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## Supplementary Information for

## Distance metrics for ranked evolutionary trees

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## Supporting Information Text

## 1. Proof of Theorem 1

Proof. Consider a ranked tree shape $T^{R}$ with $n$ leaves sampled at $m$ different sampling times. We denote the total number of change points in $T^{R}$ by $r=n+m-1$ and its ordered change point times by $\left(u_{r}, u_{r-1}, \ldots, u_{1}\right), 0=u_{r}<u_{r-1}<\cdots<u_{1}$, with time increasing into the past (rootward). The internal nodes of $T^{R}$ are labeled by the indices of their coalescent times, and all leaves of $T^{R}$ are labeled by the indices of their sampling times. We note that for convenience, internal nodes are no longer labeled $2, \ldots, n$ from the root to leaves, but they are labeled by their time-event indices (see Figure S1). Each internal node has a unique label, but the leaf nodes with the same sampling time share the same label. We define $N=\{1, \ldots, r\}$ to be a set of all node labels, $I$ to be a set of all internal node labels, and $S$ to be a set of all leaf node labels. Note that $I$ and $S$ are disjoint and contain $n-1$ and $m$ elements, respectively.

For $i \in I$, let $o_{i}=\left(x_{i, 1}, x_{i, 2}\right)$ denote the ordered pair of labels of the two immediate descendants of internal node $i$, such that $i<x_{i, 1} \leq x_{i, 2}$. We denote the set of all pairs $i$ and $o_{i}=\left(x_{i, 1}, x_{i, 2}\right)$ choices in $T^{R}$ by $X=\left\{\left(i, o_{i}\right) \mid i \in I\right\}$. Then $X$ completely specifies $T^{R}: T^{R}$ is a directed graph from the root to tips and $X$ encodes its adjacency matrix and the order of the internal node indices $i \in I$ determines internal node rankings.


Fig. S1. Example of $\phi$ mapping. (A) An example isochronous ranked tree shape. The set of internal node labels is $I=\{1,2,3,4,5,6,7\}$ and the set of leaf node labels is $S=\{8\}$. For convenience, internal nodes are labeled by their time-event indices throughout the proof. The internal node with label 2 at time $u_{2}$ has descendant nodes 3 and 7 at time $u_{3}$ and $u_{7}$, respectively $\left(o_{2}=(3,7)\right)$. The column vector $\phi\left(2, o_{2}=(3,7)\right)=(0,2,1,1,1,1,0)$ indicates the number of direct descendants of node 2 at each change point time interval. (B) An example heterochronous ranked tree shape. The set of internal node labels is $I=\{1,2,3,4,6,7,8\}$ and the set of leaf node labels is $S=\{5,9,10,11\}$. The internal node with label 3 at time $u_{3}$ has descendants node 4 and node 5 at time $u_{4}$ and $u_{5}$, respectively (o3 $=(4,5)$. The column vector $\phi\left(3, o_{3}=(4,5)\right)=(0,0,2,1,0,0,0,0,0,0)$ indicates the number of direct descendants of node 3 at each change point time interval.

We define a function $\phi: X \rightarrow\{0,1,2\}^{r-1}$ as follows:

$$
\phi_{k}\left(i, o_{i}\right)= \begin{cases}0 & \text { if } 1 \leq k<i \\ 2 & \text { if } i \leq k<x_{i, 1} \\ 1 & \text { if } x_{i, 1} \leq k<x_{i, 2} \\ 0 & \text { if } x_{i, 2} \leq k<r\end{cases}
$$

The $k$ th element of $\phi\left(i, o_{i}\right)$ is the number of immediate descendants of an internal node $i$ present at the time interval $\left(u_{k+1}, u_{k}\right)$. $\phi$ is an injective map. To prove this, let $\left(s, o_{s}\right)$ and $\left(t, o_{t}\right)$ be two elements in $X$ and let $\left(s, o_{s}\right) \neq\left(t, o_{t}\right)$. Because internal nodes of $T^{R}$ are ranked, $\left(s, o_{s}\right) \neq\left(t, o_{t}\right)$ implies $s \neq t$; without loss of generality, assume $s<t$. By the definition of the map $\phi$, the $s$ th element of $\phi\left(s, o_{s}\right)$ is $\phi_{s}\left(s, o_{s}\right)=2$, while the $s$ th element of $\phi\left(t, o_{t}\right)$ is $\phi_{s}\left(t, o_{t}\right)=0$ because $s<t$ and $t<x_{t, 1} \leq x_{t, 2}$. Thus, $\phi\left(s, o_{s}\right) \neq \phi\left(t, o_{t}\right)$ and $\phi$ is injective.

Let $\eta:\{1, \ldots, r-1\} \times\{0,1,2\}^{r-1} \rightarrow\{0,1,2\}^{r-1}$ such that for $\mathbf{y} \in\{0,1,2\}^{r-1}$, the $j$ th element of $\eta$ is

$$
\eta(k, \mathbf{y})_{j}= \begin{cases}0 & \text { if } 1 \leq j<k \\ y_{j} & \text { if } k \leq j<r\end{cases}
$$

That is, $\eta(k, \mathbf{y})$ sets all the first $k-1$ entry values of $\mathbf{y}$ to 0 . Note that the first $i-1$ elements of $\phi\left(i, o_{i}\right)$ are 0 by definition and thus, $\eta\left(i, \phi\left(i, o_{i}\right)\right)=\phi\left(i, o_{i}\right)$.

Finally, for $T^{R} \in \mathcal{T}_{n}^{R}$, define $\psi: \mathcal{T}_{n}^{R} \rightarrow M_{r-1, r-1}(\mathbb{R})$, a function that maps a ranked tree shape with $n$ leaves to a real valued square matrix of size $r-1$, with $k$ th column:

$$
\psi\left(T^{R}\right)_{\cdot, k}=\sum_{\substack{i \in I, i \leq k}} \eta\left(k, \phi\left(i, o_{i}\right)\right),
$$

where $\psi\left(T^{R}\right)_{\cdot, k}$ indicates the $k$ th column of $\psi\left(T^{R}\right)$ and $I$ is the set of all internal node labels as defined at the beginning of this section. By the definition of $\eta$, the first $k-1$ values of the $k$ th column $\psi\left(T^{R}\right)_{\cdot, k}$ are 0 , i.e., $\psi\left(T^{R}\right)$ is a lower triangular matrix. Because $\phi$ records the number of immediate descendants of a single internal node present at each time interval, $\psi\left(T^{R}\right) \cdot, k$ tracks the sum of all surviving immediate descendants of internal nodes with labels $i \leq k$ starting from time interval ( $u_{k+1}, u_{k}$ ); thus, $\psi\left(T^{R}\right)_{s, k}$, with $k \leq s$, represents the number of lineages of $T^{R}$ in $\left(u_{k+1}, u_{k}\right)$ that are still present at the time interval $\left(u_{s+1}, u_{s}\right)$. We prove that $\psi$ is an injective map. Let $T_{1}^{R}, T_{2}^{R} \in \mathcal{T}_{n}^{R}$ and $T_{1}^{R} \neq T_{2}^{R}$. Because $X=\left\{\left(i, o_{i}\right) \mid i \in I\right\}$ completely specifies $T^{R}, T_{1}^{R} \neq T_{2}^{R}$ implies that there exists an index $\ell \in\{1, \ldots, n-1\}$ such that $\left(i_{\ell}^{(1)}, o_{i_{\ell}}^{(1)}\right) \neq\left(i_{\ell}^{(2)}, o_{i_{\ell}}^{(2)}\right)$. Here, $i_{\ell}$ indicates the $\ell$ th element of $I$ sorted in increasing order. If there is more than one such index, choose $\ell$ to be the smallest of them. Without loss of generality, let $i_{\ell}^{(1)} \leq i_{\ell}^{(2)}$. Then $\psi\left(T_{1}^{R}\right)_{., i_{\ell}^{(1)}} \neq \psi\left(T_{2}^{R}\right)_{., i_{\ell}^{(1)}}$ and thus $\psi\left(T_{1}^{R}\right) \neq \psi\left(T_{2}^{R}\right)$.

Hence, $\psi$ maps each ranked tree shape $T^{R}$ to a unique matrix, i.e., given an F-matrix, if it encodes a ranked tree shape, it encodes exactly one ranked tree shape.

## 2. Proof of Proposition 2

Proof. To prove that $d_{k}^{w}, k=1,2$, is a metric, we need to prove the following properties hold for any ranked genealogies $\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}, \mathbf{g}_{3}^{R}$ with $n$ leaves:

$$
\begin{aligned}
d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right) \geq 0 & \text { non-negativity } \\
d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=d_{k}^{w}\left(\mathbf{g}_{2}^{R}, \mathbf{g}_{1}^{R}\right) & \text { symmetry } \\
d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0 \Longleftrightarrow \mathbf{g}_{1}^{R}=\mathbf{g}_{2}^{R} & \text { identity } \\
d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right) \leq d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{3}^{R}\right)+d_{k}^{w}\left(\mathbf{g}_{3}^{R}, \mathbf{g}_{2}^{R}\right) & \text { triangle inequality. }
\end{aligned}
$$

The non-negativity and symmetry are trivial. The triangle inequality follows from the Minkowski inequality of $L_{1}$ and $L_{2}$ norms. It remains to prove the identity property: $d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0$ if and only if $\mathbf{g}_{1}^{R}=\mathbf{g}_{2}^{R}$ for $k=1,2$. It is clear that $d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0$ if $\mathbf{g}_{1}^{R}=\mathbf{g}_{2}^{R}$ so we focus on $\mathbf{g}_{1}^{R}=\mathbf{g}_{2}^{R}$ if $d_{k}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0$. The following proof is for $d_{1}^{w}$. The proof for $d_{2}^{w}$ follows the same arguments.

We assume that the two genealogies have the same number of sampling events $m$ and same number of leaves $n$, so that the $\mathbf{F}$-matrices of $\mathbf{g}_{1}^{R}$ and $\mathbf{g}_{2}^{R}$ have the same dimension $(n+m-2) \times(n+m-2)$ dimension. We define $r=n+m-2$ for notational simplicity.

Because we allow only a single event at each change time point $u_{i}$, either coalescent or sampling, the first column of any F-matrix is $(2,1, \ldots, 1)$ or $(2,1, \ldots, 1,0, \ldots, 0)$. For the latter, we denote the row index of the last occurrence of 1 in the first column by $k_{1}: F_{k_{1}, 1}^{(\ell)}=1$ and $F_{k_{1}+1,1}^{(\ell)}=0$ for some index $2 \leq k_{1} \leq r$ and $\ell=1,2$.

