Problems and Results Motivated by Efficient Computation of the Independence Number

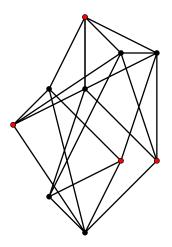
Craig Larson

Virginia Commonwealth University Richmond, VA

The University of Gent Feb. 22, 2013

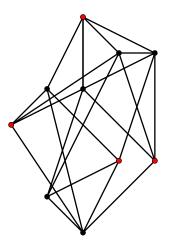
I. Introduction, Applications, Complexity

The Independence Number of a Graph



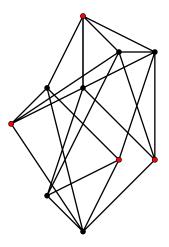
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The Independence Number of a Graph



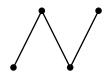
• The independence number α of a graph is the largest number of mutually non-adjacent vertices.

The Independence Number of a Graph



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Independent Sets and Chemical Properties



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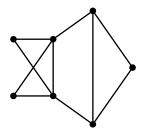
Independent Sets and Chemical Properties



The number of independent sets σ correlates both with alkane heats of formation and boiling points.

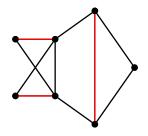
• R. Merrifield and H. Simmons, The Structure of Molecular Topological Spaces, *Theoretica Chimica Acta*, 1980.

The matching number of a graph



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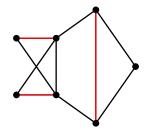
The matching number of a graph



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Let M = red.

The matching number of a graph



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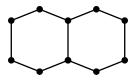
Let M=red. M is a maximum matching, and $\mu = 3$.

Molecular Stability



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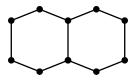
Molecular Stability



Stable benzenoids maximize their matching number



Molecular Stability



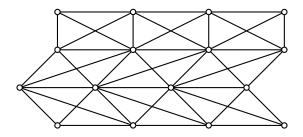
- Stable benzenoids maximize their matching number
- and minimize their independence number.
- R. Pepper, An upper bound on the independence number of benzenoid systems, *Discrete Applied Mathematics*, 2008.

Which Fullerene Isomers are Stable?

| Atoms | lsomer | # of Isomers | α | Rank | Max | Min |
|-------|--|--------------|----------|--------|-----|-----|
| 60 | $C_{60}:1(I_h)$ | 1812 | 24 | 1 | 28 | 24 |
| 70 | $C_{70}:1 (D_{5h})$ | 8149 | 29 | 1 | 33 | 29 |
| 76 | $C_{76}:1(D_2)$ | 19151 | 32 | 1 | 36 | 32 |
| 78 | $C_{78}:1(D_3)$ | 24109 | 33 | 1 (3) | 37 | 33 |
| | $C_{78}:3(C_{2v})$ | | 34 | 2 | | |
| | $C_{78}:2(C_{2v})$ | | 33 | 1 (3) | | |
| 84 | $C_{84}:22 (D_2)$ | 51592 | 36 | 1 (17) | 40 | 36 |
| | C ₈₄ :23 (D _{2d}) | | 36 | 1 (17) | | |

• S. Fajtlowicz, and C. E. Larson, Graph-theoretic Independence as a Predictor of Fullerene Stability, *Chemical Physics Letters*, 2003.

Shannon Capacity



• The zero-error capacity of a alphabet is $\lim \sqrt[n]{\alpha(G^n)}$.

• C. Shannon, The zero error capacity of a noisy channel, *IRE Transactions on Information Theory*, 1956.

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Optimal Communication Networks



• G. Brinkmann, S. Crevals, J. Frye, An independent set approach for the communication network of the GPS III system, *Discrete Applied Mathematics*, 2013.

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• Domination number: $\gamma \leq \alpha$



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• Chromatic number: $\alpha \chi \ge n$

- Domination number: $\gamma \leq \alpha$
- Clique Covering number: $\alpha \leq \bar{\omega}$
- Chromatic number: $\alpha \chi \ge n$
- Matching number: $n 2\mu \le \alpha \le n \mu$.

