

Understanding graphs locally

Annie Raymond

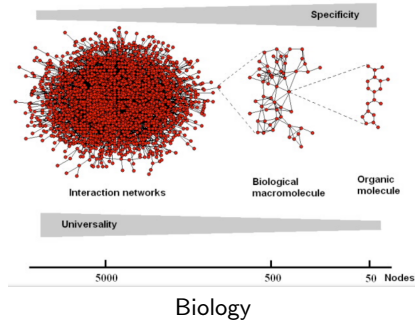
(different parts joint with Greg Blekherman,
James Saunderson, Mohit Singh,
Rekha Thomas and Fan Wei)

University of Massachusetts, Amherst

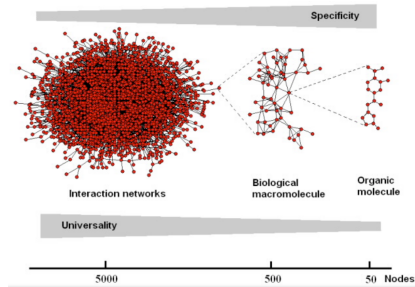
March 30, 2023

Large graphs are everywhere!

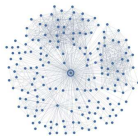
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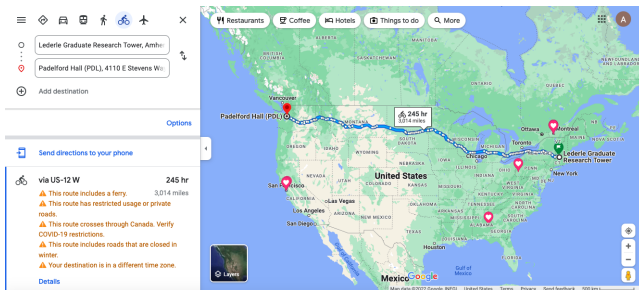
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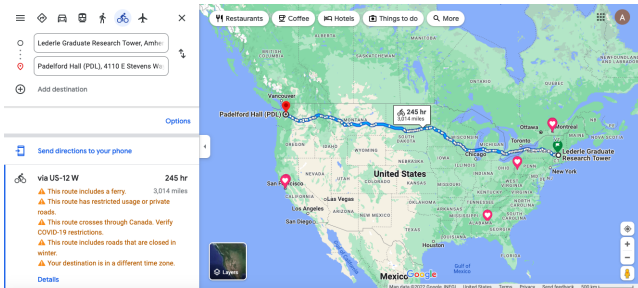
Biology



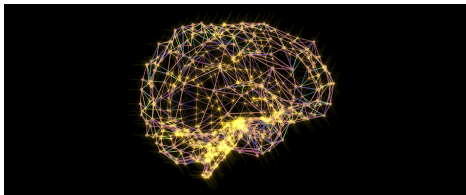
Facebook graph



Google Maps



Google Maps



Alfred Pasieka/Science Photo Library/Getty Images

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How can we understand such large graphs?

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Idea: understand the graph locally

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This raises immediately two questions:

- 1 How do global and local properties relate?
- 2 What is even possible locally? → graph profiles!

How shall we count today?

The **number of homomorphisms** from a graph H to a graph G is $\text{hom}(H; G)$ = number of maps from $V(H)$ to $V(G)$ that yield a graph homomorphism, i.e., that map every edge of H to an edge of G .

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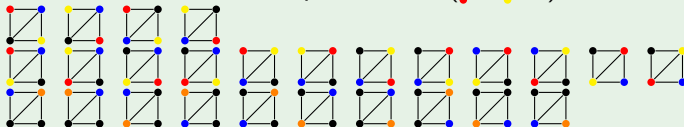
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Let $G =$ ,

- the number of homomorphisms $\text{hom}(\text{path of length 2}; G) = 26$,




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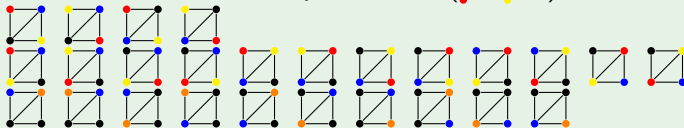
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- the homomorphism density $t(\text{path}_3; G) = \frac{26}{64}$

