The Edge Expansion of a Graph: Solution Methods and a Completely Positive Reformulation

Joint work with Akshay Gupte, Melanie Siebenhofer, and Timotej Hrga.

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Outline

Goal

Compute the edge expansion of a graph

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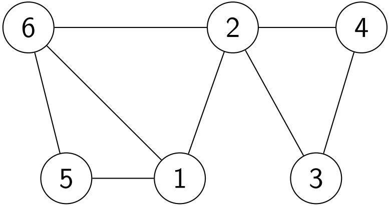
- Split & Bound
- Dinkelbach's Algorithm
- Completely Positive Formulation

Basics

- Graph $G = (V, E)$



Basics

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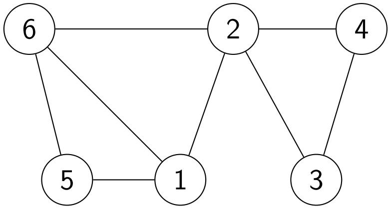
  $V = \{1, \dots, n\}$,
  $|V| = n$, $|E| = m$



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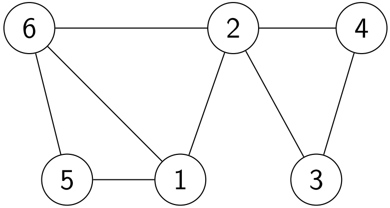
- Graph $G = (V, E)$ with $V = \{1, \ldots, n\}$, $|V| = n$, $|E| = m$
- Degree of a vertex i $d(i) \ldots \#$ neighbors of i, $d(S) = \sum_{i \in S} d(i)$ for $S \subseteq V$



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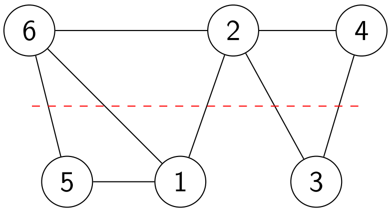
  $\partial S = \{\{i, j\} \in E \mid i \in S,\ j \notin S\}$



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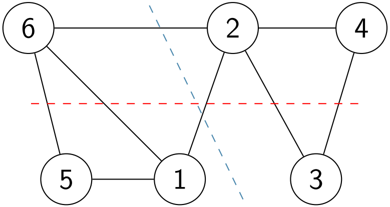
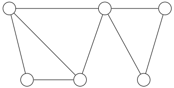


$S_1 = \{2, 4, 6\}$

$S_2 = \{2, 3, 4\}$

Minimum Cut, Minimum Cut Ratio

Aim: express connectivity
by "best" cut in graph



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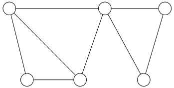

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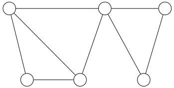

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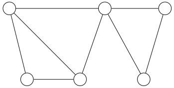

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$\min_{S \subset V} \frac{|\partial S||V|}{|S||V \setminus S|} = \min_{S \subset V} |\partial S|\left(\frac{1}{|S|} + \frac{1}{|V \setminus S|}\right)$ ... normalized cut (NP-hard)

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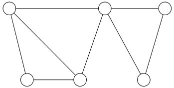

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$\min_{S \subset V} \frac{|N(S)|}{\min\{|S|,|V \setminus S|\}}$ ... vertex expansion/magnification (NP-hard)

Definition & Motivation

Edge Expansion/Cheeger Constant

$$h(G) = \min_{\substack{S \subset V \\ S \neq \emptyset}} \frac{|\partial S|}{\min\{|S|, |V \setminus S|\}} = \min_{\substack{S \subset V \\ 1 \leq |S| \leq n/2}} \frac{|\partial S|}{|S|}$$

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- $h(G)$ small: bottleneck, separating two large parts
- $h(G)$ large: any possible division has a good connection
- NP-hard to compute

Motivation:

- clustering, image segmentation
- network science, error correcting codes
- randomized approximate counting and generation (rapid mixing time)

0/1-Polytopes

Conjecture (Milena Mihail and Umesh Vazirani, 1992)

Let P be a 0/1-polytope (convex hull of 0/1-vectors),
G the 1-skeleton of P (faces of dimension 0 and 1),
then $h(G) \geqslant 1$.

Shown for

- ☑ all polytopes in dimension $\leqslant 5$ (Kaibel, 2014)
- ☑ simple 0/1-polytopes (Kaibel, 2014)
- ☑ hypersimplices (Kaibel, 2014)
- ☑ stable set polytopes (Mihail, 1992)
- ☑ matching polytopes (Mihail, 1992)
- ☑ binary matroid basis polytope (Anari et al., 2021)

Size of Cut $\leftrightarrow$ Laplacian matrix

The Laplacian matrix L of a graph $G = (V, E)$
is a matrix of dimension $n \times n$ with

$$(L)_{i,j} = \begin{cases} -1 & \{i,j\} \in E, \\ d(i) & i = j, \\ 0 & \text{else.} \end{cases}$$

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$$x^\top L x = \sum_{i=1}^{n} d(i) x_i^2 - 2 \sum_{\{i,j\} \in E} x_i x_j = \sum_{\{i,j\} \in E} (x_i - x_j)^2$$

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$\rightsquigarrow$ $|\partial S| = \mathbb{1}_S^\top L \mathbb{1}_S$ for $\mathbb{1}_S \in \{0,1\}^n$ with $(\mathbb{1}_S)_i = \begin{cases} 1 & i \in S, \\ 0 & \text{else.} \end{cases}$

$|S| = e^\top \mathbb{1}_S$ $\quad e = (1, \dots, 1)^\top$

Problem Formulation as Mixed-Integer Quadratic Program

$$
\begin{aligned}
h(G) = \min \quad & \frac{x^\top L x}{e^\top x} \\
\text{s.t.} \quad & 1 \le e^\top x \le \tfrac{n}{2} \\
& x \in \{0, 1\}^n
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$\leadsto$ can be solved with Gurobi
but only small instances

Spectral Bound – SDP Relaxation

- $x \in \{0,1\}^n$, let $X = xx^\top$, then
  - $$\operatorname{trace}(X) = \sum_{i=1}^{n} x_{ii} = \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_i = e^\top x$$

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- $X = xx^\top$ relax to $X \succcurlyeq 0$
- drop $x \in \{0, 1\}^n$

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$$= \frac{\lambda_2(L)}{2}$$

Comparison Lower Bounds

Instances: graph of grlex polytope in dimension d with $h(G) = 1$

d	n	$\lambda_2/2$
2	4	1
3	7	0.79
4	11	0.67
5	16	0.58
6	22	0.52
7	29	0.48
8	37	0.45

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d	n	$\lambda_2/2$	$\text{mincut}/\lfloor n/2 \rfloor$
2	4	1	1
3	7	0.79	1
4	11	0.67	0.80
5	16	0.58	0.63
6	22	0.52	0.55
7	29	0.48	0.50
8	37	0.45	0.44

Comparison Lower Bounds

Instances: graph of grlex polytope in dimension d with $h(G) = 1$

d	n	$\lambda_2/2$	$\text{mincut}/\lfloor n/2 \rfloor$	$\min(\ell_k)$
2	4	1	1	1
3	7	0.79	1	1
4	11	0.67	0.80	1
5	16	0.58	0.63	1
6	22	0.52	0.55	0.99
7	29	0.48	0.50	0.95
8	37	0.45	0.44	0.90

