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The first cut is the cheapest –  
improving SDP bounds for the clique number

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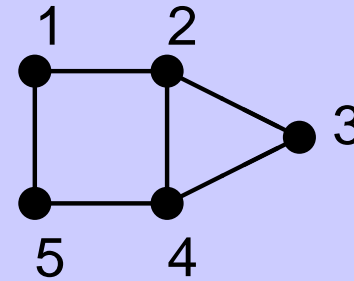
## Overview

- Maximum clique problem and StQP formulation
- Copositive relaxations for Schrijver number
- Cuts: idea and construction
- Algorithm and examples
- Graph operations and systematic test generation
- Circulant graphs and gaps
- Experimental results and outlook

# Maximum Clique Problem

Graph  $\mathcal{G} = (V, \mathcal{E})$  with vertices  $V = \{1, \dots, n\}$ , edges  $\mathcal{E} \subseteq \binom{V}{2} \dots$

loopless, undirected, unweighted



$$\text{Adjacency matrix } A_{\mathcal{G}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

**Clique:**  $S \subseteq V$  inducing complete subgraph

**clique number**  $\omega(\mathcal{G}) \dots$  size of maximum clique

Problem to determine  $\omega(\mathcal{G})$  is NP-hard

## Standard Quadratic Problem (StQP) formulation

Motzkin/Straus [1965]:

Let  $Q_G := E - A_G$ , where  $e = [1, \dots, 1]^\top$ ,  $E = ee^\top$ ,

then

$$l(G) := \min\{x^\top Q_G x : x \in \Delta\} = 1/\omega(G)$$

... (homog.) QP over standard simplex  $\Delta = \{x \in \mathbb{R}_+^n : e^\top x = 1\}$

Equivalent **copositive program** (COP):

$$l(G) = \max\{\lambda : Q_G - \lambda E \in \mathcal{C}\}.$$

Copositive matrices cone

contains psd matrices cone

and positive matrices cone

$$\mathcal{C} = \{C : x^\top C x \geq 0 \text{ for all } x \in \mathbb{R}_+^n\}$$

$$\mathcal{P} = \{P : x^\top P x \geq 0 \text{ for all } x \in \mathbb{R}^n\}$$

$$\mathcal{N} = \{N : N_{ij} \geq 0 \text{ for all } i, j \in V\}.$$

## Polynomial-time relaxations of COP

$\mathcal{K}$  ... any cone of matrices with  $\mathcal{K} \subseteq \mathcal{C}$

$$l_{\mathcal{K}}(\mathcal{G}) := \max\{\lambda : Q_{\mathcal{G}} - \lambda E \in \mathcal{K}\} \leq l(\mathcal{G})$$

In particular, for

- $\mathcal{K} = \mathcal{P}$  :  $1/l_{\mathcal{K}} = \theta$  ... Lovász number [1979]
- $\mathcal{K} = \mathcal{P} + \mathcal{N}$  :  $1/l_{\mathcal{K}} = \theta'$  ... Lovász, Schrijver [1991]
- $\mathcal{K} = \mathcal{K}^r$ ,  $r \in \mathbb{N}$  : sum-of-squares hierarchy, Parrilo [2000]
- $\mathcal{K} = \mathcal{M}^r$ ,  $r \in \mathbb{N}$  : moment-relaxation hierarchy, Lasserre [2001]
- $\mathcal{K} = \mathcal{C}^r$ ,  $r \in \mathbb{N}$  : LP hierarchy, de Klerk/Pasechnik [2002]
- $\mathcal{K} = \mathcal{Q}^r$ ,  $r \in \mathbb{N}$  : recursive hierarchy, Peña/Vera/Zuluaga [2006]
- $\mathcal{K} = \mathcal{L}^r$ ,  $r \in \mathbb{N}$  : hierarchy families, Gvozdenović/Laurent [2006]

