Extremes of the ℓ^∞-nearest ultrametric tropical polytope [Yu19]

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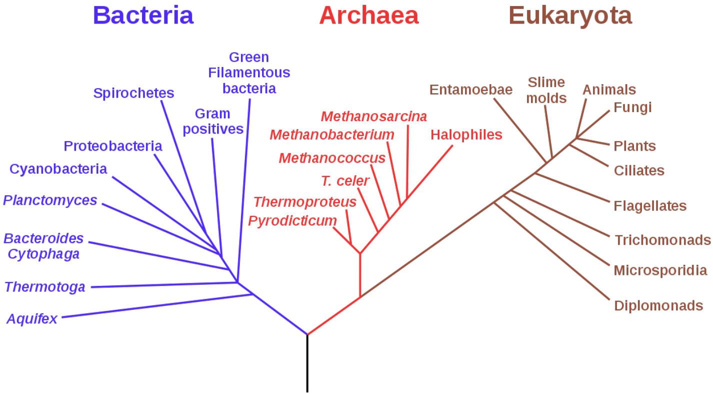
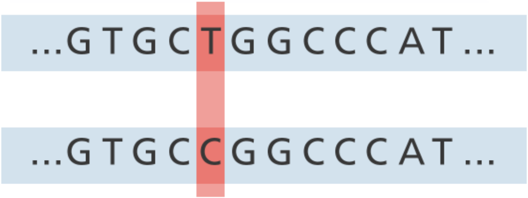
The Problem

A Phylogenetic tree encodes the evolutionary history.



The Problem

When constructing such a tree, we are usually given pair-wise distances among species (dissimilarity map).



In most cases, such distances does not correspond to a phylogenetic tree.

The Problem

- Naoko Takezaki and Masatoshi Nei. Genetic distances and reconstruction of phylogenetic trees from microsatellite dna. *Genetics*, 144(1):389-399, 1996.
- Korbinian Strimmer and Arndt Von Haeseler. Quartet puzzling: a quartet maximum-likelihood method for reconstructing tree topologies. Molecular biology and evolution, 13(7):964-969, 1996.
- Naruya Saitou and Masatoshi Nei. The neighbor-joining method: a new method for reconstructing phylogenetic trees. Molecular biology and evolution, 4(4):406-425, 1987.

The Problem

- These methods only give one or a part of the possible reconstruction.
- Goal: obtain all possible reconstructions in the ℓ^∞ sense.

The Problem

- These methods only give one or a part of the possible reconstruction.
- Goal: obtain all possible reconstructions in the ℓ^∞ sense.

Preliminary results by Bernstein:

Proposition (Ber18)

Let d be a dissimilarity map on a finite set X. The set of ultrametrics that are nearest to δ in the l^∞-norm is a tropical polytope.

- Bernstein also proposed a way to produce a set that is the superset of all the extremes of such polytope.
- My result: this set contains only the extremes when $|X| = 3$.

Tropical algebra

(max) tropical semiring $(\mathbb{R}_{\max}, \oplus, \odot)$.

- $\mathbb{R}_{\max} = \mathbb{R} \cup \{-\infty\}$;
- $x \oplus y = \max(x, y)$;
- $x \odot y = x + y$.

For $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d_{\max}$, their tropical inner product is

$$\boldsymbol{x} \cdot \boldsymbol{y} = \max_{1 \le i \le d} (x_i + y_i).$$

For $A \in \mathbb{R}^{n \times d}_{\max}$ and $\boldsymbol{x} \in \mathbb{R}^d_{\max}$, their tropical matrix-vector product is

$$A\boldsymbol{x} \in \mathbb{R}^n_{\max} \text{ and } (A\boldsymbol{x})_k = A_k \cdot x = \max_{1 \le i \le d} (A_{ki} + x_i).$$

Tropical halfspace

Definition (Tropical halfspace)

A tropical halfspace is defined by the inequality:

$$\{\boldsymbol{x} \in \mathbb{R}^d_{\max} | \boldsymbol{a} \cdot \boldsymbol{x} \leq \boldsymbol{b} \cdot \boldsymbol{x}\}, \quad a, b \in \mathbb{R}^d_{\max}.$$

Tropical cone

The following is the H-representation of a tropical cone.

