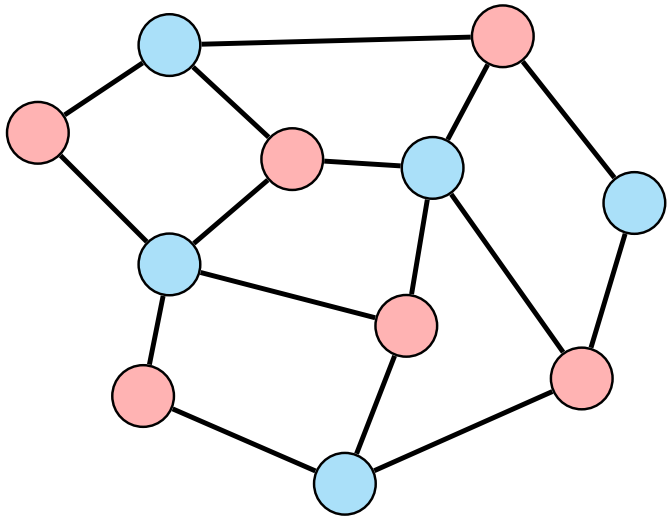
On the Graovac–Ghorbani index of bipartite graphs



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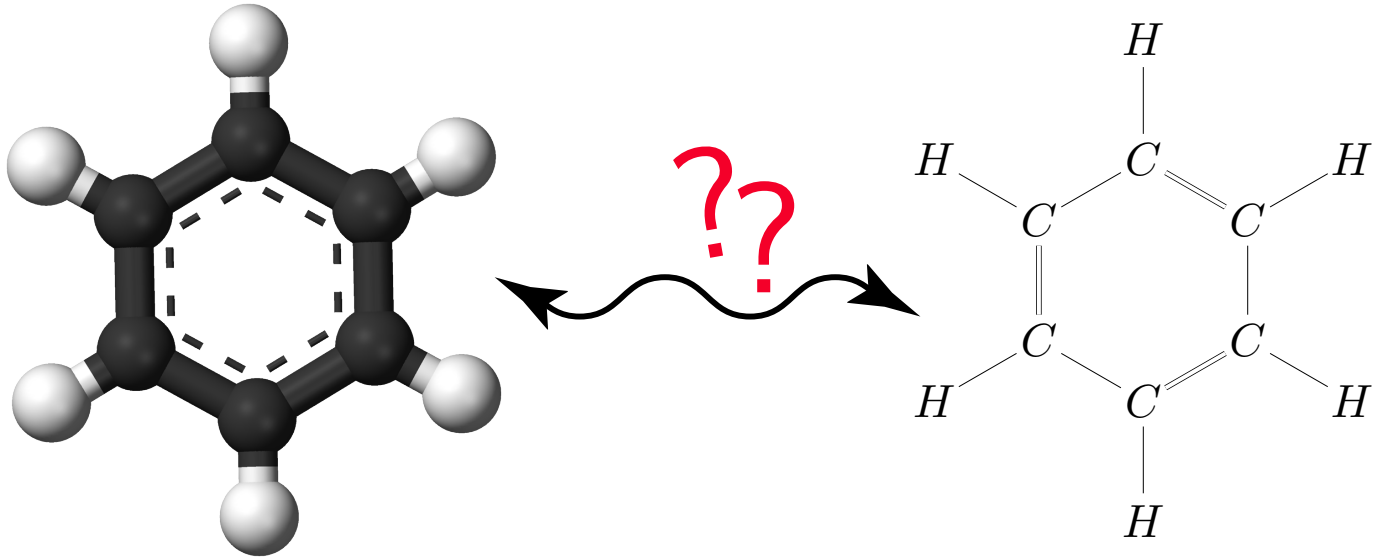
University of Ljubljana

29 September 2016

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)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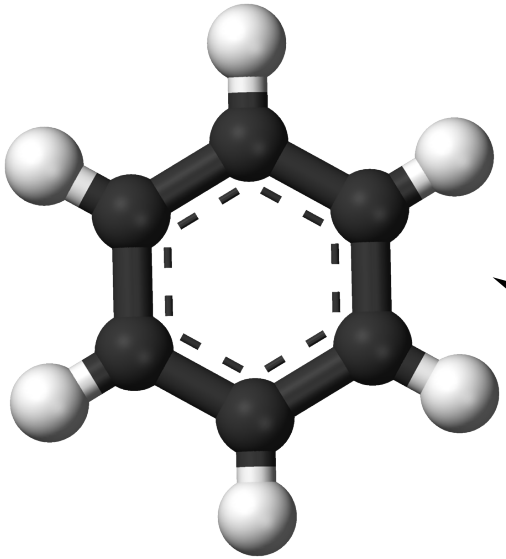

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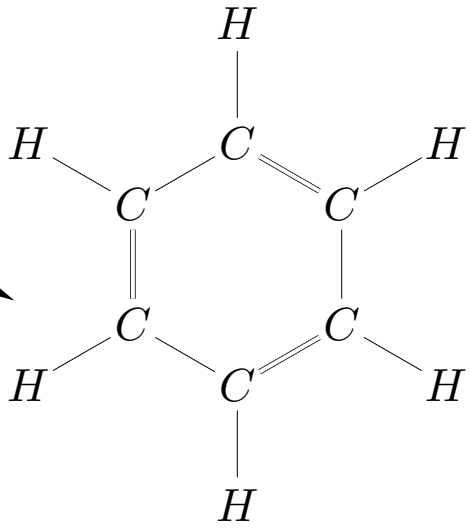

Chemical compounds:
- physicochemical,
- pharmacological,
- toxicological properties ...