Split & Bound

$$
\begin{aligned}
h_k = \min \quad & \frac{x^\top L x}{k} \\
\text{s.t.} \quad & e^\top x = k \\
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$\leadsto$

$$h(G) = \min_{1 \le k \le \frac{n}{2}} h_k$$

Split & Bound

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$\rightsquigarrow$

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ℹ computing h_k still NP-hard (Graph Bisection, BQP)

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- compute lower and upper bounds $\ell_k \le h_k \le u_k$ for all possible candidates of k

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- ℓ_k via relaxation (semidefinite programming)

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- ℓ_k via relaxation (semidefinite programming)
- u_k via heuristic (simulated annealing)

Split & Bound

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$\rightsquigarrow$

$$h(G) = \min_{1 \le k \le \frac{n}{2}} h_k$$

- ℹ computing h_k still NP-hard (Graph Bisection, BQP)
- compute lower and upper bounds $\ell_k \le h_k \le u_k$ for all possible candidates of k
- ℓ_k via relaxation (semidefinite programming)
- u_k via heuristic (simulated annealing)
- compute h_k only if needed

Split & Bound: SDP relaxation

$$h_k = \min \quad \frac{x^\top L x}{k}$$
$$\text{s.t.} \quad e^\top x = k$$
$$x \in \{0,1\}^n$$

$\rightsquigarrow$

$$h(G) = \min_{1 \le k \le \frac{n}{2}} h_k$$

ℓ_k via relaxation (semidefinite programming)

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➜ linearize with $X = xx^\top$ $\quad (X_{ij} = x_i x_j)$

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➜ relax $X - xx^\top = 0$ to $X - xx^\top \succeq 0$

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      - ➜ Schur complement $\begin{pmatrix} X & x \\ x^\top & 1 \end{pmatrix} \succeq 0$

Split & Bound: SDP relaxation

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➜ relax $X - xx^\top = 0$ to $X - xx^\top \succeq 0$

➜ Schur complement $\begin{pmatrix} X & x \\ x^\top & 1 \end{pmatrix} \succeq 0$

➜ $x_i^2 = x_i \rightsquigarrow$ add constraint $\operatorname{diag}(X) = x$

Split & Bound: SDP relaxation

$$\begin{aligned} h_k = \min \quad & \frac{x^\top L x}{k} \\ \text{s.t.} \quad & e^\top x = k \\ & x \in \{0,1\}^n \end{aligned}$$

$\rightsquigarrow$

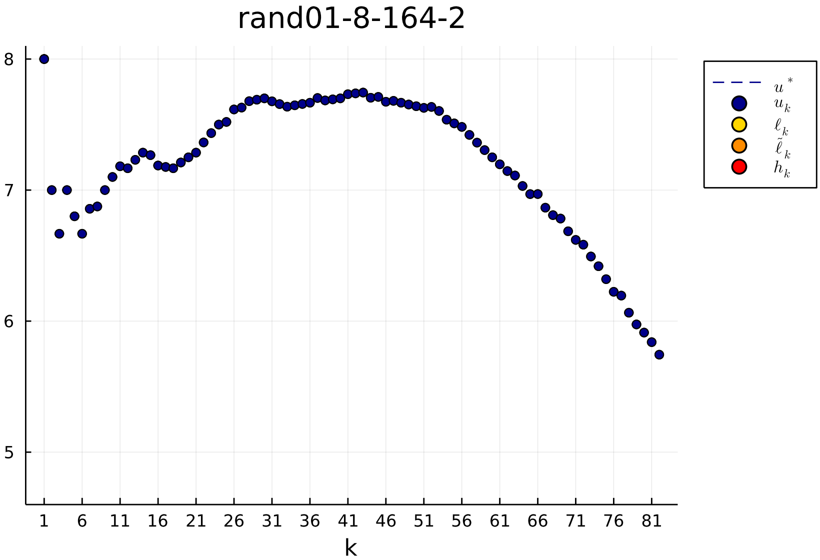
$$h(G) = \min_{1 \le k \le \frac{n}{2}} h_k$$

ℓ_k via relaxation (semidefinite programming)

$$\begin{aligned} h_k = \min \quad & \frac{1}{k}\langle L, X\rangle \\ \text{s.t.} \quad & e^\top x = k \\ & \langle J, X\rangle = k^2 \\ & X = xx^\top \\ & x = \{0,1\}^n \end{aligned}$$

$$\begin{aligned} h_k \geqslant \ell_k = \min \quad & \frac{1}{k}\langle L, X\rangle \\ \text{s.t.} \quad & e^\top x = k \\ & \langle J, X\rangle = k^2 \\ & \operatorname{diag}(X) = x \\ & \begin{pmatrix} 1 & x^\top \\ x & X \end{pmatrix} \succcurlyeq 0 \end{aligned}$$

Example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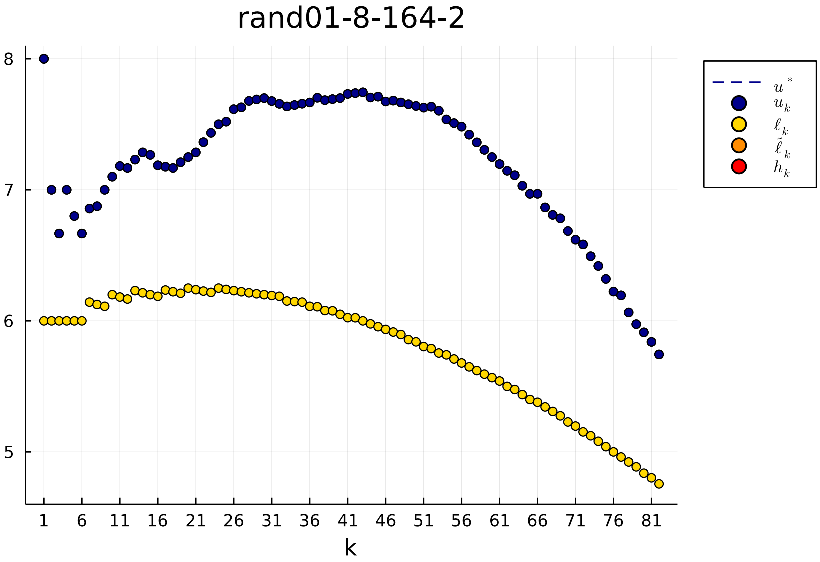
u_k
ℓ_k
$\tilde{\ell}_k$
h_k

Example



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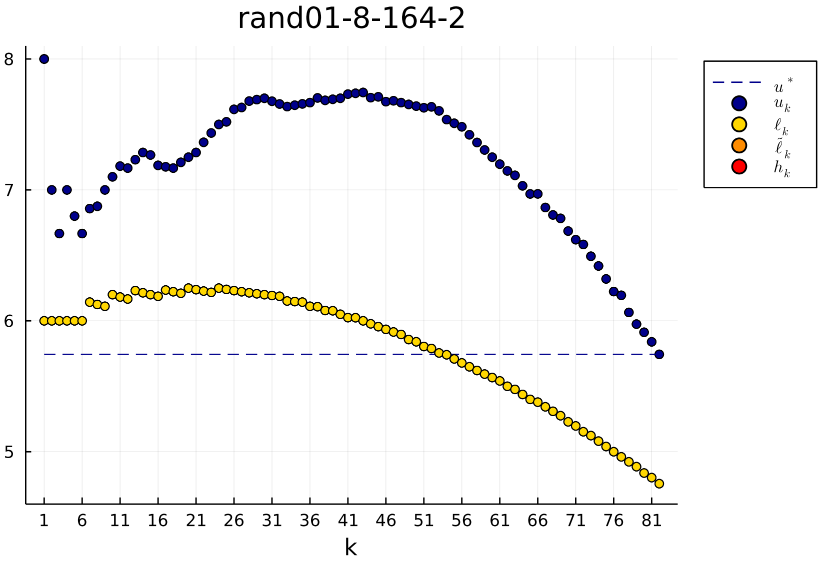
Example



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$$\begin{aligned} h_k = \min \quad & \frac{x^\top L x}{k} \\ \text{s.t.} \quad & e^\top x = k \\ & x \in \{0,1\}^n \end{aligned}$$

compute stronger lower bounds $\tilde{\ell}_k$ to have $\ell_k \leq \tilde{\ell}_k \leq h_k \leq u_k$.

