Five equivalent ways to represent a phylogenetic tree

Jiayue Qi

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Doctoral Program Computational Mathematics
Numerical Analysis and Symbolic Computation

RISC RESEARCH INSTITUTE FOR SYMBOLIC COMPUTATION JKU JOHANNES KEPLER UNIVERSITY LINZ

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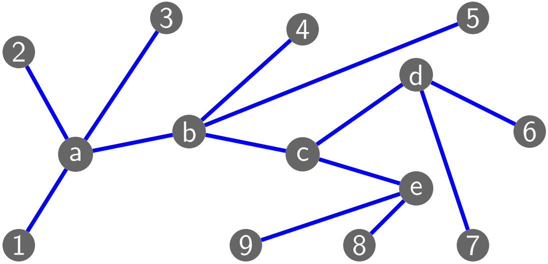
FWF Der Wissenschaftsfonds.

Five equivalent representations

- phylogenetic tree
- phylogenetic set of partitions
- phylogenetic set of cuts
- phylogenetic crossing relations
- phylogenetic equivalences of triples

Example: phylogenetic tree

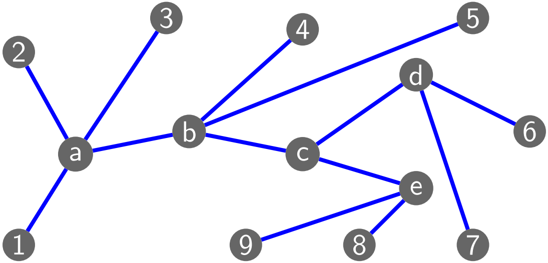


This is a phylogenetic tree with leaf set $N = \{1, 2, \cdots, 9\}$. The set of inner vertices is $V \setminus N = \{a, b, c, d, e\}$.

Definition: phylogenetic tree

- A **phylogenetic tree** with leaf set N is a tree (V, E) with no vertex of degree 2 such that $N \subset V$ is the set of leaves. We call the elements in N **labels** of the tree.
- Two phylogenetic trees are **isomorphic** iff there is a graph isomorphism between them which is the identity when restricted to the leaf set.
- In the last example, we can permute the inner vertices and obtain a phylogenetic tree that is isomorphic to the given one.

set of partitions



- For every inner vertex, we can collect the labels on each branch, respectively, forming a partion of set N.
- Then we obtain a set of partitions from the given phylogenetic tree.
- For the given tree, what partitions for N can we obtain?

running example: set of partitions

- $P = \{p_a, p_b, p_c, p_d, p_e\}$
- $p_a = \{\{1\}, \{2\}, \{3\}, \{4, 5, 6, 7, 8, 9\}\}$
- $p_b = \{\{1, 2, 3\}, \{4\}, \{5\}, \{6, 7, 8, 9\}\}$
- $p_c = \{\{1, 2, 3, 4, 5\}, \{6, 7\}, \{8, 9\}\}$
- $p_d = \{\{1, 2, 3, 4, 5, 8, 9\}, \{6\}, \{7\}\}$
- $p_e = \{\{1, 2, 3, 4, 5, 6, 7\}, \{8\}, \{9\}\}$

phylogenetic set of partitions

A set of partitions of N is **phylogenetic** iff it fulfills the following axioms:

- Each partition has at least 3 parts.
- Any cardinality-one subset of N belongs to a unique partition.
- Any subset of N belongs to at most one partition.
- For any subset $A \subset N$ that belongs to some partition, its complement $N \setminus A$ also belongs to some partition.

- Is P phylogenetic?
- Given a phylogenetic set of partitions, how to convert it back to a tree?

From partitions to tree

- VERTICES: Each partition is a vertex, each single-element set $\{x\}$ in the partition contributes to a leaf x attached to the vertex.
- EDGES: Draw an edge between vertex v_1 and v_2 iff $I \in v_1$ and $N \setminus I \in v_2$.
- From P, we can also try this method, see if we obtain a pylogenetic tree?
- Let's try it on the whiteboard.

From partitions to tree

- $P = \{p_a, p_b, p_c, p_d, p_e\}$
- $p_a = \{\{1\}, \{2\}, \{3\}, \{4, 5, 6, 7, 8, 9\}\}$
- $p_b = \{\{1, 2, 3\}, \{4\}, \{5\}, \{6, 7, 8, 9\}\}$
- $p_c = \{\{1, 2, 3, 4, 5\}, \{6, 7\}, \{8, 9\}\}$
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From partitions to tree

- The above mentioned two algorithms transfer between phylogenetic tree and phylogenetic set of partitions. Both compositions are the identity.
- These two representations are equivalent.

