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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

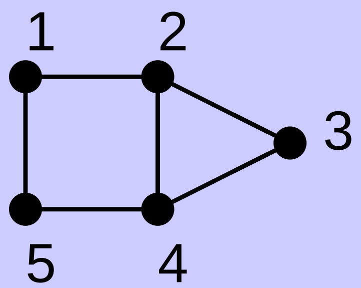
➢ Circulant graphs and gaps

➢ Experimental results and outlook

Maximum Clique Problem

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

loopless, undirected, unweighted



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 $\omega(\mathcal{G})$ ... size of maximum clique

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

Standard Quadratic Problem (StQP) formulation

Motzkin/Straus [1965]:

Let $Q_{\mathcal{G}} := E - A_{\mathcal{G}}$, where $e = [1, \dots, 1]^\top$, $E = ee^\top$,

then

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

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

Equivalent copositive program (COP):

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

Copositive matrices cone $\mathcal{C} = \left\{C : x^\top C x \geq 0 \text{ for all } x \in \mathbb{R}^n_+\right\}$
contains psd matrices cone $\mathcal{P} = \left\{P : x^\top P x \geq 0 \text{ for all } x \in \mathbb{R}^n\right\}$
and positive matrices cone $\mathcal{N} = \{N : N_{ij} \geq 0 \text{ for all } i, j \in V\}$.

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 θ'

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 $A \bullet B = \mathrm{trace}(AB)$:

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

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

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

Copositivity Cuts

For a set $\{C_1, \ldots, C_m\}$ 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

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

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) ω_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

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

$f(x) \ldots$ 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 $\{i', j'\} \in \underset{\{i,j\} \in \mathcal{E}_{\mathcal{H}}}{\operatorname{argmin}} \left\{ \frac{X^*_{i,j}}{f(T_{i,j})} \right\}$.

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

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

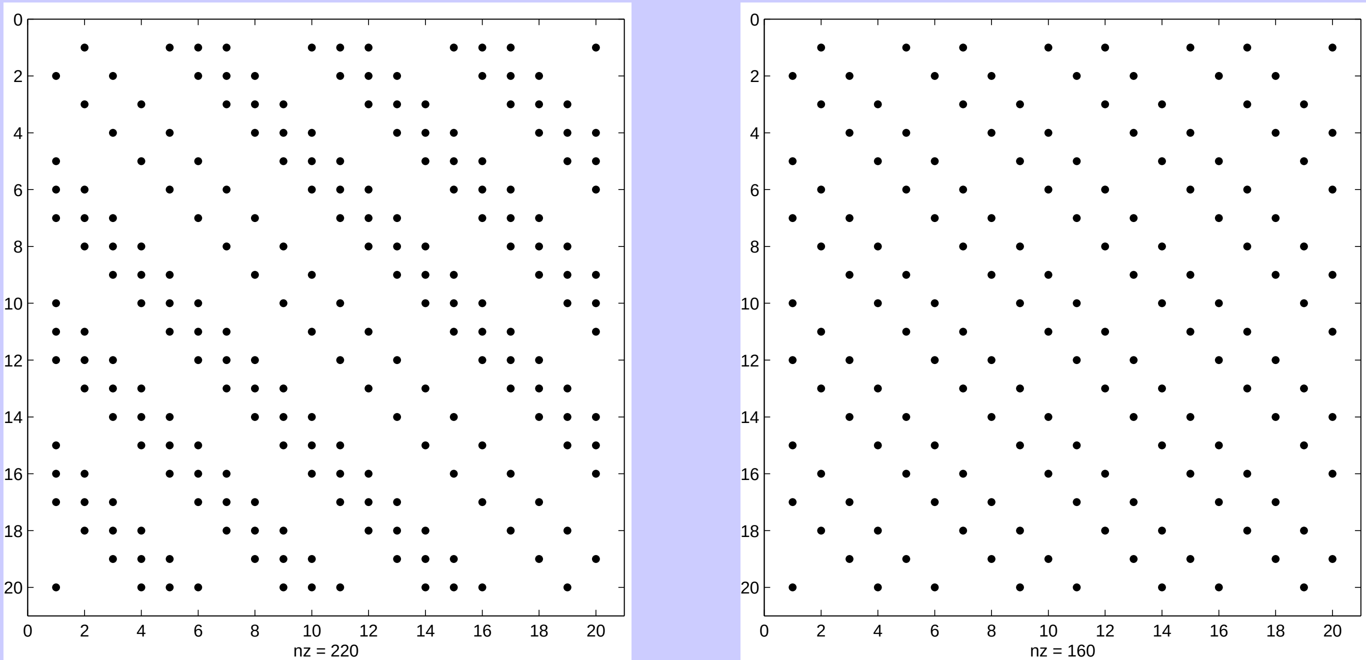
and go back to step 1.

