An inequality between the edge-Wiener index and the Wiener index of a graph

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joint work with
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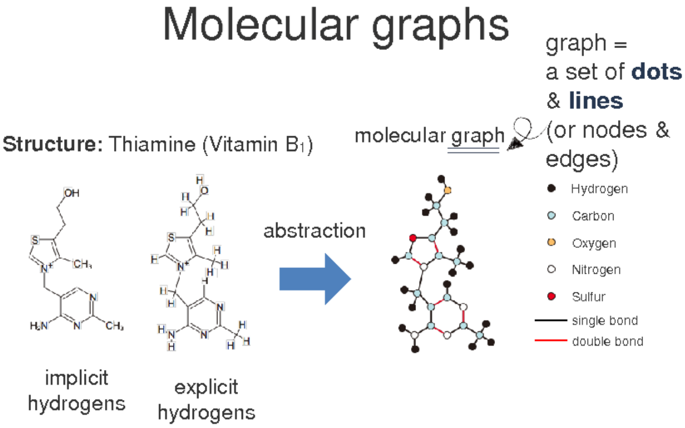
Topological indices

- derived from molecular graphs
- numerical values



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- introduced by H. Wiener, 1947
- boiling point of paraffines is in strong correlation with the graph structure of their molecules
- applications in chemistry, communication, facility location, cryptology, architecture,...

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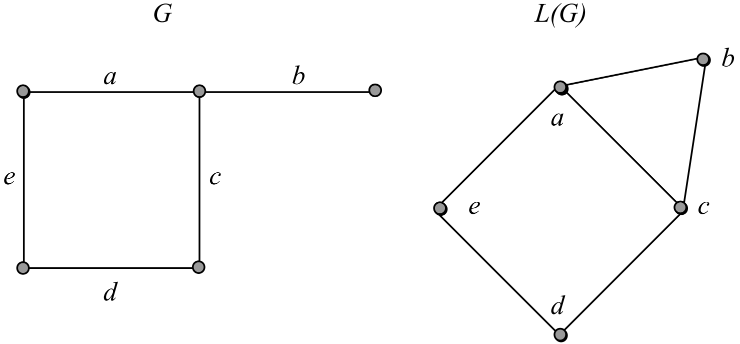
Our goal was to

- compare Wiener index with the edge-Wiener index (to improve known results)
- improve the upper bound for the edge-Wiener index
- explore the ratio between both indices (find extremal graphs)

Basic definitions

Let $L(G)$ denote the **line graph** of G:
$V(L(G)) = E(G)$ and two distinct edges $e, f \in E(G)$ adjacent in $L(G)$ whenever they share an end-vertex in G

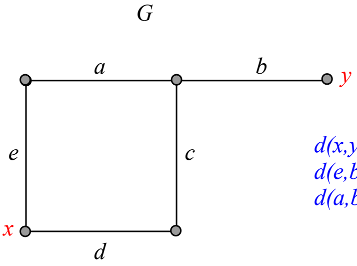


Basic definitions

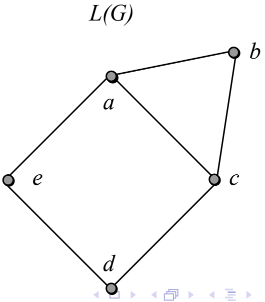
- **distance between vertices**: $d_G(u,v)$ denotes the distance (=the length of a shortest path) between vertices $u, v \in V(G)$
- **distance between edges**: $d_G(e,f) = d_{L(G)}(e,f)$,

$\Updownarrow$

$e = u_1u_2$, $f = v_1v_2$
if $e \neq f$, then $d(e,f) = \min\{d(u_i, v_j) : i, j \in \{1,2\}\} + 1$,
if $e = f$, $d(e,f) = 0$



d(x,y)=3
d(e,b)=2
d(a,b)=1



Wiener index

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

edge-Wiener index

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e,f)$$

- $W_e(G) = W(L(G))$
- sometimes in the literature slightly different definition: $W_e(G) + \binom{n}{2}$

- $\deg(u)$ = the degree of $u \in V(G)$
- $\delta(G) = \min\{deg(v) : v \in V(G)\}$

Gutman index

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

some known results

Wu, 2010

- Let G be a connected graph of order n with $\delta(G) \geq 2$. Then $W_e(G) \geq W(G)$ with equality if and only if $G \cong C_n$.