## Different formulations of $\theta'$

Schrijver bound:  $\mathcal{K}^0 = \mathcal{M}^0 = \mathcal{Q}^0 = \mathcal{P} + \mathcal{N}$

$$l'(\mathcal{G}) = \max\{\lambda : Q_{\mathcal{G}} - \lambda E \in \mathcal{K}^0\} = 1/\theta'(\mathcal{G})$$

Equivalent:  $\theta'(\mathcal{G}) = \min\{t : t Q_{\mathcal{G}} - E \in \mathcal{K}^0\}$

Dual formulation, with notation  $A \bullet B = \text{trace}(AB)$ :

$$\begin{aligned}\theta'(\mathcal{G}) &= \max\{E \bullet X : I \bullet X = 1, A_{\bar{\mathcal{G}}} \bullet X = 0, X \in \mathcal{P} \cap \mathcal{N}\} \\ &= \max\{E \bullet X : (I + A_{\bar{\mathcal{G}}}) \bullet X = 1, X \in \mathcal{P} \cap \mathcal{N}\}\end{aligned}$$

where  $\bar{\mathcal{G}} = (V, \binom{V}{2} \setminus \mathcal{E})$  is the complement graph of  $\mathcal{G}$ .

Note:  $Q_{\mathcal{G}} = E - A_{\mathcal{G}} = I + A_{\bar{\mathcal{G}}}$ , if  $I$  denotes identity matrix.

## Copositivity Cuts

For a set  $\{C_1, \dots, C_m\}$  of (known) copositive matrices

consider  $\mathcal{D} := \left\{ \sum_{j=1}^m y_j C_j : y \in \mathbb{R}_+^m \right\} \subset \mathcal{C}$

and define

$$\theta^{\mathcal{D}}(\mathcal{G}) := \min\{t : t Q_{\mathcal{G}} - E \in \mathcal{P} + \mathcal{N} + \mathcal{D}\}$$

Dual:

$$\theta^{\mathcal{D}}(\mathcal{G}) = \max\{E \bullet X : Q_{\mathcal{G}} \bullet X = 1, C_j \bullet X \geq 0 \forall j, X \in \mathcal{P} \cap \mathcal{N}\}$$

Strong duality holds (strict feasibility easy to check)

## Construction of Cuts

Let  $\mathcal{H}$  be a graph of known clique number  $\omega(\mathcal{H})$ , so that

$$1/\omega(\mathcal{H}) = \max\{\lambda : Q_{\mathcal{H}} - \lambda E \in \mathcal{C}\}$$

Consequence:

$$C_{\mathcal{H}} := \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E - A_{\mathcal{H}} \in \mathcal{C}.$$

Using this matrix for the cut ( $\mathcal{D} = \mathbb{R}_+ C_{\mathcal{H}} \subset \mathcal{C}$ ) we obtain

$$\theta^{\mathcal{H}}(\mathcal{G}) = \max\{E \bullet X : Q_{\mathcal{G}} \bullet X = 1, X \in \mathcal{P} \cap \mathcal{N}, \\ A_{\mathcal{H}} \bullet X \leq \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E \bullet X\}$$

where we simply calculated  $C_{\mathcal{H}} \bullet X$  to obtain the red inequality.

## Choice of graph $\mathcal{H}$

Let  $X^*$  be a solution of

$$\theta'(\mathcal{G}) = \max\{E \bullet X : I \bullet X = 1, A_{\overline{\mathcal{G}}} \bullet X = 0, X \in \mathcal{P} \cap \mathcal{N}\}$$

Search for graphs  $\mathcal{H}$  of known clique number which violate

$$A_{\mathcal{H}} \bullet X^* \leq \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E \bullet X^*$$

- Subgraphs of known clique number

Triangle free subgraphs,  $\omega(\mathcal{H}) = 2$

$K_4$ -free subgraphs,  $\omega(\mathcal{H}) = 3$

- Compositions of graphs with low clique number

## Subgraphs of fixed clique number

Theoretical strategy: given (small)  $\omega_0$ , find solution  $\mathcal{H}$  to

$$\max \{ A_{\mathcal{H}} \bullet X^* : \omega(\mathcal{H}) = \omega_0 \} .$$

Heuristic approach – dropping strategy:

iteratively remove edges from  $\mathcal{G}$  such that

- not too much weight of  $X^*$  is lost;
- as many  $(\omega_0 + 1)$  – cliques as possible are removed.