Graph profiles

Let $\mathcal{U} = \{H_1, H_2, \dots, H_l\}$. The (homomorphism) density profile of \mathcal{U} is

$$\mathcal{D}_{\mathcal{U}} := \text{cl}(\{(t(H_1; G), \dots, t(H_l; G)) \mid G \text{ is a graph}\})$$

and the (homomorphism) number profile of \mathcal{U} is

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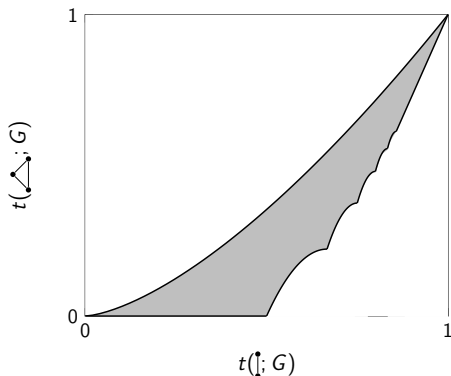
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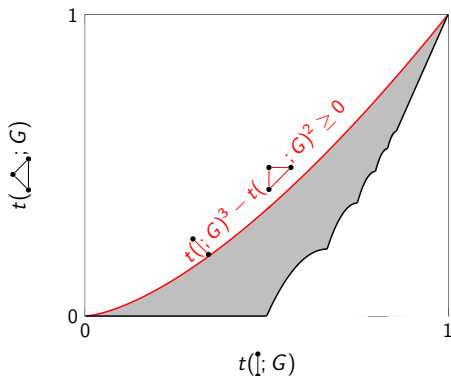
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Different techniques to certify graph inequalities

- Integer programming
- Hölder's inequality
- Entropy method
- Lagrangian method
- Cauchy-Schwarz/sums of squares
- ...

Integer programming example

Theorem (R., 2014)

The Turán inequality $t(\cdot; G) \leq 1 - \frac{1}{r-1}$ for all graphs G such that $t(K_r; G) = 0$ can be proven by studying

$$\max \sum_{e \in E(K_n)} x_e$$

$$\text{such that } \sum_{e \in E(Q)} x_e \leq \binom{r}{2} - 1 \text{ for all cliques } Q \text{ of size } r \text{ in } K_n,$$

$$x_e \in \{0, 1\} \text{ for all } e \in E(K_n).$$

Tools to certify graph inequalities with sos

- Restrict to maps that send labelled vertices to specific vertices of G

$$t \left(\begin{array}{c} \text{graph with 3 vertices labeled 2, 1, and 1} \\ \text{graph with 6 vertices labeled 3, 5, 4, 1, 2, and 6} \end{array} ; \right) = \frac{3}{6}$$

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- Symmetrization=unlabeling

$$\begin{aligned} [[t(\begin{array}{c} \text{2} \quad \bullet \quad \text{1} \\ \diagup \quad \diagdown \\ \bullet \end{array} ; G)]] &:= \frac{1}{|V(G)|^2} \sum_{1 \leq i, j \leq |V(G)|} t(\begin{array}{c} \text{j} \quad \bullet \quad \text{i} \\ \diagup \quad \diagdown \\ \bullet \end{array} ; G) \\ &= t(\begin{array}{c} \bullet \quad \bullet \\ \diagup \quad \diagdown \\ \bullet \end{array} ; G) \end{aligned}$$

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- Multiplication=gluing along vertices that have the same labels

$$t(\text{graph with 4 vertices labeled } 3, \cdot, 2, 1 ; G) \cdot t(\text{graph with 4 vertices labeled } 3, \cdot, 2, 1 ; G) = t(\text{graph with 5 vertices labeled } 3, \cdot, 2, 2, 1 ; G)$$

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From now on, when it's clear, we let $H := t(H; G)$.