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Wu, 2010

- Let G be a connected graph of order n with $\delta(G) \geq 2$. Then $W_e(G) \geq W(G)$ with equality if and only if $G \cong C_n$.
- Let G be a connected graph of size m. Then

$$\frac{1}{4}(Gut(G) - m) \leq W_e(G) \leq \frac{1}{4}(Gut(G) - m) + \binom{m}{2}.$$

- $\kappa_m(G)$ = the number of m-cliques in G

Knor, Potočnik and Škrekovski, 2014

- Let G be a connected graph. Then

$$W_e(G) \geq \frac{1}{4}\mathrm{Gut}(G) - \frac{1}{4}|E(G)| + \frac{3}{4}\kappa_3(G) + 3\kappa_4(G) \tag{1}$$

with equality in (1) if and only if G is a tree or a complete graph.

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- Let G be a connected graph of minimal degree $\delta \geq 2$. Then

$$W(L(G)) \geq \frac{\delta^2 - 1}{4} W(G).$$

- conjecture: $W(L(G)) \geq \frac{\delta^2}{4} W(G)$

main theorem

Theorem

Let G be a connected graph of minimum degree δ. Then,

$$W_e(G) \geq \frac{\delta^2}{4} W(G)$$

with equality holding if and only if G is isomorphic to a path on three vertices or a cycle.

For the proof we need...

average distance of endpoints of edges $e = u_1 u_2$ and $f = v_1 v_2$

$$s(u_1 u_2, v_1 v_2) = \frac{1}{4}\big(d(u_1, v_1) + d(u_1, v_2) + d(u_2, v_1) + d(u_2, v_2)\big)$$

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Lemma

Let G be a connected graph. Then

$$\sum_{\{e,f\} \subseteq E(G)} s(e, f) = \frac{1}{4}\Big(\mathrm{Gut}(G) - |E(G)|\Big).$$

Lemma (Knor et al.,2014)

Let u_1u_2, v_1v_2 be a pair of edges of a connected graph G. Then

$$d(u_1u_2, v_1v_2) \geq s(u_1u_2, v_1v_2) + D(u_1u_2, v_1v_2), \qquad (2)$$

where

$$D(u_1u_2, v_1v_2) = \begin{cases} -\frac{1}{2} & \text{if } u_1u_2 = v_1v_2; \\ \frac{1}{4} & \text{if the pair } u_1u_2, v_1v_2 \text{ forms a triangle;} \\ 1 & \text{if the pair } u_1u_2, v_1v_2 \text{ forms a } K_4; \\ 0 & \text{otherwise.} \end{cases}$$

Moreover, equality holds in (2) if and only if

(i) $u_1u_2 = v_1v_2$, *or*

(ii) *the pair u_1u_2, v_1v_2 forms a triangle or K_4, or*

(iii) *if u_1u_2 and v_1v_2 lie on a straight line.*

- $e, f \in E(G)$
- $D(e, f) = d(e, f) - s(e, f)$
- if $D(e, f) = \alpha$, we say that e, f forms a pair of type D_α or that the pair e, f *belongs to the set* D_α
- if $e = f$, then $D(e, f) = -\frac{1}{2}$
- $\mathcal{I} = \{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\}$

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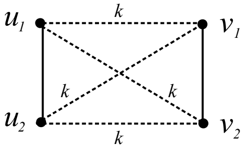
Lemma

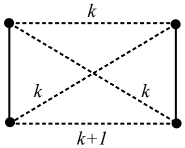
In a connected graph, every pair of distinct edges belongs to D_α for some $\alpha \in \mathcal{I}$.