Definition (Tropical cone)

A tropical cone $\mathcal{C}$ is the intersection of n halfspaces. Written as a system of inequalities:

$$A\boldsymbol{x} \leq B\boldsymbol{x}, \quad A, B \in \mathbb{R}_{\max}^{n\times d}.$$

Example:

$$\begin{aligned} x_3 &\leq x_1 + 2 \\ x_1 &\leq \max(x_2, x_3) \\ x_1 &\leq x_3 + 2 \\ x_3 &\leq \max(x_1, x_2 - 1) \end{aligned} \quad \begin{pmatrix} -\infty & -\infty & 0 \\ 0 & -\infty & -\infty \\ 0 & -\infty & -\infty \\ -\infty & -\infty & 0 \end{pmatrix} \boldsymbol{x} \leq \begin{pmatrix} 2 & -\infty & -\infty \\ -\infty & 0 & 0 \\ -\infty & -\infty & 2 \\ 0 & -1 & -\infty \end{pmatrix} \boldsymbol{x}$$

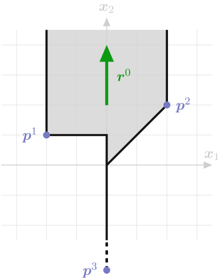
Tropical cone

The following is the V-representation of a tropical cone.

Definition (Generation of cone, extreme)

A finite set $G = \left(\boldsymbol{g}^i\right)_{i \in I} \subseteq \mathcal{C}$ of vectors is said to generate a cone $\mathcal{C}$ if $\forall \boldsymbol{x} \in \mathcal{C}$, $\boldsymbol{x} = \bigoplus_i \lambda_i \boldsymbol{g}^i, \lambda_i \in \mathbb{R}_{\max}$. The smallest such set is called the extremes of tropical cone.

Example:



$$\boldsymbol{p}_0 = (-\infty, 0, -\infty)$$

$$\boldsymbol{p}_1 = (-2, 1, 0)$$

$$\boldsymbol{p}_2 = (2, 2, 0)$$

$$\boldsymbol{p}_3 = (0, -\infty, 0)$$

Dissimilarity map

Let $X = \{x_1, \cdots, x_n\}$ be a finite set.

Definition (Dissimilarity map)

A dissimilarity map on X is a function $d : X \times X \to \mathbb{R}$. s.t. $d(x,x) = 0$ and $d(x,y) = d(y,x), \forall x, y \in X$. It can be expressed as a symmetric matrix with zero diagonal in $\mathbb{R}^{\binom{[n]}{2}}$.

Example:

$$d = \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 8 & 10 \\ 4 & 8 & 0 & 12 \\ 6 & 10 & 12 & 0 \end{pmatrix} \in \mathbb{R}^{\binom{[4]}{2}}$$

Distance

Definition (l^∞ distance)

Given two dissimilarity map d_1, d_2 on X with associated matrices D_1, D_2, define the l^∞ distance $\|d_1 - d_2\|_\infty$ to be the greatest entries in $|D_1 - D_2|$.

Example:

$$d_1 = \begin{pmatrix} 0 & 5 & 7 & 9 \\ 5 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}, d_2 = \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 8 & 10 \\ 4 & 8 & 0 & 12 \\ 6 & 10 & 12 & 0 \end{pmatrix}.$$

Then

$$\|d_1 - d_2\|_\infty = 3.$$

Rooted X-tree

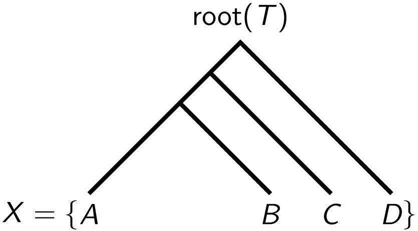
Definition (Rooted X-tree)

A rooted X-tree T is a tree with **leaf** set X and one interior vertex is designated as the root.