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

Overview

- **Molecular descriptors**:

Overview

- **Molecular descriptors**:
  - topological indices in general,

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- **Molecular descriptors**:
  - topological indices in general,
  - some results on the ABC index,

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- **An overview of our results**:

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  - bipartite graphs and the NGG index,

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  - extremals of the GG index among bipartite graphs,

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  - topological indices in general,
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- **An overview of our results**:
  - bipartite graphs and the NGG index,
  - the GG index of a long path,
  - extremals of the GG index among bipartite graphs,
  - conjectures.

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  - topological indices in general,
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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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The Wiener index

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

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Topological indices in general

The Wiener index and the Szeged index

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

$$S_Z(G) = \sum_{uv \in E(G)} n_u n_v$$

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The first Zagreb index

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2$$

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The first Zagreb index and the second Zagreb index

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2$$

$$M_2(G) = \sum_{uv \in E(G)} \deg(u) \deg(v)$$

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The atom-bond connectivity index

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

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The atom-bond connectivity index and the Graovac–Ghorbani index

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Molecular descriptors in practice

`http://www.moleculardescriptors.eu/`

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Properties

- usage: modelling thermodynamic properties of organic chemical compounds (a strong predictor of the heat of formation of alkanes and the stability of linear and branched alkanes) [Estrada et al., 1998];

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- a degree-based graph invariant

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Properties

Extremal (connected n-vertex) ...

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Extremal (connected n-vertex) ...

- ... graphs: $\max$: K_n [Chen and Guo, 2011] / $\min$: a tree

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Properties

Extremal (connected n-vertex) ...

- ... 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]

Some results on the GG index

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$$\mathrm{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$

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- usage: modelling thermodynamic properties of organic chemical compounds (a strong predictor of the entropy and the acentric factor of alkanes) [Furtula, 2016];

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$$\mathrm{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$

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

Properties

- usage: modelling thermodynamic properties of organic chemical compounds (a strong predictor of the entropy and the acentric factor of alkanes) [Furtula, 2016];
- a distance-based graph invariant

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Extremal (connected n-vertex) ...

- ... graphs: max: ??? [Furtula, 2016] / min: K_n

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Properties

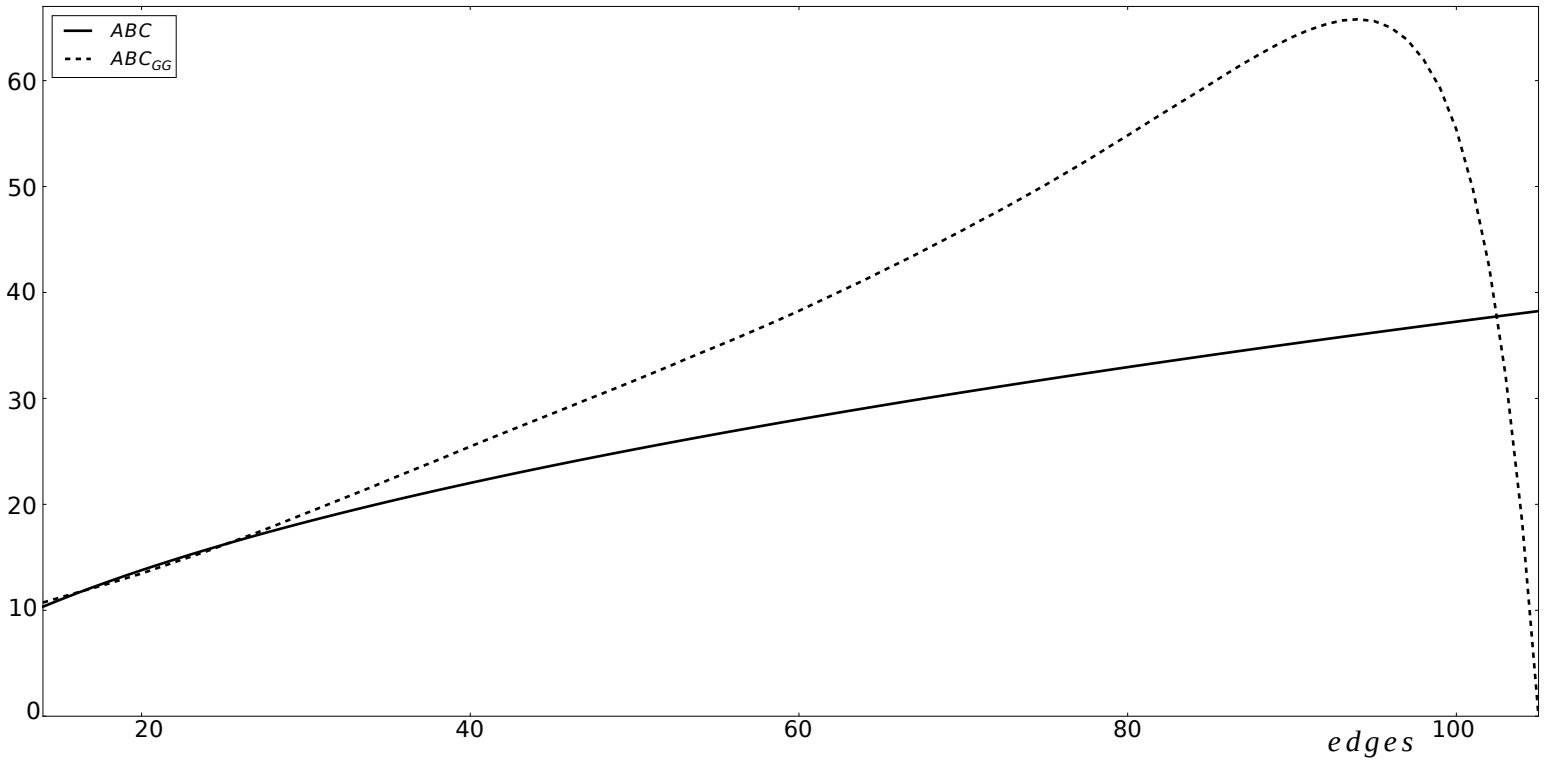
Extremal (connected n-vertex) ...

