

# Combinatorial Aspects of Tropical Geometry and its interactions with phylogenetics

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# What is tropical geometry?

- Trop. semiring  $\overline{\mathbb{R}}_{\text{tr}} := (\mathbb{R} \cup \{-\infty\}, \oplus, \odot)$ ,  $a \oplus b = \max\{a, b\}$ ,  $a \odot b = a + b$ .
- Fix  $K = \mathbb{C}\{\{t\}\}$  field of Puiseux series, with **valuation** given by **lowest exponent**, e.g.  $\text{val}(t^{-4/3} + 1 + t + \dots) = -4/3$ ,  $\text{val}(0) = \infty$ .

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$$F(\mathbf{x}) \text{ in } K[x_1^{\pm}, \dots, x_n^{\pm}] \rightsquigarrow \text{Trop}(F)(\boldsymbol{\omega}) \text{ in } \overline{\mathbb{R}}_{\text{tr}}[\omega_1^{\odot \pm}, \dots, \omega_n^{\odot \pm}]$$

$$F := \sum_{\alpha} c_{\alpha} \mathbf{x}^{\alpha} \mapsto \text{Trop}(F)(\boldsymbol{\omega}) := \bigoplus_{\alpha} -\text{val}(c_{\alpha}) \odot \boldsymbol{\omega}^{\odot \alpha} = \max_{\alpha} \{-\text{val}(c_{\alpha}) + \langle \alpha, \boldsymbol{\omega} \rangle\}$$

$$(F = 0) \text{ in } (K^*)^n \rightsquigarrow \text{Trop}(F) = \{\boldsymbol{\omega} \in \mathbb{R}^n : \max \text{ in } \text{Trop}(F)(\boldsymbol{\omega}) \text{ is } \underline{\text{not}} \text{ unique}\}$$

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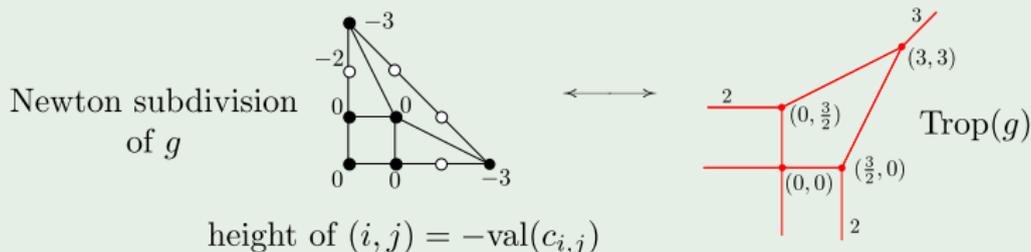
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**Example:**  $g = -t^3 x^3 + t^3 y^3 + t^2 y^2 + (4 + t^5)xy + 2x + 7y + (1 + t)$ .



Tropical Geometry is a **combinatorial shadow** of algebraic geometry

**Input:**  $X \subset (K^*)^n$  irred. of dim  $d$  defined by an ideal  $I \subset K[x_1^\pm, \dots, x_n^\pm]$ .

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- $\text{Trop}(I)$  is a polyhedral complex of *pure* dim.  $d$  & connected in codim. 1.
- **Gröbner theory:**  $\text{Trop}(I) = \{\omega \in \mathbb{R}^n \mid \text{in}_\omega(I) \neq 1\}$ .

Weight of  $\omega \in \text{mxl}$  cone =  $\#\{\text{components of } \text{in}_\omega(I)\}$  (with mult.)

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•  $(K^*)^r$  action on  $X$  via  $A \in \mathbb{Z}^{r \times n} \rightsquigarrow$  Row span  $(A)$  in all cones of  $\text{Trop}(I)$ .  
 $\rightsquigarrow$  Mod. out  $\text{Trop}(I)$  by this **lineality space** preserves the combinatorics.

• The **ends** of a curve  $\text{Trop}(X)$  in  $\mathbb{R}^2$  give a compact toric variety  $\supset \overline{X}$ .