Notations:

- $\text{root}(T)$: the root of T;
- $\text{Des}_T(v)$ the descendants of vertex v in T;
- T°: the set of interior vertices of T.

Example:

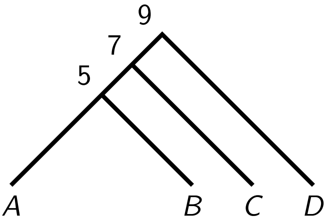


Definition (Weighting of X-tree)

Weighting of X-tree is the function $\alpha : T^\circ \to \mathbb{R}$ assigns values to each internal node of T.

The pair (T, α) induces a dissimilarity map $\delta_{T,\alpha}$ on X defined by $\delta_{T,\alpha}(x_i, x_j) = \alpha(v)$ where $v \in T^\circ$ is the vertex nearest to root(T) in the unique path from x_i to x_j.

Example:

$T, \alpha =$ 

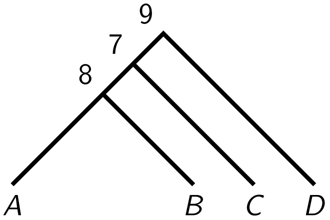
$$\delta_{T,\alpha} = \begin{pmatrix} 0 & 5 & 7 & 9 \\ 5 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

Rooted X-tree

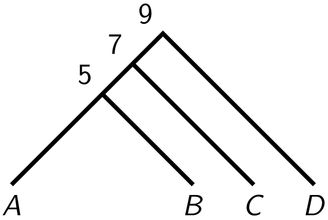
Definition (Compatibility of weighting)

α is compatible with T if $\alpha(u) \leq \alpha(v), \forall u \in \text{Des}_T(v)$.

Example:



Incompatible



Compatible

Ultrametric

Definition (Ultrametric)

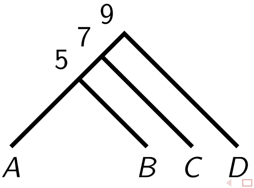
Given dissimilarity map δ on X, if $\exists\, X$-tree T and compatible α s.t. $\delta = \delta_{T,\alpha}$, δ is an ultrametric.

Example:

$$\delta = \begin{pmatrix} 0 & 5 & 7 & 9 \\ 5 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

is uniquely realized by the following tree and weighting

$T, \alpha =$



Ultrametric

Equivalent definition of ultrametric:

Definition (Ultrametric)

$\forall x_i, x_j, x_k \in X, \delta(x_i, x_k) \leq \max(\delta(x_i, x_j), \delta(x_j, x_k))$.

One reason to use ℓ^∞-norm.

Question

Proposition (Ber18)

Let d be a dissimilarity map on a finite set X. The set of ultrametrics that are nearest to δ in the l^∞-norm is a tropical polytope.

$$P(d) = \underset{\textit{ultrametric } \delta}{\operatorname{argmin}} \|\delta - d\|_\infty$$

Denote by $\mathcal{E}(d)$ the set of extremes of $P(d)$.
Can we find $\mathcal{E}(d)$?

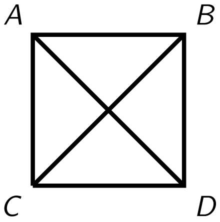
l^∞ nearest ultrametric

[CF00] gives an algorithm that computes **one** of the l^∞-nearest ultrametrics, called the maximal closest ultrametric to d, denoted by δ_m.

Example: find δ_m for

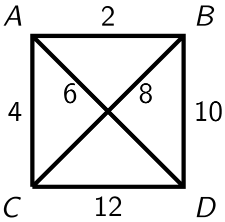
$$d = \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 8 & 10 \\ 4 & 8 & 0 & 12 \\ 6 & 10 & 12 & 0 \end{pmatrix}$$

Step 1: Draw the complete graph on vertex set $\{A, B, C, D\}$.



l^∞ nearest ultrametric

Step 2: Label the edge between x and y by $d(x, y)$.