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• Clique Number: $\alpha(G) = \omega(\overline{G})$.

- Domination number: $\gamma \leq \alpha$
- Clique Covering number: $\alpha \leq \bar{\omega}$
- Chromatic number: $\alpha \chi \ge n$
- Matching number: $n 2\mu \le \alpha \le n \mu$.

- Clique Number: $\alpha(G) = \omega(\overline{G})$.
- Covering Number: $\alpha = n \tau$.

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- ▶ Robson's algorithm is the fastest existing analyzed algorithm and runs in O(2^{.276n}).
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- ► New general algorithms may be faster San Segundo's BBMC.
 - J. M. Robson, Algorithms for Maximum Independent Sets, Journal of Algorithms 7 (1986) 425–440.

P. Östergård, A fast algorithm for the maximum clique problem, Discrete Applied Mathematics 120 (2002) 197–207.
P. San Segundo, An improved bit parallel exact maximum clique algorithm, *Optimization Letters*, 2011.

Independence number is NP-hard

The Independent Set Decision Problem:

Given a graph G and an integer k, does G have an independent set of size at least k?

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R. M. Karp, Reducibility Among Combinatorial Problems, Complexity of Computer Computations, 1972, 85–103.
M. Garey and D. Johnson, Computers and Intractability, W. H. Freeman and Company, New York, 1979.

Does P=NP?

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"My hunch is that P=NP, contrary to general belief."

• B. Bollobás, The Future of Graph Theory, Quo Vadis, Graph Theory?, 1993, 5–11 .

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II. A Structural Result

A König-Egervary graph (or KE graph) is a graph where $\alpha + \mu = n$.



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$$\alpha = 2$$
, $\mu = 2$, $n = 4$.

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A König-Egervary graph (or KE graph) is a graph where $\alpha + \mu = n$.

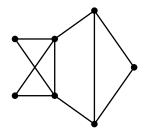


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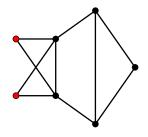
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$$\alpha = 2$$
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$$\bullet \ \alpha + \mu = \mathbf{n}.$$

The critical difference d is the maximum value of |I| - |N(I)|, for all independent sets I. An independent set I_c which realizes d is a critical independent set.

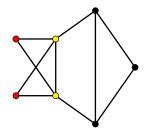


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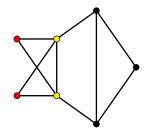
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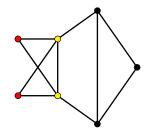
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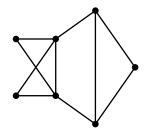


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Let I_c =red vertices, then $N(I_c)$ =yellow vertices, and $|I_c| - |N(I_c)| = 0$. The critical difference d is the maximum value of |I| - |N(I)|, for all independent sets I. An independent set I_c which realizes d is a critical independent set.

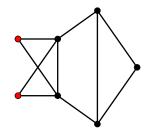


Let I_c =red vertices, then $N(I_c)$ =yellow vertices, and $|I_c| - |N(I_c)| = 0$. d = 0 and I_c is a critical independent set. A maximum critical independent set is an independent set which realizes the critical difference *d* and has maximum cardinality.



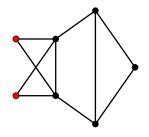
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Let $I_c = red$ vertices,

 I_c is a maximum cardinality critical independent set.

Theorem: For any graph G, there is a unique set $X \subseteq V(G)$ such that

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1.
$$\alpha(G) = \alpha(G[X]) + \alpha(G[X^c]),$$

Theorem: For any graph G, there is a unique set $X \subseteq V(G)$ such that

- 1. $\alpha(G) = \alpha(G[X]) + \alpha(G[X^c]),$
- 2. *G*[*X*] is KE,

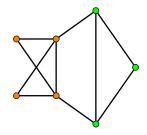
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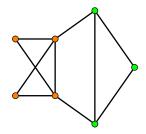
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- 3. $G[X^c]$ has the property that every non-empty independent set I has more than |I| neighbors, and

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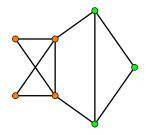
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- 4. for every maximum critical independent set J_c of G, $X = J_c \cup N(J_c)$.
- L., The Critical Independence Number and an Independence Decomposition, *European Journal of Combinatorics*, 2011.