**Conclusion:**  $\text{Trop}(I)$  sees dimension, torus actions, initial degenerations, compactifications and other *geometric invariants* of  $X$  (e.g. degree)

**Notice:**  $\text{Trop}(X)$  is highly sensitive to the embedding of  $X$ .

# Grassmannian of lines in $\mathbb{P}^{n-1}$ and the space of trees

**Definition:**  $\text{Gr}(2, n) = \{\text{lines in } \mathbb{P}^{n-1}\} := K_{\text{rk } 2}^{2 \times n} / \text{GL}_2$  (dim =  $2(n-2)$ ).

The **Plücker map** embeds  $\text{Gr}(2, n) \hookrightarrow \mathbb{P}^{\binom{n}{2}-1}$  by the list of  $2 \times 2$ -minors:

$$\varphi(X) = [p_{ij} := \det(X^{(i,j)})]_{i < j} \quad \forall X \in K^{2 \times n}.$$

Its Plücker ideal  $I_{2,n}$  is generated by the 3-term (quadratic) **Plücker eqns**:

$$p_{ij}p_{kl} - p_{ik}p_{jl} + p_{il}p_{jk} \quad (1 \leq i < j < k < l \leq n).$$

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$\rightsquigarrow$  **Tropical Plücker eqns:**  $\max\{x_{ij} + x_{kl}, x_{ik} + x_{jl}, x_{il} + x_{jk}\}$ .

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## Theorem (Speyer-Sturmfels)

The tropical Grassmannian  $\text{Trop}(\text{Gr}(2, n) \cap ((K^*)^{\binom{n}{2}} / K^*))$  in  $\mathbb{R}^{\binom{n}{2}} / \mathbb{R} \cdot \mathbf{1}$  is the **space of phylogenetic trees** on  $n$  leaves:

- all leaves are labeled 1 through  $n$  (no repetitions);
- weights on all edges (non-negative weights for internal edges).

It is cut out by the tropical Plücker equations. The lineality space is generated by the  $n$  cut-metrics  $\ell_i = \sum_{j \neq i} e_{ij}$ , modulo  $\mathbb{R} \cdot \mathbf{1}$ .

# The space of phylogenetic trees $\mathcal{T}_n$ on $n$ leaves

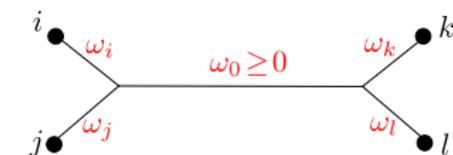
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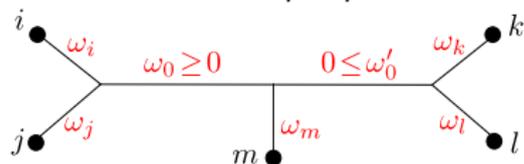
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$$\begin{cases} x_{ij} = \omega_i + \omega_j, \\ x_{ik} = \omega_i + \omega_0 + \omega_k, \dots \end{cases}$$

