

# Relaxations of Graph Partitioning and Vertex Separator Problems using Continuous Optimization

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(work with Ting Kei Pong, Hao Sun, Ningchuan Wang)

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at: THE FIELDS INSTITUTE FOR RESEARCH IN MATHEMATICAL SCIENCES

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- Model NP-hard problem using quadratic-quadratic program
- approximate/relax using eigenvalue bounds and semidefinite programming
- **bounds:** we follow approaches for eigenvalue and projected eigenvalue bounds in:
  - Hadley, Rendl, W. 1990 [1, 5]
  - Rendl, Lissner, Piacenti, (RLP) 2012 [4]
  - and
  - Semidefinite bounds in: W., Zhao 1996 [6].

# Background/Notation

Given graph  $G$  and set sizes  $m$

- $G = (N, E)$  edge-weighted undirected graph

$N = \{1, 2, \dots, n\}$  node set

$E_{ij}, ij = 1, 2, \dots, n$  edge weights

$m = \begin{pmatrix} m_1 \\ \dots \\ m_k \end{pmatrix}$  (pos. integer) set sizes, with  $m^T e = n$

Set of all Partitions  $P_m =$

$\{(S_1, \dots, S_k) : S_i \subset N, |S_i| = m_i \forall i;$   
 $S_i \cap S_j = \emptyset \forall i \neq j; \cup_i S_i = N\}$

Partition matrix  $X \in \mathbb{R}^{n \times k}$ ; col.  $X_j$  incidence vector of  $S_j$

$$X_{ij} = \begin{cases} 1 & \text{if } i \in S_j \\ 0 & \text{otherwise.} \end{cases}$$

# Partition Matrix Constraints

linear/quadratic constraints (many are redundant)

set of: zero-one; nonnegative; linear equalities;  $m$ -diagonal orthogonality type;  $e$ -diagonal orthogonality type; and gangster constraints, respectively:

$$\begin{aligned}\mathcal{Z} &:= \{X \in \mathbb{R}^{n \times k} : X_{ij} \in \{0, 1\}, \forall ij\} \\ &= \{X \in \mathbb{R}^{n \times k} : X_{ij}^2 = X_{ij}, \forall ij\}\end{aligned}$$

$$\mathcal{N} := \{X \in \mathbb{R}^{n \times k} : X_{ij} \geq 0, \forall ij\}$$

$$\begin{aligned}\mathcal{E} &:= \{X \in \mathbb{R}^{n \times k} : X\mathbf{e} = \mathbf{e}, X^T\mathbf{e} = m\} \\ &= \{X \in \mathbb{R}^{n \times k} : \|X\mathbf{e} - \mathbf{e}\|^2 + \|X^T\mathbf{e} - m\|^2 = 0\}\end{aligned}$$

$$\mathcal{D}_0 := \{X \in \mathbb{R}^{n \times k} : X^T X = \text{Diag}(m)\}$$

$$\mathcal{D}_e := \{X \in \mathbb{R}^{n \times k} : \text{diag}(XX^T) = \mathbf{e}\}$$

$$\mathcal{G} := \{X \in \mathbb{R}^{n \times k} : X_{:i} \circ X_{:j} = 0, \forall i \neq j\}, \quad \circ \text{ Hadamard prod.}$$

# Equivalent Representations of Partition Matrices

The set of partition matrices in  $\mathbb{R}^{nk}$ ,  $\mathcal{M}_m =$

$$\begin{aligned}\mathcal{M}_m &= \mathcal{E} \cap \mathcal{Z} \\ &= \mathcal{E} \cap \mathcal{D}_0 \cap \mathcal{N} \\ &= \mathcal{E} \cap \mathcal{D}_0 \cap \mathcal{D}_e \cap \mathcal{N} \\ &= \mathcal{E} \cap \mathcal{Z} \cap \mathcal{D}_0 \cap \mathcal{G} \cap \mathcal{N}\end{aligned}$$