- ... 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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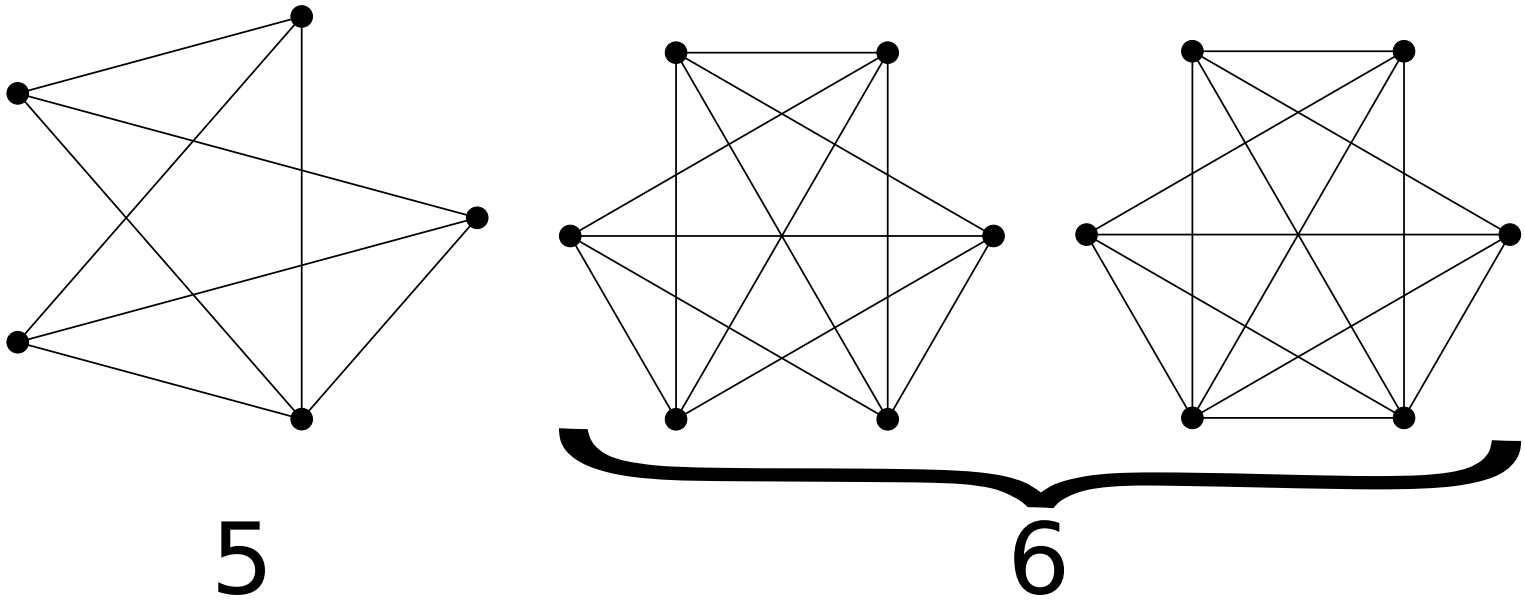

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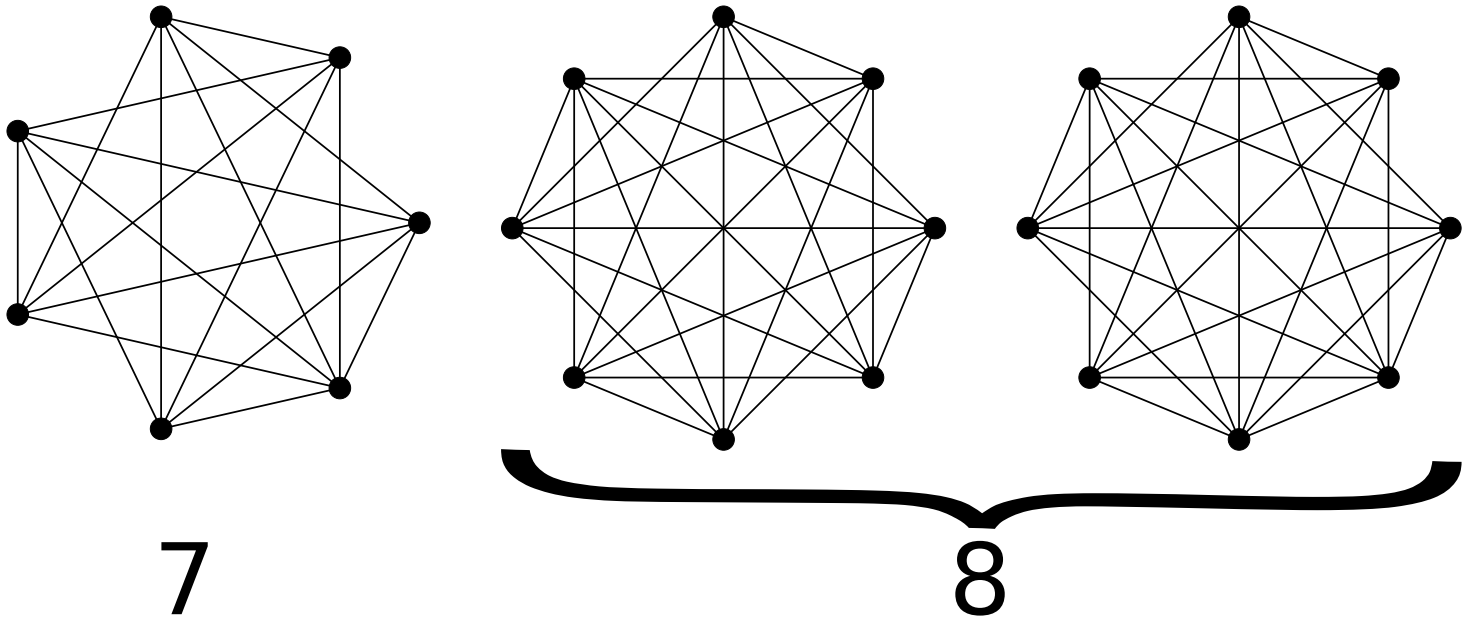