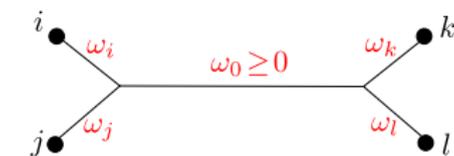


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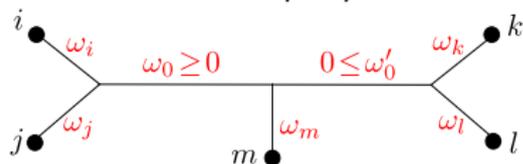
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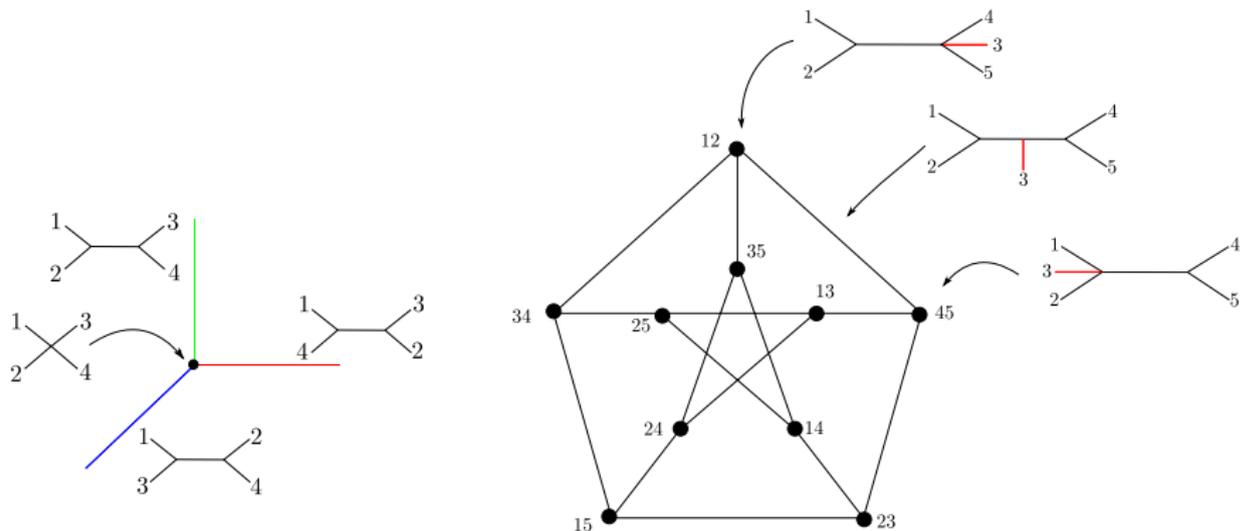
**Claim:**  $(T, \omega) \xleftrightarrow{1\text{-to-1}} \mathbf{x}$  satisfying Tropical Plücker eqns.

**Why?** (1)  $\max\{x_{ij} + x_{kl}, \underline{x_{ik} + x_{jl}}, \underline{x_{il} + x_{jk}}\} \iff$  quartet  $(ij|kl)$ .

(2) tree  $T$  is reconstructed from the list of quartets,

(3) linear algebra recovers the weight function  $\omega$  from  $T$  and  $\mathbf{x}$ .

## Examples:



$\mathcal{T}_4/\mathbb{R}^3$  has  $f$ -vector  $(1, 3)$ .  $\mathcal{T}_5/\mathbb{R}^4$  is the cone over the Petersen graph.  
 $f$ -vector =  $(1, 10, 15)$ .

$$\dim \text{Gr}(2, n) = \dim(\text{Trop}(\text{Gr}(2, n)) \cap \mathbb{R}^{\binom{n}{2}-1}) = 2(n-2).$$

# Constructing nice coordinates for $\text{Gr}(2, n)$ from tree space

- We **stratify** the classical Grassmannian by collecting points according to the vanishing of prescribed coordinates:

$$\text{Gr}_J(2, n) = \{\mathbf{p} \in \mathbb{P}^{\binom{n}{2}-1} : \mathbf{p}_{kl} = 0 \iff kl \in J\} \quad \text{for } J \in \binom{[n]}{2}.$$

**Example:** For  $J = \emptyset$  we get  $\text{Gr}_\emptyset(2, n) = \text{Gr}(2, n) \cap ((K^*)^{\binom{n}{2}}/K^*)$ .

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**Remark:** Most  $J$  will give  $\text{Gr}_J(2, n) = \emptyset$ . Meaningful  $J$ 's determine  $m$  blocks (of the rank-2 matrix in  $K^{2 \times n}$ ) of maximal linear independent columns and a (possibly empty) block of  $(0, 0)$  columns:

$$\text{Gr}_J(2, n) \ni \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \end{pmatrix} \equiv ( B_1 \mid \cdots \mid B_n \mid \mathbf{0} \ \cdots \ \mathbf{0} )$$

We identify it with a point in  $\text{Gr}_{\emptyset}(2, m)$  (pick one column per block!).

