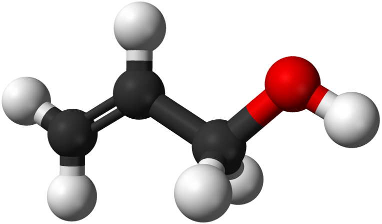
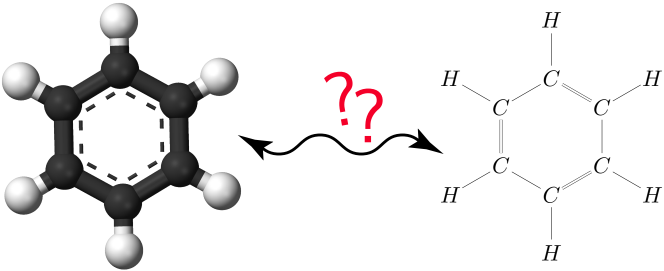
On Several Extremal Problems in Chemical Graph Theory



Barbara Ikica

FMF UL

17 January 2017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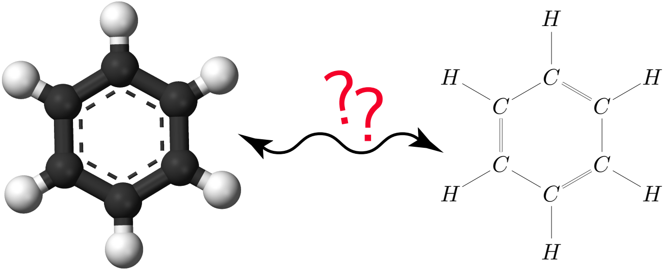

Chemical compounds:
- physicochemical,
- pharmacological,
- toxicological properties ...

Graphs:
- vertex degrees,
- vertex neighbourhoods,
- number of vertices/edges ...

Molecular descriptors

The **molecular descriptor** *is the final result of a logic and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment.*

A **topological index** *also known as a* **connectivity index** *is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound.* [Todeschini and Consonni, 2000]

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Molecular descriptors in practice

http://www.moleculardescriptors.eu/

Topological indices in general

The Wiener index

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

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Properties

- usage: a predictor of the boiling points of paraffins, a tool used for preliminary screening of potentially suitable drugs and for QSAR/QSPR modelling [Knor et al., 2016];

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- a distance-based graph invariant

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Extremal (connected n-vertex) ... [Knor et al., 2016]

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- ... **graphs**: $\max\colon P_n \;/\; \min\colon K_n$

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Extremal (connected n-vertex) … [Knor et al., 2016]

- … graphs: $\max\colon P_n \;/\; \min\colon K_n$
- … trees: $\max\colon P_n \;/\; \min\colon S_n$

Some results on the Wiener index

Problem [Plesník, 1975]

What is the maximum Wiener index among all graphs on n vertices and diameter d?

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Conjecture [DeLaViña and Waller, 2008]

Let G be a graph with diameter $d > 2$ and order $2d + 1$. Then $\mathrm{W}(G) \leq \mathrm{W}(C_{2d+1})$.

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- ... graphs: $\max$: K_n [Chen and Guo, 2011] / $\min$: a tree
- ... trees: $\max$: S_n [Furtula et al., 2009] / $\min$: **???** [Dimitrov, 2013], [Gutman et al., 2012]

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$$\boxed{n_u = |\{w \in V(G) : d(w,u) < d(w,v)\}|}$$

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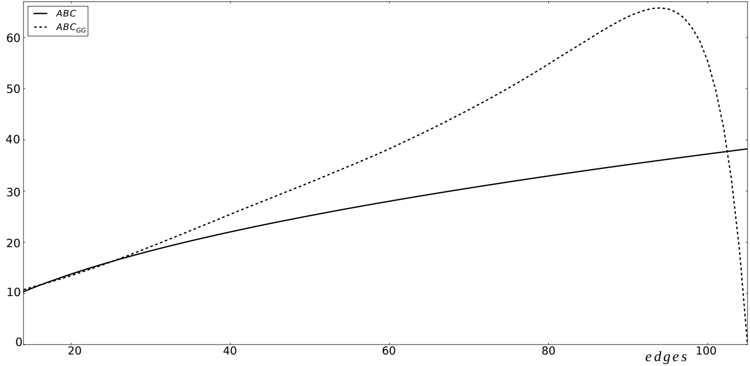
Extremal (connected n-vertex) ...

