Some problems and results on Wiener index and related graph parameters

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Based on a survey with Martin Knor and Aleksandra Tepeh

Wiener index

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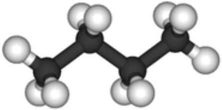

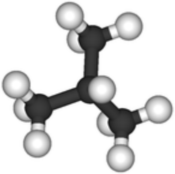

Theorem (Wiener)

For every tree T, it holds

$$W(T) = \sum_{e=uv\in E(T)} n_e(u)\, n_e(v), \tag{1}$$

where $n_e(u)$ is the number of vertices in the component of $T - e$ that contains u, and similarly define $n_e(v)$.

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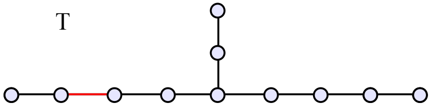

3·(1·10)
3·(2·9)
2·(3·8)
2·(4·7)

W(T)=188

Sections

1. Minimum Wiener index for chemical graphs

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2. Regular graphs vs. diameter

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6. Variable Wiener vs. Variable Szeged

1. Minimum Wiener index for chemical graphs

The forgotten problem

It is well known that

- Minimum and maximum for all graphs: K_n and P_n;
- Minimum and maximum for all trees: S_n and P_n;
- Minimum and maximum for all chemical trees: Dendrimers and P_n;

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- G is almost regular with at most three vertices of degree < 4 and these vertices induce a clique;
- Computer experiments are indicating that G is a 4-regular graph.

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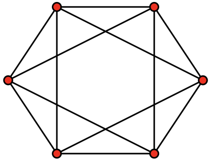

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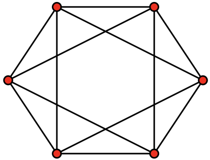
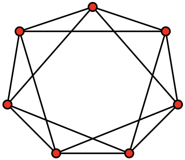
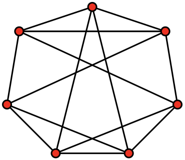


- $n = 7$:

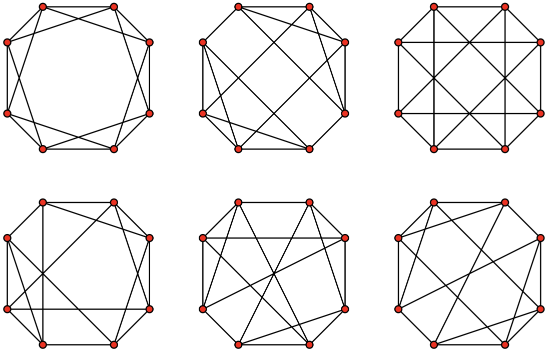




1. Minimum Wiener index for chemical graphs

The conjecture

- $n = 8$: There are 1929 such graphs and minimum Wiener index value is 40, which is attained by only 6 graphs.



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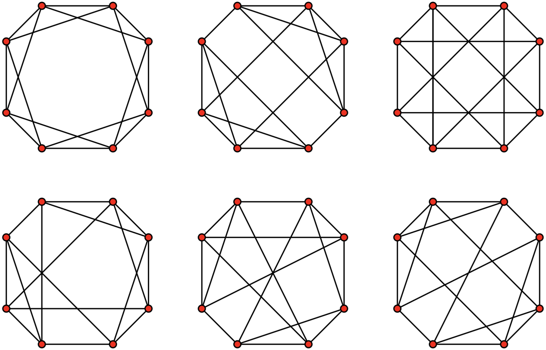

Conjecture

Every chemical graphs G on $n \geq 5$ vertices with the minimum value of Wiener index is 4-regular.

We propose the following conjectures.

Conjecture (The even case conjecture)

Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is even, then G is k-regular.

1. Minimum Wiener index for chemical graphs

Going to higher degrees

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Conjecture (The odd case conjecture)

Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is odd, then G has a unique vertex of degree smaller than k and in that case this smaller degree is $k-1$.

(Probably, it suffices to choose $n_k = k + 1$ therein.)

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Problem (The degree-diameter problem)

Determine the largest order $n(k, d)$ of a graph of (a maximum) degree k and diameter d.

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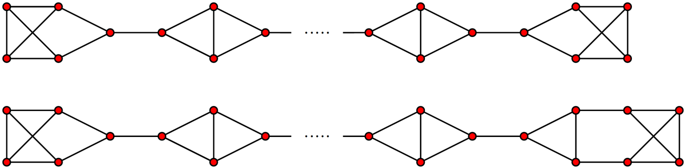

Figure: Graphs L_{4k+2} (above) and L_{4k+4} (below).

