsf{UP}(x) \neq \emptyset$ because the root and the leaves of S already have been assigned a value τ_S in the initial step. In order to construct a valid time map τ_S we must ensure $\max(\mathsf{LO}(x)) < \tau_S(x) < \min(\mathsf{UP}(x))$.

Moreover, we strengthen the bounds as follows. Put

$$\begin{aligned} \mathsf{lo}(x) &= \{\tau_T(u) \mid t(u) \in \{\square, \triangle\} \text{ and } x \preceq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))\} \\ \mathsf{up}(x) &= \{\tau_T(u) \mid \text{ where } (u,v) \in \mathcal{E} \text{ and } \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S x \ \}. \end{aligned}$$

Observe that $\max(\mathsf{lo}(x)) < \min(\mathsf{up}(x))$, since otherwise there are vertices $u, w \in V(T)$ with $\tau_T(w) \in \mathsf{lo}(x)$ and $\tau_T(u) \in \mathsf{up}(x)$ and $\tau_T(w) \geq \tau_T(u)$. However, this implies that $\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S x \preceq \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(w))$; a contradiction to (T3).

Since (D2) is satisfied for all vertices y that obtained a value $\tau_S(y) \neq *$, we have $\max(\mathsf{lo}(x)) < \min(\mathsf{UP}(x))$. Likewise because of (D3), it holds that $\max(\mathsf{LO}(x)) < \min(\mathsf{up}(x))$. Thus we set $\tau_S(x)$ to an arbitrary value such that

$$\max(\mathsf{LO}(x) \cup \mathsf{lo}(x)) < \tau_S(x) < \min(\mathsf{UP}(x) \cup \mathsf{up}(x)).$$

By construction, (D1), (D2), and (D3) are satisfied for all vertices in $V(S)$ that have already obtained a time value distinct from $*$. Moreover, for all such vertices with $x \prec_T y$ we have $\tau_S(x) > \tau_S(y)$. In each step we chose a vertex x with $\tau_S(x) = *$ that obtains then a real-valued time stamp. Hence, in each step the number of vertices that have value $*$ is reduced by one. Therefore, repeating the latter procedure will eventually assign to all vertices a real-valued time stamp such that, in particular, τ_S satisfies (D1), (D2), and (D3) and thus is indeed a time map for S. ◀

E Proof of Theorem 9

Proof. Assume that μ is time-consistent. By Theorem 7, there are two time-maps τ_T and τ_S satisfying (C1) and (C2). Let $\tau = \tau_T \cup \tau_S$ be the map from $V(T) \cup V(S) \to \mathbb{R}$. Let A' be the directed graph with $V(A') = V(S) \cup V(T)$ and set for all $x, y \in V(A')$: $(x, y) \in E(A')$ if and only if $\tau(x) < \tau(y)$. By construction A' is a DAG since τ provides a topological order on A' [17].

We continue to show that A' contains all edges of A_1.

To see that (A1) is satisfied for $E(A')$ let $(u, v) \in E(T)$. Note, $\tau(v) > \tau(u)$, since τ_T is a time map for T and by construction of τ. Hence, all edges $(u, v) \in E(T)$ are also contained in A', independent from the respective event-labels $t(u), t(v)$. Moreover, if $t(u)$ or $t(v)$ are speciation vertices or leaves, then (C1) implies that $\tau_S(\mu(u)) = \tau_T(u) > \tau_T(v)$ or $\tau_T(u) > \tau_T(v) = \tau_S(\mu(v))$. By construction of τ, all edges satisfying (A1) are contained in $E(A')$. Since τ_S is a time map for S, all edges as in (A2) are contained in $E(A')$. Finally, (C2) implies that all edges satisfying (A5) are contained in $E(A')$.

Although, A' might have more edges than required by (A1), (A2) and (A5), the graph A_1 is a subgraph of A'. Since A' is a DAG, also A_1 is a DAG.

For the converse assume that A_1 is a directed graph with $V(A_1) = V(S) \cup V(T)$ and edge set $E(A_1)$ as constructed in Def. 8 (A1), (A2) and (A5). Moreover, assume that A_1 is a DAG.

