Some problems and results on Wiener index and related graph parameters

Riste Škrekovski

University of Ljubljana
&
Faculty of Information Studies in Novo Mesto

Slovenia

19. September 2024

Based on a survey with Martin Knor and Aleksandra Tepeh

I. Part:

I. Part:
Chemical Graph Theory

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Chemical Graph Theory

- **Molecular descriptors:**

I. Part:
Chemical Graph Theory

- **Molecular descriptors:** Wiener index,

I. Part:
Chemical Graph Theory

- **Molecular descriptors:** Wiener index, Balaban Index,

I. Part: Chemical Graph Theory

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- **Carbon molecules:**

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One correspondence

A. Balaban

Re: quartic graphs Inbox ×

Balaban, Alexandru T

to me

Sun, 7 Apr, 23:22

Dar Riste,

After my 93rd anniversary, I would klike to renew our correspondence.

How are you? Please let me know .

Best wishes,

Sandy

One correspondence
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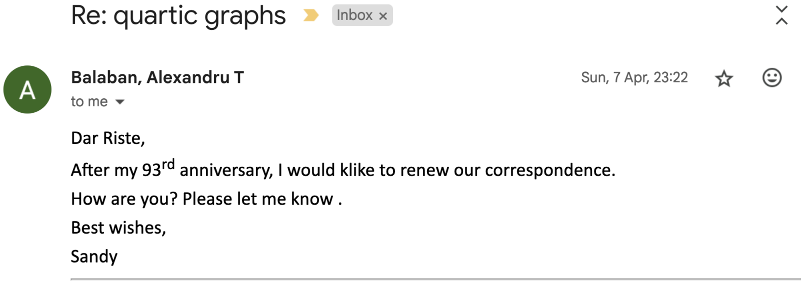
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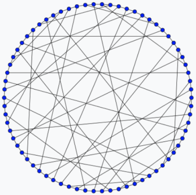
Šta da mu kažem!

Balaban cages

Balaban 10 and Balaban 11 cages

Balaban 10-cage



The Balaban 10-cage

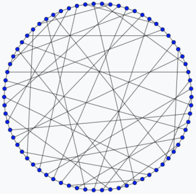
Named after	Alexandru T. Balaban
Vertices	70
Edges	105
Radius	6
Diameter	6
Girth	10
Automorphisms	80
Chromatic number	2
Chromatic index	3
Book thickness	3
Queue number	2
Properties	Cubic Cage Hamiltonian

Table of graphs and parameters

Balaban cages

Balaban 10 and Balaban 11 cages

Balaban 10-cage



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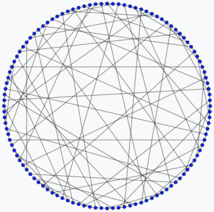

The Balaban 11-cage

Named after	Alexandru T. Balaban
Vertices	112
Edges	168
Radius	6
Diameter	8
Girth	11
Automorphisms	64
Chromatic number	3
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Table of graphs and parameters

Wiener index

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

was introduced in 1947 by the chemist H. Wiener for its correlation with the boiling point of alkane molecules $C_n H_{2n+2}$.

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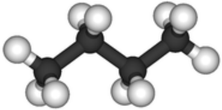

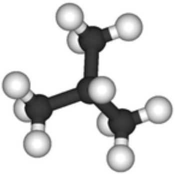

Theorem (Wiener)

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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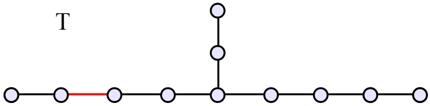

3·(1·10)
3·(2·9)
2·(3·8)
2·(4·7)

W(T)=188

Szeged index
Definition

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Another popular topological index is the Szeged index

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

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

$$\mathrm{Sz}(G) \geq W(G) \tag{2}$$

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

Definition

The variable Wiener index of a graph G

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

Variable Wiener vs. Variable Szeged

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Definition

The variable Szeged index of a graph G

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

Some others

Mostar index:

$$M(G) = \sum_{e=uv\in E(G)} |n_e(u) - n_e(v)|,$$

Gutman index

$$\mathrm{Gut}(G) = \sum_{\{u,v\}\subseteq V(G)} d(u)d(v)d(u,v).$$

II. Part:

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Survey

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Few sections:

1. Minimum Wiener index for chemical graphs

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2. Regular graphs vs. diameter

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Survey

Few sections:

1. Minimum Wiener index for chemical graphs
2. Regular graphs vs. diameter
3. Šoltés Problem

1. Minimum Wiener index for chemical graphs

The forgotten problem

It is well known that

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An "overlooked" problem

Problem

Find all the chemical graphs G on n vertices with the minimum value of Wiener index.

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We know

- G is almost regular with at most three vertices of degree < 4 and these vertices induce a clique;

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Find all the chemical graphs G on n vertices with the minimum value of Wiener index.

We know

- 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.