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Claim: $\triangle - 2\begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array} + \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \geq 0$. (Goodman bound)

Proof:

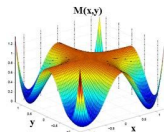
$$\begin{aligned}
 & [(\triangle - \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array} - \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array} + \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array})^2] + 2[(\begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array})^2] \\
 &= [(\triangle - \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array} - \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array} + \begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array})] + 2[\begin{array}{|c|} \hline \bullet \\ \hline \end{array} \begin{array}{|c|} \hline \bullet \\ \hline \end{array}] \\
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 \end{aligned}$$

Some sos successes

- Density profile for $\mathcal{U} = \{\text{edge}, \text{triangle}\}$ (Razborov, 2008)
- The best bound for the Turán $K_4^{(3)}$ problem (Razborov, 2014) and a solution to the problem in the ℓ_2 -norm (Balogh, Clemen, Lidický 2021)
- Every n -vertex triangle-free graph has at most $(\frac{n}{5})^5$ cycles of length 5, i.e., $\text{ind}(\text{pentagon}; G) \leq (\frac{n}{5})^5$ whenever $\text{ind}(\text{triangle}; G) = 0$ (Grzesik 2012; Hatami, Hladký, Král', Norine, Razborov 2013)
- Ramsey multiplicity bounds and results (e.g., Parczyk, Pokutta, Spiegel, Szabó 2022)
- $t_{\text{ind}}(\text{triangle}; G) + t_{\text{ind}}(\text{path of length 2}; G) \geq \frac{1}{9} - o_n(1)$ (Gilboa, Glebov, Hefetz, Linial, Morgenstern 2022)
- The smallest eigenvalue of the signless Laplacian matrix of an n -vertex graph G is at most $\frac{15n}{94}$ (Balogh, Clemen, Lidický, Norin, Volec, 2022)

Certifying polynomial inequalities with sos

A polynomial $p \in \mathbb{R}[x_1, \dots, x_n] =: \mathbb{R}[\mathbf{x}]$ is **nonnegative** if $p(x_1, \dots, x_n) \geq 0$ for all $(x_1, \dots, x_n) \in \mathbb{R}^n$



p **sum of squares (sos)**, i.e., $p = \sum_{i=1}^l f_i^2$ where $f_i \in \mathbb{R}[\mathbf{x}] \Rightarrow p \geq 0$

Hilbert (1888): Not all nonnegative polynomials are sos.

Artin (1927): Every nonnegative polynomial can be written as a (finite) sum of squares of rational functions.

Motzkin (1967, with Taussky-Todd): $M(x, y) = x^4y^2 + x^2y^4 + 1 - 3x^2y^2$ is a nonnegative polynomial but is not a sos.



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BRST (2018,2020): $\overline{\text{K}_4} - \text{K}_4 \geq 0$ is not a sum of squares or a rational sos.

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BRST (2018,2020): $\overline{K_2} - K_1 \geq 0$ is not a sum of squares or a rational sos.

RSST (2017): Graph sums of squares can be understood by doing symmetry-reduction for real polynomials.

Undecidability results

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Theorem (BRW, 2022)

Determining the validity of a polynomial inequality between weighted homomorphism densities or between weighted homomorphism numbers is undecidable.

Undecidability results - part 2

The **number of homomorphisms** from a graph H to a graph G with edge weights $\mathbf{w} : E(G) \rightarrow \mathbb{R}$, denoted as $G_{\mathbf{w}}$, is

$$\text{hom}(H; G_{\mathbf{w}}) = \sum_{\substack{\varphi: V(H) \rightarrow V(G_{\mathbf{w}}): \\ \varphi \text{ is a homomorphism}}} \prod_{\{i,j\} \in E(H)} w_{\varphi(i), \varphi(j)}.$$

We define $t(H; G_{\mathbf{w}}) = \text{hom}(H; G_{\mathbf{w}}) / |V(G_{\mathbf{w}})|^{|V(H)|}$ analogously.