- ... graphs: max: **???** [Furtula, 2016] / min: K_n
- ... trees: max: S_n [Rostami and Sohrabi-Haghighat, 2014] / min: P_n [Rostami and Sohrabi-Haghighat, 2014]

Some results on the GG index

$\max$ among connected n-vertex graphs

Computational results [Furtula, 2016]:



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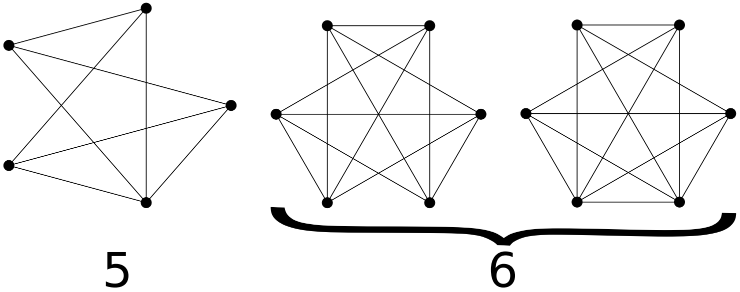

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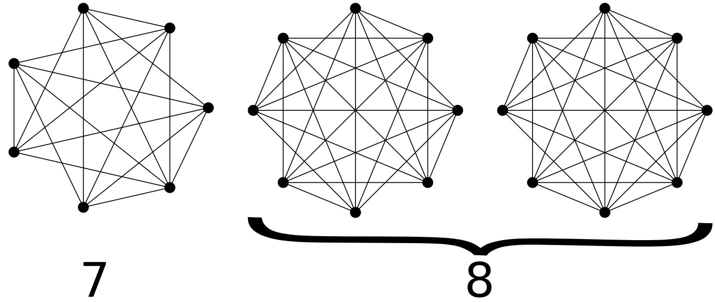

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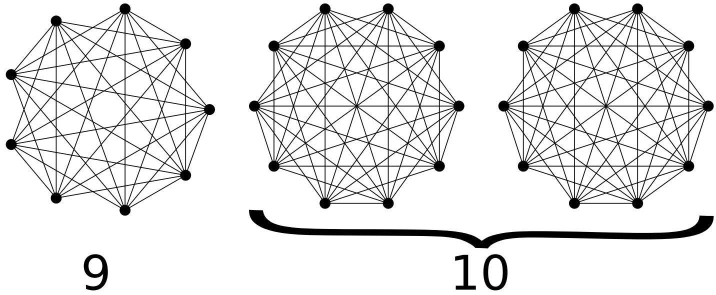
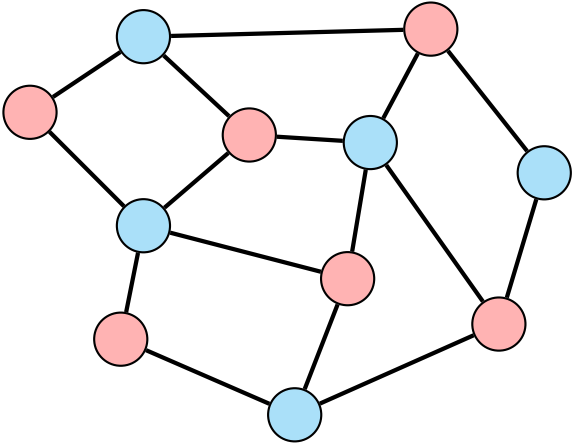
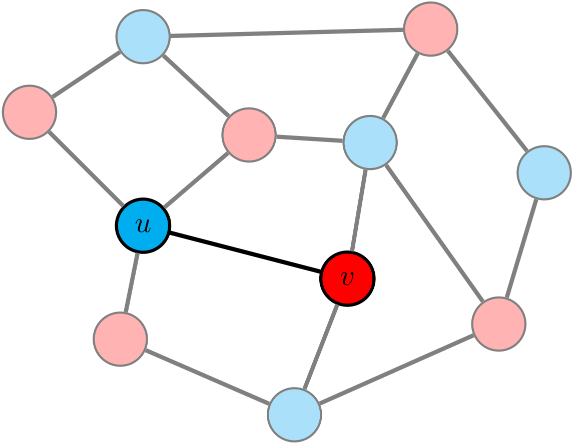


Bipartite graphs



Darko Dimitrov, B. I., Riste Škrekovski, *Remarks on the Graovac—Ghorbani index of bipartite graphs*, Appl. Math. Comput. 293 (2017) 370–376 (10.1016/j.amc.2016.08.047)

Bipartite graphs and the NGG index



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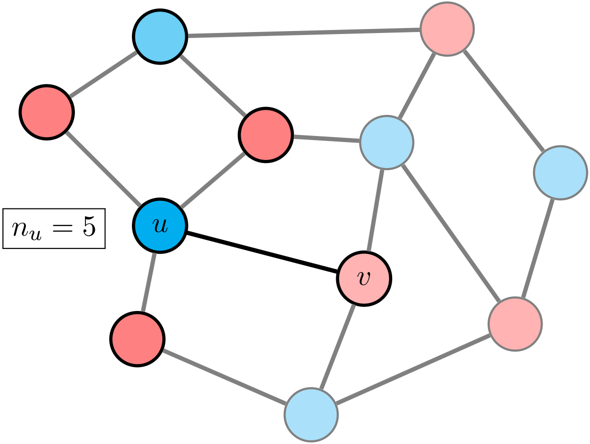