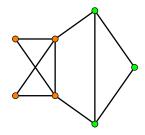
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► X is orange, X^c is green,

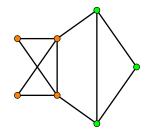


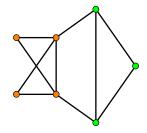
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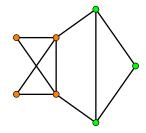
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•
$$\alpha(G) = \alpha(G[X]) + \alpha(G[X^c]) = 3.$$



- $\alpha(G) = \alpha(G[X]) + \alpha(G[X^c]) = 3.$
- Every graph decomposes into a KE graph and a graph where every independent set *I* has more than |*I*| neighbors.

For every v_i in $V = \{v_1, v_2, ..., v_n\}$, let $w(v_i) \in \{0, 1\}$,

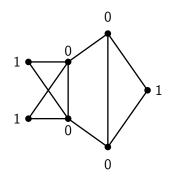
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 in $V = \{v_1, v_2, \ldots, v_n\}$, let $w(v_i) \in \{0, 1\}$,

Constraints: $w(v_i) + w(v_j) \le 1$ if v_i is adjacent to v_j

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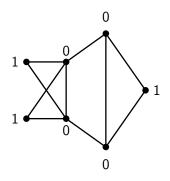
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$$\alpha = \max \sum w(v_i).$$

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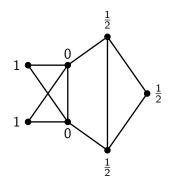
For every v_i in $V = \{v_1, v_2, ..., v_n\}$, let $w(v_i) \in [0, 1]$,

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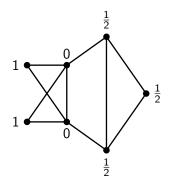
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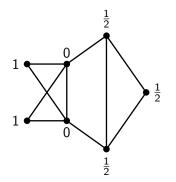


$$\alpha \leq \max \sum w(v_i).$$

A Useful Result

Theorem

(Balinsky, 1965) There is an optimal solution to VPLP with weights $w(v_i) \in \{0, 1, \frac{1}{2}\}$.

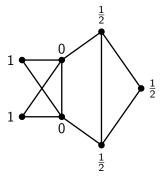


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 $\max \sum w(v_i) = 3.5.$

• G. L. Nemhauser and L. E. Trotter, "Properties of vertex packing and independence system polyhedra," in *Mathematical Programming*, 1974.

Picard-Queyranne Theorem

Theorem

(*Picard*, *Queyranne*) There are a unique maximal set of variables which are integral in optimal VPLP solutions.

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Picard-Queyranne Theorem

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(*Picard*, *Queyranne*) There are a unique maximal set of variables which are integral in optimal VPLP solutions.

Theorem

(Picard, Queyranne) If V_0 , V_1 , $V_{\frac{1}{2}}$ and V'_0 , V'_1 , $V'_{\frac{1}{2}}$ are optimal solutions with a maximum number of integral variables, then $V_0 \cup V_1 = V'_0 \cup V'_1$.

• J-C. Picard, M. Queyranne, "On the Integer-Valued Variables in the Linear Vertex Packing Problem", *Mathematical Programming*, 1977.

For a optimal solution V_0 , V_1 , $V_{\frac{1}{2}}$ of VPLP, and a critical independent set I_c , ...

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For a optimal solution V_0 , V_1 , $V_{\frac{1}{2}}$ of VPLP, and a critical independent set I_c , ...

1.
$$|V_0| + |V_1| + |V_{\frac{1}{2}}| = |I_c| + |N(I_c)| + |(I_c \cup N(I_c))^c|.$$

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2. $V_0 = N(V_1).$
3. $|I_c| - |N(I_c)| \ge |V_1| - |V_0|.$

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Optimal Solutions give Critical Independent Sets

Let V_0 , V_1 , $V_{\frac{1}{2}}$ be a feasible solution of VPLP with $N(V_1) = V_0$, and I_c be a critical independent set, ...