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:

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

Easy to prove:

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

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

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

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

Direct product $\mathcal{G}_1 * \mathcal{G}_2$: complementation, $\overline{\mathcal{G}_1 * \mathcal{G}_2} = \overline{\mathcal{G}_1} \,\overline{*}\, \overline{\mathcal{G}_2}$, 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: $$A_{\mathcal{G}_1 * \mathcal{G}_2} \leq A_{\mathcal{G}_1 \tilde{*} \mathcal{G}_2} \leq A_{\mathcal{G}_1 \overline{*} \mathcal{G}_2}\,.$$

Graph products for systematic test generation (2)

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

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

Theorem: *Multiplicativity $\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) = \theta'(\mathcal{G}_1 \overline{*} \mathcal{G}_2)$ 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 $\circ \in \{*, \tilde{*}, \overline{*}\}$.*

Idea of proof: vertex transitivity $\implies$ $\theta'(\mathcal{G}_i) = n_i / \theta'(\overline{\mathcal{G}_i})$;
for second assertion, apply Knuth's result to obtain

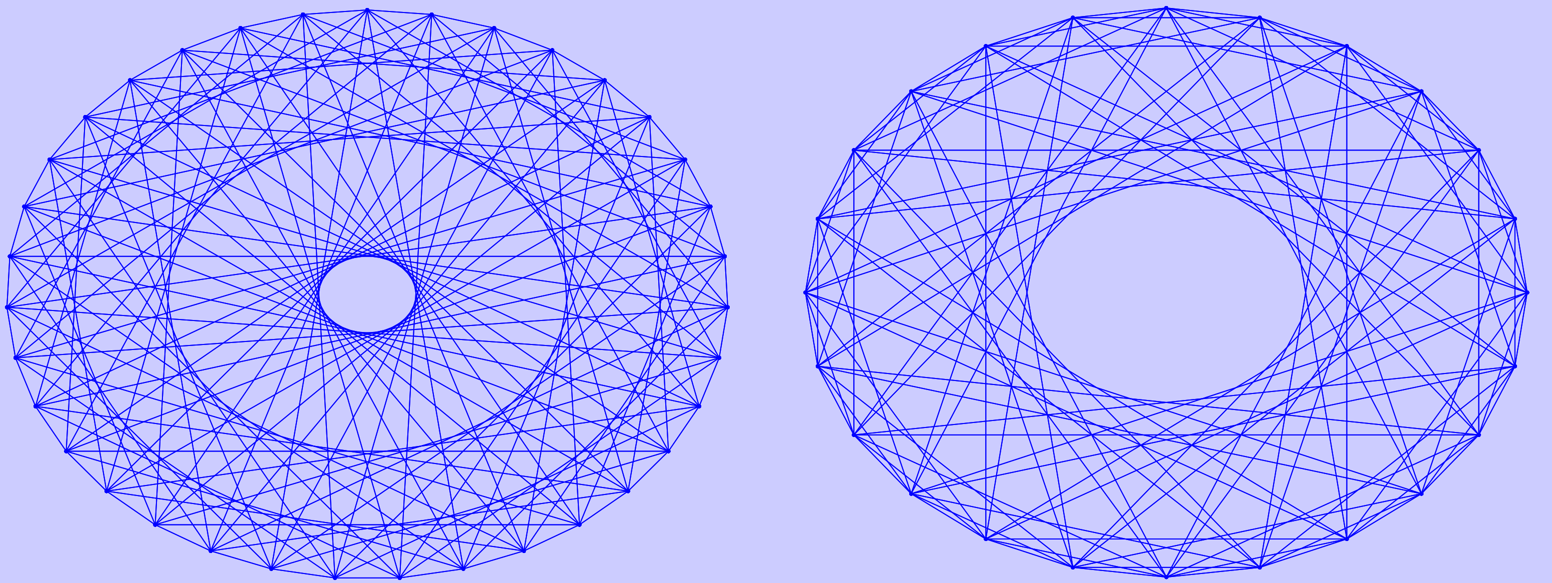
$$\theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2) = \theta(\mathcal{G}_1)\theta(\mathcal{G}_2) = \theta(\mathcal{G}_1 \overline{*} \mathcal{G}_2) \geq \theta'(\mathcal{G}_1 \overline{*} \mathcal{G}_2) \geq \theta'(\mathcal{G}_1)\theta'(\mathcal{G}_2).$$