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compute stronger lower bounds $\tilde{\ell}_k$ to have $\ell_k \leq \tilde{\ell}_k \leq h_k \leq u_k$.

Let $P \in \{0,1\}^{n \times 2}$ be a partition matrix and $x = \text{vec}(P)$.

Split & Bound

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Let $P \in \{0,1\}^{n \times 2}$ be a partition matrix and $x = \text{vec}(P)$.

$$\begin{aligned} \langle L, PP^\top \rangle &= \text{vec}(P)^\top (I_2 \otimes L)\text{vec}(P) = \\ &= x^\top (I_2 \otimes L) x = \langle I_2 \otimes L, xx^\top \rangle. \end{aligned}$$

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Replace $xx^\top$ by $\hat{X} \in \mathcal{S}^{2n}$,

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Replace $xx^\top$ by $\hat{X} \in \mathcal{S}^{2n}$,

relax $\hat{X} = xx^\top$ to $\hat{X} - xx^\top \succeq 0$, use Schur complement $\rightsquigarrow X := \begin{pmatrix} 1 & x^\top \\ x & \hat{X} \end{pmatrix} \succeq 0$.

ADMM for Graph Bisection

SDP relaxation for bisection [Henry Wolkowicz and Qing Zhao, 1999] plus nonnegativity

$$\begin{aligned}
\min_X \quad & \frac{1}{k}\langle L, X^{11} + X^{22}\rangle \\
\text{s.t.} \quad & \operatorname{trace}(X^{11}) = k,\ \langle J, X^{11}\rangle = k^2 \\
& \operatorname{trace}(X^{22}) = n - k,\ \langle J, X^{22}\rangle = (n-k)^2 \\
& \operatorname{diag}(X^{12}) = 0,\ \operatorname{diag}(X^{21}) = 0,\ \langle J, X^{12} + X^{21}\rangle = 2k(n-k), \\
& X = \begin{pmatrix} 1 & (x^1)^\top & (x^2)^\top \\ x^1 & X^{11} & X^{12} \\ x^2 & X^{21} & X^{22} \end{pmatrix} \succcurlyeq 0, \quad x^i = \operatorname{diag}(X^{ii}), \quad i = 1, 2, \\
& X \in \mathcal{S}^{2n+1}, X \geq 0.
\end{aligned}$$

ADMM for Graph Bisection

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& \operatorname{trace}(X^{22}) = n - k, \ \langle J, X^{22}\rangle = (n-k)^2 \\
& \operatorname{diag}(X^{12}) = 0, \ \operatorname{diag}(X^{21}) = 0, \ \langle J, X^{12} + X^{21}\rangle = 2k(n-k) \\
& X = \begin{pmatrix} 1 & (x^1)^\top & (x^2)^\top \\ x^1 & X^{11} & X^{12} \\ x^2 & X^{21} & X^{22} \end{pmatrix} \succcurlyeq 0, \quad x^i = \operatorname{diag}(X^{ii}), \quad i = 1,2 \\
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\end{aligned}
$$

- Can be strengthened by cutting planes from the boolean quadric polytope

ADMM for Graph Bisection

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- Can be strengthened by cutting planes from the boolean quadric polytope
- serious computational effort, standard methods for SDP not applicable.

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\end{aligned}
$$

- Can be strengthened by cutting planes from the boolean quadric polytope
- serious computational effort, standard methods for SDP not applicable.
- Apply ADMM [Frank De Meijer, Renata Sotirov, A. W., Shudian Zhao, 2023]

ADMM for Graph Bisection

The SDP has no interior $\rightsquigarrow$ apply facial reduction.
Resulting relaxation in lower dimensional space:

$$\begin{aligned} \min_R \quad & \langle \bar{L}, WRW^\top \rangle \\ \text{s.t.} \quad & \mathcal{G}(WRW^\top) = 0 \\ & (WRW^\top)_{1,1} = 1 \\ & WRW^\top \geq 0 \\ & R \succcurlyeq 0, R \in \mathcal{S}^n_+, \end{aligned}$$

where $\bar{L} := \frac{1}{2}\begin{pmatrix} 0 & 0^\top \\ 0 & I_2 \otimes L \end{pmatrix}$, $\quad \mathcal{G}$ ... Gangster operator.

ADMM for Graph Bisection

$$\mathcal{R} := \{R \in \mathcal{S}^n : R \succeq 0\},$$

$$\mathcal{X} := \left\{ X \in \mathcal{S}^{2n+1} : \begin{array}{l} \mathcal{G}(X) = 0,\ X_{1,1} = 1, \\ \mathrm{trace}(X^{11}) = k,\ \mathrm{trace}(X^{22}) = n - k, \\ \mathrm{diag}(X^{11}) + \mathrm{diag}(X^{22}) = e,\ Xu_1 = \mathrm{diag}(X), \\ 0 \le X \le J \end{array} \right\}.$$

Rewrite the facially reduced SDP relaxation:

$$\min \left\{ \langle \bar{L}, X \rangle :\ X = WRW^\top,\ R \in \mathcal{R},\ X \in \mathcal{X} \right\}.$$

ADMM for Graph Bisection

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$$\mathcal{L}_\sigma(X, R; Z) = \langle \bar{L}, X \rangle + \langle Z, X - WRW^\top \rangle + \frac{\sigma}{2} \|X - WRW^\top\|^2.$$

ADMM for Graph Bisection

$$\mathcal{L}_\sigma(X, R; Z) = \langle \bar{L}, X \rangle + \langle Z, X - WRW^\top \rangle + \frac{\sigma}{2}\|X - WRW^\top\|^2.$$

Let (R^p, X^p, Z^p) denote the p-th iterate of the ADMM. The next iterate $(R^{p+1}, X^{p+1}, Z^{p+1})$ is obtained as follows:

$$\begin{aligned} R^{p+1} &= \arg\min_{R \in \mathcal{R}} \mathcal{L}_{\sigma^p}(R, X^p; Z^p), \\ X^{p+1} &= \arg\min_{X \in \mathcal{X}} \mathcal{L}_{\sigma^p}(R^{p+1}, X; Z^p), \\ Z^{p+1} &= Z^p + \gamma \cdot \sigma^p \cdot (X^{p+1} - WR^{p+1}W^\top), \end{aligned}$$

where $\gamma \in \left(0, \frac{1+\sqrt{5}}{2}\right)$.