Theorem

 $V_0, V_1, V_{\frac{1}{2}}$ is an optimal solution of VPLP if, and only if, V_1 is a critical independent set.

Theorem

 $V_0, V_1, V_{\frac{1}{2}}$ is an optimal solution with a maximum number of integral variables if, and only if, V_1 is a maximum critical independent set.

Corollary

If V_0 , V_1 , $V_{\frac{1}{2}}$ is an optimal solution with a maximum number of integral variables then $V_0 \cup V_1 = X$, from IDT.

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Corollary

(Picard, Queyranne) There are a unique maximal set of variables which are integral in optimal VPLP solutions.

Corollary

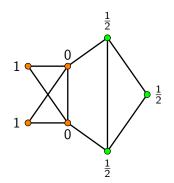
If V_0 , V_1 , $V_{\frac{1}{2}}$ is an optimal solution with a maximum number of integral variables then $V_0 \cup V_1 = X$, from IDT.

Corollary

(Picard, Queyranne) There are a unique maximal set of variables which are integral in optimal VPLP solutions.

Corollary

(Edmonds, L.) Picard-Queyranne Decomposition = Independence Decomposition



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An independent set *I* is separable if

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1. $X = I \cup N(I)$,

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$$X^{c} = V - X$$
, and

An independent set *I* is separable if

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3. $\alpha(G) = |I| + \alpha(G[X^c]).$

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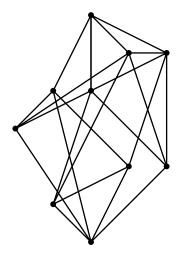
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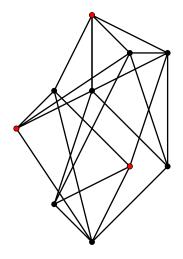
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$$X^{c} = V - X$$
, and

3. $\alpha(G) = |I| + \alpha(G[X^c]).$

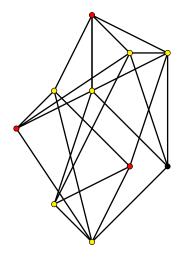
Note: critical independent sets are separable independent sets.

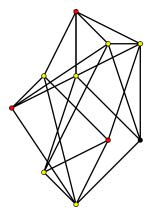


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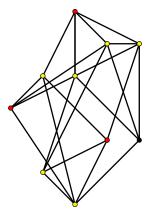
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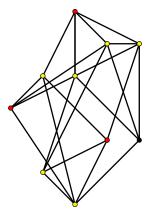
1. I = Red, N(I) = Yellow



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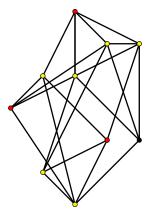
1.
$$I = \text{Red}, N(I) = \text{Yellow}$$

2. $X = I \cup N(I),$



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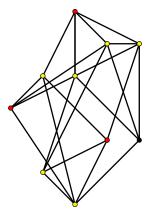
1. I = Red, N(I) = Yellow2. $X = I \cup N(I),$ 3. $X^c = \text{Black}, \text{ and}$



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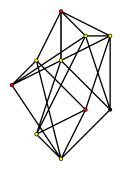
1.
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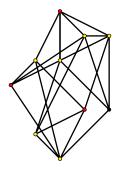
2. $X = I \cup N(I),$
3. $X^c = \text{Black}, \text{ and}$
4. $4 = \alpha(G) = |I| + \alpha(G[X^c]) = 3 + 1.$



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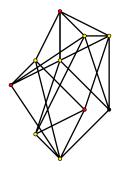
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How to Efficiently Identify Separable Independent Sets?

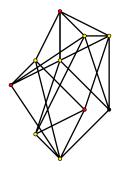
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How to Efficiently Identify Separable Independent Sets?

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What kinds of separable independent sets are there?



How to Efficiently Identify Separable Independent Sets?

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- What kinds of separable independent sets are there?
- Which kinds can be identified efficiently?