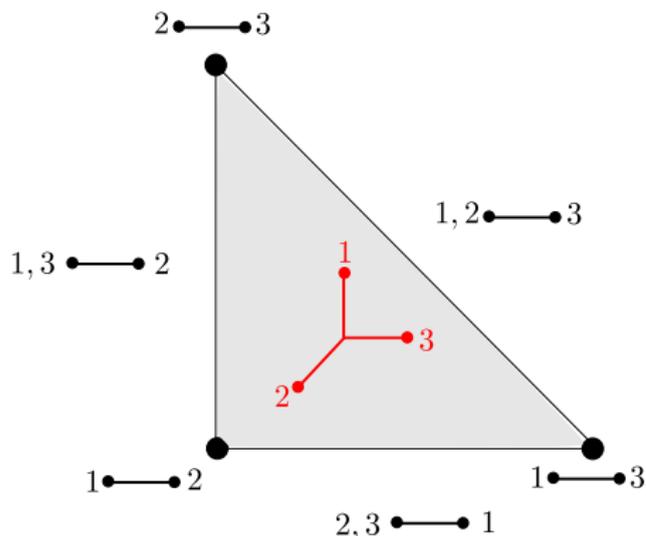
**Proposition [C.]:**  $\text{Trop}(\text{Gr}_J(2, n)) = \mathcal{T}_m$  with leaves labeled by  $B_1, \dots, B_m$ .

# How to compactify $\mathcal{T}_n$ ?

- Write  $\mathbb{TP}^{\binom{n}{2}-1} := (\mathbb{R} \cup \{-\infty\})^{\binom{n}{2}} \setminus (-\infty, \dots, -\infty) / \mathbb{R} \cdot (1, \dots, 1)$
- Compactify  $\mathcal{T}_n$  using  $\text{Trop}(\text{Gr}(2, n)) \subset \mathbb{TP}^{\binom{n}{2}-1}$ .
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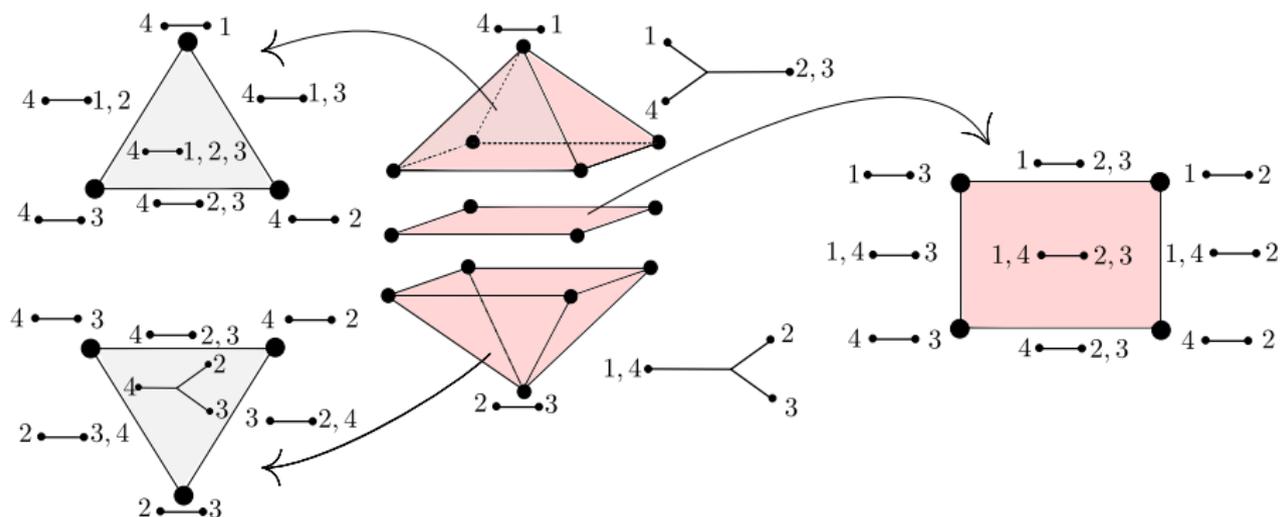
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Boundary cells in  $\overline{(14|23)} = \overline{\begin{array}{c} 1 \\ \diagdown \quad \diagup \\ 4 \quad 3 \end{array}} = \begin{array}{c} 1 \\ \diagdown \quad \diagup \\ 4 \quad 3 \end{array}$

# Choosing coordinates for $\text{Gr}(2, n)$ : from tropical to classical

Write:  $\text{Gr}(2, n) = \bigcup_{i < j} U_{ij}$ , where  $U_{ij} = \{p \in \text{Gr}(2, n) : p_{ij} \neq 0\}$ .