Hence, there is is a topological order τ on A_1 with $\tau(x) < \tau(y)$ whenever $(x, y) \in E(A_1)$. In what follows we construct the time-maps τ_T and τ_S such that they satisfy (C1) and (C2). Set $\tau_S(x) = \tau(x)$ for all $x \in V(S)$. Additionally, set for all $u \in V(T)$:

$$\tau_T(u) = \begin{cases} \tau(\mu(u)) & \text{if } t(u) \in \{\odot, \bullet\} \\ \tau(u) & \text{otherwise.} \end{cases}$$

By construction it follows that (C1) is satisfied. Due to (A2), τ_S is a valid time map for S. It follows from the construction and (A1) that τ_T is a valid time map for T. Assume now that $u \in V(T)$, $t(u) \in \{\square, \triangle\}$, and $\mu(u) = (x, y) \in E(S)$. Since τ provides a topological order we have:

$$\tau(x) \overset{(A5)}{<} \tau(u) \overset{(A5)}{<} \tau(y).$$

By construction, it follows that $\tau_S(x) < \tau_T(u) < \tau_S(y)$ satisfying (C2). ◀

F Proof of Theorem 10

Proof. Let μ be a reconcilation map for $(T; t, \sigma)$ and S and μ' be a time-consistent reconciliation map for $(T; t, \sigma)$ and S. Let A_2 and A'_2 be the auxiliary graphs that satisfy Def. 8 (A1) – (A4) for μ and μ', respectively. Since $\mu(u) = \mu'(u)$ for all $u \in V(T)$ with $t(u) \in \{\odot, \bullet\}$ and (A2) – (A4) don't rely on the explicit reconciliation map, it is easy to see that $A_2 = A'_2$.

Now we can re-use similar arguments as in the proof of Theorem 9. Assume there is a time-consistent reconciliation map $(T; t, \sigma)$ to S. By Theorem 7, there are two time-maps τ_T and τ_S satisfying (D1)-(D3). Let τ and A' be defined as in the proof of Theorem 9.

Analogously to the proof of Theorem 9, we show that A' contains all edges of A_2. Application of (D1) immediately implies that all edges satisfying (A1) and (A2) are contained in $E(A')$. By condition (D2), it yields $(u, lca_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))) \in E(A')$ and (D3) implies $(lca_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)), u) \in E(A')$. We conclude by the same arguments as before that the graph A_2 is a DAG.

For the converse, assume we are given the directed acyclic graph A_2. As before, there is is a topological order τ on A_2 with $\tau(x) < \tau(y)$ only if $(x, y) \in E(A_2)$. The time-maps τ_T and τ_S are given as in the proof of Theorem 9.

By construction, it follows that (D1) is satisfied. Again, by construction and the Properties (A1) and (A2), τ_S and τ_T are valid time-maps for S and T respectively.

Assume now that $u \in V(T)$, $t(u) \in \{\square, \triangle\}$, and $x \preceq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ for some $x \in V(S)$. Since there is a topological order on $V(A_2)$, we have

$$\tau(x) \overset{(A2)}{\geq} \tau(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))) \overset{(A3)}{>} \tau(u).$$

By construction, it follows that $\tau_S(x) > \tau_T(u)$. Thus, (D2) is satisfied.

Finally assume that $(u, v) \in \mathcal{E}$ and $\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v)) \preceq_S x$ for some $x \in V(S)$. Again, since τ provides a topological order, we have:

$$\tau(x) \overset{(A2)}{\leq} \tau(\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v))) \overset{(A4)}{<} \tau(u).$$

By construction, it follows that $\tau_S(x) < \tau_T(u)$, satisfying (D3).