If $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ have different first columns, then for some index $k_{1} \geq 2,\left(F_{k_{1}, 1}^{(1)}, F_{k_{1}, 1}^{(2)}\right)=(0,1)$ or $\left(F_{k_{1}, 1}^{(1)}, F_{k_{1}, 1}^{(2)}\right)=(1,0)$. Because $\left|F_{i, j}^{(1)} W_{i, j}^{(1)}-F_{i, j}^{(2)} W_{i, j}^{(2)}\right| \geq 0, d_{1}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0$ implies $F_{i, j}^{(1)} W_{i, j}^{(1)}=F_{i, j}^{(2)} W_{i, j}^{(2)}$ for all $i, j$. Therefore, $W_{k_{1}, 1}^{(2)}=0$ in the first case and $W_{k_{1}, 1}^{(1)}=0$ in the second case. However, this contradicts our assumption of positive time interval between two change points, and thus $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ must have the same first column.

If both $\mathbf{F}$-matrices share the same first column, then $d_{1}^{w}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=0$ implies $W_{i, 1}^{(1)}=W_{i, 1}^{(2)}$ for all $i=1, \ldots, r$. Recalling $W_{i, j}=u_{j}-u_{i+1}$, we have $u_{1}^{(1)}-u_{i+1}^{(1)}=u_{1}^{(2)}-u_{i+1}^{(2)}$. Because we assume $u_{r+1}^{(1)}=u_{r+1}^{(2)}=0$, we can traverse through $i$ in decreasing order starting from $i=r$ to get $u_{i}^{(1)}=u_{i}^{(2)}$ for all $i=1, \ldots, r+1$, which gives $\mathbf{W}^{(1)}=\mathbf{W}^{(2)}$.

Along with $\mathbf{W}^{(1)}=\mathbf{W}^{(2)}, F_{i, j}^{(1)} W_{i, j}^{(1)}=F_{i, j}^{(2)} W_{i, j}^{(2)}$ implies $F_{i, j}^{(1)}=F_{i, j}^{(2)}$ for all $i, j$, i.e., $\mathbf{F}^{(1)}=\mathbf{F}^{(2)}$, and thus $\mathbf{g}_{1}^{R}=\mathbf{g}_{2}^{R}$.

## 3. Metric spaces on heterochronous trees with different numbers of sampling events

We extend our distances to include cases in which the numbers of sampling events differ but the total number of samples remains the same.

Consider two heterochronous ranked tree shapes of $n$ leaves, $T_{1}^{R}$ and $T_{2}^{R}$, with different numbers of sampling events $m_{1}$ and $m_{2}$, respectively. In order to compute the distance between $T_{1}^{R}$ and $T_{2}^{R}$ with our metrics, we require the two ranked tree shapes to be represented as $\mathbf{F}$-matrices of the same dimension. We accomplish this by inserting artificial sampling events. The detailed steps are as follows. Note that the following formulation is done going backwards in time with time increasing from the present to the past.

For $i=1,2$, let $\mathbf{E}^{(i)}=\left(e_{m_{i}+n-1}^{(i)}, \ldots, e_{1}^{(i)}\right)$ be the vector of ordered sampling and coalescence events where $e_{m_{i}+n-1}^{(i)}$ denotes the most recent sample event $\left(e_{m_{i}+n-1}^{(i)}=s\right)$ assumed to occur at time $u_{m_{i}+n-1}^{(i)}=0 . e_{1}^{(i)}=c$ denotes the coalescent event at time $u_{1}^{(i)}$ corresponding to the most recent common ancestor of the samples in $T_{i}^{R}$. Each $e_{j}^{(i)}$ is either a sampling event $\left(e_{j}^{(i)}=s\right)$ or a coalescent event $\left(e_{j}^{(i)}=c\right)$. The event of type $c$ occurs $n-1$ times and the event of type $s$ occurs $m_{i}$ times in $\mathbf{E}^{(i)}$. In the example illustrated in Figure S2, the event vectors for $T_{1}^{R}$ (Figure S2(A)) and $T_{2}^{R}$ (Figure $\mathrm{S} 2(\mathrm{~B})$ ) are $\mathbf{E}^{(1)}=(s, c, s, c, s, c)$ and $\mathbf{E}^{(2)}=(s, s, s, c, s, c, c)$, respectively.


Fig. S2. Example of augmented F-matrix representation of ranked tree shapes. In order to compute the $d_{1}$ or $d_{2}$ distances between ranked tree shapes with equally many samples but different numbers of sampling events, such as ranked tree shapes ( $A$ ) and ( $B$ ), we insert artificial sampling events with 0 samples in order to match their dimension. (A)-(B) Two ranked tree shapes of 4 samples with different sampling events. (C) Alignment of event vectors of two trees. The $n-1$ coalescent events are aligned first by matching $i$ th coalescent event of a tree to the $i$ th coalescent event of the other tree ( $i=1, \ldots, n-1$ ). The sampling events are then matched by increasing index order in the event vector. (D) Augmentation of artificial sampling events $a$ between coalescent events or between the first sampling and the first coalescent event. (E)-(F) Augmented ranked tree shapes. (G)-(H) Augmented F-matrix representations.

We first align all $n-1$ coalescent events between the two trees by adding empty spaces when needed as depicted in Figure $\mathrm{S} 2(\mathrm{C})$. Once all the type- $c$ events are aligned, we next align the sampling events between two successive coalescent events or between $t=0$ and the first $c$ event. When aligning the events of type $s$ between the two trees, we pair the events of type $s$, starting from the most recent events. The event vector alignment is demonstrated in Figure S2(C). If one tree has more type- $s$ events than the other in a given intercoalescent interval, we insert the excess artificial sampling events, denoted by $a$ 's, in the tree with fewer type- $s$ events in that interval. We assign 0 new samples to type- $a$ events. For example, in the tree of Figure S2(A), there is only one sampling event before the first coalescent event, whereas there are three sampling events in the tree of Figure S2(B). In Figure S2(D), we illustrate how the two artificial sampling events are added to the first tree in the first interval. The resulting augmented trees are shown in Figures $S 2(\mathrm{E})$ and ( F ) along with their corresponding $\mathbf{F}$-matrix representations in Figures $\mathrm{S} 2(\mathrm{G})$ and $(\mathrm{H})$. We note that by construction, $\mathbf{F}^{(1)} \neq \mathbf{F}^{(2)}$ in these cases. Hence, $d_{i}\left(T_{1}^{R}, T_{2}^{R}\right) \neq 0$ for $i=1,2$.

Consider now two heterochronous ranked genealogies of $n$ leaves, $\mathbf{g}_{1}^{R}$ and $\mathbf{g}_{2}^{R}$, with different number of sampling events $m_{1}$ and $m_{2}$ respectively. In order to compute the distance between $\mathbf{g}_{1}^{R}$ and $\mathbf{g}_{2}^{R}$ we first augment their $\mathbf{F}$-matrix representations as with ranked tree shapes. In addition, we augment their weight matrices $W^{(1)}$ and $W^{(2)}$ by assigning a time to each augmented artificial sampling event. If $n_{a}$ artificial events are inserted between events $e_{j+1}^{(i)}$ and $e_{j}^{(i)}$, we subdivide the corresponding time interval $\left[u_{j+1}^{(i)}, u_{j}^{(i)}\right]$ into $n_{a}+1$ intervals with equal length: the times assigned to the $n_{a}$ augmented artificial events are $\left\{u_{j+1}^{(i)}+\Delta, u_{j+1}^{(i)}+2 \Delta, \ldots, u_{j+1}^{(i)}+n_{a} \Delta\right\}$, where $\Delta=\frac{u_{j}^{(i)}-u_{j+1}^{(i)}}{n_{a}+1}$.

## 4. Statistical comparison of ranked tree shape and ranked genealogy sampling distributions

We generalize the mean confusion statistics for cases when the $L_{2}$-medoid is not unique. This more general version is more appropriate for small sample spaces such as ranked tree shapes with small number of leaves.

For a given distance function $d$ defined on the space of ranked tree shapes (or ranked genealogies), let $\bar{X}$ be the $L_{2}$-medoid set of the $X_{1}, \ldots, X_{N}$ samples and let $\bar{Y}$ be the $L_{2}$-medoid set of the $Y_{1}, \ldots, Y_{N}$ samples, as defined in Equation 5 . The generalized mean confusion is defined as:

$$
\begin{align*}
C_{G}^{x, y}=\frac{1}{2} \sum_{j=1}^{N}[ & 1_{\min _{\bar{Y}}\left\{d\left(X_{j}, \bar{Y}\right)\right\} \leq \min _{\bar{X}}\left\{d\left(X_{j}, \bar{X}\right)\right\}} \frac{1}{N-|\bar{X}|} \\
& +1_{\min _{\bar{X}}\left\{d\left(Y_{j}, \bar{X}\right)\right\} \leq \min _{\bar{Y}}\left\{d\left(Y_{j}, \bar{Y}\right)\right\}} \frac{1}{N-|\bar{Y}|} \\
& -Z_{j}^{x} 1_{\min _{\bar{X}}\left\{d\left(X_{j}, \bar{X}\right)\right\}=\min _{\bar{Y}}\left\{d\left(X_{j}, \bar{Y}\right)\right\}} \frac{1}{N-|\bar{X}|} \\
& \left.-Z_{j}^{y} 1_{\min _{\bar{X}}\left\{d\left(Y_{j}, \bar{X}\right)\right\}=\min _{\bar{Y}}\left\{d\left(Y_{j}, \bar{Y}\right)\right\}} \frac{1}{N-|\bar{Y}|}\right], \tag{S1}
\end{align*}
$$

where $Z_{j}^{x}$ and $Z_{j}^{y}$ are i.i.d. Bernoulli random variables with probability 0.5 to resolve ties.

## 5. Adapting other tree metrics to ranked tree shapes and ranked genealogies

A. Other distances on ranked tree shapes. We start with two adaptations of metrics that are originally defined on the space of labeled genealogies: the BHV distance and the KC distance.

The Billera-Holmes-Vogtmann metric (BHV) metric. The BHV space (1) is obtained by representing each labeled genealogy $\mathbf{g}_{n}^{L}$ with $n$ leaves and edge set $\mathcal{E}$ by a vector in the Euclidean orthant $\mathbb{R}_{+}^{2 n-1}$, whose coordinates correspond to edge lengths. The BHV space is the union of $(2 n-3)!!$ orthants. The BHV distance ( $d_{\mathrm{BHV}}$ ) between two labeled genealogies is defined as a geodesic, the shortest path connecting two points that lies inside the BHV space. Note that unranked and labeled genealogies with positive intervals between coalescent and sample times are effectively ranked and labeled genealogies. To adapt the BHV distance to the space of ranked tree shapes, we define a modified BHV metric, $d_{\mathrm{BHV} \text {-RTS }}$ as follows:

$$
d_{\mathrm{BHV}-\mathrm{RTS}}\left(T_{1}^{R}, T_{2}^{R}\right)=d_{\mathrm{BHV}}\left(\psi\left(T_{1}^{R}\right), \psi\left(T_{2}^{R}\right)\right),
$$

where $\psi$ maps a ranked tree shape to its corresponding ranked labeled genealogy by assigning a uniquely defined label to each leaf and assigning a unit length to each change point time interval ( $u_{i}, u_{i-1}$ ).