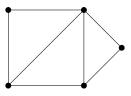
III. Efficient Computation of the Independence Number

For claw-free graphs.



• G. Minty, On maximal independent sets of vertices in claw-free graphs, Journal of Combinatorial Theory. Series B, 28 (1980) 284–304.

For perfect graphs.



• M. Chudnovsky, G. Cornuéjols, X. Liu, P. Seymour, K. Vušković, Recognizing Berge graphs, Combinatorica 25 (2005) 143–186.

For Bipartite and König-Egerváry graphs:



• König, Egerváry, 1931; Kuhn, 1955; Deming, Sterboul, 1979.

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1. P_4 -free

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- 2. (C₄, 2K₂)-free (Hertz, 1997)

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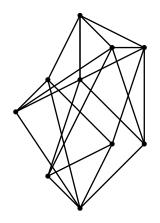
12. (P₅, bull)-free (De Simone, 1993)

- 1. P₄-free
- 2. (C₄, 2K₂)-free (Hertz, 1997)
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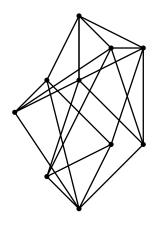
- 12. (*P*₅, bull)-free (De Simone, 1993)
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- 12. (P₅, bull)-free (De Simone, 1993)
- 13. (P₅,house)-free (Hoang, 1983)
- 14. (P₅,gem)-free (Mosca, 1997; Brandstädt, Kratsch, 2001)

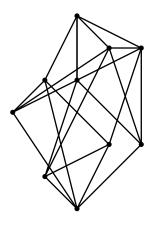
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- 15. $(P_5, K_4 e)$ -free (Arbib, Mosca, 2002; Brandstädt, 2004)



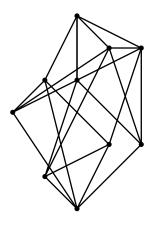
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Find New Forbidden Subgraph Characterizations

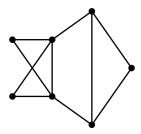


- Find New Forbidden Subgraph Characterizations
- Is it true that the independence number of P₅-free graphs can be computed efficiently?

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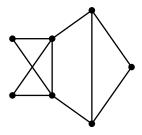
When l(G) = u(G), for an efficiently computable lower bound $l \le \alpha$ and efficiently computable upper bound $\alpha \le u$.

Given a graph G with degree sequence (d) the residue is the number of zeros at the result of the Havel-Hakimi process.



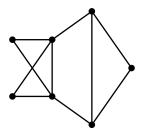
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Given a graph G with degree sequence (d) the residue is the number of zeros at the result of the Havel-Hakimi process.



▶ 4, 4, 3, 3, 2, 2, 2.

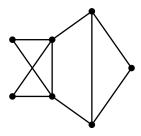
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- ► 4, 4, 3, 3, 2, 2, 2.
- ▶ 0,0,0.
- ► *R* = 3.

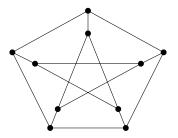
 $R \leq \alpha$ Graffiti, 1988; Favaron, Maheo, Sacle, 1991; Griggs, Kleitman, 1994.

Cvetkovíc Eigenvalues Bound

• Cvetkovic bound: $\alpha \leq \min\{\# \text{ of non-negative eigenvalues}, \# \text{ of non-positive eigenvalues}\}$

Cvetkovíc Eigenvalues Bound

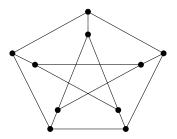
• Cvetkovic bound: $\alpha \leq \min\{\# \text{ of non-negative eigenvalues}, \# \text{ of non-positive eigenvalues}\}$



• Eigenvalues: 3, 1, 1, 1, 1, 1, -2, -2, -2, -2.

Cvetkovíc Eigenvalues Bound

• Cvetkovic bound: $\alpha \leq \min\{\# \text{ of non-negative eigenvalues}, \# \text{ of non-positive eigenvalues}\}$



- Eigenvalues: 3, 1, 1, 1, 1, 1, -2, -2, -2, -2.
- α ≤ 4.
- D. Cvetković, M. Doob, and H. Sachs, Spectra of Graphs, 3rd ed., 1995.