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

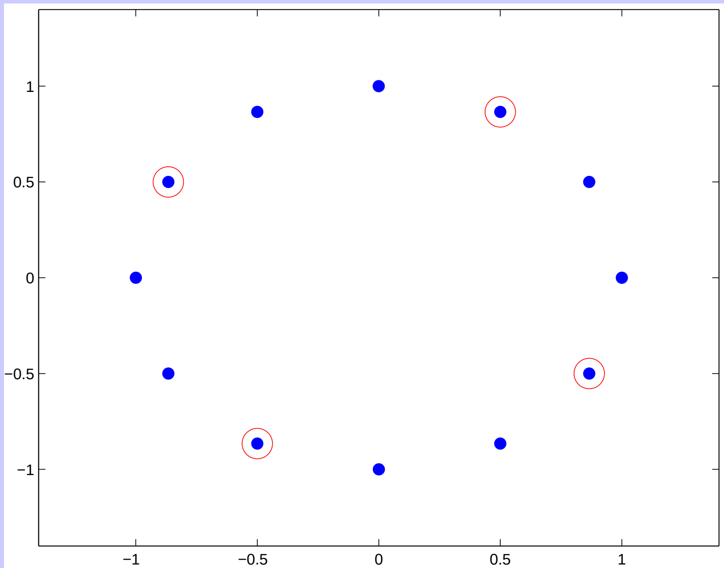
Theorem: *If $\mathcal{G}$ is a circulant graph of order n with clique number $\omega := \omega(\mathcal{G}) \geq 2$ and if there exists a maximum clique $S \subseteq V$ such that $\sum_{j \in S} \xi^j \neq 0$ for any n-th unitary root ξ, then $\theta'(\mathcal{G}) > \omega$.*

Remark: Conditions for

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

are well studied in literature.

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



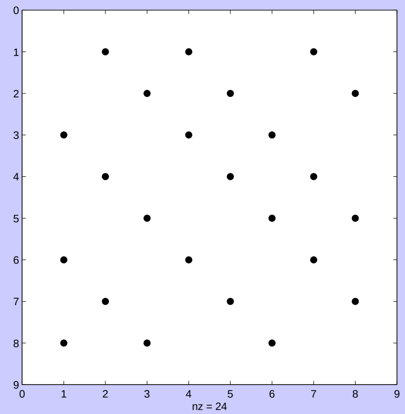
Other special cases: cycles.

Idea of proof

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

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

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



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

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

$\Longrightarrow \quad R = O$. 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 $x^d, d = 1, \ldots, 6$

Questions:

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

Simulation results

θ^{C_1}	Best improvement by one of the 14 cuts
θ^{C_2}	Best improvement by triangle free cut
θ^{C_3}	Best improvement by K_4-free cut
θ^{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]