The unique assignment of the leaf labels $\ell_{1}, \ldots, \ell_{n}$ on a ranked tree shape consists in assigning labels in increasing index order starting with leaves subtending from nodes closer to the bottom and ending with leaves subtending closer to the root (Text 6).
The Kendall-Colijn ( $\boldsymbol{K C} \boldsymbol{C}$ metric. The KC metric is another metric on labeled genealogies (2). A labeled genealogy $\mathbf{g}_{n}^{L}$ with $n$ leaves is represented by an $\frac{n(n+1)}{2}$-dimensional vector $v_{\lambda}\left(\mathbf{g}_{n}^{L}\right)$ that is a convex combination of two vectors: $(1-\lambda) m\left(\mathbf{g}_{n}^{L}\right)+\lambda M\left(\mathbf{g}_{n}^{L}\right)$, $\lambda \in[0,1] . m\left(\mathbf{g}^{L}\right)$ is a vector that concatenates $n$ repetitions of one and a vector whose entry corresponds to the number of edges between the most recent common ancestor of a pair of leaves and the root; $M\left(\mathbf{g}_{n}^{L}\right)$ is a vector that concatenates the vector of leaf branch lengths and the branch length between the most recent common ancestor of a pair of tips and the root.

The KC distance $d_{\mathrm{KC}, \lambda}$ with $\lambda>0$ between two labeled genealogies is the Euclidean norm of the difference between the two KC vector representations of the labeled genealogies. When $\lambda=0$, the KC distance becomes a distance on the space of labeled unranked topologies: $d_{\mathrm{KC}, 0}$.

To adapt the KC distance to the space of ranked tree shapes, we propose two distances. We first define a KC-based distance on ranked tree shapes, $d_{\mathrm{KC}-\mathrm{RTS}}$, as follows

$$
d_{\mathrm{KC}-\mathrm{RTS}}\left(T_{1}^{R}, T_{2}^{R}\right)=d_{\mathrm{KC}, 0}\left(\eta\left(T_{1}^{R}\right), \eta\left(T_{2}^{R}\right)\right),
$$

where $\eta$ maps a ranked tree shape to a labeled unranked tree shape by removing internal node rankings and uniquely labeling leaves following the procedure described for $d_{\text {BHV-RTS }}$.

The Colijn-Plazzotta (CP) metric. The CP metric is defined on tree shapes (3). The CP metric $d_{\mathrm{CP}}$ is defined as the Euclidean norm ( $L_{2}$-norm) of the difference between two vectors that uniquely describe the two tree shapes. Each node of a tree is labeled by an integer recursively from tips to the root. The $i$ th entry of the CP vector representing a tree shape records the frequency of the tree nodes labeled with integer $i$. We define a modified CP distance $d_{\text {CP-RTS }}$ on ranked tree shapes as

$$
d_{\mathrm{CP}-\mathrm{RTS}}\left(T_{1}^{R}, T_{2}^{R}\right)=d_{\mathrm{CP}}\left(\phi\left(T_{1}^{R}\right), \phi\left(T_{2}^{R}\right)\right),
$$

where $\phi$ returns the corresponding tree shape of a ranked tree shape by removing the labels of its internal nodes. We note that $d_{\mathrm{CP}-\mathrm{RTS}}$ is not a metric but a pseudometric: all pairs of different ranked tree shapes with the same shape will have $d_{\mathrm{CP}-\mathrm{RTS}}=0$. In addition, $d_{\mathrm{CP}-\mathrm{RTS}}$ does not account for heterochronous sampling, so we exclude $d_{\mathrm{CP}-\mathrm{RTS}}$ from our analyses on heterochronous ranked tree shapes.
B. Other distances on ranked genealogies. We now present the modified BHV and KC distances so that they can be compared to our proposed distances on ranked genealogies.

$$
d_{\mathrm{BHV}-\mathrm{RG}}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=d_{\mathrm{BHV}}\left(\eta_{2}\left(\mathbf{g}_{1}^{R}\right), \eta_{2}\left(\mathbf{g}_{2}^{R}\right)\right),
$$

where $\eta_{2}$ maps a ranked genealogy to a labeled ranked genealogy by uniquely labeling leaves as described for $d_{\mathrm{BHV} \text {-RTS }}$. Similarly,

$$
d_{\mathrm{KC}-\mathrm{RG}}\left(\mathbf{g}_{1}^{R}, \mathbf{g}_{2}^{R}\right)=d_{\mathrm{KC}, 0.5}\left(\eta_{2}\left(\mathbf{g}_{1}^{R}\right), \eta_{2}\left(\mathbf{g}_{2}^{R}\right)\right)
$$

We note that there is no adaptation of the CP metric to the space of ranked genealogies as the CP metric is defined on the space of tree shapes, and thus, does not incorporate tree branch lengths.

## 6. Unique labeling scheme of ranked tree shapes

In order to adapt other distances defined on labeled trees to ranked tree shapes, we use the following labeling scheme. We start by labeling the leaves that descend directly from the internal node with the largest rank $n$. If the node has two direct descendent leaves with different edge lengths, we label the longer leaf $\ell_{1}$ and the shorter leaf $\ell_{2}$. If the two leaves have the same edge lengths, we label them $\ell_{1}$ and $\ell_{2}$ from left to right. If the node has only one direct descendent leaf, we label it $\ell_{1}$. If there is no descending leaf, no labeling is done. We then move to the node with rank $n-1$ and continue labeling the leaves by traversing through the internal nodes in descending order of rank until all leaves are labeled. If the current node with rank $k$ has two direct descendent leaves and if the last assigned leaf label is $\ell_{j}$, we label the leaf with the longer edge $\ell_{j+1}$ and the leaf with shorter edge $\ell_{j+2}$; if the leaves have the same edge lengths, we label the pair of leaves $\ell_{j+1}$ (left) and $\ell_{j+2}$ (right). If the node $k$ has only one direct descendent leaf, we label it $\ell_{j+1}$. If the node $k$ has no direct descendent leaf, no label is assigned. Examples demonstrating our unique labeling scheme are in Figure S3.



Fig. S3. Unique labeling of ranked tree shapes and ranked genealogies. (A) Example of the unique labeling of a ranked genealogy with isochronous sampling. (B) Example of the unique labeling of a ranked genealogy with heterochronous sampling.

## 7. Beta-splitting model on labeled tree shapes

We first consider the single-parameter beta-splitting model on labeled tree shapes (4). For a parent clade of size $n$, the model chooses its child clade size to be $i$ on the left branch and $n-i$ on the right branch with probability

$$
q_{n}(i)=\frac{1}{a_{n}(\beta)} \frac{\Gamma(\beta+i+1) \Gamma(\beta+n-i+1)}{\Gamma(i+1) \Gamma(n-i+1)}
$$

where $a_{n}(\beta)$ is a normalizing constant and $i \in\{1,2, \ldots, n-1\}$. The splitting is repeated recursively in each branch independently until the tree is fully resolved. The parameter $\beta \in[-2, \infty)$ controls the degree of balance of the generated trees. With $\beta=-2$, the model generates the perfect unbalanced tree (caterpillar tree) with probability one, and with $\beta=\infty$, the model generates the perfect balanced tree with probability one. We note that Ford's alpha-model (5) is another single parameter family of models on the same class of trees as the beta-splitting model and it is not considered in this manuscript.

## 8. Alpha-Beta splitting model by Maliet et al. (6)

The alpha-beta model of Maliet et al. (6) generates labeled ranked tree shapes according to a size-biased distribution with a stick-breaking construction. The algorithm first generates $n$ independent draws $u_{1}, \ldots, u_{n}$ from a $\operatorname{Unif}(0,1)$ distribution. The $u_{i}$ 's correspond to the $n$ leaves of the tree. The first partition of the $n$ leaves (at the root) is determined by drawing a random number $R_{1} \sim \operatorname{Beta}(\beta+1, \beta+1)$. All the $n_{1}=\sum_{i=1}^{n} 1\left(u_{i}<R_{1}\right)$ are placed on the left side of the tree and the rest on the other side. Then, if $n_{1}>1$, the left branch is chosen to bifurcate with probability proportional to $n_{1}^{\alpha}$. The algorithm continues
generating beta-distributed values to bi-partition the leaves and chooses the order (ranking) proportional to their number of descendants to the $\alpha$ power until the interval $(0,1)$ is partitioned into $n$ intervals, each corresponding to an $u_{i}$ number. The pseudocode is shown below. Leaf labels are then removed to generate a ranked tree shape. The $\beta \in[-2, \infty)$ parameter determines the balance of the tree as in the beta-splitting model, and the $\alpha \in(-\infty, \infty)$ parameter regulates the relationship between subtree family size (number of descendants) and closeness to the root. More specifically, when $\alpha<0$, subtrees with small family sizes are closer to the root and when $\alpha>0$, subtrees with small family sizes are closer to the tips. When $\alpha=1$, the alpha-beta model becomes the beta-splitting model on ranked tree shapes.

```
Algorithm 1 Simulation of a labeled ranked tree shape according to alpha-beta splitting model
    Draw \(u_{1}, \ldots, u_{n} \sim U(0,1)\)
    Set \(i=1, r_{0}=0\)
    while \(i<n\) do
        Draw \(R_{i} \sim \operatorname{Beta}(1+\beta, 1+\beta)\)
        Let \(r_{1}, \ldots, r_{i}\) be the ordered permutation of \(R_{1}, \ldots, R_{i}\) such that \(r_{1}<r_{2}<\ldots<r_{i}\)
        Let \(y_{j}=\left\{\begin{array}{ll}1 & \text { if } \sum_{k=1}^{n} 1\left(u_{k} \in\left(r_{j-1}, r_{j}\right)\right)>1 \\ 0 & \text { o.w }\end{array}\right.\), for \(j=1, \ldots, i\)
        if \(\sum_{j=1}^{i} y_{j}>1\) then
            Pick \(y_{k}\) w.p. \(\frac{\left(r_{k}-r_{k-1}\right)^{\alpha y_{k}}}{\sum_{j=1}^{i}\left(r_{j}-r_{j-1}\right)^{\alpha y_{j}}}\). The partition defined by the \(u_{j}\) 's in \(\left(r_{k-1}, r_{k}\right)\) is chosen to bifurcate with ranking \(i\).
            \(i=i+1\)
```


## 9. Tajima coalescent on ranked genealogies

The Tajima coalescent is a model on ranked genealogies (Figure 1(A)). It is a Markov lumping of Kingman's n-coalescent on labeled and ranked genealogies $(7,8)$. The Tajima coalescent is a pure death process that starts with $n$ unlabeled leaves at time $t_{n+1}=0$ and proceeds backward in time, merging pairs of branches to create interior nodes labeled by their order of appearance. The merging of two branches is a coalescent event. In the Tajima coalescent, the distribution of coalescence times is the same as in the Kingman coalescent and the probability of a topology, ranked tree shape, is given by

$$
\begin{equation*}
P\left(T^{R}\right)=\frac{2^{n-c-1}}{(n-1)!} \tag{S2}
\end{equation*}
$$

where $n$ is the number of leaves, and $c$ is the number of cherries-the number of pairs of leaves that subtend from a shared interior node. The Tajima coalescent on ranked tree shapes without times corresponds to the beta-splitting model on ranked tree shapes with $\beta=0$, also called the Yule model. A full description of the Tajima coalescent process can be found in Cappello and Palacios (9).