Step 3: Define

$$d_u(x,y) = \min_{\text{path } P \text{ from } x \text{ to } y} \left(\max_{\text{edges } (i,j) \text{ of } P} d(i,j) \right) = \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 4 & 6 \\ 4 & 4 & 0 & 6 \\ 6 & 6 & 6 & 0 \end{pmatrix}$$

l^∞ nearest ultrametric

Step 4: Define

$$q = \|d_u - d\|_\infty = \left\| \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 4 & 6 \\ 4 & 4 & 0 & 6 \\ 6 & 6 & 6 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 8 & 10 \\ 4 & 8 & 0 & 12 \\ 6 & 10 & 12 & 0 \end{pmatrix} \right\|_\infty = 6$$

and let $\mathbf{1}$ be the ultrametric such that $\mathbf{1}(x, y) = 1, \forall x \neq y \in X$. Then

$$\delta_m = d_u + \frac{q}{2}\mathbf{1} = \begin{pmatrix} 0 & 5 & 7 & 9 \\ 5 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

is an ultrametric that is l^∞-nearset to d.

Bernstein's sliding-internal-node method

- $\delta_m \in P(d)$ but not necessarily $\delta_m \in \mathcal{E}(d)$;
- Start from δ_m, Bernstein's sliding-internal-node method gives $\mathcal{B}(d)$;
- $\mathcal{B}(d) \supseteq \mathcal{E}(d)$.

Mobility of nodes

Definition (Mobility)

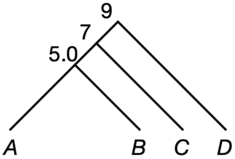
Let δ be a dissimilarity map on X and let u be an ultrametric that is closest to δ in the l^∞-norm. Let T be a resolution of the topology of u and let α be the internal nodes weighting s.t. $\delta_{T,\alpha} = u$. An internal node v of T is said to be *mobile* if there exists an ultrametric $\hat{u} \neq u$, expressible as $\hat{u} = \delta_{T,\hat{\alpha}}$ s.t.

- $\hat{u}$ is also nearest to δ in the l^∞-norm,
- $\hat{\alpha}(x) = \alpha(x), \forall x \in T^\circ, x \neq v$, and
- $\hat{\alpha}(v) \leq \alpha(v)$.

In this case, we say that $\hat{u}$ is obtained from u by sliding v down. If moreover v is no longer mobile in $\delta_{T,\hat{\alpha}}$, i.e., if $\hat{\alpha}(v) = \max\{\alpha(y) : y \in \mathrm{Des}_T(u)\}$, or $\hat{\alpha}(v)$ is the minimum value s.t. $\delta_{T,\hat{\alpha}}$ is nearest to δ in the l^∞-norm, then we say that $\hat{u}$ is obtained from u by *sliding v all the way down.*

Mobility of nodes

Example: sliding a mobile node

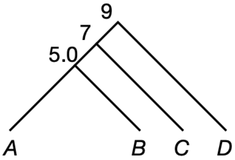


$$\begin{pmatrix} 0 & 5.0 & 7 & 9 \\ 5.0 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

$$\|\delta' - \delta\|_\infty = 3.$$

Mobility of nodes

Example: sliding a mobile node *all the way down*
Situation 1:

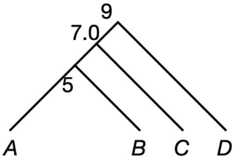


$$\begin{pmatrix} 0 & 5.0 & 7 & 9 \\ 5.0 & 0 & 7 & 9 \\ 7 & 7 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

$$\|\delta' - \delta\|_\infty = 3.$$

Mobility of nodes

Example: sliding a mobile node *all the way down*
Situation 2:

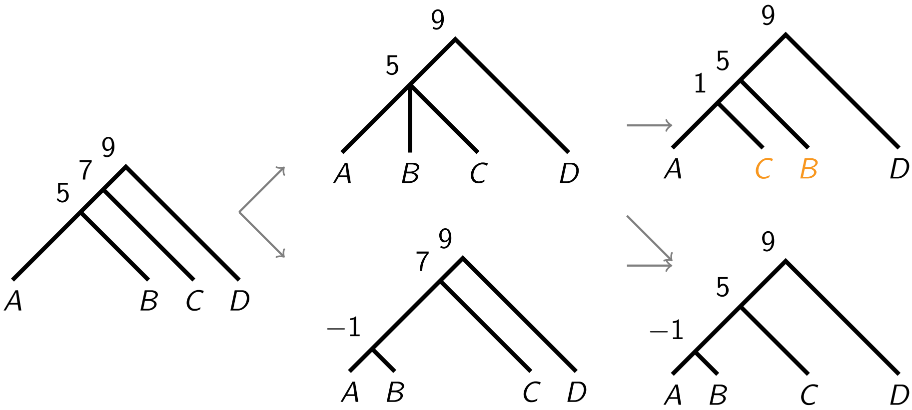


$$\begin{pmatrix} 0 & 5 & 7.0 & 9 \\ 5 & 0 & 7.0 & 9 \\ 7.0 & 7.0 & 0 & 9 \\ 9 & 9 & 9 & 0 \end{pmatrix}$$

$$\|\delta' - \delta\|_\infty = 3.$$

l^∞ nearest ultrametric

Example:



l^∞ nearest ultrametric

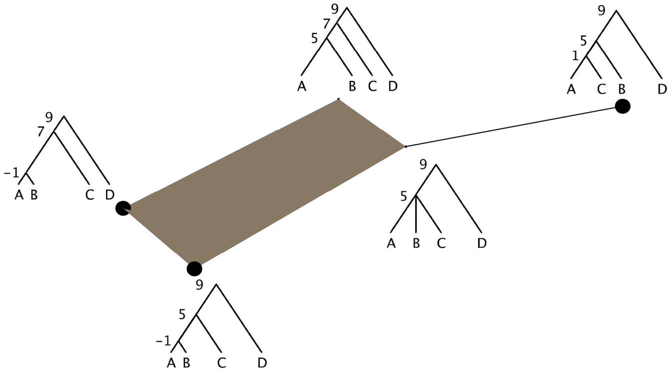
Theorem (Ber18)

Let δ be a dissimilarity map on X. Let $S_0 = \{\delta_m\}$, and for each $i \geq 1$ define S_i to be the set of ultrametrics obtained from some $u \in S_{i-1}$ by sliding a mobile internal node of a resolution of the topology of u all the way down. Then

- $\cup_i S_i$ *is a finite set, and*
- *the tropical convex hull of* $\cup_i S_i$ *is the set of ultrametrics* l^∞*-nearest to* δ*, and*
- *every vertex of this tropical polytope has at most one mobile internal node.*

l^∞ nearest ultrametric

$$d = \begin{pmatrix} 0 & 2 & 4 & 6 \\ 2 & 0 & 8 & 10 \\ 4 & 8 & 0 & 12 \\ 6 & 10 & 12 & 0 \end{pmatrix}$$



Main Theorem

Theorem (Yu19)

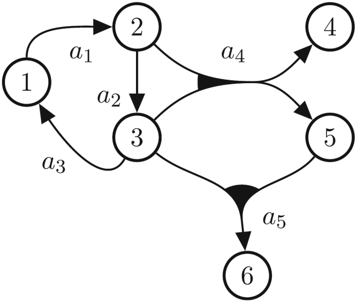
Let d be a dissimilarity map on X. Denote by $\mathcal{B}(d)$ the set generated by Bernstein's procedure and $\mathcal{E}(d)$ the set of extremes. Then $\mathcal{B}(d) = \mathcal{E}(d)$ when $|X| = 3$; $\mathcal{B}(d) \supsetneq \mathcal{E}(d)$ when $|X| \geq 4$.