ADMM for Graph Bisection

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- optimization over $\mathcal{R}$: projection onto cone of psd matrices, i.e., computing eigenvalue decomposition

ADMM for Graph Bisection

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Z^{p+1} &= Z^p + \gamma \cdot \sigma^p \cdot (X^{p+1} - WR^{p+1}W^\top),
\end{aligned}$$

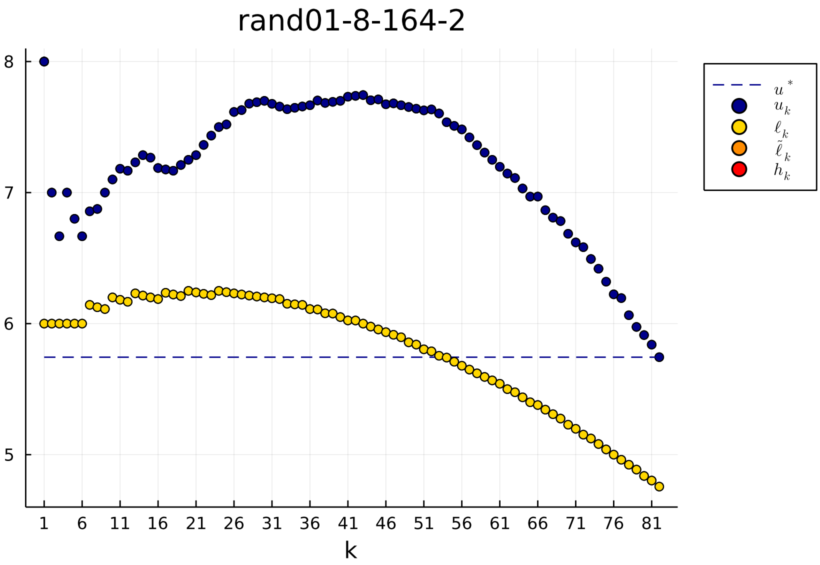
where $\gamma \in \left(0, \frac{1+\sqrt{5}}{2}\right)$.

- optimization over $\mathcal{R}$: projection onto cone of psd matrices, i.e., computing eigenvalue decomposition
- optimization over $\mathcal{X}$ with additional cutting planes: Dykstra's cyclic projection algorithm

ADMM for Graph Bisection

Initialization: Set (R^0, X^0, Z^0), σ^0 and γ. Set $p = 0$, $\mathcal{T} = \emptyset$;
Construct W;
while *stopping criteria not met* **do**
    while *stopping criteria not met* **do**
        $R^{p+1} = \mathcal{P}_{\succeq 0}\left(W^\top \left(X^p + \frac{1}{\sigma^p} Z^p\right) W\right)$;
        $X^{p+1} = \mathcal{P}_{\mathcal{X}_\mathcal{T}}\left(WR^{p+1}W^\top - \frac{1}{\sigma^p}\left(\bar{L} + Z^p\right)\right)$ using Dykstra's Algorithm;
        $Z^{p+1} = Z^p + \gamma \cdot \sigma^p \cdot (X^{p+1} - WR^{p+1}W^\top)$;
        update σ^{p+1} ;
        $p \leftarrow p + 1$;
    Compute a valid lower bound $lb(R^p, Z^p)$;
    Separate violated inequalities and add to $\mathcal{T}$;
    Cluster the cuts in $\mathcal{T}$;

Example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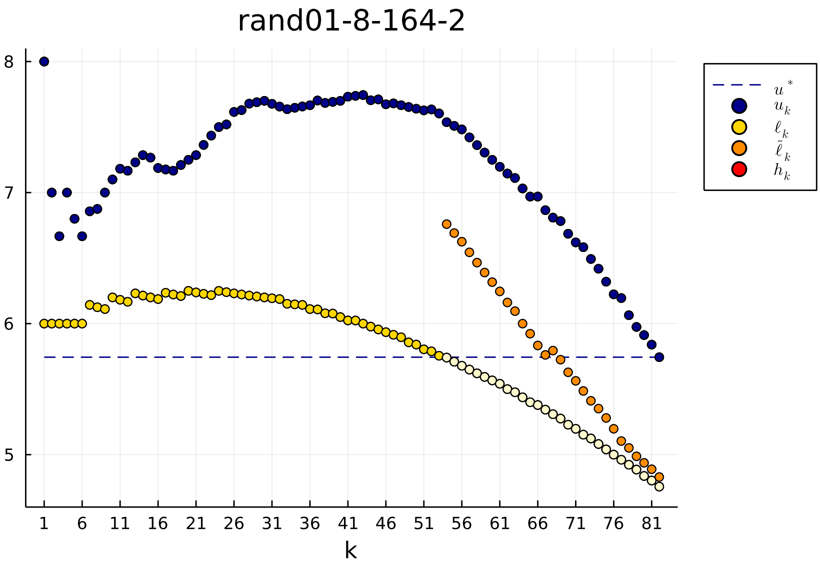
Example



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Let $\tilde{x} \in \{0,1\}$ such that $e^\top \tilde{x} = k$ and $\mu = \tilde{x}^\top L \tilde{x}$.

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Let $\tilde{x} \in \{0,1\}$ such that $e^\top \tilde{x} = k$ and $\mu = \tilde{x}^\top L \tilde{x}$. Consider $x \in \{0,1\}^n$. Then

$$
x^\top L x + \mu \| e^\top x - k \|^2 \begin{cases} = x^\top L x & \text{if } e^\top x = k \\ \geq \mu & \text{if } e^\top x \neq k \end{cases}
$$

Computing h_k

$$\begin{aligned} h_k = \min \quad & \tfrac{1}{k} x^\top L x \\ \text{s.t.} \quad & e^\top x = k \\ & x \in \{0,1\}^n \end{aligned}$$

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$$\begin{aligned} h_k &= \frac{1}{k} \min\{x^\top L x + \mu \|e^\top x - k\|^2 \colon x \in \{0,1\}^n\} \\ &= \frac{1}{k} \min\{x^\top (L + \mu e e^\top) x - 2\mu k e^\top x + \mu k^2 \colon x \in \{0,1\}^n\} \end{aligned}$$

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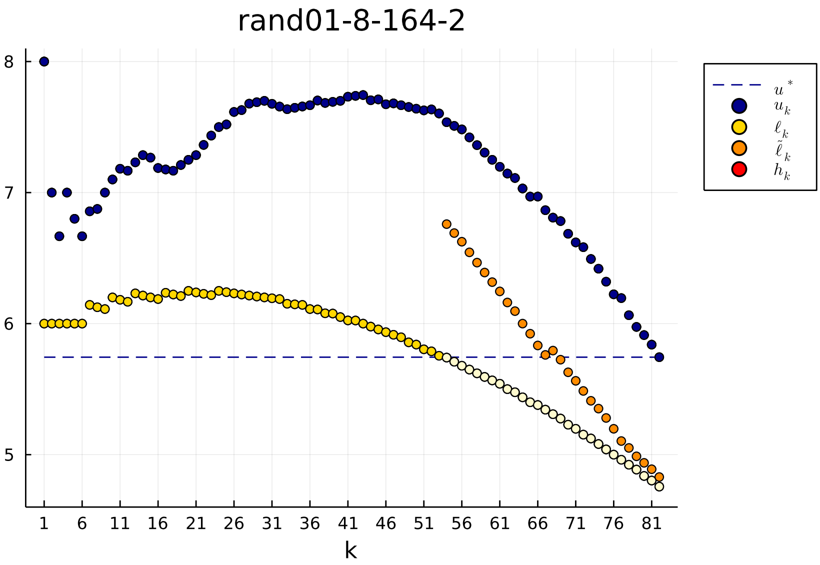
➤ unconstrained binary quadratic program $\rightsquigarrow$ can be solved, e.g., with BiqMac or BiqCrunch.