Criterion of choosing an edge: **minimize**  $K(i, j) = \frac{X_{i,j}^*}{f(T_{i,j})}$  with

$T_{ij}(\mathcal{G}) \dots$  number of  $(\omega_0 + 1)$  - cliques of  $\mathcal{G}$  with  $\{i, j\}$  as an edge.

$f(x) \dots$  some positive increasing function, e.g.  $x^d$ ,  $\exp(x)$ , etc.

# Algorithm

**Initialization.** Let  $\mathcal{H} = \mathcal{G}$ .

**Step 1.** Compute  $T_{ij}(\mathcal{H})$  for all edges  $\{i, j\} \in \mathcal{E}_{\mathcal{H}}$ .

**Step 2.** If  $T_{ij}(\mathcal{H}) = 0$  for all  $\{i, j\} \in \mathcal{E}_{\mathcal{H}}$ , then STOP and return  $\mathcal{H}$ .

Otherwise, let  $\{i', j'\} \in \operatorname{argmin}_{\{i, j\} \in \mathcal{E}_{\mathcal{H}}} \left\{ \frac{X_{i, j}^*}{f(T_{i, j})} \right\}$ .

**Step 3.** Remove  $\{i', j'\}$ , i.e. put

$$\mathcal{E}_{\mathcal{H}} = \mathcal{E}_{\mathcal{H}} \setminus \{\{i', j'\}\}$$

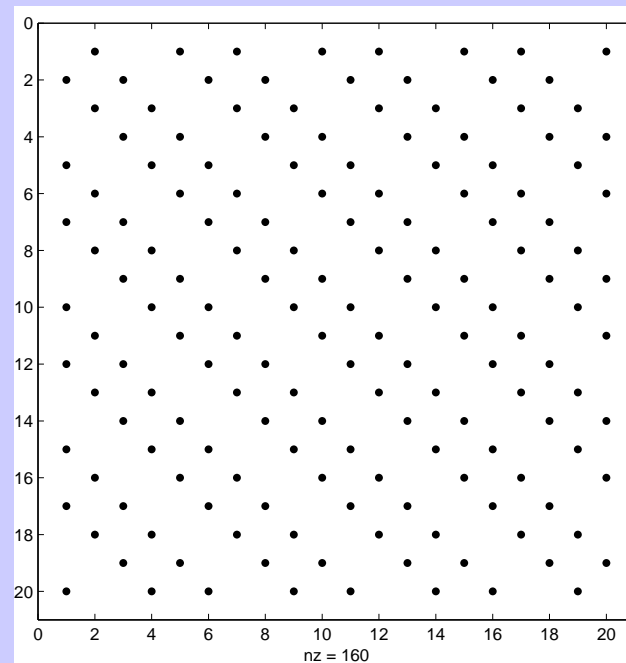
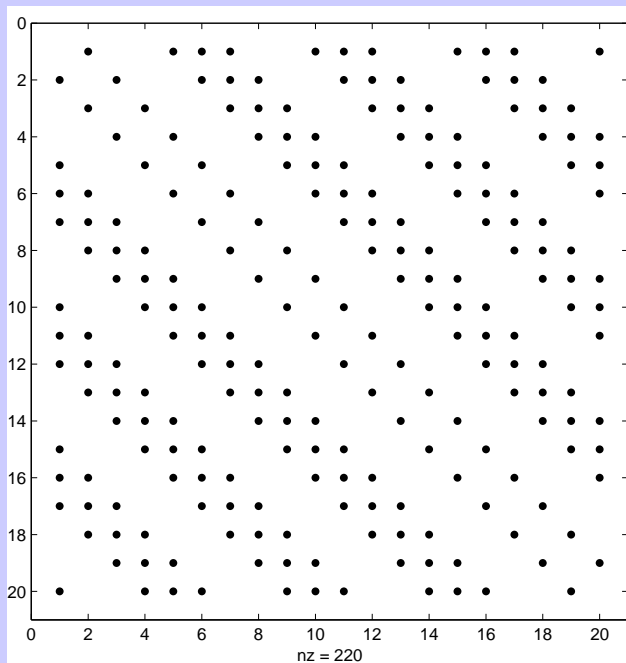
and go back to step 1.