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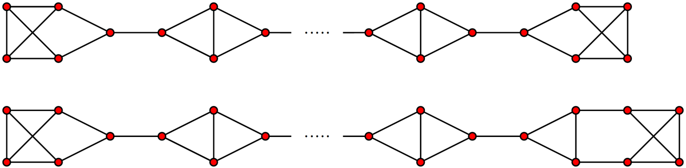

Figure: Graphs L_{4k+2} (above) and L_{4k+4} (below).

Y.-Z. Chen, X. Li, X.-D. Zhang recently confirmed the last conjecture for $r = 3$ with extremal graphs being L_n.

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3. Šoltés problem
The original problem

Math. Slovaca 41, 1991, No. 1, 11—16

TRANSMISSION IN GRAPHS : A BOUND AND VERTEX REMOVING

ĽUBOMÍR ŠOLTÉS

ABSTRACT. The transmission of a graph G is the sum of all distances in G. Strict upper bound on the transmission of a connected graph with a given number of vertices and edges is provided. Changes of the transmission caused by removing a vertex are studied.

1. Introduction

All graphs considered in this paper are undirected without loops and multiple edges. For all terminology on graphs not explained here we refer to [1].

If S is set, then $|S|$ denotes the *cardinality of* S. Given a graph G, $V(G)$ and $E(G)$ denote its *vertex-set* and *edge-set*, respectively. The cardinalities $|v(G)|$ and $|E(G)|$ are often denoted n and m, respectively. If v and w are the vertices of G, then $d_G(v, w)$ or, briefly, $d(v, w)$ denotes *the distance from v to w in G*, $ec_G(v)$ or $ec(v)$ denotes *the eccentricity of* v.

The transmission of a vertex v of a graph G is defined by

$$\sigma_G(v) = \sum_{w \in V(G)} d_G(v, w).$$

3. Šoltés problem
The original problem

of n for $q \leq 1$, then we can restrict ourselves to the case when v is an endvertex (it follows from (Dj)). Hence (4) holds and we immediately get

$$F_f(G, v) = -(2q\sigma(v) + (q-1)\,\sigma(G-v)),$$

which is minimal if and only if G is the path on n vertices. We wil not deal here with further technical details.

Eventually the following unsolved problem is presented.

Problem. Find all such graphs G that the equality $\sigma(G) = \sigma(G-v)$ holds for all their vertices v. We know just one such graph — the cycle on 11 vertices.

REFERENCES

[1] BEHZAD, M.—CHARTRAND, G.—LESNIAK – FOSTER, L.: Graphs and Digrphs. Weber & Schmidt, Boston 1979.

[2] ENTRINGER, R. C. JACKSON, D. E. SNYDER, D. A.: Distance in graphs. Czech Math. J., 26 (101), 1976, 283—296.

[3] [illegible]

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- for each $c \geq 5$, there is a unicyclic graph G with a cycle of length c and a vertex that satisfies the Šoltés property;
- for every graph G there are infinitely many graphs H such that G is an induced subgraph of H and $W(H) = W(H - v)$ for some $v \in V(H) \setminus V(G)$.

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More precisely:

- infinitely many cactus graphs with exactly k cycles of length at least 7 that contain exactly $2k$ vertices satisfying the Šoltés property; and
- infinitely many cactus graphs with exactly k cycles of length 5 or 6 that contain exactly k vertices satisfying the Šoltés property.

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Conjecture

If G is a Šoltés graph, then it is regular.

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If G is a Šoltés graph, then G is vertex-transitive.

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The cycle on eleven vertices is the only Šoltés graph.

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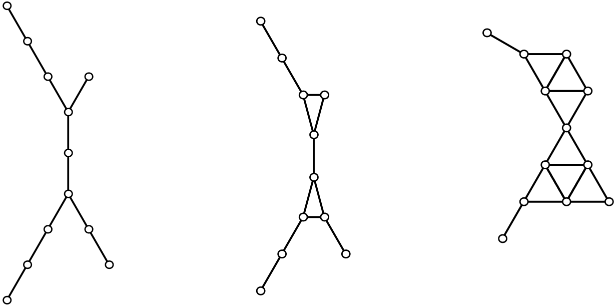

Figure: Graph, its line graph, and its second iterated line graph

4. Ratio of Wiener index of its line graphs

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and explicitly stated the case $k = 1$ as a problem.