Example



rand01-8-164-2
8
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36
41
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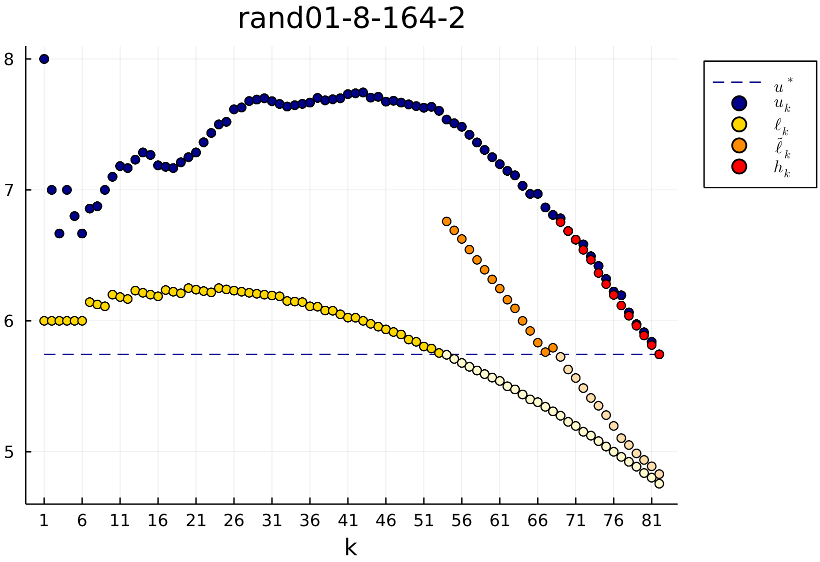
51
56
61
66
71
76
81
k
u^*
u_k
ℓ_k
$\tilde{\ell}_k$
h_k

Example



rand01-8-164-2
8
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k
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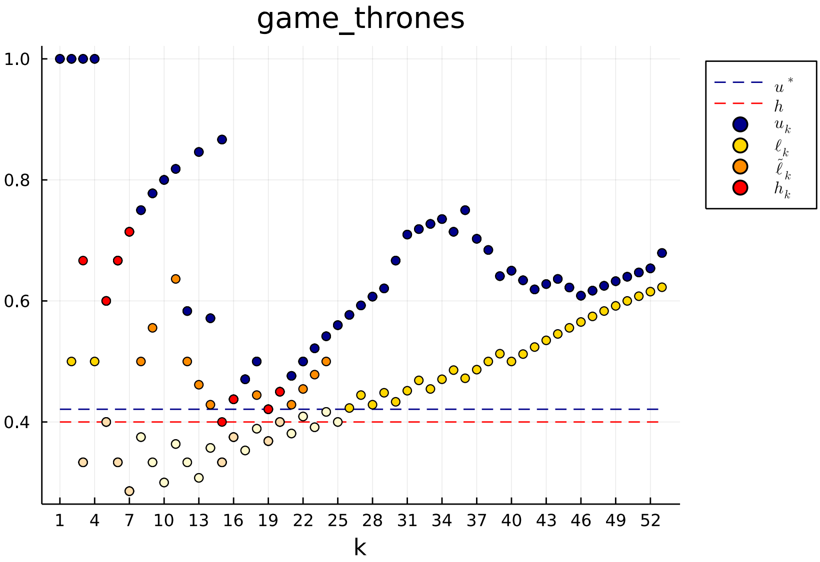
game_thrones
1.0
0.8
0.6
0.4
1 4 7 10 13 16 19 22 25 28 31 34 37 40 43 46 49 52
k
u^*
h
u_k
ℓ_k
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Outline

Goal

Compute the edge expansion of a graph

- Split & Bound
- Dinkelbach's Algorithm
- Completely Positive Formulation

Idea by Dinkelbach

Let $\mathcal{F} = \{x \in \{0,1\}^n \mid 1 \leqslant e^\top x \leqslant \frac{n}{2}\}$.

By Definition:

1. $\exists x \in \mathcal{F} : \frac{x^\top L x}{e^\top x} = h(G)$
2. $\forall x \in \mathcal{F} : \frac{x^\top L x}{e^\top x} \geqslant h(G)$

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$$\begin{aligned} P(\gamma) = \min \quad & x^\top L x - \gamma e^\top x \\ \text{s.t.} \quad & x \in \mathcal{F} \end{aligned}$$

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1. $\exists x \in \mathcal{F} : \frac{x^\top Lx}{e^\top x} = h(G) \quad \Leftrightarrow \quad \exists x \in \mathcal{F} : x^\top Lx - \gamma e^\top x = 0$
2. $\forall x \in \mathcal{F} : \frac{x^\top Lx}{e^\top x} \geqslant h(G) \quad \Leftrightarrow \quad \forall x \in \mathcal{F} : x^\top Lx - \gamma e^\top x \geqslant 0$

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Cases

$\gamma = h(G)$:

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Cases

$\gamma = h(G)$: $\quad P(\gamma) = 0$

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Cases

$\gamma = h(G)$: $\quad P(\gamma) = 0$

$\gamma > h(G)$:

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Cases

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\end{aligned}
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$$\begin{aligned} P(\gamma) = \min \quad & x^\top L x - \gamma e^\top x \\ \text{s.t.} \quad & x \in \mathcal{F} \end{aligned}$$

➥ find zero of P

Cases

$\gamma = h(G)$: $P(\gamma) = 0$
$\gamma > h(G)$: $P(\gamma) < 0$
$\gamma < h(G)$: $P(\gamma) > 0$

1. start with $x_1 \in \mathcal{F}$, set $\gamma_1 = \frac{x_1^\top L x_1}{e^\top x_1} \geqslant h(G)$
2. compute $P(\gamma_1)$ by solving the Binary Quadratic Problem, get x_2 and $\gamma_2 = \frac{x_2^\top L x_2}{e^\top x_2}$

↻ iterate until $P(\gamma_t) = 0$

Instance			Split & Bound	Dinkelbach	Gurobi
	n	$h(G)$	time (s)	time (s)	time (s)
grlex-11	67	1.0000	148	4.4	2.0
grlex-12	79	1.0000	280.4	4.6	2.0
grlex-13	92	1.0000	14037.2	4.1	2.3
grevlex-11	67	3.6667	193.9	10412.3	1460.7
grevlex-12	79	3.9231	1315.5	11861.7	8624.9
grevlex-13	92	4.0000	2246.3	29.4	-
polbooks	105	0.3654	540	128.7	3.3
football	115	1.0702	399.9	25.8	31.2
celegansneural	297	1.0000	389.3	80.6	22.0
sp_office	92	3.3696	19.3	858.7	522.2
revolution	141	0.0962	1595.6	639.0	1.3
malaria_genes_HVR1	307	0.2377	62943.4	425.8	7.8