## Cut of a partition

- $\delta(S_i, S_j)$  - set of edges between sets  $S_i, S_j$
- $\delta(S) = \cup_{i < j < k} \delta(S_k, S_j)$  - set of edges with endpoints in distinct partition sets  $S_1, \dots, S_{k-1}$
- The minimum of the cardinality  $|\delta(S)|$  is denoted  
(objective)  $\text{cut}(m) = \min\{|\delta(S)| : S \in P_m\}$

## $\mathcal{G}$ has a vertex separator

graph  $G$  has a vertex separator if there exists  $S \in P_m$  with  $\delta(S) = \emptyset$ , i.e.,  $\text{cut}(m) = 0$ .

(see (RLP) [4], Hager, Hungerford 2013 [2] for relationship with bandwidth of graph and other applications)

# Trace Representation of Cut Problem

- $B := \begin{bmatrix} ee^T & -I_{k-1} & 0 \\ 0 & & 0 \end{bmatrix} \in \mathbb{S}^k$ ,  
 $\mathbb{S}^k$  -  $k \times k$  symm. matrices with trace inner-product.
- $A = (a_{ij})$  - adjacency matrix,  $a_{ij} = \begin{cases} 1 & \text{if } E_{ij} \neq 0 \\ 0 & \text{otherwise} \end{cases}$
- $L := \text{Diag}(Ae) - A = \sum_{ij \in E(G)} (e_i - e_j)(e_i - e_j)^T$  -  
Laplacian ( $e_i$  unit vectors)

## Quadratic objective for $\text{cut}(m)$

Proposition RLP [4, Prop. 2] For partition  $S \in P_m$ , and associated partition matrix  $X \in \mathcal{M}_m$ , the cardinality of the partition is

$$|\delta(S)| = \frac{1}{2} \text{trace } AXBX^T = \frac{1}{2} \text{trace}(-L)XBX^T$$



# Basic Eigenvalue Bound

## Relaxed problem

$$\begin{aligned} \text{cut}(m) &\geq p_{\text{eig}}^*(m) \\ &:= \min \quad \frac{1}{2} \text{trace } AXBX^T \quad (A \text{ or } -L) \\ &\quad \text{s.t.} \quad X \in \mathcal{D}_O \end{aligned}$$

$\mathcal{D}_O = \{X \in \mathbb{R}^{n \times k} : X^T X = M := \text{Diag}(m)\}$   
(orthogonal type cols for  $X$ )

## Hoffman-Wielandt '53 [3] bound/Theorem

$C, D$  symmetric order  $n, k$ , resp.,  $k \leq n$ . Then

$$\min \{ \text{trace } CXDX^T : X^T X = I_k \} =$$

$$\min \left\{ \sum_{i=1}^k \lambda_i(D) \lambda_{\phi(i)}(C) : \phi : N \rightarrow \{1, \dots, k\} \text{ is an injection} \right\}.$$

minimum attained for  $X = (p_{\phi(1)}, \dots, p_{\phi(k)}) Q^T$ , where  $p_{\phi(i)}$  normalized eigenvector to  $\lambda_{\phi(i)}(C)$  and cols of

$Q = [q_1 \ \dots \ q_k]$  contains normalized eigenvectors  $q_i$  of  $\lambda_i(D)$ .



# Basic Eigenvalue Bound II

## Lemma (RLP)

$k$ -ordered eigs of  $\tilde{B} := M^{1/2}BM^{1/2}$  satisfy

$$\lambda_1(\tilde{B}) \leq \lambda_2(\tilde{B}) \leq \dots \leq \lambda_{k-2}(\tilde{B}) < \lambda_{k-1}(\tilde{B}) = 0 < \lambda_k(\tilde{B}).$$

## Basic Eigenvalue Bound, apply Hoffman-Wielandt Theorem

Let  $-\lambda_1(L) \geq -\lambda_2(L) \geq \dots \geq -\lambda_n(L)$  denote ordered  $n$  eigenvalues of  $-L$ ;  $-\lambda(L)$  denotes corresponding vector of eigenvalues.