Can fix  $p_{ij} = 1$ , so

$$\text{Trop}(U_{ij}) = \{x \in \text{Trop}(\text{Gr}(2, n)) : x_{ij} = 0\} \in \overline{\mathbb{R}}^{\binom{n}{2}-1}.$$

Now change coordinates to  $u_{kl} := p_{kl}/p_{ij}$  for  $kl \neq ij$ . The **Plücker eqns**

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yield the dependency  $u_{kl} = u_{ik}u_{jl} - u_{il}u_{jk}$ .

**Conclusion:** We parameterize  $U_{ij}$  by the  $2(n-2)$  coordinates

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**BIG ISSUE:** these coordinates are not well adapted to the tree space.

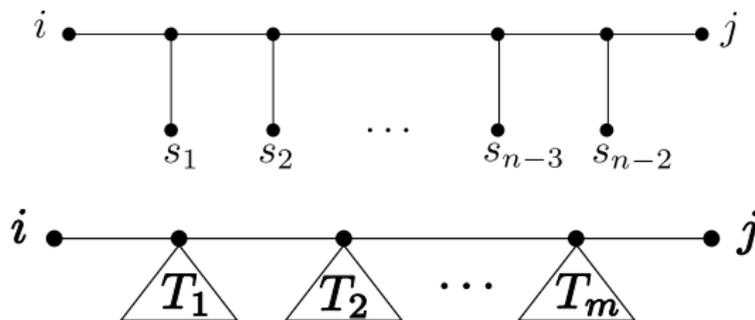
- We view  $\text{Trop}(\text{Gr}(2, n)) = \bigcup_{T \in \mathcal{T}_n} \overline{\mathcal{C}_T}$  inside  $\mathbb{T}^{\binom{n}{2}-1}$ .

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For each valid  $J$ , we pick  $ij \notin J$  and view each tree in “caterpillar form”



**Figure:** From left to right: the caterpillar tree on  $n$  leaves with endpoint leaves  $i$  and  $j$ , and the path from leaf  $i$  to  $j$  on a tree arranged in caterpillar-like form. The labeled triangles indicate subtrees of the original tree. The backbone of the caterpillar tree is the chain graph with  $m + 2$  nodes given by the horizontal path from  $i$  to  $j$ . The trees  $T_1, \dots, T_m$  need not be trivalent.

**GOAL:** Adapt our choice of  $2(n-2)$  coords.  $I \in \binom{[n]}{2}$  for  $U_{ij} \subset \text{Gr}_J(2, n)$

to:

- (1) the indexing pair  $ij$ ,
- (2) the tree  $T$  and,
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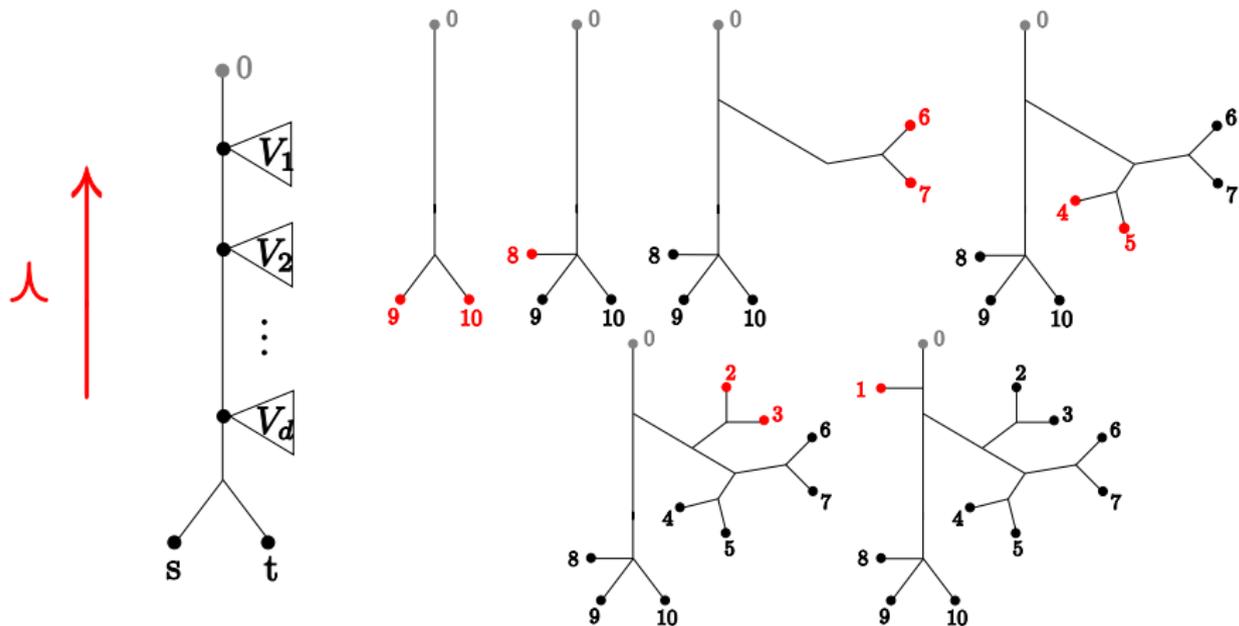
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We do so by first constructing a suitable partial order  $\preceq$  on  $[n] \setminus \{i, j\}$ :