All types of pairs of two edges

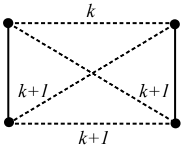
D_1



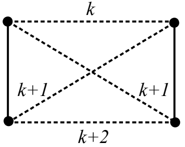
$D_{\frac{3}{4}}$



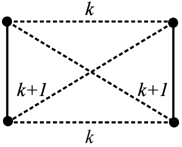
$D_{\frac{1}{4}}$



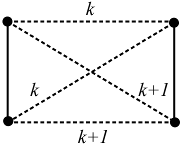
D_0



$D'_{\frac{1}{2}}$



$D''_{\frac{1}{2}}$



$$
\begin{aligned}
W_e(G) &= \sum_{\{e,f\}\subseteq E(G)} d(e,f) \\
&= \sum_{\{e,f\}\subseteq E(G)} s(e,f) + \sum_{\{e,f\}\subseteq E(G)} D(e,f)
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Proposition

Let G be a connected graph. Then

$$W_e(G) = \frac{\mathrm{Gut}(G)}{4} - \frac{|E(G)|}{4} + |D_1| + \frac{1}{4}|D_{\frac{1}{4}}| + \frac{1}{2}|D_{\frac{1}{2}}| + \frac{3}{4}|D_{\frac{3}{4}}|.$$

Case 1: *G is non-regular*

G has a vertex $w \in V(G)$ of degree at least $\delta + 1$. By previous proposition:

$$\begin{aligned} 4W_e(G) &= \mathrm{Gut}(G) - |E(G)| + 4|D_1| + |D_{\frac{1}{4}}| + 2|D_{\frac{1}{2}}| + 3|D_{\frac{3}{4}}| \\ &\geq \mathrm{Gut}(G) - |E(G)| \end{aligned}$$

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&\geq \mathrm{Gut}(G) - |E(G)| \\
&= \sum_{\{u,v\}\subseteq V(G)} \deg(u)\deg(v)\, d(u,v) - |E(G)| \\
&\geq \delta^2 \sum_{\{u,v\}\in V(G)\setminus\{w\}} d(u,v) + \\
&\quad (\delta+1) \sum_{u\in V(G)\setminus\{w\}} \deg(u) d(u,w) - |E(G)|
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&\geq \delta^2 W(G) + \sum_{u\in V(G)\setminus\{w\}} \deg(u) - |E(G)| \\
&\geq \delta^2 W(G).
\end{aligned}$$

Equality is attained if G is isomorphic P_3.

Case 2: *G is regular*

Lemma

In a 2-connected graph G, we have

$$2|D'_{\frac{1}{2}}| + |D_{\frac{1}{4}}| \geq |E(G)|.$$

Moreover, equality holds if and only if G is a cycle.

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Lemma

Suppose that $G \neq K_2$ is a regular graph containing bridges. Then every end-block of G contains an edge e such that for every bridge b the pair e, b is in $D''_{\frac{1}{2}}$.

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- if G contains a bridge $\Rightarrow |D''_{\frac{1}{2}}| \geq 2|B|$
- $4W_e(G) \geq ... \geq \delta^2 W(G)$
- equality is obtained if G is a cycle.

Upper bound for $W_e(G)$

Dankelmann, 2009

$W(L(G)) \leq \frac{4n^5}{5^5} + O(n^{\frac{9}{2}})$

Mukwembi, 2012

Let G be a connected graph on n vertices. Then

$$\mathrm{Gut}(G) \leq \frac{2^4}{5^5} n^5 + O(n^4).$$

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Theorem

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problem by Dobrynin and Mel'nikov, 2012

Estimate the ratio $W(L^i(G))/W(G)$, where $L^i(G)$ stands for an *iterated line graph*, defined inductively as

$$L^i(G) = \begin{cases} G & \text{if } i = 0, \\ L(L^{i-1}(G)) & \text{if } i > 0. \end{cases}$$

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Theorem

Among all connected graphs on n vertices, the fraction $\frac{W_e(G)}{W(G)}$ *is minimum for the star* S_n, *in which case* $\frac{W_e(G)}{W(G)} = \frac{n-2}{2(n-1)}$.

THANK YOU