## First Example

$C_5$  ... 5-cycle,  $K_r$  ... complete graph of size  $r$

$\mathcal{G}_r := K_r * C_5$  ... direct product, i.e.

$$A_{\mathcal{G}_r} = A_{K_r} \otimes I_5 + E_r \otimes A_{C_5}$$



Adjacency of  $\mathcal{G}_4$  and the corresponding cut-matrix  $\mathcal{H}_4$

## First example, continued

Well known:

$$\theta'(C_5) = \sqrt{5}, \quad \omega(C_5) = 2$$

Easy to prove:

$$\theta'(K_r * C_5) = \sqrt{5} r, \quad \omega(K_r * C_5) = 2r$$

Algorithm delivers for small  $r$ :

$$\theta^{\mathcal{H}_r}(K_r * C_5) = 2r$$

Result can be proven for all  $r$ , if  $\mathcal{H}_r$  defined via  $A_{\mathcal{H}_r} := E_r \otimes A_{C_5}$ .

Example where cutting with a triangle free graph gives arbitrary large improvement of  $\theta'$ , so that even  $\lfloor \theta' \rfloor \gg \theta^{\mathcal{H}}$ .

## Graph cosums for systematic test generation

Direct sum of  $\mathcal{G}_1 = (V_1, \mathcal{E}_1)$  and  $\mathcal{G}_2 = (V_2, \mathcal{E}_2)$  with  $V_1 \cap V_2 = \emptyset$ :

$$\mathcal{G} = (V_1 \cup V_2, \mathcal{E}_1 \cup \mathcal{E}_2), \quad A_{\mathcal{G}} = \begin{pmatrix} A_{\mathcal{G}_1} & O \\ O & A_{\mathcal{G}_2} \end{pmatrix}.$$

**Cosum:** complement of direct sum of complements,

$$Q_{\mathcal{G}_1 \oplus \mathcal{G}_2} = \begin{pmatrix} Q_{\mathcal{G}_1} & O \\ O & Q_{\mathcal{G}_2} \end{pmatrix}$$

(recall  $Q_{\mathcal{G}} = I + A_{\overline{\mathcal{G}}}$ ). Then  $\omega(\mathcal{G}_1 \oplus \mathcal{G}_2) = \omega(\mathcal{G}_1) + \omega(\mathcal{G}_2)$  and

**Theorem:**  $\theta'(\mathcal{G}_1 \oplus \mathcal{G}_2) = \theta'(\mathcal{G}_1) + \theta'(\mathcal{G}_2)$ .

Thus: increase gap  $\theta'(\mathcal{G}) > \omega(\mathcal{G})$  by multiplying:  $\mathcal{G} \oplus \mathcal{G} \cdots \oplus \mathcal{G}$ .

## Graph products for systematic test generation (1)

Direct **co**product of  $\mathcal{G}_1 = (V_1, \mathcal{E}_1)$  and  $\mathcal{G}_2 = (V_2, \mathcal{E}_2)$  with  $V_1 \cap V_2 = \emptyset$ :

$$\mathcal{G}_1 \bar{*} \mathcal{G}_2 = (V = V_1 \times V_2, \mathcal{E} \subseteq \mathcal{E}_1 \times \mathcal{E}_2), \quad Q_{\mathcal{G}_1 \bar{*} \mathcal{G}_2} = Q_{\mathcal{G}_1} \otimes Q_{\mathcal{G}_2},$$

where  $A \otimes B$  is Kronecker (tensor) product of  $A$  and  $B$ .