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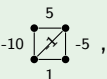
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Let $G_{\mathbf{w}} =$  ,

• $\text{hom}(H; G) = 142$

$$2(100 + 25 + 25 + 1 + 1) + 2(-10 \cdot 5 - 5 \cdot 5 - 5 \cdot 1 - 10 \cdot 1 + 1 \cdot 10 + 1 \cdot 5 - 1 \cdot 5 - 1 \cdot 1) = 142$$




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• $t(\text{path}_3; G_{\mathbf{w}}) = \frac{142}{64}$ (the expected weight of a random map)

Undecidability results - part 3

All these results build on the following solution to Hilbert's 10th problem:

Given a Diophantine equation with any number of unknown quantities and with rational integral numerical coefficients: To devise a process according to which it can be determined in a finite number of operations whether the equation is solvable in rational integers.

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Theorem (Matiyasevich 1970 (Davis, Putnam, Robinson), Tarski 1948)

Given $k \in \mathbb{N}$ and $p \in \mathbb{Z}[x_1, \dots, x_k]$, the problem of determining whether $p(x_1, \dots, x_k) \geq 0$ for every $x_1, \dots, x_k \in \mathbb{Z}$ is undecidable.

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In contrast, given $k \in \mathbb{N}$ and $p \in \mathbb{Z}[x_1, \dots, x_k]$, the problem of determining whether $p(x_1, \dots, x_k) \geq 0$ for all $x_1, \dots, x_k \in \mathbb{R}$ is decidable.

Simplifying graph profiles

Definition

The **tropicalization** of $\mathcal{S} \subseteq \mathbb{R}'_{\geq 0}$ is

$$\text{trop}(\mathcal{S}) := \lim_{k \rightarrow 0} \log_{\frac{1}{k}}(\mathcal{S}).$$

Theorem (BRST20)

$\text{trop}(\mathcal{D}_{\mathcal{U}}) = \text{cl}(\text{conv}(\log(\mathcal{D}_{\mathcal{U}})))$ which is a closed convex cone in $\mathbb{R}'_{\leq 0}$ determined by linear inequalities corresponding to the pure binomial inequalities valid on $\mathcal{D}_{\mathcal{U}}$. Similarly for $\mathcal{N}_{\mathcal{U}}$ (except $\mathbb{R}'_{\geq 0}$).

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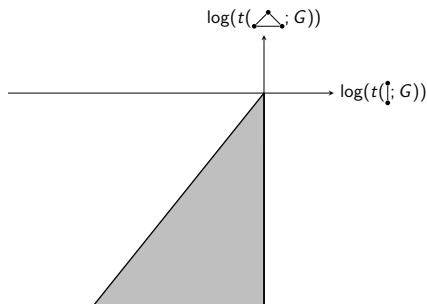
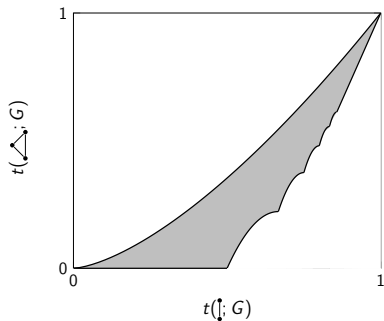
$\text{trop}(\mathcal{D}_{\mathcal{U}}) = \text{cl}(\text{conv}(\log(\mathcal{D}_{\mathcal{U}})))$ which is a closed convex cone in $\mathbb{R}_{\leq 0}^I$ determined by linear inequalities corresponding to the pure binomial inequalities valid on $\mathcal{D}_{\mathcal{U}}$. Similarly for $\mathcal{N}_{\mathcal{U}}$ (except $\mathbb{R}_{\geq 0}^I$).

$$x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_I^{\alpha_I} - x_1^{\beta_1} x_2^{\beta_2} \cdots x_n^{\beta_n} \geq 0$$

$$\rightarrow \alpha_1 y_1 + \alpha_2 y_2 + \cdots + \alpha_n y_n - \beta_1 y_1 - \beta_2 y_2 - \cdots - \beta_n y_n \geq 0$$

where $y_i = \log x_i$.

Tropicalization example



$$t(\text{path}; G)^3 - t(\text{triangle}; G)^2 \geq 0$$

becomes

$$3 \log(t(\text{path}; G)) - 2 \log(t(\text{triangle}; G)) \geq 0$$

Tropicalizations we computed

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Conjecture (BRST2020): $\text{trop}(\mathcal{N}_{\mathcal{U}})$ is a rational polyhedral cone.