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$$\frac{W(L(K_n))}{W(K_n)} = \binom{n-1}{2}.$$

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case $k = 1$

In 2015 this problem was solved for the minimum and $k = 1$.

Theorem (M. Knor, R.Š., A. Tepeh)

Among all connected graphs G on n vertices, the fraction

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is minimum for the star S_n.

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Recently, the same problem was solved for the maximum and $k = 1$.

Theorem (J. Sedlar & R.Š.)

Among all connected graphs G on n vertices, the fraction

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is maximum for K_n.

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Trees & generalization

Theorem (M. Knor, K. Hriňáková, R.Š.)

Let $k \geq 3$. Then the path P_n attains the minimum value of

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Conjecture (M. Knor, K. Hriňáková, R.Š.)

Let n be a large number and $k \geq 2$. Among all graphs G on n vertices,

$$\frac{W(L^k(G))}{W(G)},$$

attains the maximum for K_n, and it attains the minimum for P_n.

4. Ratio of Wiener index of its line graphs

Ghebleh's mail

Mamad Ghebleh <mgh... 23 Jan 2024, 14:42

to hrinakova, knor, me

Dear Professors Hriňáková, Knor, Škrekovski,

Happy new year! I hope this email finds you well. We recently were able to settle your conjecture on the minimum value of the ratio W(L^2(G))/W(G) and submitted the paper few weeks ago. It will probably come to you for refereeing, but nonetheless, we will appreciate any comments you may have on this manuscript (attached).

Sincerely yours,
M. Ghebleh and A. Kanso

4. Ratio of Wiener index of its line graphs

Ghebleh's paper

On the Second-Order Wiener Ratios of Iterated Line Graphs

Mohammad Ghebleh and **Ali Kanso**

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Kuwait University, P.O. Box 5969, Safat 13060, Kuwait

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January 22, 2024

Abstract

The Wiener index $W(G)$ of a graph G is the sum of distances between all unordered pairs of its vertices. Dobrynin and Mel'nikov [in: Distance in Molecular Graphs – Theory, 2012, p. 85–121] propose the study of estimates for extremal values of the ratio $R_k(G) = W(L^k(G))/W(G)$ where $L^k(G)$ denotes the kth iterated line graph of G. Hriňáková, Knor and Škrekovski [Art Discrete Appl. Math. 1 (2018) #P1.09] prove that for each $k \geqslant 3$, the path P_n has the smallest value of the ratio R_k among all trees of large order n, and they conjecture that the same holds for the case $k = 2$. We give a counterexample of every order $n \geqslant 22$ to this conjecture.

5. Wiener index for directed graphs
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In a digraph D here the distances $d_D(u, v)$ and $d_D(v, u)$ may be different. Therefore we sum the distances over ordered pairs of vertices:

$$W(D) = \sum_{(u,v) \in V(D) \times V(D)} d_D(u, v).$$

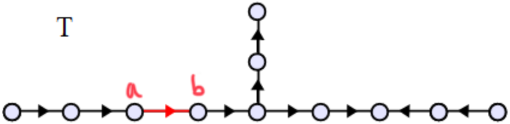
Wiener Theorem for directed graphs

Theorem

Let T be a directed tree with the arc set $A(T)$. Then

$$W(T) = \sum_{ab \in A(T)} t(a)s(b),$$

where $t(a)$ denotes the number of vertices that reach a, and $s(b)$ denotes the number of vertices reachable from b.



3·6 = 18

Wiener index vs. betweenness centrality

The Wiener index - betweenness centrality relation claims that

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Directed graph version:

Theorem

For any digraph D of order n

$$W(D) = \sum_{x \in V(D)} B(x) + p(D),$$

where $p(D)$ denotes the number of ordered pairs (u, v) such that there exists a directed path from u to v in D.

For strongly connected digraphs, $p(D) = 2\binom{n}{2}$.

Some easy facts and results about oriented graphs:

5. Wiener index for directed graphs

Basic properties

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- $W(\overrightarrow{C_n}) = n\binom{n}{2}$ has the maximum Wiener index between all digraphs
- A directed bipartite graph G with bipartition L, R gets its minimum Wiener index if all edges are oriented from L to R.