Thus τ_T and τ_S are valid time maps satisfying (D1)-(D3). ◀

Algorithm 2 Compute $\ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ for all $u \in V(T)$

1: **function** ComputeLcaSigma$((T;t,\sigma), S)$
2: $\quad \ell(u) \leftarrow \emptyset$ for all $u \in V(T)$ $\quad\triangleright$ "$\emptyset$" means uninitialized
3: $\quad A \leftarrow$ empty stack
4: $\quad A.push(\rho_T)$
5: $\quad$ **while** A is not empty **do**
6: $\quad\quad u \leftarrow A.pop()$
7: $\quad\quad$ **if** $t(u) = \odot$ **then** $\ell(u) \leftarrow \sigma(u)$
8: $\quad\quad$ **else if** $\ell(v) = \emptyset$ for some child v of u **then** $A.push(u)$, $A.push(v)$
9: $\quad\quad$ **else**
10: $\quad\quad\quad \ell(u) \leftarrow \mathrm{lca}_S(\{\ell(v) \mid (u,v) \in E(T) \text{ and } t((u,v)) = 0\})$
11: $\quad$ **return** ℓ

G Algorithm 2, Proof of Lemma 11 and Theorem 12

Proof of Lemma 11. Let $u \in V(T)$. In what follows, we show that $\ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. In fact, the algorithm is (almost) a depth first search through T that assigns the (species tree) vertex $\ell(u)$ to u if and only if every child v of u has obtained an assignment $\ell(v)$ (cf. Line (9) - (10)). That there are children v with non-empty $\ell(v)$ at some point is ensured by Line (7). That is, if $t(u) = \odot$, then $\ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) = \sigma(u)$. Now, assume there is an interior vertex $u \in V(T)$, where every child v has been assigned a value $\ell(v)$, then

$$\begin{aligned}
\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) &= \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(\{\sigma_{T_{\overline{\mathcal{E}}}}(v) \mid (u,v) \in E(T) \text{ and } t(u,v) = 0\})) \\
&= \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(\{\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) \mid (u,v) \in E(T) \text{ and } t(u,v) = 0\})) \\
&= \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(\{\ell(v) \mid (u,v) \in E(T) \text{ and } t(u,v) = 0\}))
\end{aligned}$$

The latter is achieved by Line (10).

Since T is a tree and the algorithm is in effect a depth first search through T, the while loop runs at most $O(V(T) + E(T))$ times, and thus in $O(V(T))$ time.

The only non-constant operation within the while loop is the computation of lca_S in Line (10). Clearly lca_S of a set of vertices $C = \{c_1, c_2 \dots c_k\}$, where $c_i \in V(S)$, for all $c_i \in C$ can be computed as sequence of lca_S operations taking two vertices: $\mathrm{lca}_S(c_1, \mathrm{lca}_S(c_2, \dots \mathrm{lca}_S(c_{k-1}, c_k)))$, each taking $O(\lg(|V(S)|))$ time. Note however, that since Line (10) is called exactly once for each vertex in T, the number of lca_S operations taking two vertices is called at most $|E(T)|$ times through the entire algorithm. Hence, the total time complexity is $O(|V(T)| \lg(|V(S)|))$. ◀

Proof of Theorem 12. In order to produce a time-consistent reconciliation map, we first construct some valid reconciliation map μ from $(T;t,\sigma)$ to S. Using the lca-map ℓ from Algorithm 2, μ will be adjusted to become time-consistent, if possible.

By assumption, there is a reconciliation map from $(T;t,\sigma)$ to S. The for-loop (Line (3)-(5)) ensures that each vertex $u \in V$ obtained a value $\mu(u)$. We continue to show that μ is a valid reconciliation map satisfying (M1)-(M3).

Assume that $t(u) = \odot$, in this case $\ell(u) = \sigma(u)$, and thus (M1) is satisfied. If $t(u) = \bullet$, it holds that $\mu(u) = \ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$, thus satisfying (M2i). Note that $\rho_S \succ_S \ell(u)$, and hence, $\mu(u) \in F$ by Line (5), implying that (M2ii) is satisfied. Now, assume $t(u) = \triangle$ and $(u,v) \in \mathcal{E}$. By assumption, we know there exists a reconciliation map from T to S, thus by

(Σ2):

$\sigma_{T_{\overline{\mathcal{E}}}}(u) \cap \sigma_{T_{\overline{\mathcal{E}}}}(v) = \emptyset$

It follows that, $\ell(u)$ is incomparable to $\ell(v)$, satisfying (M2iii).