BR22: If \mathcal{U} contains only chordal series-parallel graphs, then $\text{trop}(\mathcal{N}_{\mathcal{U}})$ and $\text{trop}(\mathcal{D}_{\mathcal{U}})$ is a rational polyhedral cone.

Some consequences of the tropicalization of paths (BR22)

- $\max\{c \in \mathbb{R} : \text{hom}(P_m; G) \geq \text{hom}(P_n; G)^c \text{ for all graphs } G\}$

$$= \begin{cases} \frac{m}{n+1} & \text{when } m \text{ is even and } n \text{ is odd and } m \leq n \\ \frac{km - (m-1)}{k(n-1) + 2k - n} & \text{when } m \text{ and } n \text{ are both even and } m \leq n \\ \frac{m}{n} & \text{when } m \text{ is odd and } m \leq n \\ 1 & \text{when } m \geq n \end{cases}$$

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- C_5 is strongly common (Behague, Morrison, Noel 2022)

Future directions

- What are the strengths and limitations of different techniques to prove graph inequalities?
- Computing graph profiles in more than two dimensions (and even computing more in two dimensions!)
- Is the tropicalization of $\mathcal{N}_{\mathcal{U}}$ always a polyhedral rational cone?
- Is determining the validity of a **pure binomial** inequality between homomorphism numbers decidable?

Thank you!

Tropicalization of homomorphism numbers of paths

Theorem (BR, 2021)

The following inequalities hold for homomorphism numbers of paths into any graph G with no isolated vertices:

- *log-convexity between odd paths:*
 $\text{hom}(P_a; G)^{c-b} \text{hom}(P_c; G)^{b-a} \geq \text{hom}(P_b; G)^{c-a}$ for $a \leq b \leq c$, a, c odd
- *log-convexity for odd and even paths, even middle:*
 $\text{hom}(P_a; G)^{c-b} \text{hom}(P_c; G)^{b-a} \geq \text{hom}(P_b; G)^{c-a}$ for $a \leq b \leq c$, a odd, b, c even
- *“weak convexity” for odd and even path, odd middle:*
 $\text{hom}(P_a; G)^{\frac{c}{2}} \text{hom}(P_c; G) \geq \text{hom}(P_b; G)^{\frac{c}{2}}$ for $a \leq b \leq c$, a, b odd, c even
- *non-decreasing:*
 $\text{hom}(P_a; G) \leq \text{hom}(P_b; G)$ for $a \leq b$
- *log-subadditivity:*
 $\text{hom}(P_a; G) \text{hom}(P_b; G) \leq \text{hom}(P_{a+b}; G)$

Moreover, any pure binomial inequality in paths can be deduced in a finite way from the above inequalities. In particular, for a binomial inequality where the largest path has v vertices, only inequalities involving paths on at most $2v$ vertices need to be considered.

Example of how to deduce an inequality

Suppose we want to recover $\text{hom}(P_3; G)^3 \geq \text{hom}(P_4; G)^2$. We know:

- ① $\text{hom}(P_3; G) \text{hom}(P_5; G) \geq \text{hom}(P_4; G)^2$ (log-convexity)
- ② $\text{hom}(P_3; G) \text{hom}(P_7; G) \geq \text{hom}(P_5; G)^2$ (log-convexity)
- ③ $\text{hom}(P_4; G)^2 \geq \text{hom}(P_8; G)$ (log-subadditivity)
- ④ $\text{hom}(P_8; G) \geq \text{hom}(P_7; G)$ (non-decreasing)

So we have

$$\begin{aligned} & \text{hom}(P_3; G)^3 \text{hom}(P_5; G)^2 \text{hom}(P_7; G) \\ &= (\text{hom}(P_3; G) \text{hom}(P_5; G))^2 (\text{hom}(P_3; G) \text{hom}(P_7; G)) \\ &\geq \text{hom}(P_4; G)^4 \text{hom}(P_5; G)^2 \\ &\geq \text{hom}(P_4; G)^2 \text{hom}(P_5; G)^2 \text{hom}(P_8; G) \\ &\geq \text{hom}(P_4; G)^2 \text{hom}(P_5; G)^2 \text{hom}(P_7; G) \end{aligned}$$

and so $\text{hom}(P_3; G)^3 \geq \text{hom}(P_4; G)^2$.