Pad the 0 eigenvalue of  $\tilde{B}$  with further zeros to get an ordered vector of length  $n$  and denote it by  $\hat{\lambda}(\tilde{B})$ . Then

$$\text{cut}(m) \geq 0 > p_{\text{eig}}^* = -\lambda(L)^T \hat{\lambda}(\tilde{B})$$

# Two Projected Eigenvalue Bound

## Relaxed problem

$$\begin{aligned} \text{cut}(m) &\geq p_{\text{projeig}}^*(m) \\ &:= \min_{X \in \mathcal{D}_0 \cap \mathcal{E}} \frac{1}{2} \text{trace } AXBX^T \quad (A \text{ or } -L) \end{aligned}$$

$$\mathcal{D}_0 = \{X \in \mathbb{R}^{n \times k} : X^T X = M := \text{Diag}(m)\} \text{ (orthog type)}$$

$$\mathcal{E} = \{X \in \mathbb{R}^{n \times k} : Xe = e, X^T e = m\} \text{ (linear row/col sums)}$$

# Special Parametrization of $X \in \mathcal{E}$

$\tilde{m} = \sqrt{m}$ ;  $n \times n, k \times k$  orthogonal matrices  $P, Q$

$$P = \begin{bmatrix} \frac{1}{\sqrt{n}} \mathbf{e} & V \end{bmatrix} \in \mathcal{O}_n, \quad Q = \begin{bmatrix} \frac{1}{\sqrt{n}} \tilde{m} & W \end{bmatrix} \in \mathcal{O}_k. \quad (*)$$

LEMMA: Rendl and W. 1990 [5]

Let  $\tilde{M} = \text{Diag}(\tilde{m})$ . Suppose that  $X \in \mathbb{R}^{n \times k}$  and  $Z \in \mathbb{R}^{(n-1) \times (k-1)}$  are related by

$$X = P \begin{bmatrix} 1 & 0 \\ 0 & Z \end{bmatrix} Q^T \tilde{M}. \quad (*)$$

Then the following holds:

- 1  $X \in \mathcal{E}$ .
- 2  $X \in \mathcal{N} \Leftrightarrow VZW^T \geq -\frac{1}{n} \mathbf{e} \tilde{m}^T$
- 3  $X \in \mathcal{D}_0 \Leftrightarrow Z \in \mathcal{O}_{(n-1) \times (k-1)}$

Conversely, if  $X \in \mathcal{E}$ , then there exists  $Z$  such that the representation (\*) holds.



## THEOREM

$V, W$  as above,  $\hat{X} := \frac{1}{n}em^T \in \mathbb{R}^{n \times k}$

$Q: \mathbb{R}^{(n-1) \times (k-1)} \rightarrow \mathbb{R}^{n \times k}$ ,  $Q(Z) = VZW^T \tilde{M}$

Then:

$\hat{X} \in \mathcal{E}$ , and  $Q$  is invertible  $\mathbb{R}^{(n-1) \times (k-1)} \leftrightarrow \mathcal{E} - \hat{X}$

Equivalently,  $\mathcal{E}$  can be parametrized using  $\hat{X} + VZW^T \tilde{M}$ .