1. Minimum Wiener index for chemical graphs

Graphs of small order

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Small n

- $n = 1, 2, \ldots, 5$: K_n

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Graphs of small order

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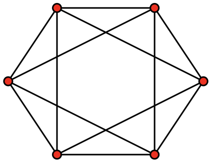
- $n = 1, 2, \ldots, 5$: K_n
- $n = 6$:



Small n

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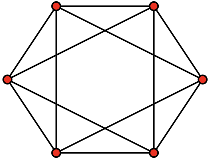
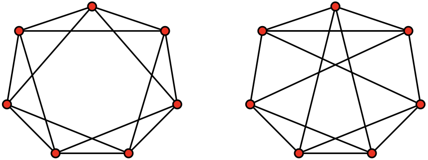
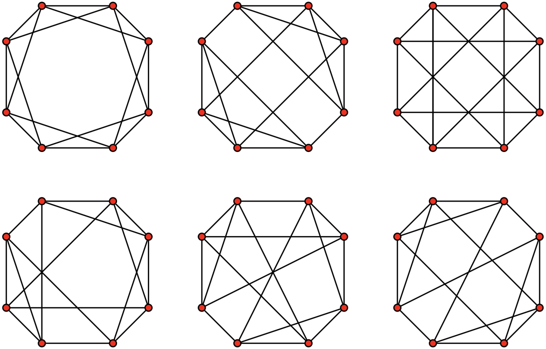


- $n = 7$:



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.



1. Minimum Wiener index for chemical graphs

Conjecture

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

1. Minimum Wiener index for chemical graphs

Going to higher degrees

We think the following may hold:

Conjecture (The even case)

Let G be a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index among such graphs. If kn is even, then G is k-regular.

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We assume $n >> k+1$.

2. Regular graphs vs. diameter

Minumum values

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Among all r-regular graphs on n vertices, the minimum Wiener index is attained by a graph with the minimum possible diameter.

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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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Petersen graph appears in $n(3, 2)$, J_5 appears in $n(3, 3)$,
Heawood graph does not appear there but it is a cage graph Cage(3,6).

2. Regular graphs vs. diameter

Maximum values

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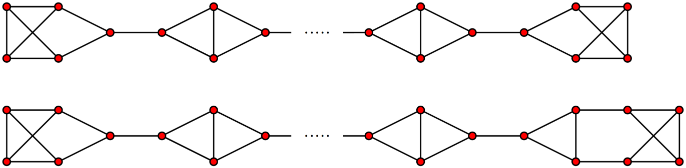

Figure: Graphs L_{4k+2} (above) and L_{4k+4} (below).

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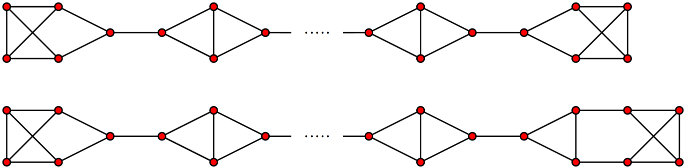

Figure: Graphs L_{4k+2} (above) and L_{4k+4} (below).

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

3. Šoltés problem

This is Snježa

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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.

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We say v satisfies Soltés property if (3) holds,

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The weaker version

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The weaker version

Theorem (M. Knor, S. Majstorović, R. Š.)

There exist infinitely many graphs G with a particular vertex v such that

$$W(G) = W(G - v)$$

holds.

3. Šoltés problem
The weaker version

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There exist infinitely many graphs G with a particular vertex v such that

$$W(G) = W(G - v)$$

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- for each $n \geq 9$, there is a unicyclic graph G on n vertices containing a vertex v that satisfies the Šoltés property;
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More precisely:

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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 $v \in V(H) \setminus V(G)$.

3. Šoltés problem

Together with Nino Bašić and Martin Knor we worked on constructing cubic graphs with many Soltés vertices.

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On regular graphs with Šoltés vertices*

Nino Bašić †

FAMNIT, University of Primorska, Koper, Slovenia and
IAM, University of Primorska, Koper, Slovenia and
Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

Martin Knor ‡

Slovak University of Technology in Bratislava, Slovakia

Riste Škrekovski

3. Šoltés problem

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

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Conjecture

The cycle C_{11} is the only Šoltés graph.

3. Šoltés problem

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Kriva je

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Kriva je

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Kriva je

Do not drink and work!

3. Šoltés problem

For a general (regular) graph G, the values

$$W(G - u) \qquad \text{and} \qquad W(G - v)$$

might be significantly different for two different vertices u and v from G.

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However, $W(G-u)$ and $W(G-v)$ are equal if vertices u and v belong to the same vertex orbit.

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However, $W(G-u)$ and $W(G-v)$ are equal if vertices u and v belong to the same vertex orbit.

A computer search on publicly available collections of vertex-transitive graphs **did not** reveal any Soltés graph.

3. Šoltés problem

Šoltés problem is a balance between opposites:

3. Šoltés problem

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Figure: Yin-Yang

3. Šoltés problem

Snowball effect

3. Šoltés problem
Snowball effect

Some more people became interested:

3. Šoltés problem
Snowball effect

Some more people became interested: *Dragan Stevanović,*

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We got snowball effect thanks to Snježa!

THE END ☺

3. Šoltés problem
Last slide

Stijn Cambie:

3. Šoltés problem

Last slide

Stijn Cambie: At this point I do not even dare to conjecture

3. Šoltés problem

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Last slide

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Last slide

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`Šta da mu kažem!`