## 10. Distributions on branching or coalescent times of heterochronous genealogies



Fig. S4. Heterochronous genealogy. Example of a ranked genealogy with heterochronous sampling. $s_{4}, \ldots, s_{1}$ and $t_{8}, \ldots, t_{2}$ indicate sampling times (red dotted lines) and coalescent times (blue dotted lines), respectively. $u_{11}, \ldots, u_{1}$ are the ordered times of change points where the number of lineages changes due to either a sampling event or a coalescent event. The time increases backwards in time starting with $u_{11}=0$ as the present time. $I_{0, k}$ is the interval that ends with a coalescent event at $t_{k}$. $I_{i, k}$ $(i>0)$ represents the interval that ends with a sampling time within the interval $\left(t_{k+1}, t_{k}\right)$. For $k=n$, we adopt the convention $t_{n+1}=0$.

The ranked tree shape and ranked genealogy of time-stamped samples are termed heterochronous ranked tree shapes and heterochronous genealogies, respectively (Figure S4). Here, we assume that samples are collected at times $s_{m}, s_{m-1}, \ldots, s_{1}$, with $s_{m}=t_{n+1}=0$ (the present), and $s_{j}<s_{j-1}$ for $j=m, \ldots, 2$. At time $s_{j}, n_{j}$ lineages are sampled, and $\sum_{j=1}^{m} n_{j}=n$.

The $\lambda(t)$-heterochronous-coalescent (10) describes the distribution of coalescent times conditioned on collecting $n_{m}, n_{m-1}, \ldots, n_{1}$ samples at times $s_{m}, s_{m-1}, \ldots, s_{1}$. As before, $t_{n+1}, t_{n}, \ldots, t_{2}$ denote the coalescent times, except that the subindex no longer indicates the number of lineages. Instead, the subindex indicates the rank order of the coalescent events going forward in time (tipward) from the root at $t_{2}$. Define $\left(u_{n+m-1}, u_{n+m-2}, \ldots, u_{1}\right)$ as the vector of change points (coalescent or sampling times), with $0=u_{n+m-1}<u_{n+m-2}<\cdots<u_{1}=t_{2}$. To state the density of coalescent times according to the $\lambda(\mathrm{t})$-heterochronouscoalescent, going backwards in time (rootward), we denote the intervals that end with a coalescent event at $t_{k}$ by $I_{0, k}$, and the intervals that end with a sampling time within the interval $\left(t_{k+1}, t_{k}\right)$ as $I_{i, k}$, where $i$ is an index tracking the sampling events in $\left(t_{k+1}, t_{k}\right)$. More specifically,

$$
\begin{aligned}
I_{0, k} & =\left(\max \left\{t_{k+1}, s_{j}\right\}, t_{k}\right] \text { for } s_{j}<t_{k} \\
I_{i, k} & =\left(\max \left\{t_{k+1}, s_{j+i}\right\}, s_{j+i-1}\right] \text { for } s_{j+i-1}>t_{k+1} \text { and } s_{j}<t_{k}
\end{aligned}
$$

with $k=2, \ldots, n$ and $i$ ranges from 1 to the number of sampling events in $\left(t_{k+1}, t_{k}\right)$. An example of the annotated time intervals using $I_{0, k}$ and $I_{i, k}$ is shown in Figure S4.

The conditional density of $t_{k-1}$ is the product of the conditional density of $t_{k-1} \in I_{0, k}$ and the probability of not having a coalescent event during the period of time spanned by intervals $I_{1, k}, \ldots, I_{m, k}$. That is, for $k=2, \ldots, n$,

$$
\begin{align*}
& P\left[t_{k-1} \mid t_{k}, \mathbf{s}, \mathbf{n}, N_{e}(t)\right]=\frac{C_{0, k-1}}{N_{e}\left(t_{k-1}\right)} \\
& \times \exp \left[-\left\{\int_{I_{0, k-1}} \frac{C_{0, k-1} d t}{N_{e}(t)}+\sum_{i=1}^{m} \int_{I_{i, k-1}} \frac{C_{i, k-1} d t}{N_{e}(t)}\right\}\right], \tag{S3}
\end{align*}
$$

where $C_{i, k}=\binom{n_{i, k}}{2}$.

## 11. Embeddings in MDS

We chose MDS in two dimensions to visualize matrices of pairwise distances. In general, our metrics are well explained in the MDS visualization; however, the other distances are usually poorly represented in this space. In this section, we propose a measure of distortion and correlation to assess how well the embedding preserves the pairwise distances for each metric. In our examples, the distortion measure shown in Table S15 suggests that our $d_{2}$ metric has the best MDS embedding in general of all distance functions considered with our $d_{1}$ metric a close second. Similarly, the correlation measure shown in Table S16 confirms that our $d_{1}$ and $d_{2}$ metrics, with near perfect correlations, have far better embedding in the 2 -dimensional MDS space than the other distances considered.
A. Distortion. To assess our distances and their MDS embeddings in two dimensions, we compute the following distortion statistic (11) defined as follows:

$$
\text { distortion }=\text { expansion } \times \text { contraction }
$$

where expansion and contraction are defined as follows. For a given sample of ranked tree shapes $\mathcal{T}_{S}=\left\{T_{1}^{R}, T_{2}^{R}, \ldots, T_{s}^{R}\right\}$ with $n$ leaves in $\mathcal{T}_{n}^{R}$,

$$
\text { expansion }=\max _{\substack{T_{i}^{R}, T_{j}^{R} \in \mathcal{T}_{S} ; \\ i \neq j}} \frac{d_{\mathrm{MDS}}\left(T_{i}^{R}, T_{j}^{R}\right)}{d\left(T_{i}^{R}, T_{j}^{R}\right)},
$$

where $d_{\text {MDS }}$ is the $L_{2}$-Euclidean distance in the reduced MDS space and $d$ is any distance function on ranked tree shapes, and

$$
\text { contraction }=\max _{\substack{T_{i}^{R}, T_{j}^{R} \in \mathcal{T}_{S} \\ i \neq j}} \frac{d\left(T_{i}^{R}, T_{j}^{R}\right)}{d_{\mathrm{MDS}}\left(T_{i}^{R}, T_{j}^{R}\right)} .
$$

The distortion on the ranked genealogies is defined similarly. The comparison of distortions for simulated ranked tree shapes and ranked genealogies can be found in Table S15.
B. Correlation. As a second measure for assessing our distances and their MDS embeddings in two dimensions, we compute the Pearson correlation coefficient between the two vectors of pairwise distances between sampled ranked tree shapes, one from using any distance functions $d$ on ranked tree shapes and the other from the $L_{2}$-Euclidean distance $d_{\text {MDS }}$ in the reduced MDS space:

$$
\text { correlation }=\frac{\sum_{i=2}^{s} \sum_{j=1}^{i}\left(d\left(T_{i}^{R}, T_{j}^{R}\right)-\mu_{d}\right)\left(d_{\mathrm{MDS}}\left(T_{i}^{R}, T_{j}^{R}\right)-\mu_{d_{\mathrm{MDS}}}\right)}{\sqrt{\sum_{i=2}^{s} \sum_{j=1}^{i}\left(d\left(T_{i}^{R}, T_{j}^{R}\right)-\mu_{d}\right)^{2} \sum_{i=2}^{s} \sum_{j=1}^{i}\left(d_{\mathrm{MDS}}\left(T_{i}^{R}, T_{j}^{R}\right)-\mu_{\left.d_{\mathrm{MDS}}\right)^{2}}\right.}},
$$

where $s$ is the number of sampled ranked tree shapes. $\mu_{d_{\mathrm{MDS}}}$ and $\mu_{d}$ are the mean of the pairwise distances using $L_{2}$-Euclidean distance in the MDS space and using any distance functions $d$ on the sampled ranked tree shapes, respectively. The comparisons of correlations for simulated ranked tree shapes and ranked genealogies appear in Table S16.

(C)

(B)

$$
\mathbf{F}=\left(\begin{array}{ccccccc}
2 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 3 & 0 & 0 & 0 & 0 & 0 \\
1 & 2 & 4 & 0 & 0 & 0 & 0 \\
1 & 2 & 3 & 5 & 0 & 0 & 0 \\
1 & 2 & 3 & 4 & 6 & 0 & 0 \\
1 & 2 & 3 & 3 & 5 & 7 & 0 \\
1 & 1 & 2 & 2 & 4 & 6 & 8
\end{array}\right)
$$

(D)

$$
\mathbf{F}=\left(\begin{array}{cccc:cccc:c:c}
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 2 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 2 & 3 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hdashline 1 & 2 & 2 & 4 & 4 & 0 & 0 & 0 & 0 & 0 \\
1 & 2 & 2 & 3 & 3 & 5 & 0 & 0 & 0 & 0 \\
1 & 2 & 2 & 2 & 2 & 4 & 6 & 0 & 0 & 0 \\
1 & 1 & 1 & 1 & 1 & 3 & 5 & 7 & 0 & 0 \\
\hdashline 1 & 1 & 1 & 1 & 1 & 1 & 3 & 5 & 5 & 0 \\
\hdashline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2
\end{array}\right)
$$

Fig. S5. Bijection of ranked tree shapes and F-matrices for isochronous and heterochronous trees. (A) Example of a ranked genealogy with isochronous sampling. (B) The corresponding $\mathbf{F}$-matrix that encodes the ranked tree shape information of the tree in (A). (C) Example of a ranked genealogy with heterochronous sampling. (D) The corresponding F-matrix of the heterochronous ranked tree shape in (C). Blue dotted lines indicate coalescent events and red dotted lines represent sampling events. In (C), coalescent times are denoted by $\left\{t_{k}\right\}_{k=2}^{8}$, sampling times by $\left\{s_{k}\right\}_{k=1}^{4}$, and the number of lineages changes at change points $\left\{u_{k}\right\}_{k=1}^{11}$.
$\left(\begin{array}{cccccccccc}u_{1}-u_{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u_{1}-u_{3} & u_{2}-u_{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u_{1}-u_{4} & u_{2}-u_{4} & u_{3}-u_{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ u_{1}-u_{5} & u_{2}-u_{5} & u_{3}-u_{5} & u_{4}-u_{5} & 0 & 0 & 0 & 0 & 0 & 0 \\ u_{1}-u_{6} & u_{2}-u_{6} & u_{3}-u_{6} & u_{4}-u_{6} & u_{5}-u_{6} & 0 & 0 & 0 & 0 & 0 \\ u_{1}-u_{7} & u_{2}-u_{7} & u_{3}-u_{7} & u_{4}-u_{7} & u_{5}-u_{7} & u_{6}-u_{7} & 0 & 0 & 0 & 0 \\ u_{1}-u_{8} & u_{2}-u_{8} & u_{3}-u_{8} & u_{4}-u_{8} & u_{5}-u_{8} & u_{6}-u_{8} & u_{7}-u_{8} & 0 & 0 & 0 \\ u_{1}-u_{9} & u_{2}-u_{9} & u_{3}-u_{9} & u_{4}-u_{9} & u_{5}-u_{9} & u_{6}-u_{9} & u_{7}-u_{9} & u_{8}-u_{9} & 0 & 0 \\ u_{1}-u_{10} & u_{2}-u_{10} & u_{3}-u_{10} & u_{4}-u_{10} & u_{5}-u_{10} & u_{6}-u_{10} & u_{7}-u_{10} & u_{8}-u_{10} & u_{9}-u_{10} & 0 \\ u_{1} & u_{2} & u_{3} & u_{4} & u_{5} & u_{6} & u_{7} & u_{8} & u_{9} & u_{10}\end{array}\right)$