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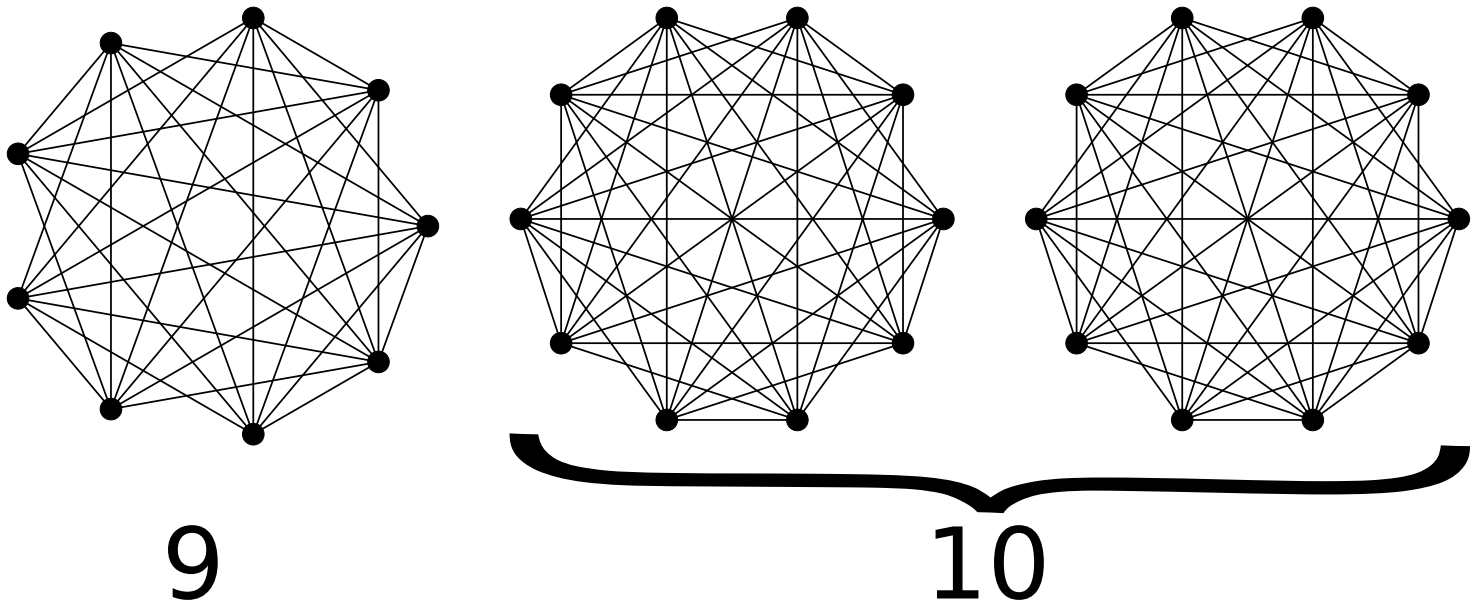

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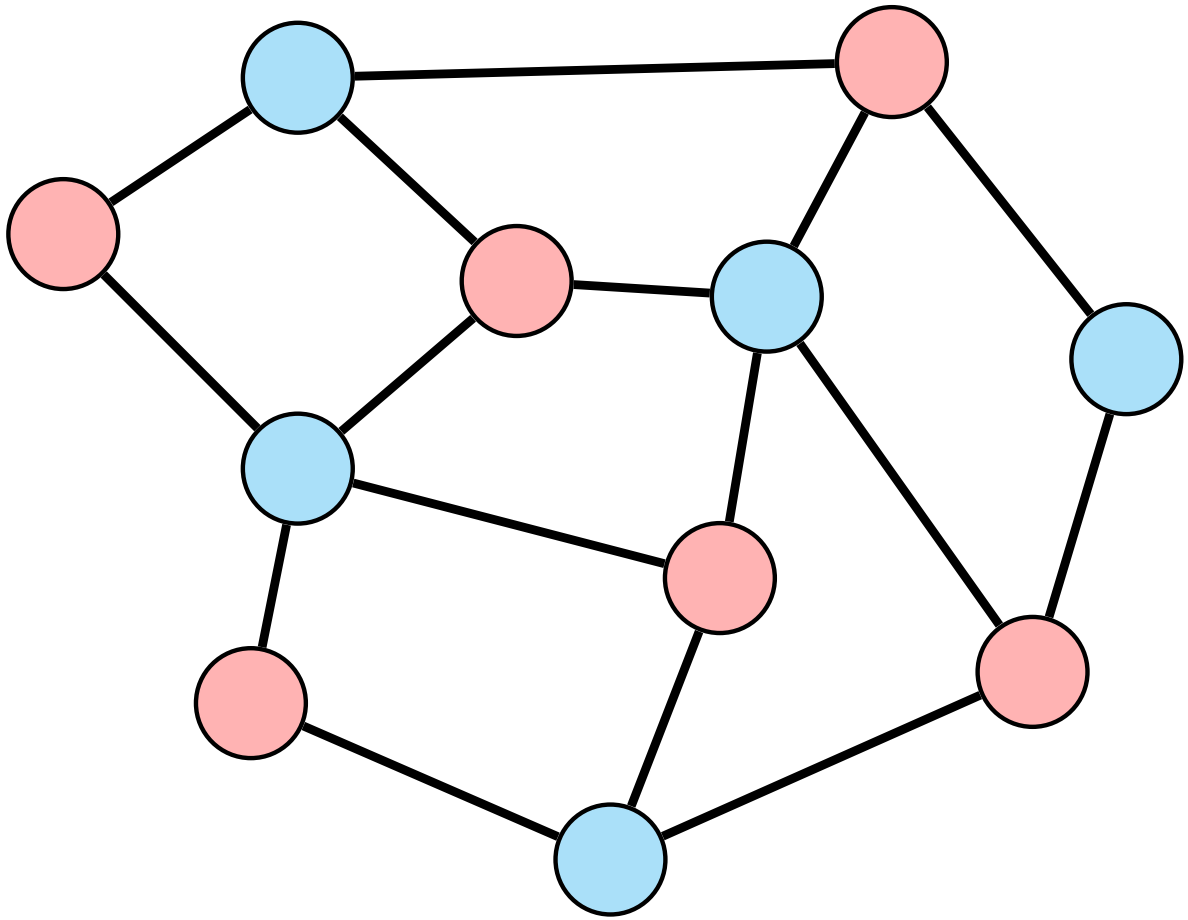