Example of how to deduce an inequality

Suppose we want to recover $\text{hom}(P_3; G)^3 \geq \text{hom}(P_4; G)^2$.

Equivalently, we can recover $3y_3 - 2y_4 \geq 0$ where $y_i := \log(\text{hom}(P_i; G))$.

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① $y_3 - 2y_4 + y_5 \geq 0$ (log-convexity)

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③ $2y_4 - y_8 \geq 0$ (log-subadditivity)

④ $-y_7 + y_8 \geq 0$ (non-decreasing)

So we have

$$\begin{array}{rcl} 2 \cdot (& y_3 & -2y_4 & +y_5 & & & \geq 0) \\ + (& y_3 & & -2y_5 & +y_7 & & \geq 0) \\ + (& & & & -y_7 & +y_8 & \geq 0) \\ + (& & 2y_4 & & & -y_8 & \geq 0) \\ \hline & 3y_3 & -2y_4 & & & & \geq 0 \end{array}$$

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Checking the validity of a pure binomial in paths is equivalent to checking if there exists a conical combination that yields it.

Some important properties of $\mathcal{N}_{\mathcal{U}}$ and $\text{trop}(\mathcal{N}_{\mathcal{U}})$

- $\mathcal{N}_{\mathcal{U}}$ has the Hadamard property since
$$\text{hom}(H; G_1) \cdot \text{hom}(H; G_2) = \text{hom}(H; G_1 \times G_2)$$
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- Any extreme ray of the dual cone $\text{trop}(\mathcal{N}_{\mathcal{U}})^*$ is spanned by a vector with at most one negative coordinate (BR 2021). For example, this means that we know the following inequality is redundant:

$$\text{hom}(P_{2a+1}; G) \text{hom}(P_{2(a+b+c)+1}; G) \geq \text{hom}(P_{2a+c+1}; G) \text{hom}(P_{2(a+b)+c+1}; G).$$

$\text{trop}(\mathcal{N}_{\mathcal{U}})$ when $\mathcal{U} = \{\bullet, \vdots, \triangle, \square, \dots, K_l\}$

Theorem (BRST 2020)

Let $\mathcal{U} = \{K_1, \dots, K_l\}$ where K_i is a complete graph on i vertices. Let

$$Q_{\mathcal{U}} = \left\{ \mathbf{y} \in \mathbb{R}^l \mid \begin{array}{l} i \cdot y_{i-1} - (i-1) \cdot y_i \geq 0 \quad 2 \leq i \leq l \\ y_l \geq 0 \end{array} \right\}$$

where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

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Proof.

Claim 2: The extreme rays of $Q_{\mathcal{U}}$ are $\mathbf{r}_i = (r_1, \dots, r_l)$ for $1 \leq i \leq l$ where

$$r_j = \begin{cases} j & \text{if } j \leq i, \\ 0 & \text{if } j > i. \end{cases}$$

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where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

Proof.

Claim 2: The extreme rays of $Q_{\mathcal{U}}$ are $\mathbf{r}_i = (r_1, \dots, r_l)$ for $1 \leq i \leq l$ where

$$r_j = \begin{cases} j & \text{if } j \leq i, \\ 0 & \text{if } j > i. \end{cases}$$

l constraints in l variables, and $\mathbf{r}_i = (1, 2, \dots, i, 0, \dots, 0)$ satisfies all but the i th constraint at equality (which it still satisfies).

$$\text{trop}(\mathcal{N}_{\mathcal{U}}) = \{\bullet, \vdots, \triangle, \square, \dots, K_I\}$$

Theorem (BRST 2020)

Let $\mathcal{U} = \{K_1, \dots, K_I\}$ where K_i is a complete graph on i vertices. Let

$$Q_{\mathcal{U}} = \left\{ \mathbf{y} \in \mathbb{R}^I \mid \begin{array}{l} i \cdot y_{i-1} - (i-1) \cdot y_i \geq 0 \quad 2 \leq i \leq I \\ y_I \geq 0 \end{array} \right\}$$

where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

Proof.