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• $2 = Residue \le \alpha \le Cvetkovic = 2$



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•
$$2 = Residue \le \alpha \le Cvetkovic = 2$$

• Independence Number Theory implies $\alpha = 2$.

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For connected graphs with minimum degree \geq 3 and maximum degree \leq n-2,

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• Residue predicts α for 6 out of 8 graphs of order 6.

For connected graphs with minimum degree \geq 3 and maximum degree \leq n - 2,

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- Residue predicts α for 38 out of 88 graphs of order 7.

For connected graphs with minimum degree \geq 3 and maximum degree \leq n - 2,

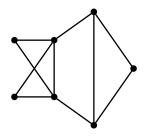
- Residue predicts α for 6 out of 8 graphs of order 6.
- Residue predicts α for 38 out of 88 graphs of order 7.
- Residue predicts α for 411 out of 2079 graphs of order 8.

For connected graphs with minimum degree \geq 3 and maximum degree \leq n - 2,

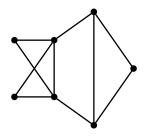
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- Residue predicts α for 11620 out of 76783 graphs of order 9.

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- Residue predicts α for 11620 out of 76783 graphs of order 9.
- \blacktriangleright Residue predicts α for 501793 out of 5005243 graphs of order 10



$$\alpha = residue = 3$$



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• Characterize the Graphs where $\alpha = residue$

Lovász Theta Function

• The Lovász number of a graph G is:

$$\vartheta(G) = \max[1 - \frac{\lambda_1(A)}{\lambda_n(A)}]$$

over all real matrices A with $a_{ij} = 0$ if $v_i \sim v_j$ in G, with eigenvalues $\lambda_1(A) \geq \ldots \lambda_n(A)$

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 $\alpha \leq \vartheta = 4$

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 $\alpha \leq \vartheta = \mathbf{4}$

• L. Lovász, On the Shannon capacity of a graph, *IEEE Transactions on Information Theory*, 1979.

• D. Knuth, The sandwich theorem, Electronic Journal of Combinatorics 1 (1994).

For all simple graphs,



For *all* simple graphs,

• ϑ predicts α for 34 out of 34 graphs of order 5.

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For *all* simple graphs,

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- ϑ predicts α for 156 out of 156 graphs of order 6.

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- ϑ predicts α for 34 out of 34 graphs of order 5.
- ϑ predicts α for 156 out of 156 graphs of order 6.
- ϑ predicts α for 1044 out of 1044 graphs of order 7.

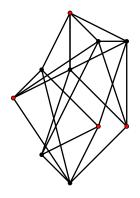
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- ϑ predicts α for 12346 out of 12346 graphs of order 8.

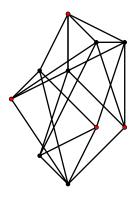
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- ϑ predicts α for 274668 out of 274668 graphs of order 9.

Problem 4



Problem 4



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• Characterize Graphs Where $\alpha = Lovász$ Theta.

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1. Residue Lower Bound

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- 1. Residue Lower Bound
- 2. Cvetkovic Upper Bound

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- 3. Lovász Theta Upper Bound

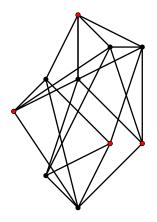
- 1. Residue Lower Bound
- 2. Cvetkovic Upper Bound
- 3. Lovász Theta Upper Bound
- 4. Even minus Even Horizontal Lower Bound

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- 1. Residue Lower Bound
- 2. Cvetkovic Upper Bound
- 3. Lovász Theta Upper Bound
- 4. Even minus Even Horizontal Lower Bound
- 5. Fractional Independence Upper Bound

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- 2. Cvetkovic Upper Bound
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- 4. Even minus Even Horizontal Lower Bound
- 5. Fractional Independence Upper Bound
- 6. 50 Efficiently Computable Bounds are Known

Problem 5



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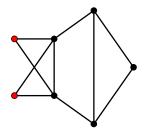
Find More Efficiently Computable Bounds for α .