Thus, two objective functions

$$\frac{1}{2} \text{trace } AXBX^T =$$

$$\frac{1}{2} \text{trace}(A\hat{X}B\hat{X}^T + (V^T AV)Z(W^T \tilde{M}B\tilde{M}W)Z^T + 2V^T A\hat{X}B\tilde{M}WZ^T)$$

and

$$\frac{1}{2} \text{trace}((-L)XBX^T) = \frac{1}{2} \text{trace}(V^T(-L)V)Z(W^T \tilde{M}B\tilde{M}W)Z^T.$$

# Two Projected Eigenvalue Bounds

Let

$$\hat{A} = V^T A V, \hat{L} = V^T (-L) V, \hat{B} = W^T \tilde{M} B \tilde{M} W, \\ \alpha = \text{trace } A \hat{X} B \hat{X}^T, C = 2V^T A \hat{X} B \tilde{M} W.$$

Then:

$$\begin{aligned} \text{cut}(m) \geq p_{\text{proj eig}, A}^* &= \frac{1}{2} \left\{ \alpha + \min_{\phi \text{ injective}} \left\{ \sum_{i=1}^k \lambda_i(\hat{B}) \lambda_{\phi(i)}(\tilde{A}) \right\} + \right. \\ &\quad \left. \min_{0 \leq \hat{X} + V Z W^T \tilde{M}} \text{trace } C Z^T \right\} \\ &\geq p_{\text{eig}}^* \end{aligned}$$

$$\begin{aligned} \text{cut}(m) \geq p_{\text{proj eig}, L}^* &= \frac{1}{2} \min_{\phi \text{ injective}} \left\{ \sum_{i=1}^k \lambda_i(\hat{B}) \lambda_{\phi(i)}(\tilde{L}) \right\} \\ &\geq p_{\text{eig}}^* \end{aligned}$$

and note eigenvalues of  $V^T L V$  are  $n - 1$  nonzero eigenvalues of  $L$ .

# Attainment for Quadratic Terms

let  $Q \in \mathbb{R}^{k-1 \times k-1}$  be orthog. with cols consisting of eigenvectors of  $\hat{B}$  corresponding to eigenvalues of  $\hat{B}$  in nondecreasing order;

let  $P_A, P_L \in \mathbb{R}^{n-1 \times k-1}$  have orthonormal cols consisting of  $k-1$  eigenvectors of  $\hat{A}, \hat{L}$ , respectively, corresponding to eigenvalues in nonincreasing order where the columns correspond to the largest  $k-2$  followed by the smallest. Then the minimal scalar product terms in  $P_{proj, A}^*, P_{proj, L}^*$  are attained by resp.

$$Z_A = P_A Q^T, Z_L = P_L Q^T.$$

Get two approx. solutions using  $Q$ :

$$X_A = \hat{X} + V Z_A W^T \tilde{M}, \quad X_L = \hat{X} + V Z_L W^T \tilde{M},$$

# Feasible Solutions; Upper Bounds

## Using an approx. solution $\bar{X}$

Find nearest (Frobenius norm) feas. soln (use strong polytime LP)

Recall:  $X \in \mathcal{E} \cap \mathcal{Z}$  implies that  $Xe = e$ ,  $X^T e = m$ , and  $X^T X = \text{Diag}(m)$ . Therefore:

$$\begin{aligned}\|\bar{X} - X\|_F^2 &= \text{trace}(\bar{X}^T \bar{X} + X^T X - 2\bar{X}^T X) \\ &= n + n + 2 \text{trace}(-\bar{X}^T X).\end{aligned}$$

## Finding nearest feasible solution; a strong polytime LP

Solve the transportation problem:

$$\begin{aligned}\max \quad & \text{trace} \bar{X}^T X \\ \text{s.t.} \quad & Xe = e \\ & X^T e = m \\ & X \geq 0\end{aligned}$$

# Node-Arcs for a Random Adjacency Matrix

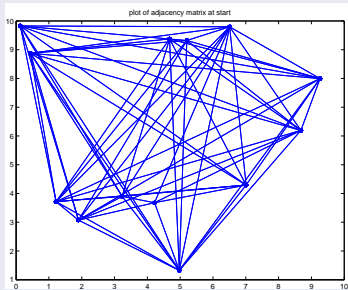
node $i$												
1	2	3	4	5	7	8	9	10	11	12	13	
2	3	4	8	9	10	11	12	13	14			
3	6	7	8	9	10	11	12	13	14			
4	7	8	9	11	13	14						
5	6	7	9	10	12	13						
6	7	9	10	12	13							
7	8	10	12	13								
8	9	10	11	12	14							
9	10	13	14									
10	11	12	14									
11	12											
12	13	14										