Sketch of proof

- Enumerate all possible cases when $|X| = 3$;
- Inductively construct counterexamples when $|X| \geq 4$.

Characterization of extremes

A point in the tropical polytope corresponds to a directed hypergraph, called tangent directed hypergraph.
Example:



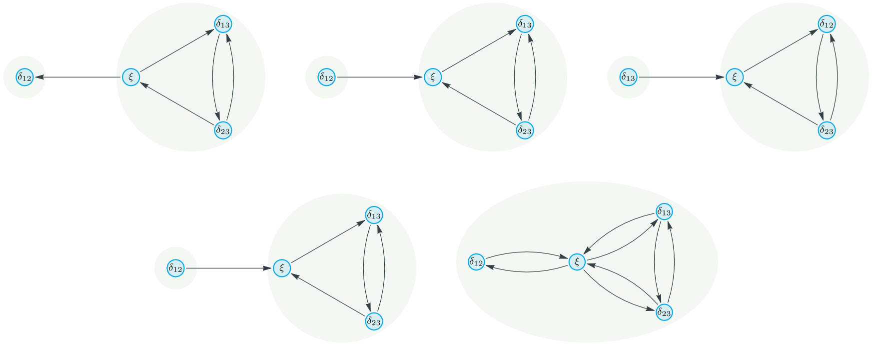
Characterization of extremes

Theorem (AGG10)

Let $\mathcal{C}$ be a tropical cone. A vector $\boldsymbol{v} \in \mathcal{C}$ is extreme iff. the set of the **strongly connected components** *of the tangent directed hypergraph at $\boldsymbol{v} \in \mathcal{C}$, partially ordered by the reachability relation, admits a greatest element.*

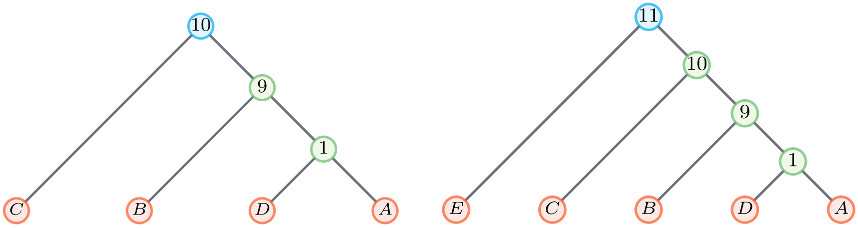
Sketch of proof

Enumerate all possible cases when $|X| = 3$



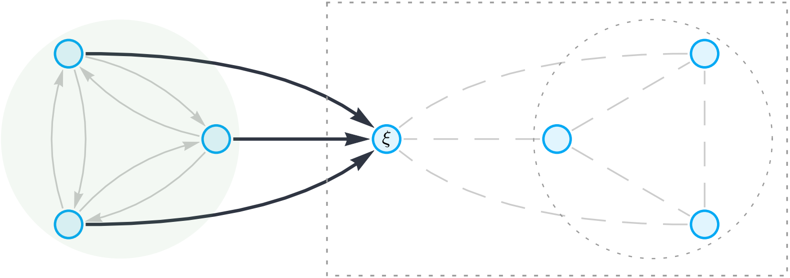
Sketch of proof

Inductively construct counterexamples when $|X| \geq 4$



Sketch of proof

Inductively construct counterexamples when $|X| \geq 4$



Extra n nodes (an SCC)

Original $\binom{n}{2} + 1$ nodes

(include the auxiliary variable node)

Further direction

- A direct method to generate all extremes based on enumerating the tangent hypergraphs.

References

1. L. Yu. Extreme rays of the ℓ^{∞}-nearest ultrametric tropical polytope. To appear on Linear Algebra and Appl.
2. S. Gaubert and R. Katz. The Minkowski theorem for max-plus convex sets. Linear Algebra and Appl., 421:356–369, (2007).
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Thank You!