5. Wiener index for directed graphs
Extremal orientations

Let $W_{\max}(G)$ and $W_{\min}(G)$ be the maximum possible and the minimum possible, respectively, Wiener index among all digraphs obtained by orienting the edges of a graph G.

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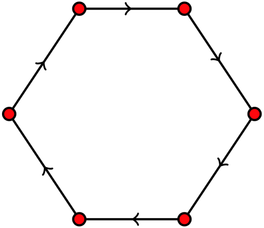

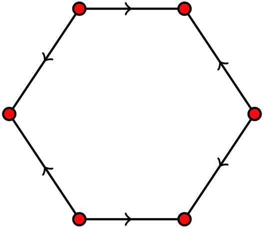

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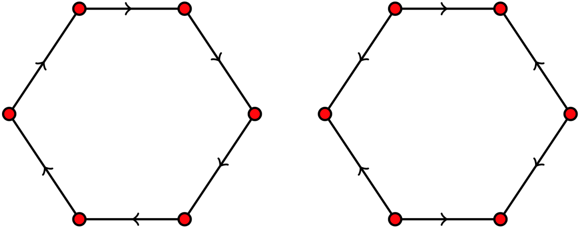

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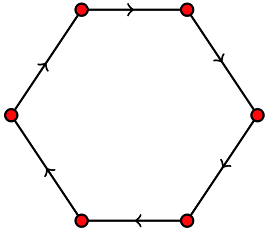

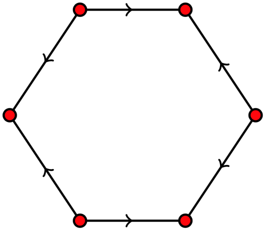

$W_{\max} = 6 \cdot \binom{6}{2} = 90$

$W_{\min} = 6 \cdot 1 = 6$

5. Wiener index for directed graphs
Extremal orientations

Problem

For a given graph G find

$$W_{\max}(G) \quad \textit{and} \quad W_{\min}(G).$$

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Problem

What is the complexity of determing $W_{\max}$ and $W_{\min}$?

5. Wiener index for directed graphs

Extremal orientations

- One may expect that the maximum value $W_{\max}$ is always achieved at some strongly connected orientation.

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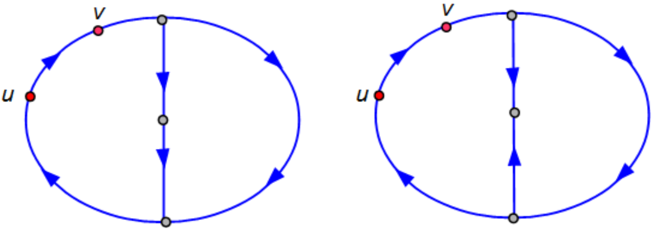

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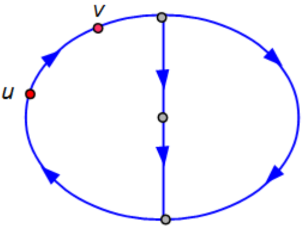

- Maybe, the minimum value $W_{\min}$ is always achieved at some acyclic orientation.

5. Wiener index for directed graphs
Acyclic orientations

For the minimum value, the following may hold:

Conjecture (Acyclic orientation conjecture)

For every graph G, the value $W_{\min}(G)$ is achieved for some acyclic orientation of G.

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Conjecture (Acyclic orientation conjecture)

For every graph G, the value $W_{\min}(G)$ is achieved for some acyclic orientation of G.

This conjecture is true for

- bipartite graphs,
- unicyclic graphs,
- the Petersen graph,
- prismes.

5. Wiener index for directed graphs

Grid graphs

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Find an orientation in the grid $G_{n,m}$ that has the maximal Wiener index.

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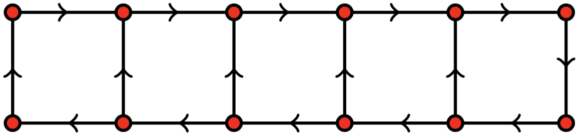
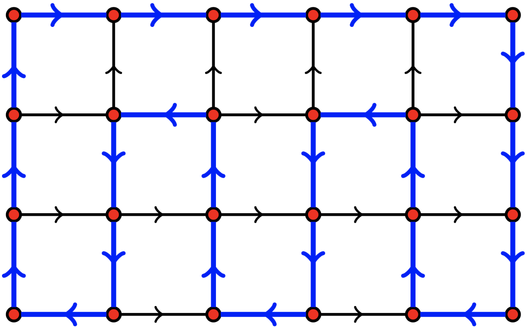


5. Wiener index for directed graphs
Grid graphs

Is this an optimal orientation for the 6×4 grid



6. Variable Wiener vs. Variable Szeged

Szeged index

Another popular topological index is the Szeged index

$$\mathrm{Sz}(G) = \sum_{e=uv\in E} n_e(u)\cdot n_e(v),$$

where $n_e(u)$ is the number of vertices strictly closer to u than v, and analogously, $n_e(v)$ is the number of vertices strictly closer to v.