Table: Existing edges node  $i$  to node  $j$



# Random Ex.; Proj. Eigenvalue Lower Bound

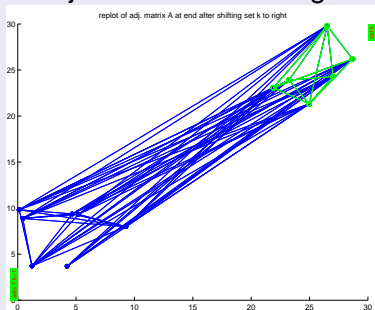
Adjacency Matrix,  $m = (4 \ 2 \ 1 \ 6)$ ,  $k = 4, n = 13$



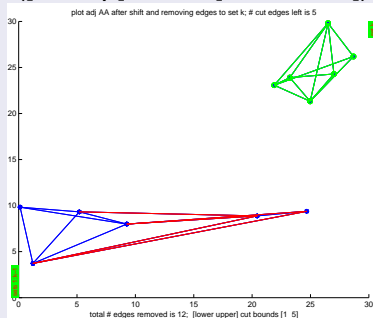
total edges: 61

# Bounds, Feas. Sol., $m = (4 \ 2 \ 1 \ 6)$ , $k = 4$ , $n = 13$

Adj. after shift set  $k$  right



Adj. after delet. edges;  
([low up] bnds: [0.76067 5])



# Random Problems

$imax = 35; k = 6$

$n$  is 144 and  $m$  is [28 17 28 32 34 5]

best projection lower and upper bounds are: 5092 5495

relative gap is: 0.076131

$n$  is 94 and  $m$  is [3 17 14 32 19 9]

best projection lower and upper bounds are 1672 1890

relative gap is 0.1224

$imax = 35; k = 8$

$n$  is 188 and  $m$  is [31 27 26 34 7 6 35 22]

best projection lower and upper bounds are 7558 8285

relative gap is 0.091776

An equivalent quadratically constrained quadratic problem

$$\begin{aligned} \text{cut}(m) \geq p_{SDP}^* = \min & \quad \frac{1}{2} \text{trace } AXBX^T && (A \text{ or } (-L)) \\ \text{s.t.} & \quad X \circ X = X \\ & \quad \|Xe - e\|^2 = 0 \\ & \quad \|X^T e - m\|^2 = 0 \\ & \quad X_{:i} \circ X_{:j} = 0 \quad \forall i \neq j. \end{aligned}$$

where  $\circ$  is the Hadamard (elementwise) product

# Semidefinite Lower Bounds

## Quadratic Model

We can use the various equality (quadratic) constraints in the representation and use the quadratic objective function. The Lagrangian relaxation for this quadratic-quadratic problem is equivalent to a semidefinite program, SDP. The dual of this is the SDP relaxation. Adding redundant constraints can help.

## Alternatively: directly by lifting process

linearize quadratic terms using the matrix

$$Y_X := \begin{pmatrix} 1 \\ \text{vec}(X) \end{pmatrix} (1 \text{ vec}(X))^T,$$

$\text{vec}(X)$  is vector formed from the columns of  $X$ .

$Y_X \succeq 0$  and is rank one, the hard constraint that is relaxed.