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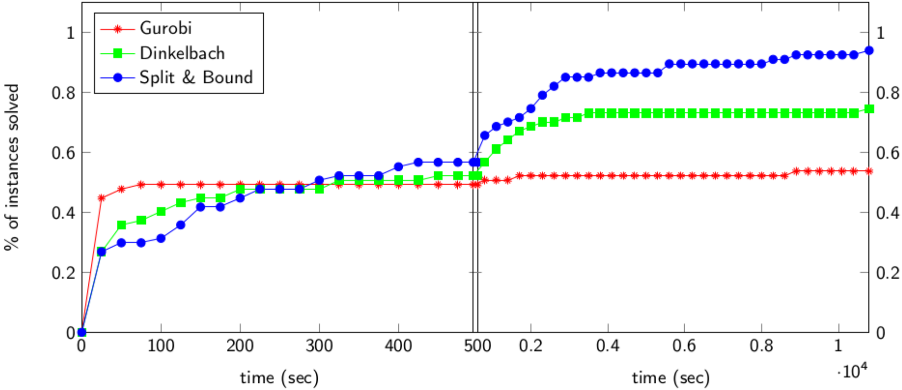
	n	$h(G)$	time (s)	time (s)	gap (rel.)
rand01-9-278-0	278	10.0719	17542.8	-	0.953
rand01-9-278-1	278	9.0000	8153.3	103.7	0.954
rand01-9-278-2	278	9.9209	31125.4	-	0.957
rand01-10-281-0	281	28.9000	1807.9	-	0.975
rand01-10-281-1	281	27.7929	1776.4	-	0.973
rand01-10-281-2	281	27.7500	2435.7	1103.5	0.972

Performance Comparison – 3 Exact Algorithms



ℹ Time limit set to 3 hours.

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Set of Completely Positive Matrices

$$\mathcal{CP}^n = \{X \in \mathcal{S}^n : X = \sum_{i=1}^{t} a_i a_i^\top,\ a_i \geq 0 \ \ \forall i \in \{1, \dots, t\}\}$$

Convexification techniques for quadratic fractional programs

$$\min_{x \in \mathcal{X}} \frac{x^\top B x + b^\top x + b_0}{x^\top A x + a^\top x + a_0}$$

Theorem (He, Liu, Tawarmalani, 2024)

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Theorem (He, Liu, Tawarmalani, 2024)

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$$q(x) = x^\top Ax + a^\top x + a_0 > 0 \quad \forall x \in \mathcal{X} \subseteq \mathbb{R}n,$$

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Convexification techniques for quadratic fractional programs

$$\min_{x \in \mathcal{X}} \frac{x^\top Bx + b^\top x + b_0}{x^\top Ax + a^\top x + a_0} = \min_{(\rho, y, Y) \in \mathcal{G}} \langle B, Y \rangle + b^\top y + b_0 \rho$$

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➠ $\mathrm{conv}(\mathcal{F})$ **?**

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➟ $\mathrm{conv}(\mathcal{F})$ **?**

$$\mathcal{X} = \mathbb{R}^n_{\geqslant 0} \Rightarrow \mathrm{conv}(\mathcal{F}) = \left\{(1, x, X) : \begin{pmatrix} X & x \\ x^\top & 1 \end{pmatrix} \in \mathcal{CP}^{n+1}\right\}$$

Convexification techniques for quadratic fractional programs

$$\min_{x\in\mathcal{X}} \frac{x^\top Bx + b^\top x + b_0}{x^\top Ax + a^\top x + a_0} = \min_{(\rho,y,Y)\in\mathrm{conv}(\mathcal{G})} \langle B, Y\rangle + b^\top y + b_0\rho$$

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↪ not bounded ☹

$$\min_{x \in \mathcal{X} \cap \mathcal{L}} \frac{x^\top Bx + b^\top x + b_0}{x^\top Ax + a^\top x + a_0}$$

Theorem (He, Liu, Tawarmalani, 2024)

Let $\mathcal{L} = \{x \in \mathbb{R}^n : Cx = d\}$, $\mathcal{X} \subseteq \mathbb{R}^n$, $\mathcal{X} \cap \mathcal{L} \neq \emptyset$ *bounded,*

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Binary variables $x \in \{0, 1\}^n$

- $x, z \in \mathbb{R}^n_{\geqslant 0}$, $x_i + z_i = 1$ ☞ constraints in $\mathcal{L}$
- $Y_{i,i+n} = 0$ ☞ description of $\operatorname{conv}(\mathcal{G}')$
- non-negative variables ➜ completely positive cone

Convexification of the edge expansion problem

$$
\begin{aligned}
h(G) = \ \min\ & \frac{x^\top L x}{e^\top x} \\
\text{s.t.}\ & e^\top x + s = \lfloor \tfrac{n}{2} \rfloor \\
& e^\top x - t = 1 \\
& x \in \{0,\, 1\}^n \\
& s, t \geqslant 0
\end{aligned}
$$

Convexification of the edge expansion problem

$$
\begin{aligned}
h(G) = \min \ & \frac{x^\top L x}{e^\top x} \\
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\end{aligned}
$$

- $\mathcal{F} = \left\{ \left(1, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}^\top \right) : \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \in \mathbb{R}^{2n+2}_{\geqslant 0} \right\}$

- $C = \begin{pmatrix} e_n^\top & 0_n^\top & 1 & 0 \\ e_n^\top & 0_n^\top & 0 & -1 \\ I_n & I_n & 0_n & 0_n \end{pmatrix}, \ d = \begin{pmatrix} \lfloor \frac{n}{2} \rfloor \\ 1 \\ e_n \end{pmatrix}$

  $M = \begin{pmatrix} C & -d \end{pmatrix}$

- $y^\top = \begin{pmatrix} y_x^\top & y_z^\top & y_s & y_t \end{pmatrix}$

  $$Y = \begin{pmatrix} Y_{xx} & Y_{xz} & Y_{xs} & Y_{xt} \\ Y_{zx} & Y_{zz} & Y_{zs} & Y_{zt} \\ Y_{sx} & Y_{sz} & Y_{ss} & Y_{st} \\ Y_{tx} & Y_{tz} & Y_{ts} & Y_{tt} \end{pmatrix} \in \mathcal{S}^{2n+2}$$

  $$\widetilde{Y} = \begin{pmatrix} Y & y \\ y^\top & \rho \end{pmatrix}$$

Convexification of the edge expansion problem

$$h(G) = \min \frac{x^\top L x}{e^\top x}$$
$$\text{s.t.} \quad e^\top x + s = \lfloor \tfrac{n}{2} \rfloor$$
$$e^\top x - t = 1$$
$$x \in \{0, 1\}^n$$
$$s, t \geqslant 0$$

$$= \min \langle L, Y_{xx} \rangle$$
$$\text{s.t.} \quad (\rho, y, Y) \in \text{conv}(\mathcal{G}') \left\{ \right.$$

- $\mathcal{F} = \left\{ \left(1, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}^\top \right) : \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \in \mathbb{R}^{2n+2}_{\geqslant 0} \right\}$
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Convexification of the edge expansion problem

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& s, t \geqslant 0
\end{aligned}
$$

$$
\begin{aligned}
= \min\ & \langle L, Y_{xx} \rangle \\
\text{s.t.}\ & (\rho, y, Y) \in \operatorname{conv}(\mathcal{G}') \begin{cases} e^\top y_x = 1 \\ \operatorname{diag}(Y_{xz}) = 0_n \\ \langle M^\top M, \widetilde{Y} \rangle = 0 \\ \widetilde{Y} \in \mathcal{CP}^{2n+3} \end{cases}
\end{aligned}
$$

- $\mathcal{F} = \left\{ \left(1, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}, \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix}^\top \right) : \begin{pmatrix} x \\ z \\ s \\ t \end{pmatrix} \in \mathbb{R}^{2n+2}_{\geqslant 0} \right\}$