Direct product  $\mathcal{G}_1 * \mathcal{G}_2$ : complementation,  $\overline{\mathcal{G}_1 * \mathcal{G}_2} = \overline{\mathcal{G}_1} \bar{*} \overline{\mathcal{G}_2}$ , or via

$$A_{\mathcal{G}_1 * \mathcal{G}_2} = (I_{V_1} + A_{\mathcal{G}_1}) \otimes (I_{V_2} + A_{\mathcal{G}_2}) - I_V = I_{V_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes (I_{V_2} + A_{\mathcal{G}_2}).$$

Lexicographic (left) product  $\mathcal{G}_1 \tilde{*} \mathcal{G}_2$ : increase **last term** above,

$$A_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2} := I_{V_1} \otimes A_{\mathcal{G}_2} + A_{\mathcal{G}_1} \otimes E_{V_2}.$$

Immediate:  $A_{\mathcal{G}_1 * \mathcal{G}_2} \leq A_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2} \leq A_{\mathcal{G}_1 \bar{*} \mathcal{G}_2}$ .

## Graph products for systematic test generation (2)

Knuth [1994]:  $\theta(\mathcal{G}_1 * \mathcal{G}_2) = \theta(\mathcal{G}_1 \bar{*} \mathcal{G}_2) = \theta(\mathcal{G}_1)\theta(\mathcal{G}_2)$ .

**Theorem:**  $\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) \leq \theta'(\mathcal{G}_1 * \mathcal{G}_2) \leq \theta'(\mathcal{G}_1 \tilde{*} \mathcal{G}_2) \leq \theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_2)$ .

**Theorem:** *Multiplicativity  $\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) = \theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_2)$  holds if all graphs are vertex-transitive, or if  $\theta(\mathcal{G}_i) = \theta'(\mathcal{G}_i)$ .*

*In latter case, also  $\theta(\mathcal{G}_1 \circ \mathcal{G}_2) = \theta'(\mathcal{G}_1 \circ \mathcal{G}_2)$  for  $\circ \in \{*, \tilde{*}, \bar{*}\}$ .*

Idea of proof: vertex transitivity  $\implies \theta'(\mathcal{G}_i) = n_i/\theta'(\bar{\mathcal{G}}_i)$ ;