Now assume that $u, v \in V$ and $u \prec_{T_{\overline{\mathcal{E}}}} v$. Note that $\sigma_{T_{\overline{\mathcal{E}}}}(u) \subseteq \sigma_{T_{\overline{\mathcal{E}}}}(v)$. It follows that $\ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u)) \preceq_S \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(v)) = \ell(v)$. By construction, (M3) is satisfied. Thus, μ is a valid reconciliation map.

By Theorem 10, two time maps τ_T and τ_S satisfying (D1)-(D3) only exists if the auxiliary graph A build on Line (6) is a DAG. Thus if A contains a cycle, no such time-maps exists and the statement "No time-consistent reconciliation map exists." is returned (Line (7)). On the other hand, if A is a DAG, the construction in Line (8)-(11) is identical to the construction used in the proof of Theorem 10. Hence correctness of this part of the algorithm follows directly from the proof of Theorem 10.

Finally, we adjust μ to become a time-consistent reconciliation map.. By the latter arguments, τ_T and τ_S satisfy (D1)-(D3) w.r.t. to μ. Note, that μ is chosen to be the "lowest point" where a vertex $u \in V$ with $t(u) \in \{\square, \triangle\}$ can be mapped, that is, $\mu(u)$ is set to $(p(x), x)$ where $x = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$. However, by the arguments in the proof of Theorem 7, there is a unique edge $(y, z) \in W$ on the path from x to ρ_S such that $\tau_S(y) < \tau_T(u) < \tau_S(z)$. The latter is ensured by choosing a different value for distinct vertices in $V(A)$, see comment in Line (9). Hence, Line (14) ensures, that $\mu(u)$ is mapped on the correct edge such that (C2) is satisfied. It follows that adjusted μ is a valid time-consistent reconciliation map.

We are now concerned with the time-complexity. By Lemma 11, computation of ℓ in Line (1) takes $O(|V|\log(|W|))$ time and the for-loop (Line (3)-(5)) takes $O(|V|)$ time. We continue to show that the auxiliary graph A (Line (6)) can be constructed in $O(|V|\log(|W|))$ time.

Since we know $\ell(u) = \mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u))$ for all $u \in V$ and since T and S are trees, the subgraph with edges satisfying (A1)-(A3) can be constructed in $O(|V|+|W|+|E|+|F)|) = O(|V|+|W|)$ time. To ensure (A4), we must compute for a possible transfer edges $(u, v) \in \mathcal{E}$ the vertex $\mathrm{lca}_S(\sigma_{T_{\overline{\mathcal{E}}}}(u) \cup \sigma_{T_{\overline{\mathcal{E}}}}(v))$. which can be done in $O(\log(|W|))$ time. Note, the number of transfer edges is bounded by the number of possible transfer event $O(|V|)$. Hence, generating all edges satisfying (A4) takes $O(|V|(\log(|W|))$ time. In summary, computing A can done in $O(|V| + |W| + |V|(\log(|W|)) = O(|V|(\log(|W|))$ time.

To detect whether A contains cycles one has to determine whether there is a topological order τ on $V(A)$ which can be done via depth first search in $O(|V(A)| + |E(A)|)$ time. Since $|V(A)| = |V| + |W|$ and $O(|E(A)|) = O(|F| + |E| + |W| + |V|)$ and S, T are trees, the latter task can be done in $O(|V| + |W|)$ time. Clearly, Line (10)-(11) can be performed on $O(|V| + |W|)$ time.

Finally, we have to adjust μ according to τ_T and τ_S. Note, that for each $u \in V$ with $t(u) \in \{\square, \triangle\}$ (Line (12)) we have possibly adjust μ to the next edge $(p(x), x)$. However, the possibilities for the choice of $(p(x), x)$ is bounded by by the height of S, which is in the worst case $\log(|W|)$. Hence, the for-loop in Line (12) has total-time complexity $O(|V|\log(|W|))$.

In summary, the overall time complexity of Algorithm 1 is $O(|V|\log(|W|))$. ◀

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