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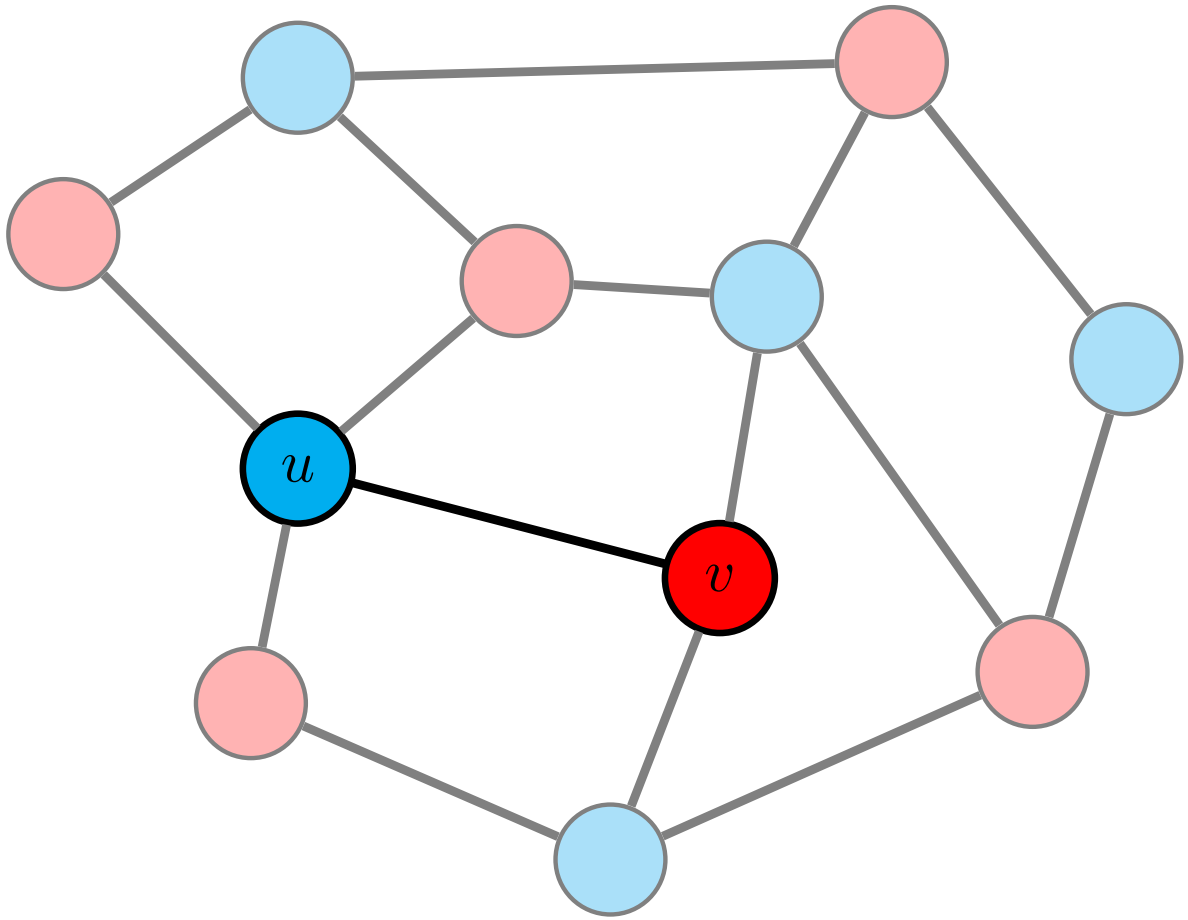