Fig. S6. Example of the weight matrix $\mathbf{W}$. The weight matrix associated with the example heterochronous ranked genealogy and its $\mathbf{F}$-matrix in Figures $\mathrm{S} 5(\mathrm{C})$ and (D). In the last row, $u_{11}$ is suppressed because we set the initial sampling time to be $u_{11}=0$.
(A) $\boldsymbol{d}_{1}$
(B) $\boldsymbol{d}_{2}$
$\left.\begin{array}{l}T_{1}^{R} \\ T_{2}^{R} \\ T_{3}^{R} \\ T_{4}^{R} \\ T_{5}^{R}\end{array} \begin{array}{ccccc}T_{1}^{R} & T_{2}^{R} & T_{3}^{R} & T_{4}^{R} & T_{5}^{R} \\ 0 & 2 & 3 & 2 & 1 \\ & 0 & 1 & 2 & 3 \\ & & 0 & 1 & 2 \\ & & & 0 & 1 \\ & & & & 0\end{array}\right]$
$\left[\begin{array}{ccccc}T_{1}^{R} & T_{2}^{R} & T_{3}^{R} & T_{4}^{R} & T_{5}^{R} \\ 0 & 1.41 & 1.73 & 1.41 & 1 \\ & 0 & 1 & 1.41 & 1.73 \\ & & 0 & 1 & 1.41 \\ & & & 0 & 1 \\ & & & & 0\end{array}\right]$

| (C) | $\boldsymbol{d}_{\text {BHV-RTS }}$ |  |  |  |  |  |  | $d_{\text {KC-RTS }}$ |  |  |  | (E) | $d_{\text {CP-RTS }}$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $T_{1}^{R}$ | $T_{2}^{R}$ | $T_{3}^{R}$ | $T_{4}^{R}$ | $T_{5}^{R}$ |  | $T_{1}^{R}$ | $T_{2}^{R}$ | $T_{3}^{R}$ | $T_{4}^{R}$ | $T_{5}^{R}$ |  | $T_{1}^{R}$ | $T_{2}^{R}$ | $T_{3}^{R}$ | $T_{4}^{R}$ | $T_{5}^{R}$ |
| $T_{1}^{R}[0$ | 0 | 2.45 | 3.74 | 3.46 | 2.45 |  | 0 |  | 3.61 |  |  |  | 0 | 2 | 2 | 2 | 2.45 |
| $T_{2}^{R}$ |  | 0 | 3.46 | 3.74 | 3.74 |  |  | 0 | 2.45 | 2.83 | 2.65 |  |  | 0 | 0 | 0 | 2 |
| $T_{3}^{R}$ |  |  | 0 | 2.45 | 2.45 |  |  |  | 0 | 2.45 | 2.65 |  |  |  | 0 | 0 | 2 |
| $T_{4}^{R}$ |  |  |  |  | 2.45 |  |  |  |  | 0 | 2.65 |  |  |  |  | 0 | 2 |
| $T_{5}^{R}[$ |  |  |  |  | 0 |  |  |  |  |  | 0 | L |  |  |  |  | 0 ] |


$T_{5}^{R}$

Fig. S7. Comparisons of metrics applied to isochronous ranked tree shapes with $\boldsymbol{n}=\mathbf{5}$.


Fig. S8. MDS representation of distances between 4,000 simulated isochronous ranked tree shapes of $\boldsymbol{n}=100$ leaves, aggregated from four different alpha-beta splitting models. 1,000 isochronous ranked tree shapes were simulated for each of pairs of $(\alpha, \beta)$ values in $\{(-1,0),(-1,-1.5),(+1,0),(+1,-1.5)\}$. Different $\alpha$ generates different distributions of internal node ranking while different $\beta$ generates different distributions of tree balance. (A) MDS of the $d_{1}$ metric. (B) MDS of the $d_{2}$ metric. (C) $L_{2}$-medoid trees from each distribution using the $d_{1}$ metric. MDS plots for (D) $d_{\mathrm{BHV} \text {-RTS }}$, ( E ) $d_{\mathrm{KC} \text {-RTS }}$, and (F) $d_{\mathrm{CP} \text {-RTS. }}$. In each MDS plot, the triangle represents the $L_{2}$-medoid tree of 1,000 points for a specified model.


Fig. S9. MDS representation of distances between 2,000 simulated heterochronous ranked tree shapes of $\boldsymbol{n}=\mathbf{1 0 0}$ with different sampling events. (A) MDS of the $d_{1}$ metric. (B) MDS of the $d_{2}$ metric. (C) $L_{2}$-medoid trees from each distribution using the $d_{1}$ metric. MDS plots for (D) $d_{\mathrm{BHV} \text {-RTS }}$ and (E) $d_{\mathrm{KC}}$-RTs. To demonstrate that our metrics are sensitive to sampling schedules, we simulated trees with $n=100$ leaves under heterochronous sampling with two sampling scenarios. For the first set of trees (the "Single" distribution), we selected 90 samples at time 0 and the remaining 10 samples at distinct times with sampling times drawn uniformly at random from ( $0,10^{4}$ ], i.e., $\mathbf{n}=(90,1,1,1,1,1,1,1,1,1,1)$. In the second set of trees (the "Double" distribution), 80 samples were drawn at time 0 and the remaining 20 were sampled in pairs at ten distinct random sampling times drawn uniformly from ( $0,10^{4}$ ], i.e., $\mathbf{n}=(80,2,2,2,2,2,2,2,2,2,2)$. We generated 1,000 coalescent trees per sampling scheme assuming a constant effective population size trajectory of $N_{0}=10^{4}$. We then removed leaf labels to produce the $2,000 \times 2,000$ distance matrices with all applicable distances. Our metrics and $d_{\text {BHV-RTS }}$ show a clear separation between the two distributions along the first two MDS axes. The total distance explained in the two-dimensional space is higher using our metrics, $66.5 \%$ and $76.4 \%$ for $d_{1}$ and $d_{2}$, respectively, compared to $13.5 \%$ of $d_{\text {BHV-RTS. }}$. $d_{\mathrm{KC}}$-RTS exhibits less discrimination than the other three distances. The confusion matrices in Table S7 and the confusion statistics in Table S8 confirm that our metrics distinguish different sampling schemes better than the other two metrics compared.

Table S1. Summary of dispersions for ranked tree shapes. Comparison of dispersion (Eq. 6) of ranked tree shape distribution using distance functions between ranked tree shapes. (A) Isochronous ranked tree shapes simulated from the beta-splitting model with varying $\beta$ parameters (Figure 4). (B) Isochronous ranked tree shapes simulated from the alpha-beta splitting model with varying $\alpha$ parameters and fixed $\beta=0$ (Figure 5). (C) Heterochronous ranked tree shapes simulated from different sampling schemes (Figure S9). Note that $d_{\mathrm{CP}-\mathrm{RTs}}$ does not account for heterochronous sampling, so we exclude $d_{\text {CP-RTS }}$ from our analyses on heterochronous ranked tree shapes (Text 5).
(A) Isochronous ranked tree shapes, beta-splitting model

|  | $d_{1}$ | $d_{2}$ | $d_{\text {BHV-RTS }}$ | $d_{\text {KC-RTS }}$ | $d_{\text {CP-RTS }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | 5541.21 | 117.14 | 377.84 | 128.20 | 8.51 |
| Yule | 5889.31 | 119.40 | 363.33 | 182.52 | 8.97 |
| AB | 6579.90 | 127.37 | 345.82 | 271.78 | 9.58 |
| PDA | 6966.50 | 133.24 | 304.49 | 490.98 | 10.48 |
| Unbalanced | 4391.36 | 90.88 | 154.44 | 944.90 | 12.50 |

(B) Isochronous ranked tree shapes, alpha-beta splitting model

|  | $d_{1}$ | $d_{2}$ | $d_{\text {BHV-RTS }}$ | $d_{\text {KC-RTS }}$ | $d_{\text {CP-RTS }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | 4701.27 | 90.81 | 85.33 | 110.76 | 8.95 |
| $\alpha=-1$ | 7202.89 | 135.70 | 110.64 | 126.06 | 9.00 |
| $\alpha=0$ | 7719.71 | 150.57 | 262.18 | 172.73 | 8.96 |
| $\alpha=1$ | 6084.73 | 122.77 | 363.17 | 182.49 | 9.06 |
| $\alpha=2$ | 5668.18 | 115.80 | 376.98 | 179.18 | 9.08 |

(C) Heterochronous ranked tree shapes, different sampling schemes

|  | $d_{1}$ | $d_{2}$ | $d_{\text {BHV-RTS }}$ | $d_{\text {KC-RTS }}$ | $d_{\text {CP-RTS }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Single | 10359.43 | 277.88 | 350.26 | 230.17 | - |
| Double | 10423.86 | 238.90 | 324.47 | 257.65 | - |

Table S2. Comparison of metrics: discrimination of isochronous ranked tree shapes under different beta-splitting models. We compare the performance of different distances on ranked tree shapes according to how well they separate trees simulated from the beta-splitting distribution of ranked tree shapes with different balance parameters $\beta$. Rows indicate the sampling distribution and columns indicate the $L_{2}$-medoid of each distribution. Each matrix corresponds to a different distance metric. Entry ( $i, j$ ) corresponds to the percentage of trees simulated from the $i$ th distribution that are closer to the $j$ th $L_{2}$-medoid than to the medoids of any other columns. The color scheme of the $L_{\mathbf{2}}$-medoids follows Figure 4. The mean diagonal values are 83.28, 82.02, 20.32, 70.50, and 74.96 for matrices (A)-(E), respectively.
(A)
Balanced
Yule
AB $\left[\begin{array}{ccccc}\boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} \\ 85.9 & 14.0 & 0.1 & 0 & 0 \\ 22.9 & 64.4 & 12.7 & 0 & 0 \\ 1.1 & 19.7 & 73.6 & 5.6 & 0 \\ 0 & 0 & 7.2 & 92.5 & 0.3 \\ 0 & 0 & 0 & 0 & 100.0\end{array}\right]$
(B)