for second assertion, apply Knuth's result to obtain

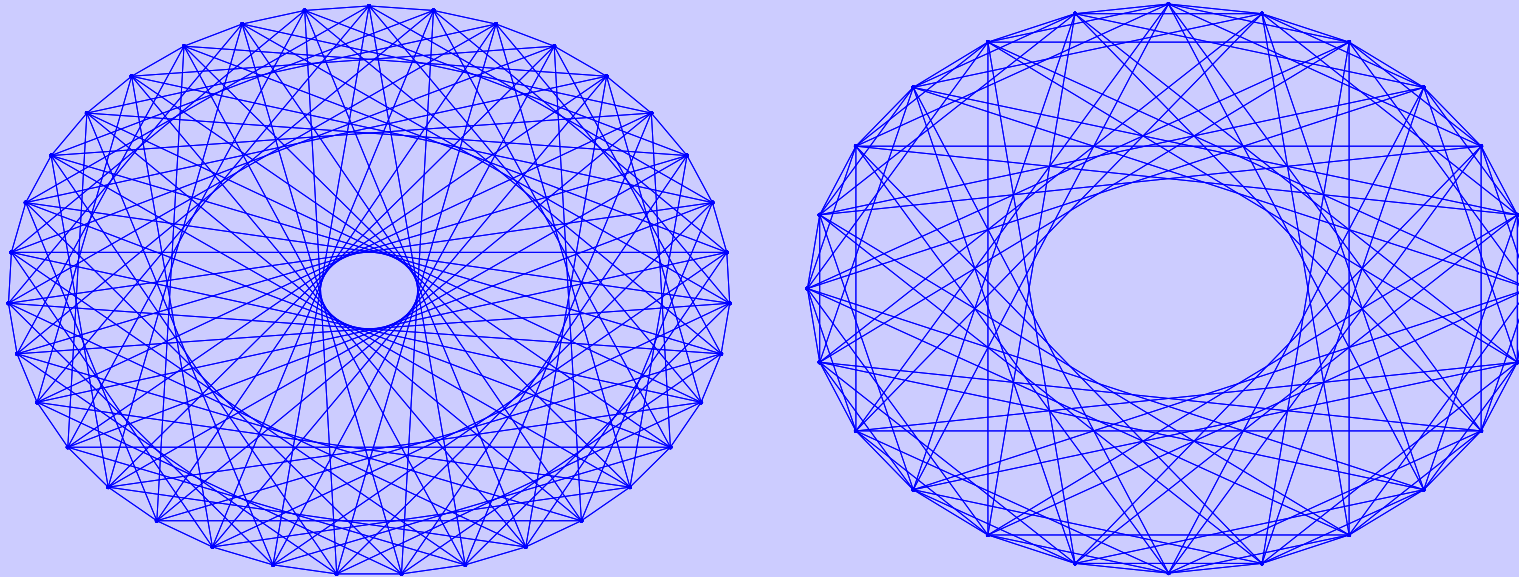
$$\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) = \theta(\mathcal{G}_1)\theta(\mathcal{G}_2) = \theta(\mathcal{G}_1 \bar{*} \mathcal{G}_2) \geq \theta'(\mathcal{G}_1 \bar{*} \mathcal{G}_2) \geq \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2).$$

Again increase gap  $\lfloor \theta' \rfloor > \theta^{\mathcal{H}} \geq \omega$  by  $\mathcal{G} \mapsto K_r * \mathcal{G}$ , in ex.:  $\mathcal{G} = C_5$ .

# Circulant Graphs

Toeplitz graph:  $A_{i,j} = A_{1,|j-i|+1}$

Circulant graph:  $A_{1,j+1} = A_{1,n-j+1}, 1 \leq j \leq n - 1$



Two examples of circulant graphs

## Gap of Schrijver bound for circulant graphs

**Theorem:** If  $\mathcal{G}$  is a circulant graph of order  $n$  with clique number  $\omega := \omega(\mathcal{G}) \geq 2$  and if there exists a **maximum clique**  $S \subseteq V$  such that  $\sum_{j \in S} \xi^j \neq 0$  for any  $n$ -th unitary root  $\xi$ , then  $\theta'(\mathcal{G}) > \omega$ .

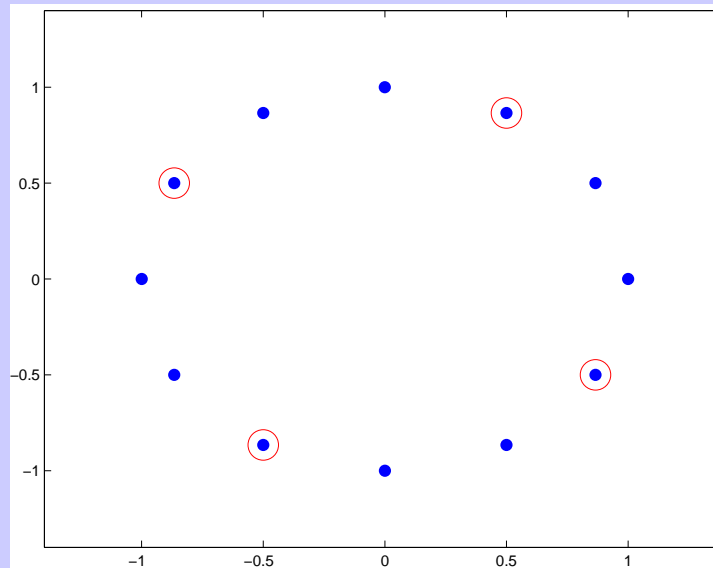
**Remark:** Conditions for

$$\sum_{0 \leq j_1 < \dots < j_\omega < n} \xi^{j_l} = 0$$

are well studied in literature.