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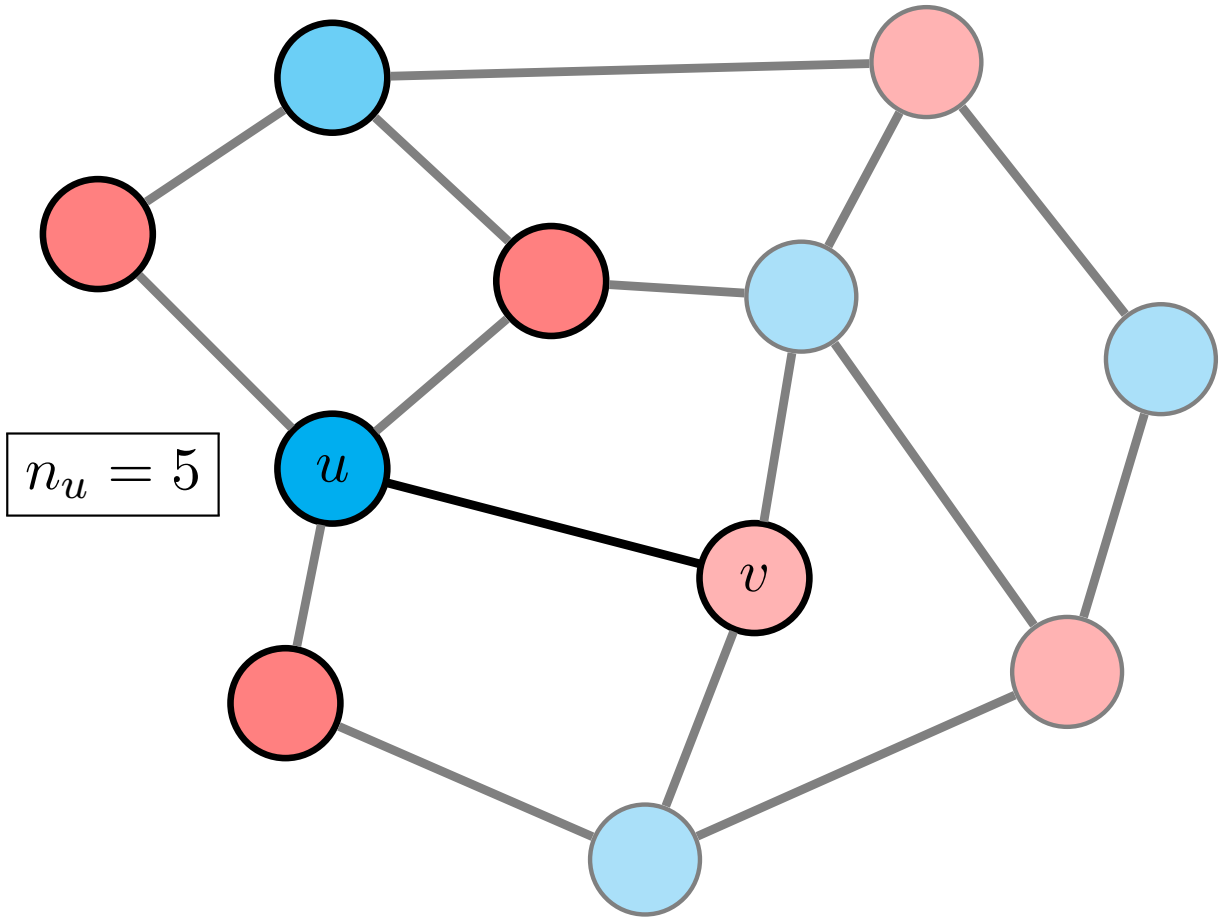

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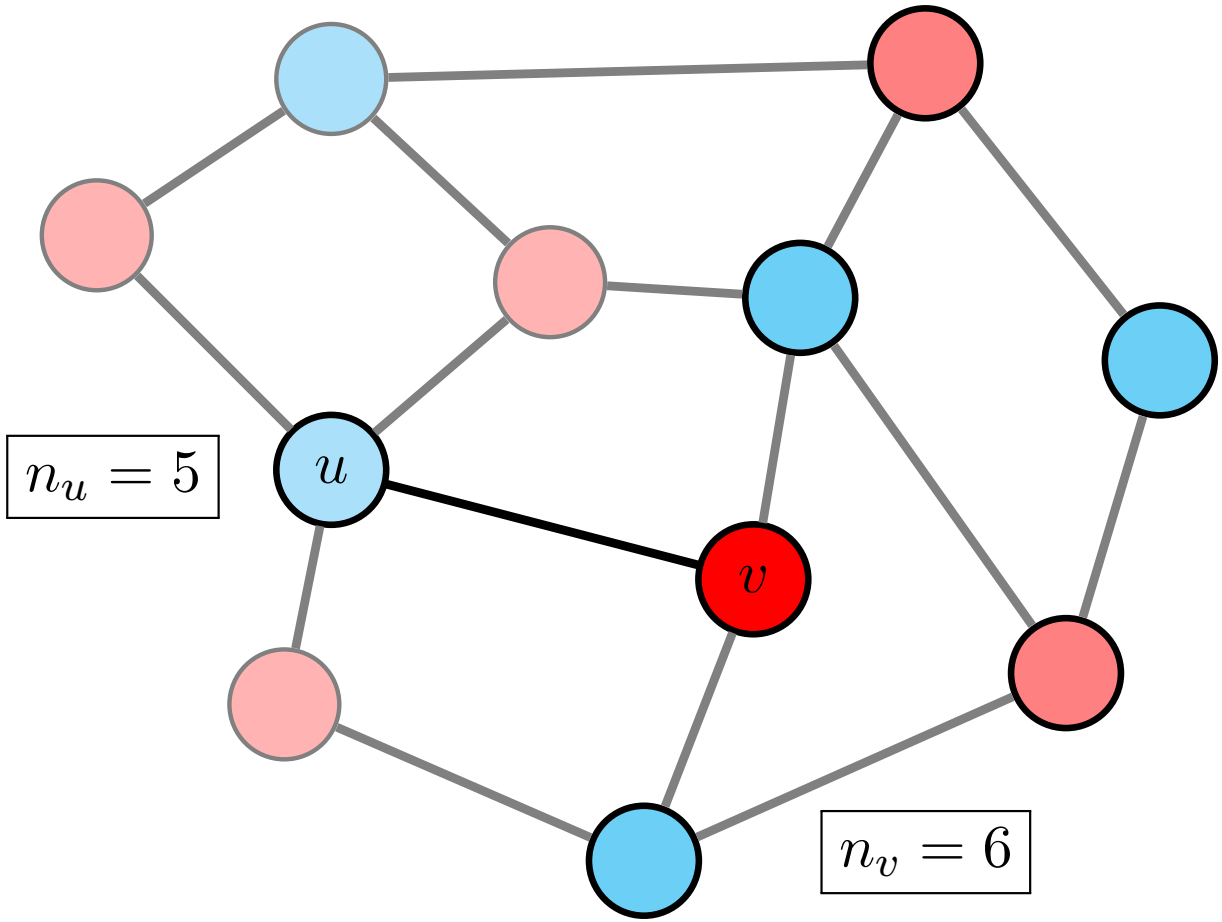