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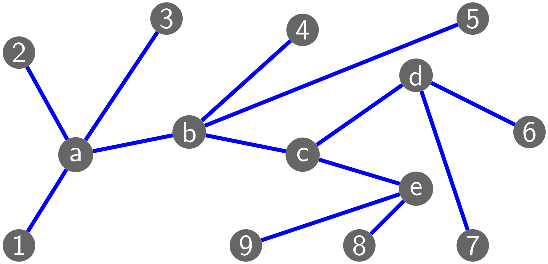
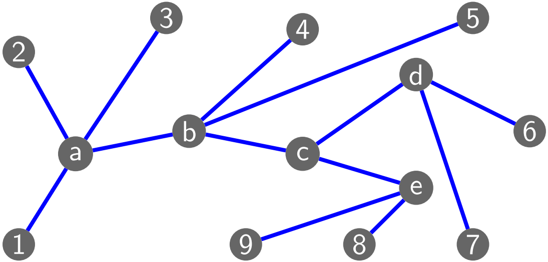
running example: set of cuts



- A **cut of** N is a partition of N into two subsets I, J such that cardinality of both I and J are bigger than one.
- Starting from a phylogenetic tree with leaf set N, for each inner edge, we can collect the labels on two sides of the edge respectively, forming a cut of N.
- Then we obtain a set of cuts.

running example: set of cuts



Let's see what we will obtain from this given tree!

running example: set of cuts

- C_{ab}: $\{\{1,2,3\},\{4,5,6,7,8,9\}\}$
- C_{bc}: $\{\{1,2,3,4,5\},\{6,7,8,9\}\}$
- C_{cd}: $\{\{1,2,3,4,5,8,9\},\{6,7\}\}$
- C_{ce}: $\{\{1,2,3,4,5,6,7\},\{8,9\}\}$
- We obtain the set $C = \{C_{ab}, C_{bc}, C_{cd}, C_{ce}\}$.
- We say that a set of cut C is **phylogenetic** iff for any two cuts $\{I_1, J_1\}$, $\{I_2, J_2\}$ in C, (at least) one of these four sets is empty: $I_1 \cap I_2$, $I_1 \cap J_2$, $J_1 \cap I_2$, $J_1 \cap J_2$.
- Is C in our running example phylogenetic?
- We have an algorithm converting from a phylogenetic set of cuts to a phylogenetic tree. Both compositions are the identity.
- These two representations are equivalent.

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Crossing relations

- A **crossing relation** is a set X of a pair of cardinality-two subsets of N. We denote as $(i, j \mid k, l)$ the element $\{\{i, j\}, \{k, l\}\}$ and we call it a **cross** of X.
- Starting from a set of cuts C, we can construct a crossing relation X_C as follows: $(i, j \mid k, l) \in X_C$ iff $i, j \in I$ and $k, l \in J$ for some cut $\{I, J\} \in C$.
- We say X is **phylogenetic** iff it fulfills the following axioms:

X1 If $(i, j \mid k, l) \in X$, $(i, k \mid j, l) \notin X$.

X2 If $(i, j \mid k, l), (i, j \mid k, m) \in X$ and $l \neq m$, then $(i, j \mid l, m) \in X$.

X3 If $(i, j \mid k, l) \in X$ and m is distinct from i, j, k, l, then $(i, j \mid k, m) \in X$ or $(i, m \mid k, l) \in X$. (Note that here "or" means at least one incident should happen.)

recall: phylogenetic set of cuts

- $C = \{C_{ab}, C_{bc}, C_{cd}, C_{ce}\}$.
- C_{ab}: $\{\{1, 2, 3\}, \{4, 5, 6, 7, 8, 9\}\}$
- C_{bc}: $\{\{1, 2, 3, 4, 5\}, \{6, 7, 8, 9\}\}$
- C_{cd}: $\{\{1, 2, 3, 4, 5, 8, 9\}, \{6, 7\}\}$
- C_{ce}: $\{\{1, 2, 3, 4, 5, 6, 7\}, \{8, 9\}\}$

running example: crossing relations

- Starting from the set of cuts C in our running example, we obtain a crossing relation X_C containing the following elements.
- $i, j \in \{1, 2, 3\}$ and $k, l \in \{4, 5, 6, 7, 8, 9\}$ (45 crosses);
- $i, j \in \{1, 2, 3, 4, 5\}$ and $k, l \in \{6, 7, 8, 9\}$ (60 crosses);
- $i, j \in \{1, 2, 3, 4, 5, 8, 9\}$ and $\{k, l\} = \{6, 7\}$ (21 crosses);
- $i, j \in \{1, 2, 3, 4, 5, 6, 7\}$ and $\{k, l\} = \{8, 9\}$ (21 crosses).
- We can check that X_C is a phylogenetic crossing relation.
- We also have an algorithm converting from phylogenetic crossing relation to a phylogenetic set of cuts. The two compositions are both the identity.
- These two representations are equivalent.