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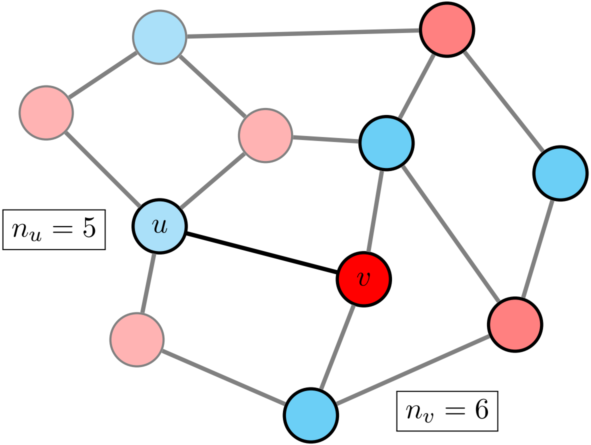

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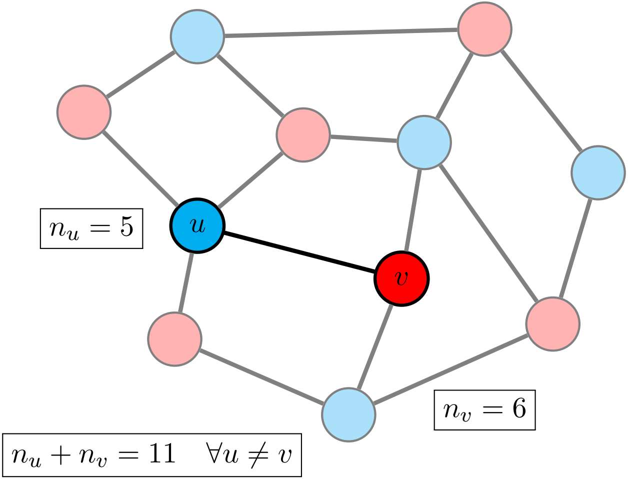

The normalized Graovac-Ghorbani index

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Proposition

Let G be a bipartite graph on n vertices. Then

$$\mathrm{GG}(G) = \mathrm{NGG}(G)\sqrt{n-2}.$$

The GG index of a long path

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$$\lim_{n \to \infty} \mathrm{NGG}(P_n) = \pi.$$

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$$\lim_{n\to\infty} \mathrm{NGG}(P_n) = \pi.$$

Corollary

$$\mathrm{GG}(P_n) \sim \pi\sqrt{n-2}.$$

Extremals of the GG index among bipartite graphs

Theorem

Amongst all bipartite graphs on n vertices, the **maximum** GG index is uniquely attained by $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

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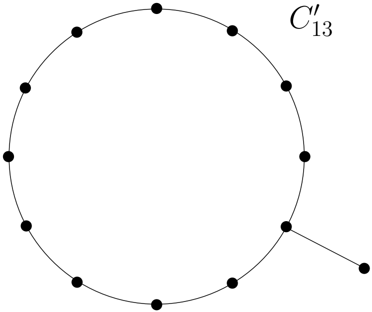

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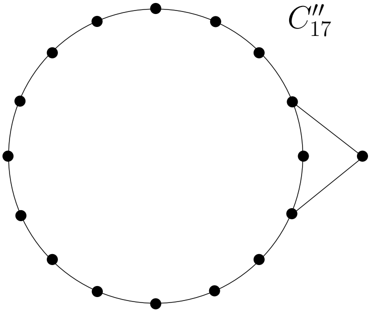

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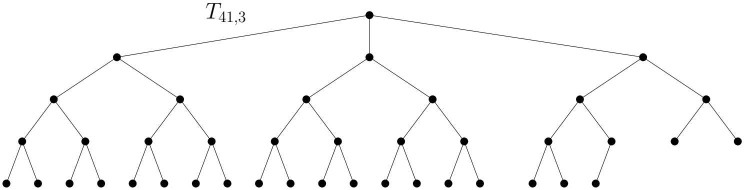

Maximizing the ABC index subject to ...[1]

The ABC index

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} \sqrt{\frac{\deg(u) + \deg(v) - 2}{\deg(u)\deg(v)}}$$

[1]Based on joint work with D. Dimitrov and R. Škrekovski (*Remarks on maximum atom-bond connectivity index with given graph parameters*, accepted for publication in DAM subject to minor modifications).