$L_{2}$-medoid
A Balanced

- Yule
- AB
$\triangle \mathrm{PDA}$
A Unbalanced
(C)
Balanced $\left[\begin{array}{c}\boldsymbol{d} \\ \text { Yule }\end{array}\left[\begin{array}{ccccc}\boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} \\ \text { Unbalanced } \\ \text { AB }\end{array}\left[\begin{array}{ccccc} \\ \text { PDA }\end{array}\left[\begin{array}{ccccc} \\ 0.5 & 0.2 & 0 & 0.2 & 99.1 \\ 0.5 & 0.1 & 0.2 & 0.2 & 99.0 \\ 0.2 & 0 & 0 & 0.3 & 99.5 \\ 0 & 0 & 0 & 0.1 & 99.9\end{array}\right]\right.\right.\right.$
(D)
$d_{\text {KC-RTS }}$

(E) $\quad d_{\text {CP-RTS }}$
$\left[\begin{array}{ccccc}\boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} \\ 77.1 & 22.5 & 0.4 & 0 & 0 \\ 29.8 & 51.3 & 18.7 & 0.2 & 0 \\ 4.8 & 26.4 & 57.7 & 11.1 & 0 \\ 0 & 0.5 & 10.7 & 88.8 & 0 \\ 0 & 0 & 0 & 0.1 & 99.9\end{array}\right]$

Table S3. Summary of the pairwise mean confusion statistics and associated $P$ values for isochronous ranked tree shapes under different beta-splitting models. Each entry in the table contains a pair of values: the mean confusion statistic of two ranked tree shape sampling distributions (Eq. 8) and its associated $P$ value (Eq. 9). The simulated distributions of ranked tree shapes for the off-diagonal entries are the same as those considered in Figure 4 and Table S2. The diagonal entries represent the tests of true null cases, where we generated additional 1,000 random ranked tree shapes per each $\beta$-value and computed the mean confusion statistic between two samples drawn from the same distribution.
(A) $d_{1}$

|  | Balanced | Yule | AB | PDA | Unbalanced |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | $0.4935,0.4628$ |  |  |  |  |
| Yule | $0.1850,0.0001$ | $0.4990,0.5088$ |  |  |  |
| AB | $0.0360,0.0001$ | $0.1675,0.0001$ | $0.5025,0.6396$ |  |  |
| PDA | $0.0005,0.0001$ | $0.0110,0.0001$ | $0.0640,0.0001$ | $0.5105,0.8766$ |  |
| Unbalanced | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0015,0.0001$ | $0.5245,0.9919$ |

(B) $d_{2}$

|  | Balanced | Yule | AB | PDA | Unbalanced |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | $0.5040,0.7583$ |  |  |  |  |
| Yule | $0.2025,0.0001$ | $0.5015,0.6240$ |  |  |  |
| AB | $0.0405,0.0001$ | $0.1755,0.0001$ | $0.4960,0.3915$ |  |  |
| PDA | $0.0015,0.0001$ | $0.0125,0.0001$ | $0.0695,0.0001$ | $0.5020,0.6494$ |  |
| Unbalanced | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0015,0.0001$ | $0.4720,0.0087$ |

(C) $d_{\text {BHV-RTS }}$

|  | Balanced | Yule | AB | PDA | Unbalanced |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | $0.4900,0.2052$ |  |  |  |  |
| Yule | $0.4795,0.0452$ | $0.4760,0.0194$ |  |  |  |
| AB | $0.4570,0.0001$ | $0.4685,0.0028$ | $0.4955,0.4076$ |  |  |
| PDA | $0.4695,0.0033$ | $0.4700,0.0041$ | $0.4825,0.0639$ | $0.5150,0.9245$ |  |
| Unbalanced | $0.4950,0.3609$ | $0.4990,0.4886$ | $0.4990,0.4864$ | $0.4990,0.5025$ | $0.5085,0.8043$ |

(D) $d_{\mathrm{KC} \text {-RTS }}$

|  | Balanced | Yule | AB | PDA | Unbalanced |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | $0.5015,0.5973$ |  |  |  |  |
| Yule | $0.2815,0.0001$ | $0.4940,0.3448$ |  |  |  |
| AB | $0.0945,0.0001$ | $0.2145,0.0001$ | $0.4880,0.1071$ |  |  |
| PDA | $0.0675,0.0001$ | $0.0900,0.0001$ | $0.1650,0.0001$ | $0.4760,0.0126$ |  |
| Unbalanced | $0.0400,0.0001$ | $0.0460,0.0001$ | $0.0535,0.0001$ | $0.0765,0.0001$ | $0.5115,0.8692$ |

(E) $d_{\mathrm{CP}-\mathrm{RTS}}$

|  | Balanced | Yule | AB | PDA | Unbalanced |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Balanced | $0.4935,0.3205$ |  |  |  |  |
| Yule | $0.2590,0.0001$ | $0.5150,0.9263$ |  |  |  |
| AB | $0.0755,0.0001$ | $0.2555,0.0001$ | $0.5015,0.6544$ |  |  |
| PDA | $0.0035,0.0001$ | $0.0260,0.0001$ | $0.1110,0.0001$ | $0.5035,0.7410$ |  |
| Unbalanced | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0005,0.0001$ | 0.47500 .0274 |

Table S4. Comparison of metrics: discrimination of isochronous ranked tree shapes under different alpha-beta splitting models with a fixed beta value. We compare the performance of different distances on ranked tree shapes according to how well they separate trees simulated from the alpha-beta splitting distribution of ranked tree shapes with different parameter values $\alpha$ which regulates the internal node ranking of a given tree shape. The format of the matrices follows Table S2. The simulation values and the color scheme of the $L_{2}$-medoids follow Figure 5. The mean diagonal values are $75.40,76.94,20.14,36.48$, and 19.56 for matrices (A)-(E), respectively.

$$
\begin{gathered}
(\mathrm{A}) \\
\alpha=-2 \\
\alpha=-1 \\
\alpha=0 \\
\alpha=1 \\
\alpha=2
\end{gathered}\left[\begin{array}{ccccc}
\boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} & \boldsymbol{\Delta} \\
95.6 & 4.4 & 0 & 0 & 0 \\
30.4 & 69.0 & 0.6 & 0 & 0 \\
0 & 0.6 & 86.0 & 12.8 & 0.6 \\
0 & 0 & 4.9 & 61.4 & 33.7 \\
0 & 0 & 0 & 35.0 & 65.0
\end{array}\right]
$$

(B)
$\Delta \quad \begin{gathered}d_{2} \\ \Delta\end{gathered} \Delta \quad L_{2}$-medoid


- $\alpha=-2$
$\Delta \alpha=-1$
- $\alpha=0$
- $\alpha=1$
- $\alpha=2$

| (C) | $d_{\text {BHV-RTS }}$ |  |  |  |  | (D) | $d_{\text {KC-RTS }}$ |  |  |  |  | (E) | $\boldsymbol{d}_{\text {CP-RTS }}$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\Delta$ | A | $\Delta$ | $\Delta$ | A |  | A | A | A | A | A |  | $\Delta$ | A | $\Delta$ | A | A |
| $\alpha=-2$ | 97.5 | 2.5 | 0 | 0 | 0 |  | 71.5 | 28.5 | 0 | 0 | 0 |  | 29.6 | 13.1 | 17.0 | 14.4 | 25.9 |
| $\alpha=-1$ | 97.1 | 2.9 | 0 | 0 | 0 |  | 71.4 | 28.5 | 0 | 0 | 0.1 |  | 31.4 | 13.5 | 15.3 | 11.2 | 28.6 |
| $\alpha=0$ | 88.2 | 11.7 | 0.1 | 0 | 0 |  | 34.2 | 34.1 | 17.3 | 1.5 | 12.9 |  | 29.9 | 12.3 | 15.3 | 14.3 | 28.2 |
| $\alpha=1$ | 80.1 | 18.2 | 1.6 | 0.1 | 0 |  | 1.3 | 2.9 | 35.7 | 19.6 | 40.5 |  | 28.8 | 11.1 | 17.3 | 11.1 | 31.7 |
| $\alpha=2$ | 80.2 | 18.4 | 1.2 | 0.1 | 0.1 |  | 1.5 | 3.8 | 32.2 | 17.0 | 45.5 |  | 28.2 | 13.9 | 16.9 | 12.7 | 28.3 |

Table S5. Summary of the pairwise mean confusion statistics and associated $P$ values for isochronous ranked tree shapes under different alpha-beta splitting models. The format of the table follows Table S3. The simulated distributions of ranked tree shapes for the off-diagonal entries are the same as those considered in Figure 5 and Table S4. The diagonal entries represent the tests of true null cases, where we generated additional 1,000 random ranked tree shapes per each $\alpha$-value.
(A) $d_{1}$

|  | $\alpha=-2$ | $\alpha=-1$ | $\alpha=0$ | $\alpha=1$ | $\alpha=2$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | $0.4845,0.1206$ |  |  |  |  |
| $\alpha=-1$ | $0.1740,0.0001$ | $0.5020,0.6866$ |  |  |  |
| $\alpha=0$ | $0.0000,0.0001$ | $0.0060,0.0001$ | $0.5175,0.9541$ |  |  |
| $\alpha=1$ | $0.0000,0.0001$ | $0.0005,0.0001$ | $0.0915,0.0001$ | $0.4970,0.4946$ |  |
| $\alpha=2$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0505,0.0001$ | $0.3430,0.0001$ | $0.4900,0.2482$ |

(B) $d_{2}$

|  | $\alpha=-2$ | $\alpha=-1$ | $\alpha=0$ | $\alpha=1$ | $\alpha=2$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | $0.4970,0.5093$ |  |  |  |  |
| $\alpha=-1$ | $0.1520,0.0001$ | $0.4990,0.5878$ |  |  |  |
| $\alpha=0$ | $0.0000,0.0001$ | $0.0045,0.0001$ | $0.5120,0.8818$ |  |  |
| $\alpha=1$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0795,0.0001$ | $0.5035,0.7277$ |  |
| $\alpha=2$ | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0415,0.0001$ | $0.3400,0.0001$ | $0.4805,0.0777$ |

(C) $d_{\text {BHV-RTS }}$

|  | $\alpha=-2$ | $\alpha=-1$ | $\alpha=0$ | $\alpha=1$ | $\alpha=2$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | $0.4930,0.2680$ |  |  |  |  |
| $\alpha=-1$ | $0.4980,0.4308$ | $0.5075,0.7598$ |  |  |  |
| $\alpha=0$ | $0.4995,0.5020$ | $0.4990,0.4879$ | $0.5160,0.9350$ |  |  |
| $\alpha=1$ | $0.4995,0.4940$ | $0.4995,0.5025$ | $0.4975,0.4313$ | $0.4890,0.1853$ |  |
| $\alpha=2$ | $0.4995,0.5217$ | $0.4995,0.5303$ | $0.4950,0.3698$ | $0.4675,0.0019$ | $0.4965,0.4360$ |