Five equivalent representations

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phylogenetic equivalent classes of triples

- A **triple** in N is a cardinality-three subset of N. We denote the set of all triples in N by $\binom{N}{3}$.
- We say an equivalence relation $\sim$ on $\binom{N}{3}$ is **phylogenetic** if the following two axioms are fulfilled.

E1 For any subset $Q \subseteq N$ of cardinality 4, either all 4 triples in $\binom{Q}{3}$ are equivalent, or there are two equivalence classes, each containing two triples of $\binom{Q}{3}$.

E2 If i, j, k, l, m are pairwise distinct, and $\{i, j, k\} \sim \{i, j, l\}$, then $\{i, j, k\} \sim \{i, j, m\}$ or $\{i, k, l\} \sim \{m, k, l\}$.

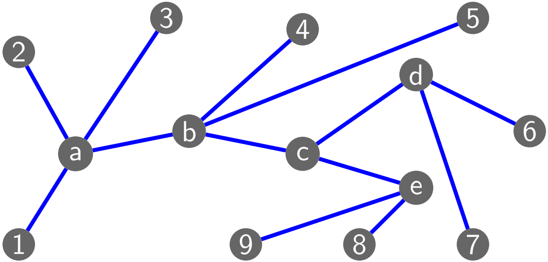
example: equivalences of triples

- Let $N = \{1, 2, 3, 4, 5\}$. We define an equivalence relation E with three distinct classes as follows:
- $\{1, 2, 3\} \sim \{1, 2, 4\} \sim \{1, 2, 5\}$
- $\{1, 4, 5\} \sim \{2, 4, 5\} \sim \{3, 4, 5\}$
- $\{1, 3, 4\} \sim \{1, 3, 5\} \sim \{2, 3, 4\} \sim \{2, 3, 5\}$
- We can check that it is phylogenetic.
- Starting from a phylogenetic equivalence relation E of triples in $\binom{N}{3}$, we can construct a crossing relation on N X_E as follows.
- Cross $(i, j \mid k, l) \in X_E$ iff $\{i, j, k\} \sim \{i, j, l\} \not\sim \{i, k, l\} \sim \{j, k, l\}$.
- Continue with the above example, we obtain a crossing relation containing the following elements:

from crossing relation to equivalences of triples

- $(1,2 \mid 3,4), (1,2 \mid 3,5), (1,2 \mid 4,5), (1,3 \mid 4,5), (2,3 \mid 4,5)$.
- We can check that it is phylogenetic.
- Starting from a phylogenetic crossing relation X in N, we can define equivalences of triples E_X on $\binom{N}{3}$ as follows.
- First, define a relation R_X on $\binom{N}{3}$ as follows: $(t_1, t_2) \in R_X$ iff $t_1 = t_2$ or $\mid t_1 \cap t_2 \mid = 2$ and – say $t_1 = \{i,j,k\}$, $t_2 = \{i,j,l\}$ – neither $ik \mid jl$ nor $il \mid jk$ is in X.
- E_X is defined to be the transitive closure of R_X.
- Starting from a phylogenetic crossing relation, via the above construction, we actually will obtain a phylogenetic equivalences of triples.
- Composition of the two transformations are both the identity.
- These two representations are equivalent.

more comments?



From set of partitions to equivalences of triples.

Five equivalent representations ?

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meta-level overview

- Edges? Vertices?
- Macro level? Micro level?
- macro level + focusing on edges $\Longrightarrow$ set of cuts. (Each cut corresponds to an edge.)
- micro level + focusing on edges $\Longrightarrow$ crossing relation.
- macro level + focusing on vertices $\Longrightarrow$ set of partitions. Each partition corresponds to a vertex.
- micro level + focusing on vertices $\Longrightarrow$ equivalent classes of triples. Each class corresponds to a vertex.

Thank You