... given edge-connectivity

Theorem [Zhang et al., 2016]

Let G be a connected graph on n vertices with edge-connectivity $k \geq 2$. Then $\boxed{\mathrm{ABC}(G) \leq \mathrm{ABC}(K_n(k))}$ with equality if and only if $\boxed{G \cong K_n(k)}$.

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$$\boxed{K_n(k) = K_k \vee (K_1 + K_{n-k-1})}$$

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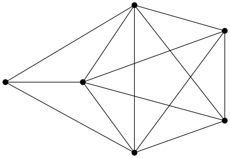

$K_6(3)$

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Theorem

Let G be a connected graph on n vertices with edge-connectivity $k = 1$. Then $\boxed{\mathrm{ABC}(G) \leq \mathrm{ABC}(K_n(1))}$ with equality if and only if $\boxed{G \cong K_n(1)}$.

... given chromatic number χ

Theorem [Zhang et al., 2016]

Let G be an n-vertex connected graph with chromatic number $\chi = 2$. Then $\boxed{\mathrm{ABC}(G) \leq \mathrm{ABC}(T_{n,\chi})}$ with equality if and only if $\boxed{G \cong T_{n,\chi}}$[2].

---

[2] $T_{n,l}$ denotes a complete l-partite graph of order n with $|t_i - t_j| \leq 1$, where t_i is the number of vertices in the i-th partition set of $T_{n,l}$.

... given chromatic number χ

Theorem [Zhang et al., 2016]

Let G be an n-vertex connected graph with chromatic number $\chi = 2$. Then $\boxed{\mathrm{ABC}(G) \leq \mathrm{ABC}(T_{n,\chi})}$ with equality if and only if $\boxed{G \cong T_{n,\chi}}$[2].

Theorem

Let G be an n-vertex connected graph with chromatic number $\chi \geq 2$ and suppose that χ divides n. Then $\boxed{\mathrm{ABC}(G) \leq \mathrm{ABC}(T_{n,\chi})}$ with equality if and only if $\boxed{G \cong T_{n,\chi}}$.

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Maximizing the Wiener index subject to a given diameter[3]

The Wiener index

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

[3] Based on joint work with Q. Sun, R. Škrekovski and V. Vukasinović.

Large-diameter graphs

Double broom

The *double broom* $D(n, a, b)$ consists of a path on $n - a - b$ vertices together with a independent vertices adjacent to one of its endpoints and b independent vertices adjacent to the other endpoint.

Large-diameter graphs

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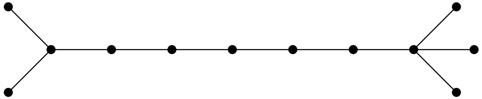

$D(12,2,3)$

Large-diameter graphs

Theorem

Let G be a graph of order n and let $\boxed{d = n - c}$ be its diameter. Here, $c \geq 3$ is a constant such that $n \geq \frac{1}{6}(7c^3 - 18c^2 + 23c - 6)$. Then $\boxed{W(G) \leq W(D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil))}$ with equality if and only if $\boxed{G \cong D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil)}$.

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Proposition

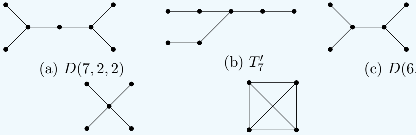
Let G be a graph of order n. If the diameter of G is $\boxed{d = n - 1}$, then $\boxed{W(G) \leq W(D(n, 1, 1))}$ with equality if and only if $\boxed{G \cong D(n, 1, 1)(\cong P_n)}$. If the diameter of G is $\boxed{d = n - 2}$, then $\boxed{W(G) \leq W(D(n, 1, 2))}$ with equality if and only if $\boxed{G \cong D(n, 1, 2)}$.

Large-diameter graphs

Proposition

Let G be a graph on n vertices with diameter equal to $d = n - 3$.

- If $n \geq 8$, then $W(G) \leq W(D(n,2,2))$ with equality if and only if $G \cong D(n,2,2)$.
- If $n = 7$, then $W(G) \leq W(D(7,2,2)) = W(T_7')$ with equality if and only if $G \cong D(7,2,2)$ or $G \cong T_7'$.
- If $n = 6$, then $W(G) \leq W(D(6,2,2))$ with equality if and only if $G \cong D(6,2,2)$.
- If $n = 5$, then $W(G) \leq W(S_5)$ with equality if and only if $G \cong S_5$.
- If $n = 4$, then $W(G) \leq W(K_4)$ with equality if and only if $G \cong K_4$.



(a) $D(7,2,2)$ (b) T_7' (c) $D(6,2,2)$ (d) S_5 (e) K_4

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