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• When the graph has a vertex v of degree n - 1, and α of G - N[v] can be computed efficiently. (So $\alpha(G) = \alpha(G - N[v])$)

- ▶ When the graph has a vertex v of degree n 1, and α of G N[v] can be computed efficiently. (So $\alpha(G) = \alpha(G N[v])$)
- When the graph has twin vertices v and w (that is, N[v] = N[w]) and α of G − v can be computed efficiently. So α(G) = α(G − v)).

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- When the graph has a simplicial vertex (that is, a vertex v, where N[v] is complete. So α(G) = α(G − v)).



When G has a non-empty critical independent set, and α of $G[X^c]$ can be computed efficiently.

 \bullet L., A note on critical independence reductions, Bulletin of the ICA 51 (2007) 34–46.

G is α -reducible if it is possible to efficiently find a smaller order graph *G'* such that $\alpha(G)$ can be computed in terms of $\alpha(G')$.

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- 2. Maximum degree = n 1.
- 3. Has twin vertices.

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- 4. Has a simplicial vertex.

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- 2. Maximum degree = n 1.
- 3. Has twin vertices.
- 4. Has a simplicial vertex.
- 5. Has a non-empty critical independent set.

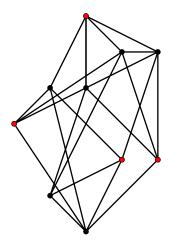
G is α -reducible if it is possible to efficiently find a smaller order graph *G'* such that $\alpha(G)$ can be computed in terms of $\alpha(G')$.

- 1. Is disconnected.
- 2. Maximum degree = n 1.
- 3. Has twin vertices.
- 4. Has a simplicial vertex.
- 5. Has a non-empty critical independent set.
- 6. Has a foldable vertex (Fomin, Grandoni, Kratsch, 2006).

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- 4. Has a simplicial vertex.
- 5. Has a non-empty critical independent set.
- 6. Has a foldable vertex (Fomin, Grandoni, Kratsch, 2006).
- 7. Has a magnet (Leveque, de Werra, 2012).

Problem 6



Find new α -reductions.

IV. The Independence Number Project

Joint Work with Patrick Gaskill

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The main idea is to find the smallest graphs whose independence number cannot be efficiently computed (according to existing Independence Number Theory) and use these graphs to help extend the theory.

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- Then we generated all graphs with n = 5, and checked if:

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- the best upper bound equals the best lower bound.
- Then we generated all graphs with $n = 6, \ldots$
- Then we generated all graphs with $n = 7, \ldots$
- Then we generated all graphs with $n = 8, \ldots$

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- Then we generated all graphs with n = 5, and checked if:
 - they were reducible (and α could be computed in terms of the independence number of a graph with n < 5),

- \blacktriangleright they had an $\alpha\text{-property, or}$
- the best upper bound equals the best lower bound.
- Then we generated all graphs with $n = 6, \ldots$
- Then we generated all graphs with $n = 7, \ldots$
- Then we generated all graphs with $n = 8, \ldots$
- Then we generated all graphs with $n = 9, \ldots$



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It has no n − 1 vertices, no foldable vertices, no simplicial vertices, no magnets, or any other α-reductions,



- But we got stuck at n = 10.
- For this graph (I?bbrr[ko), α = 4 but the best lower bound = 3,
- It has no n − 1 vertices, no foldable vertices, no simplicial vertices, no magnets, or any other α-reductions,
- It has a claw, a bull, a chair, a co-chair, a house, a P₅, a P, a co-P, a gem, and a diamond.



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- It demands new theory.

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1. Characterize of and Efficiently Identify Separable Independent Sets

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3. Efficiently characterize graphs where $\alpha = residue$.

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6. Find new α -reductions, especially one that applies to I?bbrr[ko.

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Sage: sagemath.org



- Sage: sagemath.org
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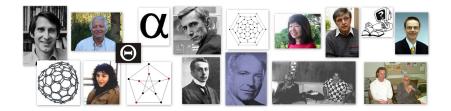
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Thank You!



The Independence Number Project:

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