(D) $d_{\mathrm{KC}-\mathrm{RTS}}$

|  | $\alpha=-2$ | $\alpha=-1$ | $\alpha=0$ | $\alpha=1$ | $\alpha=2$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | $0.5060,0.7526$ |  |  |  |  |
| $\alpha=-1$ | $0.5000,0.5893$ | $0.5070,0.7606$ |  |  |  |
| $\alpha=0$ | $0.3395,0.0001$ | $0.3350,0.0001$ | $0.4940,0.3101$ |  |  |
| $\alpha=1$ | $0.1420,0.0001$ | $0.1210,0.0001$ | $0.4065,0.0001$ | $0.4895,0.2360$ |  |
| $\alpha=2$ | $0.0610,0.0001$ | $0.0780,0.0001$ | $0.3425,0.0001$ | $0.4885,0.0001$ | $0.4860,0.1200$ |

(E) $d_{\text {CP-RTS }}$

|  | $\alpha=-2$ | $\alpha=-1$ | $\alpha=0$ | $\alpha=1$ | $\alpha=2$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\alpha=-2$ | $0.5090,0.8159$ |  |  |  |  |
| $\alpha=-1$ | $0.4920,0.2788$ | $0.5020,0.6775$ |  |  |  |
| $\alpha=0$ | $0.4890,0.1934$ | $0.4970,0.4219$ | $0.5080,0.7847$ |  |  |
| $\alpha=1$ | $0.4925,0.2898$ | $0.4865,0.1333$ | $0.5035,0.6906$ | $0.4870,0.1825$ |  |
| $\alpha=2$ | $0.4895,0.1984$ | $0.4975,0.4956$ | $0.4990,0.5067$ | $0.5120,0.9041$ | $0.5105,0.8784$ |

Table S6. Comparison of metrics: discrimination of isochronous ranked tree shapes under different alpha-beta splitting models. We compare the performance of different distances on ranked tree shapes according to how well they separate trees simulated from the alpha-beta splitting distribution of ranked tree shapes with different parameter values $\alpha$ and $\beta$. The format of the matrices follows Table S2. The simulation values and the color scheme of the $L_{2}$-medoids follow Figure S 8 . The respective mean separation indices (mean diagonal) are 89.8, 89.8, 25.4, 78.8, and 49.5 for $d_{1}, d_{2}, d_{\text {BHV-RTS }}, d_{\text {KC-RTS }}$, and $d_{\text {CP-RTS }}$.


Table S7. Comparison of metrics: heterochronous ranked tree shapes with different sampling schemes. We compare the performance of different distances on ranked tree shapes according to how well they separate trees simulated from the heterochronous Tajima coalescent with different sampling sequences $s$ and $n$. The format of the matrices follows Table S2. The simulation values and the color scheme of the $L_{2}$-medoids follow Figure S9. The mean diagonal values are 99.85, 99.90, 95.60, and 56.60 for matrices (A)-(D), respectively.

| (A) | $d_{1}$ |  | (B) | $d_{2}$ |  | $L_{2}$-medoid |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\Delta$ | A |  | - | A |  |
| Single | 100.0 | 0 |  | 99.9 | 0.1 | $\triangle$ Single |
| Double | 0.3 | 99.7 | L |  | 99.9 | - Double |
| (C) | $d_{\text {BHV-RTS }}$ |  | (D) | $d_{\text {KC-RTS }}$ |  |  |
|  | A | A |  | A | A |  |
| Single | 92.1 | 7.9 |  |  | 6.1 |  |
| Double | 0.9 | 99.1 |  |  |  |  |

Table S8. Summary of the pairwise mean confusion statistics and associated $P$ values for heterochronous ranked tree shapes under different sampling schemes. The format of the table follows Table S3. The simulated distributions of ranked tree shapes for the off-diagonal entries are the same as those considered in Figure S9 and Table S7. The diagonal entries represent the tests of true null cases, where we generated additional 1,000 random ranked tree shapes per each sampling scenario.
(A) $d_{1}$

|  | Single | Double |
| :--- | :---: | :---: |
| Single | $0.5175,0.9782$ |  |
| Double | $0.0015,0.0001$ | $0.5065,0.7484$ |

(B) $d_{2}$

|  | Single | Double |
| :--- | :---: | :---: |
| Single | $0.5215,0.9832$ |  |
| Double | $0.0010,0.0001$ | $0.5075,0.8271$ |

(C) $d_{\text {BHV-RTS }}$

|  | Single | Double |
| :--- | :---: | :---: |
| Single | $0.5135,0.9413$ |  |
| Double | $0.0440,0.0001$ | $0.4935,0.2702$ |

(D) $d_{\text {KC-RTS }}$

|  | Single | Double |
| :--- | :---: | :---: |
| Single | $0.4860,0.1288$ |  |
| Double | $0.4340,0.0001$ | $0.5000,0.6279$ |

Table S9. Summary of dispersion comparisons for ranked genealogies. Comparison of dispersion of ranked genealogies using distance functions between ranked genealogies. (A) Isochronous ranked genealogies simulated from different population trajectories under neutral coalescent model (Figure 6). (B) Heterochronous ranked genealogies of real and simulated human influenza A/H3N2 virus data from different geographical regions (Figure 8).
(A) Isochronous ranked genealogies, different demographic models

|  | $d_{1}^{w}$ | $d_{2}^{w}$ | $d_{\text {BHV-RG }}$ | $d_{\text {KC-RG }}$ |
| :--- | :---: | :---: | :---: | :---: |
| Constant | 6420771.00 | 142726.04 | 33007.42 | 391150.52 |
| Exponential | 1331068.00 | 24847.09 | 1397.17 | 4743.48 |
| Logistic | 1744504.00 | 39291.83 | 8751.45 | 109258.59 |

(B) Heterochronous ranked genealogies, human influenza $A / H 3 N 2$ virus

|  | $d_{1}^{w}$ | $d_{2}^{w}$ | $d_{\text {BHV-RG }}$ | $d_{\text {KC-RG }}$ |
| :--- | :---: | :---: | :---: | :---: |
| New York - New York | 3368.28 | 53.41 | 3.90 | 88.91 |
| New York - Southeast Asia | 4581.15 | 65.93 | 9.21 | 263.54 |
| Southeast Asia - Southeast Asia | 6370.47 | 85.97 | 6.93 | 152.59 |
| Southeast Asia - New York | 5547.11 | 77.86 | 8.20 | 259.08 |

Table S10. Comparison of metrics: isochronous ranked genealogies under different demographic models. We compare the performance of different distances on ranked genealogies according to how well they separate trees simulated from the $\lambda(t)$-coalescent with different population histories. The format of the matrices follows Table S2. The simulation values and the color scheme of the $L_{2}$-medoids follow Figure 6. The mean diagonal values are 99.80, 99.87, 33.40, and 73.97 for matrices (A)-(D), respectively.

| (A) |  | $d_{1}^{w}$ |  | (B) |  | $d_{2}^{w}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $\Delta$ | A | A |  | A | A | A |  |
| Uniform | 99.6 | 0.4 | 0 |  | 99.7 | 0.3 | 0 |  |
| Exponential | 0 | 99.9 | 0.1 |  | 0 | 99.9 | 0.1 |  |
| Logistic | 0 | 0.1 | 99.9 |  |  |  | 100.0 | $L_{2}$-medoid |
|  |  |  |  | (D) $\boldsymbol{d}_{\text {KC-RG }}$ |  |  |  | - Uniform |
| (C) | $\boldsymbol{d}_{\text {BHV-RG }}$ |  |  |  |  |  |  | - Exponential |
|  | $\Delta$ | A | A |  | $\Delta$ | A | - | - Logistic |
| Uniform |  | 99.9 | 0 |  | 60.0 | 1.0 | 39.0 |  |
| Exponential | 0 | 100.0 | 0 |  | 0 | 100.0 | 0 |  |
| Logistic | 0 | 99.9 | 0.1 |  | 4.4 | 33.7 | 61.9 |  |

Table S11. Summary of the pairwise mean confusion statistics and associated $P$ values for isochronous ranked genealogies under different demographic models. The format of the table follows Table S3. The simulated distributions of ranked genealogies for the off-diagonal entries are the same as those considered in Figure 6 and Table S10. The diagonal entries represent the tests of true null cases, where we generated additional 1,000 random ranked genealogies per each demographic scenario.

|  | $(\mathrm{A}) \boldsymbol{d}_{\mathbf{1}}^{\boldsymbol{w}}$ |  |  |
| :--- | :---: | :---: | :---: |
|  | Uniform | Exponential | Logistic |
| Uniform | $0.4910,0.2565$ |  |  |
| Exponential | $0.0020,0.0001$ | $0.4870,0.1493$ |  |
| Logistic | $0.0005,0.0001$ | $0.0010,0.0001$ | $0.5015,0.5805$ |

(B) $d_{2}^{w}$

|  | Uniform | Exponential | Logistic |
| :--- | :---: | :---: | :---: |
| Uniform | $0.5010,0.6534$ |  |  |
| Exponential | $0.0015,0.0001$ | $0.4840,0.1144$ |  |
| Logistic | $0.0005,0.0001$ | $0.0005,0.0001$ | $0.5125,0.9081$ |

(C) $d_{\text {BHV-RG }}$

|  | Uniform | Exponential | Logistic |
| :--- | :---: | :---: | :---: |
| Uniform | $0.4990,0.4722$ |  |  |
| Exponential | $0.4995,0.5093$ | $0.5135,0.8979$ |  |
| Logistic | $0.4995,0.4875$ | $0.4995,0.5139$ | $0.5030,0.8152$ |

(D) $d_{\mathrm{KC}-\mathrm{RG}}$

|  | Uniform | Exponential | Logistic |
| :--- | :---: | :---: | :---: |
| Uniform | $0.4890,0.1819$ |  |  |
| Exponential | $0.1335,0.0001$ | $0.5070,0.8513$ |  |
| Logistic | $0.2220,0.0001$ | $0.1685,0.0001$ | $0.5060,0.7667$ |