From direct lifting (can use  $A$  or  $-L$ ?)

$$\begin{aligned}\text{trace } AXBX^T &= \langle AXB, X \rangle = \text{vec}(X)^T (\text{vec } AXB) = \\ &= \text{vec}(X)^T (B \otimes A) \text{vec}(X) = \text{trace}(B \otimes A) (\text{vec}(X) \text{vec}(X)^T)\end{aligned}$$

The objective function becomes  $\text{trace } AXBX^T = \text{trace } L_A Y_X$ ,

$$L_A := \begin{bmatrix} 0 & 0 \\ 0 & B \otimes A \end{bmatrix}$$

$B \otimes A$  is the Kronecker product

Relax the rank one restriction

$$\begin{aligned} \text{cut}(m) \geq p_{SDP}^* &:= \min && \text{trace } L_A Y \\ &&& \text{s.t. } \text{arrow}(Y) = e_0 \\ &&& \text{trace } D_1 Y = 0 \\ &&& \text{trace } D_2 Y = 0 \\ &&& \mathcal{G}_J(Y) = 0 \\ &&& Y_{00} = 1 \\ &&& Y \succeq 0, \end{aligned}$$

(RGP)

# Linear Transformations

## arrow operator

acting  $(kn + 1) \times (kn + 1)$  matrix  $Y$

$$\text{arrow}(Y) := \text{diag}(Y) - (0, Y_{0,1:kn})^T$$

represents the 0, 1 constraints; guarantees diagonal and 0-th row (or column) are identical;

## Gangster operator $\mathcal{G}_J : \mathcal{S}_{kn+1} \rightarrow \mathcal{S}_{kn+1}$

shoots “holes” in a matrix

$$(\mathcal{G}_J(Y))_{ij} := \begin{cases} Y_{ij} & \text{if } (i, j) \text{ or } (j, i) \in J \\ 0 & \text{otherwise,} \end{cases}$$

$$J := \left. \begin{array}{l} \{(i, j) : i = (p-1)n + q, j = (r-1)n + q, \\ \text{for } p < r, p, r \in \{1, \dots, k\} \\ q \in \{1, \dots, n\} \} \end{array} \right\}$$

represents the (Hadamard) orthogonality of the cols

# Linear Transformations

## The norm constraints

represented by the  $(kn + 1) \times (kn + 1)$  matrices

$$D_1 := \begin{bmatrix} n & -\mathbf{e}_k^T \otimes \mathbf{e}_n^T \\ -\mathbf{e}_k \otimes \mathbf{e}_n & (\mathbf{e}_k \mathbf{e}_k^T) \otimes I_n \end{bmatrix}$$

and

$$D_2 := \begin{bmatrix} \bar{\mathbf{m}}^T \bar{\mathbf{m}} & -\bar{\mathbf{m}}^T \otimes \mathbf{e}_n^T \\ -\bar{\mathbf{m}} \otimes \mathbf{e}_n & I_k \otimes (\mathbf{e}_n \mathbf{e}_n^T) \end{bmatrix}.$$

## Loss of Slater's condition

all  $D_1, D_2, Y \succeq 0$ ,

both  $\text{trace } YD_1 = 0, \text{trace } YD_2 = 0$ ; therefore, range of  $Y$  subset intersection of nullspaces of  $D_1, D_2$ .

feasible set of (RGP) has no strictly feasible points; implies numerical difficulties for interior-point methods.

Fix: apply facial reduction.



## Facial Reduction;

$$Y = \hat{V}Z\hat{V}^T \in \mathbb{S}^{kn+1}, Z \in \mathbb{S}^{(n-1)(k-1)+1}$$

$$V_j \in \mathbb{R}^{j \times j-1}$$

$$V_j \mathbf{e} = 0, V_j^T V_j = \text{Diag}(w) \succ 0, \text{ e.g.,}$$

$$V_j := \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ 0 & 1 & \dots & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & 1 \\ -1 & \dots & \dots & 0 & -1 \end{bmatrix}_{j \times (j-1)}.$$