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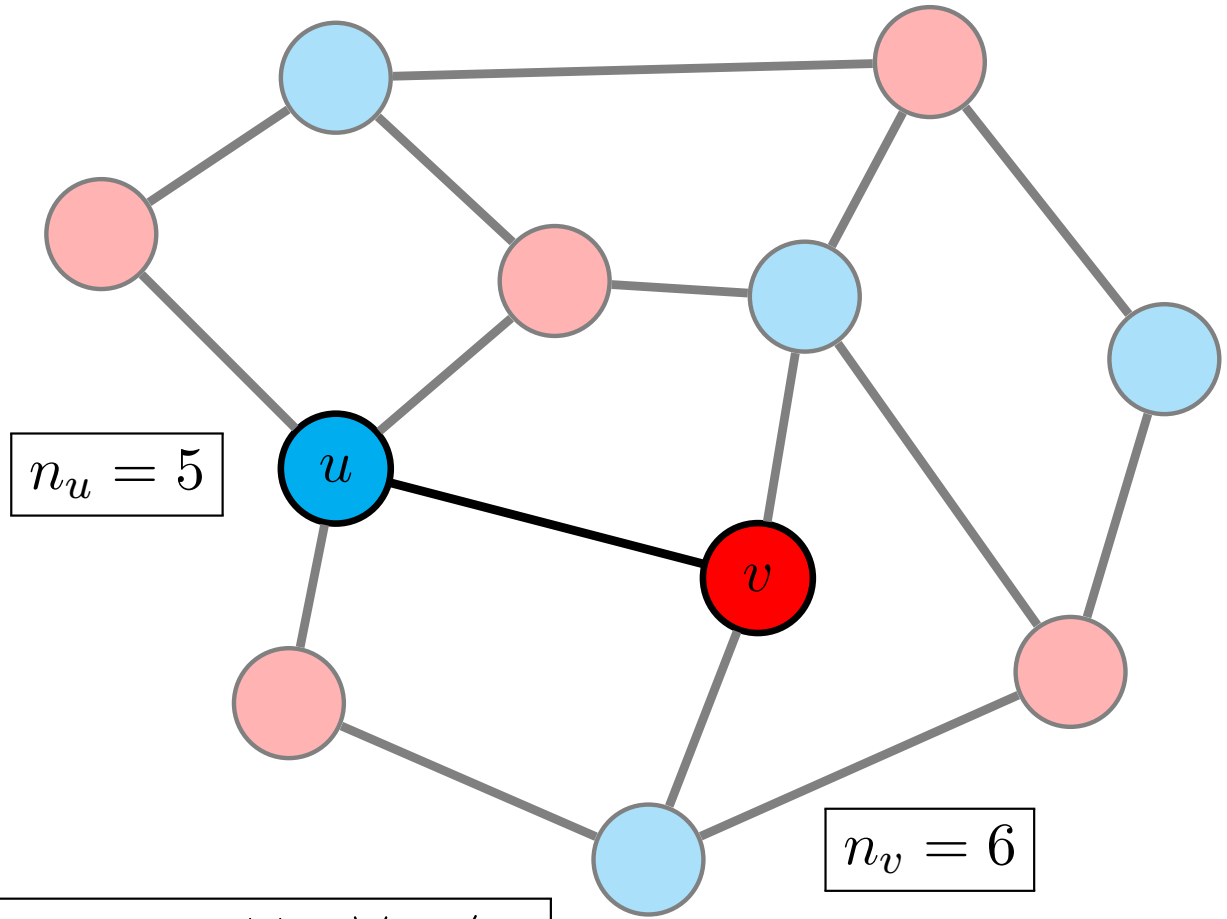

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The normalized Graovac-Ghorbani index

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$$\mathrm{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}$$

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The normalized Graovac-Ghorbani index

The NGG index

$$\mathrm{NGG}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{n_u n_v}}$$

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The normalized Graovac-Ghorbani index

The NGG index

$$\mathrm{NGG}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{n_u n_v}}$$

Proposition

Let G be a bipartite graph on n vertices. Then

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

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Proposition

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

The GG index of a long path

Proposition

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

Corollary

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

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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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- P_n for $n < 8$,

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Theorem

Amongst all bipartite graphs on n vertices, the **minimum** GG index is uniquely attained by

- P_n for $n < 8$,
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Amongst all bipartite graphs on n vertices, the **minimum** GG index is uniquely attained by

- P_n for $n < 8$,
- C_n for even $n \geq 8$,
- C'_n for odd $8 \leq n \leq 15$,

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Amongst all bipartite graphs on n vertices, the **minimum** GG index is uniquely attained by

- P_n for $n < 8$,
- C_n for even $n \geq 8$,
- C'_n for odd $8 \leq n \leq 15$,
- C''_n for odd $n \geq 17$.