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This is well known:

Theorem (A. Dobrynin, I. Gutman, S. Klavžar, A. Rajapakse)

For every graph G we have

$$\mathrm{Sz}(G) \geq W(G) \tag{3}$$

and equality holds if and only if every block of G is a complete graph.

6. Variable Wiener vs. Variable Szeged

Variable variations

Definition

The variable Wiener index of a graph G

$$W^{\alpha}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)^{\alpha}.$$

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$$\mathrm{Sz}^{\alpha}(G) = \sum_{e=uv \in E(G)} [n_e(u) \cdot n_e(v)]^{\alpha}.$$

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Problem

When

$$\mathrm{Sz}^{\alpha}(G) \geq W^{\alpha}(G)?$$

6. Variable Wiener vs. Variable Szeged

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For trees we have

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Using Karamata's inequality, one can show the following statement:

Theorem (M. Knor, K. Hriňáková, R.Š.)

Let T be a tree on n vertices. Then

1. $W^\alpha(T) \le \mathrm{Sz}^\alpha(T)$ *if* $\alpha > 1$,
2. $W^\alpha(T) \ge \mathrm{Sz}^\alpha(T)$ *if* $0 \le \alpha < 1$.

Moreover, equalities hold if and only if $n = 2$.

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Moreover, equalities hold if and only if $n = 2$.

Theorem (M. Knor, K. Hriňáková, R.Š.)

Let G be a bipartite graph on n vertices and $\alpha > 1$. Then

$$W^\alpha(G) \leq \mathrm{Sz}^\alpha(G)$$

with equality if and only if $n = 2$.

6. Variable Wiener vs. Variable Szeged

Negative α's

Negative α's are easy. ☺

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Let G be a non-complete graph. Then for every $\alpha < 0$ we have

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Hence, if $\alpha < 0$,

$$\mathrm{Sz}^{\alpha}(G) \le m < W^{\alpha}(G).$$

□

6. Variable Wiener vs. Variable Szeged

The stronger and the weaker conjectures

Conjecture (M. Knor, K. Hriňáková, R.Š.)

For every non-complete graph G there is a constant $\alpha_G \in (0, 1]$ such that

$$\begin{array}{lcll} \mathrm{Sz}^{\alpha}(G) & > & W^{\alpha}(G) & \text{if } \alpha > \alpha_G \\ \mathrm{Sz}^{\alpha}(G) & = & W^{\alpha}(G) & \text{if } \alpha = \alpha_G \\ \mathrm{Sz}^{\alpha}(G) & < & W^{\alpha}(G) & \text{if } \alpha < \alpha_G . \end{array}$$

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Conjecture

For every non-complete graph G *and* $\alpha > 1$ *we have* $\mathrm{Sz}^\alpha(G) > W^\alpha(G)$.

The weaker conjecture was solved by Kovijanić Vukićević and Bulatović and simulationously and independently by Cambie and Haslegrave.

6. Variable Wiener vs. Variable Szeged

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- graphs with diameter 3 and n vertices and m edges satisfying $m < \frac{1}{2}\binom{n}{2}$
- almost every graph in $G_{n,p}$ (or $G_{n,m}$)
- but in general this conjecture is false!

6. Variable Wiener vs. Variable Szeged

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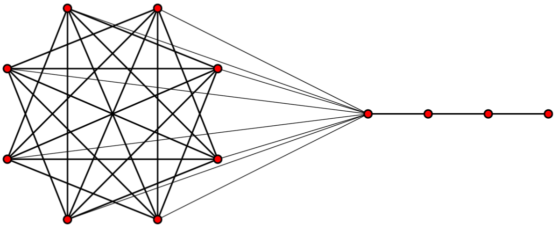
Example $G_{8,3}$:



6. Variable Wiener vs. Variable Szeged

Problem

Is the last conjecture true for traingle-free graphs?

THE END ☺