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Completely positive reformulation → Strong relaxation

$$
\begin{aligned}
h(G) = \min\ & \langle L, Y_{xx} \rangle \\
\text{s.t.}\ & e^\top y_x = 1 \\
& \operatorname{diag}(Y_{xz}) = 0_n \\
& \langle M^\top M, \widetilde{Y} \rangle = 0 \\
& \widetilde{Y} \in \mathcal{CP}^{2n+3}
\end{aligned}
$$

⚠ optimization over $\mathcal{CP}$ NP-hard

Completely positive reformulation → Strong relaxation

$$
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h(G) \geqslant \min\ & \langle L, Y_{xx} \rangle \\
\text{s.t.}\ & e^\top y_x = 1 \\
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& \langle M^\top M, \widetilde{Y} \rangle = 0 \\
& \widetilde{Y} \geq 0,\ \widetilde{Y} \succeq 0
\end{aligned}
$$

⚠ optimization over $\mathcal{CP}$ NP-hard ☞ relax to DNN

Completely positive reformulation → Strong relaxation

$$
\begin{aligned}
h(G) \geqslant \min\ & \langle L, Y_{xx} \rangle \\
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& \operatorname{diag}(Y_{xz}) = 0_n \\
& \langle M^\top M, \widetilde{Y} \rangle = 0 \\
& \widetilde{Y} \geq 0,\ \widetilde{Y} \succeq 0
\end{aligned}
$$

- ⚠ optimization over $\mathcal{CP}$ NP-hard ☞ relax to DNN
- ⚠ DNN relaxation has no Slater point ☞ facial reduction

Completely positive reformulation → Strong relaxation

$$
\begin{aligned}
h(G) \geqslant \min\ & \langle L, Y_{xx}\rangle \\
\text{s.t.}\ & e^\top y_x = 1 \\
& \operatorname{diag}(Y_{xz}) = 0_n \\
& \langle M^\top M, \widetilde{Y}\rangle = 0 \\
& \widetilde{Y} \geq 0,\ \widetilde{Y} \succeq 0
\end{aligned}
$$

- optimization over $\mathcal{CP}$ NP-hard ☞ relax to DNN
- DNN relaxation has no Slater point ☞ facial reduction
  - $\widetilde{Y} \succeq 0$ ➟ $\langle M^\top M, \widetilde{Y}\rangle = 0 \Leftrightarrow M\widetilde{Y} = 0$

Completely positive reformulation → Strong relaxation

$$
\begin{aligned}
h(G) \geqslant \min\ & \langle L, Y_{xx}\rangle & = \min\ & \langle L, Y_{xx}\rangle \\
\text{s.t.}\ & e^\top y_x = 1 & \text{s.t.}\ & e^\top y_x = 1 \\
& \operatorname{diag}(Y_{xz}) = 0_n & & \operatorname{diag}(Y_{xz}) = 0_n \\
& \langle M^\top M, \widetilde{Y}\rangle = 0 & & \widetilde{Y} = WRW^\top \geqslant 0 \\
& \widetilde{Y} \geq 0,\ \widetilde{Y} \succeq 0 & & R \succeq 0
\end{aligned}
$$

- optimization over $\mathcal{CP}$ NP-hard ☞ relax to DNN
- DNN relaxation has no Slater point ☞ facial reduction
  - $\widetilde{Y} \succeq 0$ ➟ $\langle M^\top M, \widetilde{Y}\rangle = 0 \Leftrightarrow M\widetilde{Y} = 0$
  - columns of $W \in \mathbb{R}^{(2n+3)\times(n+1)}$ orthonormal basis of $\ker(M)$
    - ➟ $\{\widetilde{Y} \succeq 0 : M\widetilde{Y} = 0\} = \{WRW^\top : R \succeq 0\}$
      - ➟ dimension of psd variable $2n+3 \to n+1$ ☺

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & \begin{pmatrix} e_n^\top & 0_{n+2}^\top \end{pmatrix} y = 1 \\
& \operatorname{diag}(Y_{xz}) = 0 \\
& W R W^\top \geqslant 0, R \succeq 0
\end{aligned}
\tag{DNN-PFR}
$$

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\
& \operatorname{diag}(Y_{xz}) = 0 \\
& WRW^\top \geqslant 0, R \succeq 0
\end{aligned}
\qquad \text{(DNN-PFR)}
$$

Strengthening

- $\widetilde{Y} \in \mathcal{CP}^{2n+3} \Leftrightarrow (\rho, y, Y) \in \rho \operatorname{conv}\left(\left\{(1, \bar{x}, \bar{x}\bar{x}^\top) : \bar{x} \in \mathbb{R}^{2n+2}_{\geqslant 0}\right\}\right)$, $\bar{x} = (x^\top, z^\top, s, t)$

$$\begin{aligned} \min \quad & \langle L, Y_{xx} \rangle \\ \text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\ & \operatorname{diag}(Y_{xz}) = 0 \\ & WRW^\top \geqslant 0, R \succeq 0 \end{aligned} \tag{DNN-PFR}$$

Strengthening

- $\widetilde{Y} \in \mathcal{CP}^{2n+3} \Leftrightarrow (\rho, y, Y) \in \rho \operatorname{conv}\left(\{(1, \bar{x}, \bar{x}\bar{x}^\top) : \bar{x} \in \mathbb{R}^{2n+2}_{\geqslant 0}\}\right), \ \bar{x} = (x^\top, z^\top, s, t)$
- $x, z \in \{0,1\}^n$ → BQP inequalities

→ ❶ scaled BQP inequalities for y_x, y_z

$$\begin{aligned} X_{ij} &\leqslant x_i \\ X_{ij} + X_{ik} - X_{jk} &\leqslant x_i \\ x_i + x_j - X_{ij} &\leqslant 1 \\ x_i + x_j + x_k - X_{ij} - X_{ik} - X_{jk} &\leqslant 1 \end{aligned} \quad \Rightarrow \quad \begin{aligned} Y_{ij} &\leqslant y_i \\ Y_{ij} + Y_{ik} - Y_{jk} &\leqslant y_i \\ y_i + y_j - Y_{ij} &\leqslant \rho \\ y_i + y_j + y_k - Y_{ij} - Y_{ik} - Y_{jk} &\leqslant \rho \end{aligned}$$

❷ $\operatorname{diag}(Y_{xx}) = y_x, \ \operatorname{diag}(Y_{zz}) = y_z$

$$\begin{aligned} \min \quad & \langle L, Y_{xx} \rangle \\ \text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\ & \operatorname{diag}(Y_{xz}) = 0 \\ & WRW^\top \geqslant 0, R \succeq 0 \end{aligned} \tag{DNN-PFR}$$

Theorem (Hrga, Siebenhofer, W., 2024$^+$)

- (DNN-PFR) *has a Slater feasible point.*
- *every feasible point* $\widetilde{Y}$ *satisfies*
  - ☑ $\frac{1}{\lfloor \frac{n}{2} \rfloor} \leqslant \rho \leqslant 1$
  - ☑ $y_x + y_z = \rho e_n$
  - ☑ $1 \leqslant \langle E, Y_{xx} \rangle \leqslant \lfloor \frac{n}{2} \rfloor$
  - ☑ *upper bounds for* $\widetilde{Y}$
  - ☑ $Y_{ij} \leqslant y_i \quad \forall i,j \in [2n]$
  - ☑ $y_i + y_j - Y_{ij} \leqslant \rho \quad \forall i,j \in [2n]$

➥ add BQP: $Y_{ij} + Y_{ik} - Y_{jk} \leqslant y_i \quad \forall i,j,k \in [2n]$

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\
& \operatorname{diag}(Y_{xz}) = 0 \\
& Y_{ij} + Y_{ik} - Y_{jk} \leqslant y_i \quad \forall i, j, k \in [2n] \\
& WRW^\top \geqslant 0, \; R \succeq 0
\end{aligned}
\tag{DNN-PFRC}
$$

only variable is R, $\widetilde{Y} = WRW^\top$ for easier notation only.