## Definition

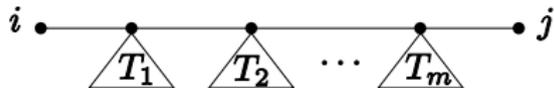
Let  $i, j$  be a pair of indices, and let  $\preceq$  be a partial order on the set  $[n] \setminus \{i, j\}$ . Let  $T$  be a tree on  $n$  leaves arranged in caterpillar form with backbone  $i-j$ . We say that  $\preceq$  has the *cherry property on  $T$*  with respect to  $i$  and  $j$  if the following conditions hold:

- (i) Two leaves of different subtrees  $T_a$  and  $T_b$  can't be compared by  $\preceq$ .
- (ii) The partial order  $\preceq$  restricts to a total order on the leaf set of each  $T_a$ ,  $a = 1, \dots, m$ .
- (iii) If  $k \prec l \prec v$ , then either  $\{k, l\}$  or  $\{l, v\}$  is a cherry of the quartet  $\{i, k, l, v\}$  (and hence also of  $\{j, k, l, v\}$ ).



**Figure:** Inductive definition of the order  $\preceq_a$  on the leaves of the subtree  $T_a$  ( $s \prec_a t$ ,  $t$  is maximal) by example. We add one leaf or one cherry at a time so that the corresponding new leaf or leaves are smaller than the previous ones in the order  $\preceq_a$ . When adding a cherry, we arbitrarily order its two leaves as well. The grey dot with label 0 in  $T_a$  is internal in  $T$ . Broken leaf edges, such as the one in the third tree from the left, should be thought of as straight edges. The edge adjacent to the grey node with label 0 could be contracted.

- Fix two indices  $\{i, j\}$ , a “caterpillar like” tree  $T$  with backbone  $i-j$ , and a vanishing set  $J$ . Fix a partial order  $\preceq$  on  $[n] \setminus \{i, j\}$  having the cherry property on  $T$ . Let  $I \subset \binom{[n]}{2}$  be a set of size  $2(n-2)$  not containing  $ij$ .



- $J(ij) := J \cap \{ik, jk : k \neq i, j\}$ , and

## Definition

We say that  $I$  is *compatible with  $\preceq$  and  $J(ij)$*  if for each index  $a = 1, \dots, m$  and each leaf  $k \in T_a$ , exactly one of the following condition holds:

- $ik$  and  $jk \in I$ , and for all  $l \prec k$  we have  $il$  or  $jl \in J(ij)$ ; or
- $ik \notin I$ ,  $jl \in I$  for all  $l \in T_a$ , and there exists  $t \prec k$  in  $T_a$  where  $it, jt \notin J(ij)$ . If  $t$  is the maximal element with this property, then  $kt \in I$ ; or
- $jk \notin I$ ,  $il \in I$  for all  $l \in T_a$  and there exists  $t \prec k$  in  $T_a$  where  $it, jt \notin J(ij)$ . If  $t$  is the maximal element with this property, then  $kt \in I$ .