Table S12. Comparison of metrics: human influenza A/H3N2 virus from different regions. We compare the performance of different distances on ranked genealogies according to how well they separate trees from human influenza $A$ virus from different regions. The format of the matrices follows Table S2. The simulation values and the color scheme of the $L_{2}$-medoids follow Figure 8 . The mean diagonal values are 99.9, 99.9, 28.9, and 65.6 for matrices (A)-(D), respectively.
(A)
NY - NY
NY - SEA
SEA - SEA
SEA - NY $\left[\begin{array}{cccc}\boldsymbol{\Delta} & \boldsymbol{d}_{1}^{w} & \boldsymbol{\Delta} & \boldsymbol{\Delta} \\ 99.8 & 0.2 & 0.0 & 0.0 \\ 0.1 & 99.9 & 0.0 & 0.0 \\ 0.0 & 0.0 & 100.0 & 0.0 \\ 0.0 & 0.0 & 0.1 & 99.9\end{array}\right]$
(B)

| $d_{2}^{w}$ |  |  |  | $L_{2}$-medoid |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| A | - | A | A |  |  |
| 99.8 | 0.2 | 0.0 | 0.0 | 4 | New York - New York |
| 0.1 | 99.9 | 0.0 | 0.0 | $\triangle$ | New York - Southeast Asia |
| 0.0 | 0.0 | 100.0 | 0.0 | 4 | Southeast Asia - Southeast Asia |
| 0.0 | 0.0 | 0.1 | 99.9 |  | Southeast Asia - New York |


| (C) | $d_{\text {BHV-RG }}$ |  |  |  | (D) | $d_{\text {KC-RG }}$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | A | - | A | - |  | A | - | A | - |
| NY - NY | 100.0 | 0.0 | 0.0 | 0.0 |  | 99.7 | 0.3 | 0.0 | 0.0 |
| NY - SEA | 98.7 | 0.1 | 1.2 | 0.0 |  | 46.8 | 38.2 | 11.6 | 3.4 |
| SEA - SEA | 84.6 | 0.2 | 15.2 | 0.0 |  | 0.0 | 0.8 | 99.1 | 0.1 |
| SEA - NY | 98.7 | 0.0 | 1.1 | 0.2 |  | 55.6 | 13.0 | 6.1 | 25.3 |

Table S13. Summary of the pairwise mean confusion statistics and associated $P$ values for heterochronous ranked genealogies sampled from two posterior distributions of human influenza A/H3N2 virus (NY-NY and SEA-SEA) and two sets of simulated trees (NY-SEA and SEANY). The format of the table follows Table S3. The simulated distributions of ranked genealogies for the off-diagonal entries are the same as those considered in Figure 8 and Table S12. The diagonal entries represent the tests of true null cases, where we generated additional 1,000 random ranked genealogies per each scenario.
(A) $d_{1}^{w}$

|  | NY - NY | NY - SEA | SEA - SEA | SEA - NY |
| :--- | :---: | :---: | :---: | :---: |
| NY - NY | $0.4985,0.7797$ |  |  |  |
| NY - SEA | $0.0015,0.0001$ | $0.4965,0.4107$ |  |  |
| SEA - SEA | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.4780,0.0365$ |  |
| SEA - NY | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0005,0.0001$ | $0.5030,0.6356$ |

(B) $d_{2}^{w}$

|  | NY - NY | NY - SEA | SEA - SEA | SEA - NY |
| :--- | :---: | :---: | :---: | :---: |
| NY - NY | $0.4925,0.3424$ |  |  |  |
| NY - SEA | $0.0015,0.0001$ | $0.5075,0.8267$ |  |  |
| SEA - SEA | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.4915,0.2798$ |  |
| SEA - NY | $0.0000,0.0001$ | $0.0000,0.0001$ | $0.0005,0.0001$ | $0.4850,0.1196$ |

(C) $d_{\text {BHV-RG }}$

|  | NY - NY | NY - SEA | SEA - SEA | SEA - NY |
| :--- | :---: | :---: | :---: | :---: |
| NY - NY | $0.4890,0.1764$ |  |  |  |
| NY - SEA | $0.4995,0.5242$ | $0.4720,0.0034$ |  |  |
| SEA - SEA | $0.4240,0.0001$ | $0.3025,0.0001$ | $0.5000,0.5256$ |  |
| SEA - NY | $0.4990,0.5154$ | $0.1435,0.0001$ | $0.4225,0.0001$ | $0.5005,0.5278$ |

(D) $d_{\mathrm{KC}-\mathrm{RG}}$

|  | NY - NY | NY - SEA | SEA - SEA | SEA - NY |
| :--- | :---: | :---: | :---: | :---: |
| NY - NY | $0.4820,0.0632$ |  |  |  |
| NY - SEA | $0.2395,0.0001$ | $0.4955,0.3624$ |  |  |
| SEA - SEA | $0.0005,0.0001$ | $0.0625,0.0001$ | $0.4860,0.1215$ |  |
| SEA - NY | $0.2810,0.0001$ | $0.2540,0.0001$ | $0.0355,0.0001$ | $0.5160,0.9560$ |

Table S14. The NCBI GenBank accession numbers for the HA sequences used in the analysis of human influenza A/H3N2 virus from different geographical regions.
(A) New York

| CY000001 | CY000017 | CY000025 | CY000057 | CY000177 | CY000065 | CY0000089 | CY000097 |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| CY000145 | CY000209 | CY000217 | CY000233 | CY000257 | CY000265 | CY000345 | CY000353 | CY000361 |
| CY000033 | CY000401 | CY000409 | CY000417 | CY000433 | CY000441 | CY0000489 | CY000545 |  |
| CY000753 | CY000761 | CY000777 | CY000873 | CY000769 | CY000933 | CY000941 | CY000965 |  |
| CY001088 | CY000049 | CY001072 |  |  |  |  |  |  |
| CY001317 | CY001333 | CY001325 | CY001061 | CY001293 | CY001045 | CY000137 | CY001237 | CY001144 |
| CY001640 | CY000073 | CY001736 | CY002032 | CY002072 | CY001301 |  |  |  |
| CY002240 | CY002264 | CY000865 | CY002424 | CY002408 | CY002416 | CY002456 | CY002472 | CY002488 |
| CY002480 | CY002504 | CY002608 | CY002712 | CY002720 | CY002728 | CY002736 | CY002784 | CY002776 |
| CY003056 | CY003096 | CY003104 | CY003120 | CY003144 | CY003160 | CY003168 | CY003192 | CY003112 |
| CY003040 | CY003344 | CY003424 | CY003656 | CY003777 | CY006115 | CY006147 | CY006291 | CY006371 |
| CY006435 | CY007643 | CY008884 | CY008868 | CY009260 | CY009244 | CY013805 | CY019165 | CY019173 |
| CY019189 | CY019253 | CY019285 | CY019293 | CY019811 | EF473618 | EF473619 | EF473625 | CY020533 |
| EU501484 | EU502299 | EU502307 | EU502310 | EU502316 |  |  | CY002248 |  |

(B) Southeast Asia

| DQ865945 | DQ865949 | DQ865951 | DQ865955 | DQ865957 | DQ865958 | DQ865959 | DQ865961 | DQ865962 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| DQ865970 | AB281195 | AB281200 | AB281205 | AB281210 | AB281215 | AB281232 | AB281235 | AB281238 |
| AB281241 | AB281244 | AB281247 | AB281250 | EF566141 | EF566142 | EF566155 | EF566164 | EF566173 |
| EF566176 | EF566224 | EF566227 | EF566229 | EF566332 | EF566361 | EF566362 | EF566365 |  |
| EF566053 | EF566067 | EF566068 | EF566074 | EU501124 | EU501125 | EU501126 | EU501127 |  |
| EU501168 | EU501171 | EU501172 | EU501174 | EU501176 | EU501177 | EU501221 | EU501279 |  |
| EU501283 | EU501308 | EU501312 | EU501317 | EU501318 | EU501319 | EU501320 | EU501321 |  |
| EU501373 | EU501374 | EU501375 | EU501385 | EU501441 | EU501458 | EU501459 | EU501460 |  |
| EU501462 | EU501463 | EU501464 | EU501465 | EU501466 | EU501467 | EU501474 | EU501531 |  |
| EU501542 | EU501544 | EU501545 | EU501546 | EU501547 | EU501548 | EU501558 | EU501622 |  |
| EU501774 | EU501787 | EU501788 | EU501789 | EU501790 | EU501791 | EU501792 | EU501793 |  |
| EU501800 | EU502344 | EU514639 | EU514653 | EU514654 | EU514667 | FJ229884 | FJ561060 |  |
| FJ865283 | FJ865284 | CY091149 | CY091157 | CY091165 | CY091229 | CY091245 | CY091253 |  |
| CY091437 | CY091445 | CY091453 | CY091469 | CY091485 |  | CY091261 |  |  |

Table S15. Summary of distortions. Comparison of distortion (Text 11A) using distance functions between ranked trees shapes and ranked genealogies.
(A) Comparison of distortions on ranked tree shapes. The simulated data used for computation are the same considered for Table S1

|  | $d_{1}$ | $d_{2}$ | $d_{\text {BHV-RTS }}$ | $d_{\text {KC-RTS }}$ | $d_{\text {CP-RTS }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Isochronous <br> ranked tree shapes <br> (beta splitting) | 5582.02 | 2369.98 | 8586.00 | 14331.64 | 27721.77 |
| Isochronous <br> ranked tree shapes <br> (alpha-beta splitting) | 3979.43 | 3028.30 | 10941.54 | 23989.64 | 5446.20 |
| Heterochronous <br> ranked tree shapes | 2343.93 | 2969.33 | 4553.04 | 12034.03 | - |

(B) Comparison of distortions on ranked genealogies. The simulated data used for computation are the same considered for Table S9.

|  | $d_{1}^{w}$ | $d_{2}^{w}$ | $d_{\text {BHV-RG }}$ | $d_{\text {KC-RG }}$ |
| :---: | :---: | :---: | :---: | :---: |
| Isochronous <br> ranked genealogies | 6751.44 | 1836.89 | 18569.28 | 13716.09 |
| Heterochronous <br> ranked genealogies | 13938.84 | 7196.04 | 16197.56 | 3368.99 |

Table S16. Summary of correlations. Comparison of correlation (Text 11B) between original distances and Euclidean distances in 2dimensional MDS comparisons.
(A) Comparison of correlations of original distances and Euclidean distances in two-dimensional MDS plots on ranked tree shapes. The simulated data used for computation are the same considered for Table S1.

|  | $d_{1}$ | $d_{2}$ | $d_{\text {BHV-RTS }}$ | $d_{\text {KC-RTS }}$ | $d_{\text {CP-RTS }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Isochronous <br> ranked tree shapes <br> (beta splitting) | 0.998 | 0.998 | 0.401 | 0.982 | 0.988 |
| Isochronous <br> ranked tree shapes <br> (alpha-beta splitting) | 0.998 | 0.999 | 0.648 | 0.518 | 0.909 |
| Heterochronous <br> ranked tree shapes | 0.984 | 0.986 | 0.634 | 0.734 | - |

(B) Comparison of correlations of original distances and Euclidean distances in two-dimensional MDS plots on ranked genealogies. The simulated data used for computation are the same considered for Table S9.

|  | $d_{1}^{w}$ | $d_{2}^{w}$ | $d_{\text {BHV-RG }}$ | $d_{\text {KC-RG }}$ |
| :---: | :---: | :---: | :---: | :---: |
| Isochronous <br> ranked genealogies | 0.981 | 0.954 | 0.527 | 0.946 |
| Heterochronous <br> ranked genealogies | 0.980 | 0.955 | 0.096 | 0.844 |

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