E.g., if  $n$  is a prime number then always  $\theta'(\mathcal{G}) > \omega(\mathcal{G})$ .

Other special cases: cycles.

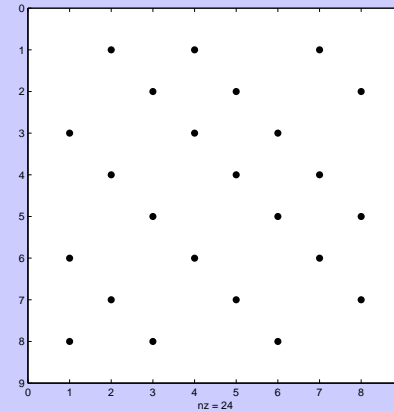


## Idea of proof

Assume  $\theta'(\mathcal{G}) = \omega = \omega(\mathcal{G})$ , then write

$$Q_{\mathcal{G}} - \frac{1}{\omega}E = RR + N, \quad R = R^{\top} \text{ with columns } r_j, \quad N \in \mathcal{N}.$$

If  $S = \{j_1, \dots, j_{\omega}\}$  maximum clique  
 $\Rightarrow S_k := \{[j_1 + k]_n, \dots, [j_{\omega} + k]_n\}$   
 also maximum clique.



Show:  $S$  maximum clique  $\implies \sum_{j \in S} r_j = o$ .

Due to assumption on  $S$  guaranteed that  $[S_0 \dots S_{n-1}]$  full rank

$\implies R = O$ . But then  $Q_{\mathcal{G}} - \frac{1}{\omega}E = N \in \mathcal{N}$ , contradiction!

## Simulation

- 250 random circulant graphs of size 31 and 43
- Triangle free and  $K_4$ -free subgraphs
- Seven choices of  $f(x)$  for the dropping strategy  
 $\exp(x)$  and  $x^d, d = 1, \dots, 6$

Questions:

- Which of the 14 strategies works best?
- Benefit of applying simultaneous cuts?

## Simulation results

$\theta^{C_1}$  Best improvement by one of the 14 cuts

$\theta^{C_2}$  Best improvement by triangle free cut

$\theta^{C_3}$  Best improvement by  $K_4$ -free cut

$\theta^C$  Simultaneous cut with all 14 matrices

Number of instances where certain bounds are actually different

Size	$\theta > \theta'$	$\theta > \theta^C$	$\theta' > \theta^C$	$\theta' > \theta^{C_2}$	$\theta' > \theta^{C_3}$	$\theta^{C_1} > \theta^C$
31	84	164	115	73	76	34
43	158	194	88	59	49	29
Both	242	358	203	132	125	63

## Simulation results - summary

- Whenever  $A_{\mathcal{H}} \bullet X^* > \left(1 - \frac{1}{\omega(\mathcal{H})}\right) E \bullet X^*$  then  $\theta' > \theta^{\mathcal{H}}$
- Strong correlation between values of  $A_{\mathcal{H}} \bullet X^*$  and  $\theta^{\mathcal{H}}$   
But not one to one!
- None of the 14 strategies works best!  
 $K_4$ -free not necessarily better than triangle free  
Different  $f(x)$  work best for different graphs
- Recommendation:  
Use different strategies to obtain several cuts  
(computationally cheap)  
Apply simultaneous cuts

## More results and future research

Already done:

- Further examples based on graph products
- Comparison with other bounds from the literature
- Valid cuts based on cosum decompositions  $\mathcal{H} = \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_p$

Further Research:

- Better heuristics for compound graphs
- Combine with other cheap methods, e.g. triangle inequalities – Dukanović/Rendl [2006]