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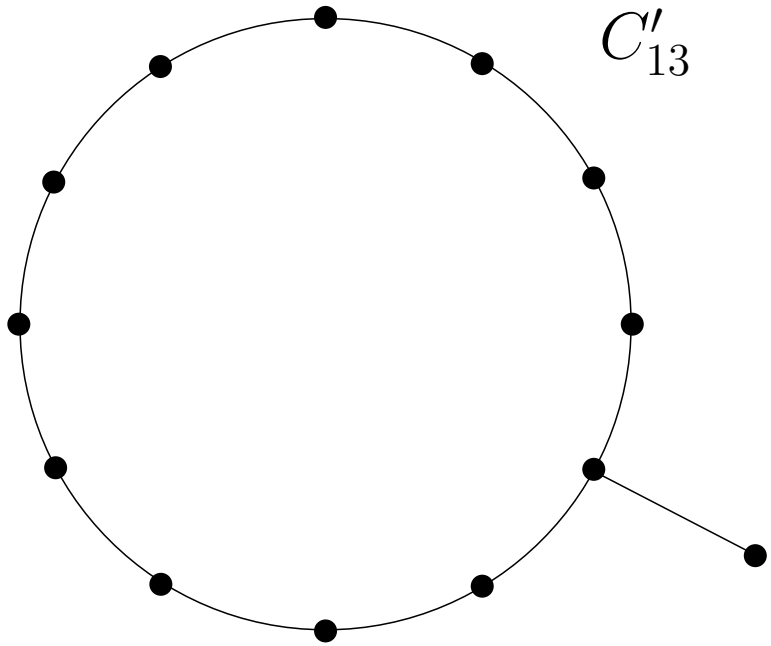

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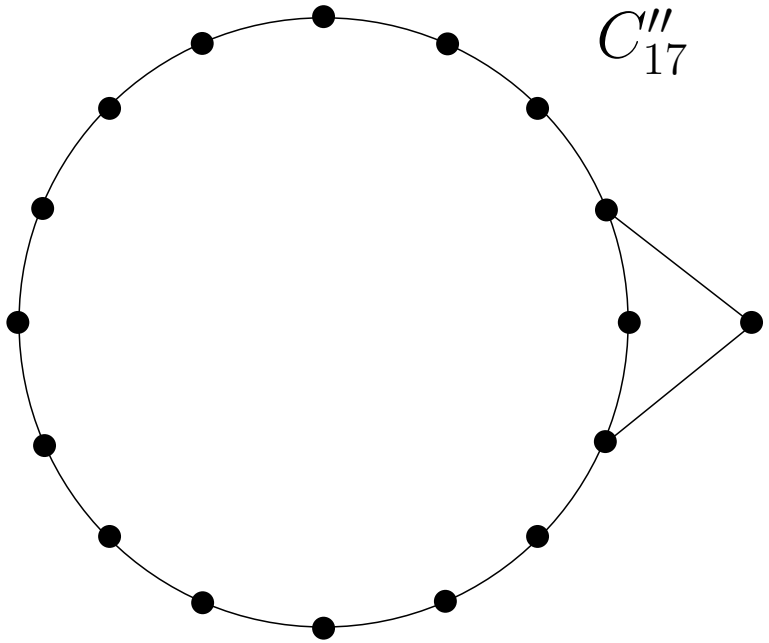

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Let G be a tree with **maximal** GG index amongst all trees on n vertices with maximum degree $\Delta \leq n-1$. Then G is an almost dendrimer $T_{n,\Delta}$.

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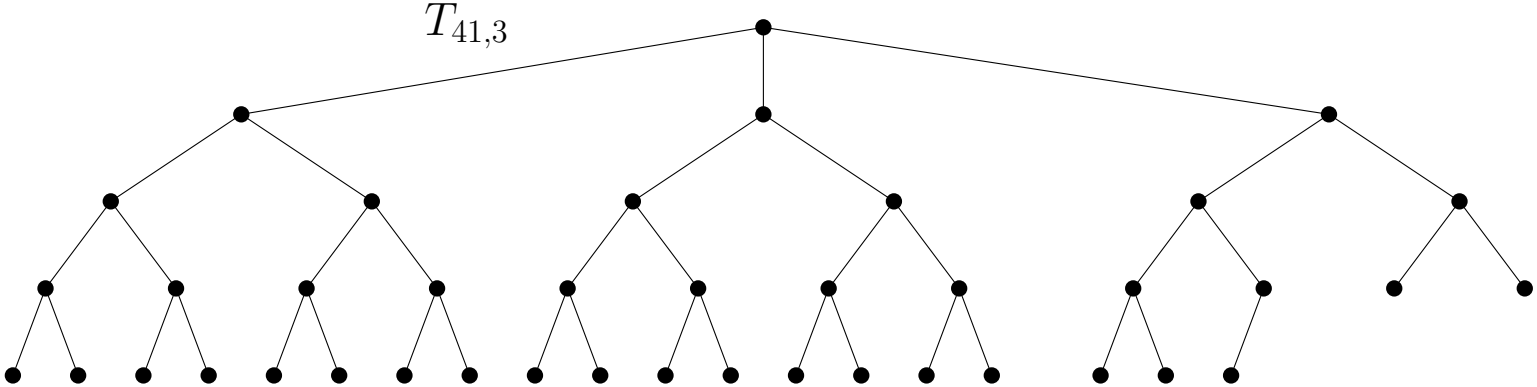

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