Range of  $\hat{V}$  forms basis for range (any)  $\hat{Y} \in \text{relint } F$

$$\hat{V} := \begin{bmatrix} 1 & 0 \\ \frac{1}{n}m \otimes \mathbf{e}_n & V_k \otimes V_n \end{bmatrix}$$

Constraints for  $X \in \mathcal{E}$  eliminated;  $Z \in \mathbb{S}^{(n-1)(k-1)+1}$

$$\begin{aligned} \min \quad & \text{trace } \hat{V}^T L_A \hat{V} Z \\ \text{s.t.} \quad & \text{arrow}(\hat{V} Z \hat{V}^T) = 0 \\ & \mathcal{G}_J(\hat{V} Z \hat{V}^T) = 0 \\ & (\hat{V} Z \hat{V}^T)_{00} = 1 \\ & Z \succeq 0 \end{aligned}$$

Slater's CQ now holds (strict feasibility).

But are we done? Are the constraints onto?

Projected onto range of gangster;  $\bar{J} = J \cup (0, 0)$

$$\begin{aligned} \min \quad & \text{trace} \left( \hat{V}^T L_A \hat{V} \right) Z \\ \text{s.t.} \quad & \mathcal{G}_{\bar{J}}(\hat{V}Z\hat{V}^T) = \mathcal{G}_{\bar{J}}(E_{00}) \\ & Z \succeq 0 \end{aligned}$$

Dual program (also satisfies Slater)

$$\begin{aligned} \max \quad & W_{00} \\ \text{s.t.} \quad & \hat{V}^T \mathcal{G}_{\bar{J}}(W) \hat{V} \preceq \hat{V}^T L_A \hat{V} \end{aligned}$$

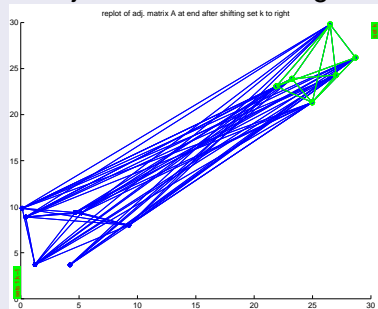
Doubly Nonnegative

A stronger relaxation adds the nonnegativity elementwise:

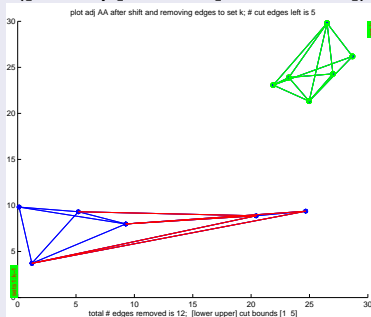
$$\hat{V}Z\hat{V}^T \geq 0.$$

SDP Bounds;  $m = (4 \ 2 \ 1 \ 6)$ ,  $k = 4$ ,  $n = 13$

Adj. after shift set  $k$  right



Adj. after delet. edges;  
([low up] bnds: [0.76067 5])



lower bnds: [ Proj L and A; SDP; Doubly Nonneg.]

$[-0.52065 \ 0.76067 \ 2.9057 \ 4.8603]$

rounded up:  $[0 \ 1 \ 3 \ 5]$ .

Therefore,  $5$  is optimal value.

Random Ex;  $n = 85$ ,  $k = 6$ ,  $m = [18\ 20\ 11\ 18\ 11\ 7]$

### Proj. Eig. Bounds

$n$  is 85 and  $m$  is 18 20 11 18 11 7

best projection lower and upper bounds are 1518 1714

relative gap is 0.12129

### SDP Bounds



sdp lower and upper bounds are 1556 1726

current best lower/upper bounds are: 1556 1714

relative gap is 0.096636

- Model NP hard problems using quadratic-quadratic models
- First Relaxations lead to eigenvalue problems
- Lagrangian Relaxation leads to SDP problem and the dual is the SDP (strong) relaxation
- The Slater condition typically fails for SDP relaxations (facial reduction is needed for stability)

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Thanks for your attention!

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