**Theorem [C.-Häbich-Werner]:** The coordinates  $I$  are well adapted as liftings of points from  $\mathcal{C}_T \cap \text{Trop}(\text{Gr}_J(2, n))$  to  $\text{Gr}_J(2, n)$ .

**Why pick these compatibility properties?** Fix  $T$  as in the figure. For each  $a = 1, 2, 3$ , we let  $l_a := \{kl \in I : k \text{ or } l \in T_a\}$ . Thus,  $I = l_1 \sqcup l_2 \sqcup l_3$ .

- $|T_1| = 1$ , so  $l_1 = \{i1, j1\}$  independently of  $J$ .
- If  $i2$  or  $j2 \in J$ , then  $l_3 = \{i2, j2, i3, j3\}$  in agreement with condition (i).

On the contrary, if  $i2, j2 \notin J$  then we can choose between

$l_3 = \{i2, j2, j3, 32\}$  (since (ii) is satisfied) or  $l_3 = \{i2, j2, i3, 32\}$  (by (iii)).

- Choice of  $l_2$ , depends on  $J_2(ij) := \{ik \in J : k \in T_2\} \cup \{jk \in J : k \in T_2\}$ .

**Example 1:** If  $\emptyset \neq J_2(ij) \subseteq \{i4, j4\}$ , then we can take either

$l_2 = \{i4, j4, i5, j5, i6, 65, i7, 76\}$  or  $l_2 = \{i4, j4, i5, j5, j6, 65, j7, 76\}$ .

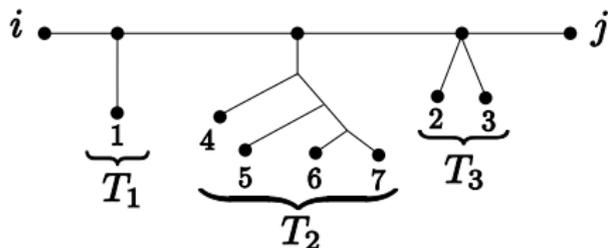
Notice that in both cases  $i5, j5 \in l_2$  by condition (i).

**Example 2:** If  $\emptyset \neq J_2(ij) \subseteq \{i7, j7\}$ , we can take either

$l_2 = \{i4, j4, i5, 54, i6, 65, i7, 76\}$  or  $l_2 = \{i4, j4, j5, 54, j6, 65, j7, 76\}$ .

**Example 3:** Finally, assume  $J_2(ij) = \{j5, j6\}$ . Then, we may choose

$l_2 = \{i4, j4, i5, 54, i6, 64, i7, 74\}$  or  $l_2 = \{i4, j4, j5, 54, j6, 64, j7, 74\}$ .



- $i = 1, j = 2$ ,

- $\prec$  is the natural order on  $\{3, \dots, 7\}$ .

## Example: Coordinate changes when $n = 4$ and $i = 1, j = 2$ .

- If  $T$  is the quartet  $(13|24)$  or  $(14|23)$ , we pick our coordinates to be  $u_{13}, u_{23}, u_{14}, u_{24}$ . We derive the value of  $u_{34}$  from  $u_{34} = u_{13}u_{24} - u_{14}u_{23}$ .
- If  $T$  is the quartet  $(12|34)$ , then the choice of coordinates depends on  $J$ . We choose the order  $3 \prec 4$ :

(1) If  $13, 23 \notin J$ , we take  $I = \{13, 23, 34, 14\}$ . The expression for  $u_{24}$  is

$$u_{24} = u_{13}^{-1}(u_{34} + u_{14}u_{23})$$

**Note:** we must have  $u_{13} \neq 0$  (this follows from  $13 \notin J$ ).

(2) If  $13$  or  $23 \in J$ , then  $I = \{13, 23, 14, 24\}$  and  $u_{34} = u_{13}u_{24} - u_{14}u_{23}$ .

### References:

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