Claim 3: The extreme rays of $Q_{\mathcal{U}}$ are in $\text{trop}(\mathcal{N}_{\mathcal{U}})$, and hence $Q_{\mathcal{U}} = \text{trop}(\mathcal{N}_{\mathcal{U}})$.

$$\text{trop}(\mathcal{N}_{\mathcal{U}}) = \{\cdot, \vdots, \triangle, \square, \dots, K_l\}$$

Theorem (BRST 2020)

Let $\mathcal{U} = \{K_1, \dots, K_l\}$ where K_i is a complete graph on i vertices. Let

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where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

Proof.

Claim 3: The extreme rays of $Q_{\mathcal{U}}$ are in $\text{trop}(\mathcal{N}_{\mathcal{U}})$, and hence $Q_{\mathcal{U}} = \text{trop}(\mathcal{N}_{\mathcal{U}})$.

To realize \mathbf{r}_i , let G_n be an i -partite complete graph where each part has $\frac{n}{i}$ vertices (i.e., a Turán graph) with a disjoint copy of K_l .

$$\text{trop}(\mathcal{N}_{\mathcal{U}}) = \{\cdot, \vdots, \triangle, \square, \dots, K_I\}$$

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Let $\mathcal{U} = \{K_1, \dots, K_I\}$ where K_i is a complete graph on i vertices. Let

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Proof.

Claim 3: The extreme rays of $Q_{\mathcal{U}}$ are in $\text{trop}(\mathcal{N}_{\mathcal{U}})$, and hence $Q_{\mathcal{U}} = \text{trop}(\mathcal{N}_{\mathcal{U}})$.

To realize \mathbf{r}_i , let G_n be an i -partite complete graph where each part has $\frac{n}{i}$ vertices (i.e., a Turán graph) with a disjoint copy of K_I .

Then as $n \rightarrow \infty$, $\frac{\log \text{hom}(K_j; G_n)}{\log n} \rightarrow j$ if $j \leq i$ and $\frac{\log \text{hom}(K_j; G_n)}{\log n} \rightarrow 0$ if $j > i$.



$$\text{trop}(\mathcal{N}_{\mathcal{U}}) = \{\bullet, \vdots, \triangle, \square, \dots, K_l\}$$

Theorem (BRST 2020)

Let $\mathcal{U} = \{K_1, \dots, K_l\}$ where K_i is a complete graph on i vertices. Let

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where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

Consequence: Every pure binomial inequality involving complete graphs can be deduced in a finite way from the inequalities above.

$$\text{trop}(\mathcal{N}_{\mathcal{U}}) = \{\cdot, \cdot, \cdot, \cdot, \cdot, \dots, K_I\}$$

Theorem (BRST 2020)

Let $\mathcal{U} = \{K_1, \dots, K_I\}$ where K_i is a complete graph on i vertices. Let

$$Q_{\mathcal{U}} = \left\{ \mathbf{y} \in \mathbb{R}^I \mid \begin{array}{l} i \cdot y_{i-1} - (i-1) \cdot y_i \geq 0 \quad 2 \leq i \leq I \\ y_I \geq 0 \end{array} \right\}$$

where $y_i = \log(\text{hom}(K_i; G))$. Then $\text{trop}(\mathcal{N}_{\mathcal{U}}) = Q_{\mathcal{U}}$.

Consequence: Every pure binomial inequality involving complete graphs can be deduced in a finite way from the inequalities above.

For example, the general Kruskal-Katona inequalities $\text{hom}(K_p; G)^q \geq \text{hom}(K_q; G)^p$ for any $2 \leq p < q$ can be recovered from the set of inequalities $\text{hom}(K_{i-1}; G)^i \geq \text{hom}(K_i; G)^{i-1}$