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\
& \operatorname{diag}(Y_{xz}) = 0 \\
& Y_{ij} + Y_{ik} - Y_{jk} \leqslant y_i \quad \forall i, j, k \in [2n] \\
& WRW^\top \geqslant 0, \ R \succeq 0
\end{aligned} \tag{DNN-PFRC}
$$

only variable is R, $\widetilde{Y} = WRW^\top$ for easier notation only.

$$
\begin{aligned}
\min \quad & \langle \widetilde{L}, WRW^\top \rangle \\
\text{s.t.} \quad & \langle A_0, WRW^\top \rangle = 1 \\
& \langle A_i, WRW^\top \rangle = 0 \qquad \forall i \in [n] \\
& \langle B_{ijk}, WRW^\top \rangle \leq 0 \qquad \forall i, j, k \in [2n] \\
& \langle E_{ij}, WRW^\top \rangle \geqslant 0 \qquad \forall i, j \in [n] \\
& R \succeq 0
\end{aligned}
$$

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\
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& Y_{ij} + Y_{ik} - Y_{jk} \leqslant y_i \quad \forall i, j, k \in [2n] \\
& WRW^\top \geqslant 0, \; R \succeq 0
\end{aligned}
\tag{DNN-PFRC}
$$

only variable is R, $\widetilde{Y} = WRW^\top$ for easier notation only.

$$
\begin{aligned}
\min \quad & \langle W^\top \widetilde{L} W, R \rangle \\
\text{s.t.} \quad & \langle W^\top A_0 W, R \rangle = 1 \\
& \langle W^\top A_i W, R \rangle = 0 \qquad \forall i \in [n] \\
& \langle W^\top B_{ijk} W, R \rangle \leq 0 \qquad \forall i, j, k \in [2n] \\
& \langle W^\top E_{ij} W, R \rangle \geqslant 0 \qquad \forall i, j \in [n] \\
& R \succeq 0
\end{aligned}
$$

$$
\begin{aligned}
\min \quad & \langle L, Y_{xx} \rangle \\
\text{s.t.} \quad & (e_n^\top \quad 0_{n+2}^\top) y = 1 \\
& \operatorname{diag}(Y_{xz}) = 0 \\
& Y_{ij} + Y_{ik} - Y_{jk} \leqslant y_i \quad \forall i, j, k \in [2n] \\
& WRW^\top \geqslant 0, \; R \succeq 0
\end{aligned} \tag{DNN-PFRC}
$$

only variable is R, $\widetilde{Y} = WRW^\top$ for easier notation only.

$$
\begin{aligned}
\min \quad & \langle \widetilde{L}, WRW^\top \rangle \\
\text{s.t.} \quad & \mathcal{A}(WRW^\top) = b \\
& \mathcal{B}(WRW^\top) \leqslant 0 \\
& WRW^\top \geqslant 0 \\
& R \succeq 0
\end{aligned}
$$

Computing (DNN-PFR) and (DNN-PFRC)

➥ augmented Lagrangian method on dual

$$\begin{aligned} \max \quad & b^\top \nu \\ \text{s.t.} \quad & W^\top\left(\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \widetilde{L}\right) W + Z = 0 \\ & \nu \in \mathbb{R}^{n+1},\ \nu \geq 0,\ S \geq 0,\ Z \succeq 0 \end{aligned} \qquad \text{(DNN-DFRC)}$$

$$\begin{aligned} \mathcal{L}_\alpha(\nu,\mu,S,Z;R) = {} & b^\top \nu - \left\langle W^\top\left(\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \widetilde{L}\right) W + Z, R \right\rangle \\ & - \frac{1}{2\alpha}\left\| W^\top\left(\mathcal{A}^\top \nu - \mathcal{B}^\top \mu + S - \widetilde{L}\right) W + Z \right\|^2 \end{aligned}$$

- ℹ Initialize R_0, $\alpha_0 > 0$
- ❶ $(\nu_k, \mu_k, S_k, Z_k) = \arg\min \mathcal{L}_{\alpha_k}(\nu, \mu, S, Z; R_k)$ ➜ quasi-Newton method
- ❷ $R_{k+1} = R_k - \frac{1}{\alpha_k}\left(W^\top\left(\mathcal{A}^\top \nu_k - \mathcal{B}^\top \mu_k + S_k - \widetilde{L}\right) W + Z_k\right)$
- ❸ iteratively add violated BQP cuts, few violated $\rightarrow$ decrease α_{k+1}
- ⚙ post processing to obtain valid lower bound

Numerical results - with cuts

Instance	n	UB	(DNN-PFR) gap (%)	(DNN-PFR) time (s)	(DNN-PFRC) gap (%)	(DNN-PFRC) time (s)	(DNN-PFRC) cuts
rand01-9-278-0	278	10.07	11.7	878.5	2.8	760.7	2204
rand01-9-278-1	278	9.00	10.6	1180.1	7.8	2922.7	4272
rand01-9-278-2	278	9.92	12.8	763.3	1.6	1737.8	3091
rand01-10-281-0	281	28.90	4.1	408.3	0.8	680.6	2068
rand01-10-281-1	281	27.79	4.8	1103.3	0.5	858.7	2233
rand01-10-281-2	281	27.75	4.7	418.1	0.8	693.2	1997
grlex-23	277	1.00	2.3	1415.0	1.2	1455.7	1278
grlex-24	301	1.00	1.0	1542.0	0.0	1663.3	968
grlex-25	326	1.00	5.9	2231.8	3.9	2250.9	443
grevlex-25	326	7.72	18.7	2544.0	5.8	2984.0	2317
grevlex-26	352	7.94	21.0	2169.6	5.5	4133.8	2373
grevlex-27	379	8.13	19.4	2747.3	6.0	3515.5	1450
polbooks	105	0.37	14.9	114.2	3.0	175.6	1033
football	115	1.07	9.4	86.4	0.0	118.1	382
celegansneural	297	1.00	8.2	2595.9	3.6	3844.4	841
sp-office	92	3.37	7.1	64.9	2.4	89.8	1333
revolution	141	0.10	21.0	242.2	7.9	233.7	1110
malariagenes-HVR1	307	0.24	52.3	3225.4	4.4	2620.7	1608

Summary

- Edge Expansion – NP-hard
- 2 Exact Solution Approaches
  - Split & Bound
  - Dinkelbach's Algorithm
- Equivalent formulation using Completely Positive Matrices
- Doubly Non-Negative Relaxation & Augmented Lagrangian
- Code available at Melanie Siebenhofer's github repository
  https://github.com/melaniesi/EdgeExpansion.jl,
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Summary

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Thank you!

Akshay Gupte (Edinburgh), Timotej Hrga & Melanie Siebenhofer (Klagenfurt)