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

A. Tepeh

joint work with
M. Knor and R. Škrekovski
Topological indices

- derived from molecular graphs
- numerical values

Molecular graphs

Structure: Thiamine (Vitamin B₁)
The Wiener index, defined as the sum of distances between all unordered pairs of vertices in a graph, is one of the most popular molecular descriptors.
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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)
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**: $d_G(e, f) = d_{L(G)}(e, f)$,

\[
d(e, f) = \begin{cases} 
\min \{d(u_i, v_j) : i, j \in \{1, 2\}\} + 1, & \text{if } e \neq f, \\
0, & \text{if } e = f,
\end{cases}
\]

\[d(x, y) = 3, \quad d(e, b) = 2, \quad d(a, b) = 1\]
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- $W_e(G) = W(L(G))$
- sometimes in the literature slightly different definition: $W_e(G) + \binom{n}{2}$
- $\text{deg}(u) =$ the degree of $u \in V(G)$
- $\delta(G) = \min\{\text{deg}(v) : v \in V(G)\}$

<table>
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<th>Gutman index</th>
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<td>$\text{Gut}(G) = \sum_{{u,v}\subseteq V(G)} \text{deg}(u) \text{deg}(v) , d(u, v)$</td>
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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 $G \cong C_n$. 
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 $G \cong C_n$.
- 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

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

with equality in (1) if and only if $G$ is a tree or a complete graph.
\( \kappa_m(G) \) = the number of \( m \)-cliques in \( G \)

**Knor, Potočnik and Škrekovski, 2014**

- Let \( G \) be a connected graph. Then

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W_e(G) \geq \frac{1}{4} \text{Gut}(G) - \frac{1}{4} |E(G)| + \frac{3}{4} \kappa_3(G) + 3 \kappa_4(G)
\]  

(1)

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

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

Let $G$ be a connected graph of minimum degree $\delta$. 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 $f = v_1 v_2$

$s(u_1 u_2, v_1 v_2) = \frac{1}{4} (d(u_1, v_1) + d(u_1, v_2) + d(u_2, v_1) + d(u_2, v_2))$
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The average distance of endpoints of edges $e = u_1u_2$ and $f = v_1v_2$

$$s(u_1u_2, v_1v_2) = \frac{1}{4} \left( d(u_1, v_1) + d(u_1, v_2) + d(u_2, v_1) + d(u_2, v_2) \right)$$

**Lemma**

Let $G$ be a connected graph. Then

$$\sum_{\{e,f\} \subseteq E(G)} s(e, f) = \frac{1}{4} \left( \text{Gut}(G) - |E(G)| \right).$$
Lemma (Knor et al., 2014)

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

\[
d(u_1u_2, v_1v_2) \geq s(u_1u_2, v_1v_2) + D(u_1u_2, v_1v_2),
\]

(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 $D_\alpha$ or that the pair $e, f$ belongs to the set $D_\alpha$
• if $e = f$, then $D(e, f) = -\frac{1}{2}$
• $I = \{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\}$
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**Lemma**

In a connected graph, every pair of distinct edges belongs to $D_\alpha$ for some $\alpha \in \mathcal{I}$.
### All types of pairs of two edges

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- **$D_1$**
  - $u_1$ to $v_1$: $k$ edges
  - $u_2$ to $v_2$: $k$ edges

- **$D_{rac{3}{4}}$**
  - $u_1$ to $v_1$: $k$ edges
  - $u_2$ to $v_2$: $k$ edges

- **$D_{rac{1}{4}}$**
  - $u_1$ to $v_1$: $k$ edges
  - $u_2$ to $v_2$: $k+1$ edges
\[ W_e(G) = \sum_{\{e,f\} \subseteq E(G)} d(e, f) \]
\[ = \sum_{\{e,f\} \subseteq E(G)} s(e, f) + \sum_{\{e,f\} \subseteq E(G)} D(e, f) \]
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**Proposition**

Let \( G \) be a connected graph. Then

\[ W_e(G) = \frac{\text{Gut}(G)}{4} - \frac{|E(G)|}{4} + |D_1| + \frac{1}{4} |D_{\frac{1}{4}}| + \frac{1}{2} |D_{\frac{1}{2}}| + \frac{3}{4} |D_{\frac{3}{4}}|. \]
Case 1: $G$ is non-regular

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

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

$$\geq \text{Gut}(G) - |E(G)|$$
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$$\geq \delta^2 \sum_{\{u,v\} \in V(G) \setminus \{w\}} d(u,v) +$$

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\geq \text{Gut}(G) - |E(G)|
= \sum\limits_{\{u,v\} \subseteq V(G)} \deg(u)\deg(v)\,d(u,v) - |E(G)|
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(\delta + 1) \sum\limits_{u \in V(G) \setminus \{w\}} \deg(u)d(u, w) - |E(G)|
\geq \delta^2 W(G) + \sum\limits_{u \in V(G) \setminus \{w\}} \deg(u) - |E(G)|
\geq \delta^2 W(G).
\]

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.*
### Case 2: $G$ is regular

**Lemma**

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

- 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 $W_e(G)$

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Dankelmann, 2009

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

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Let $G$ be a connected graph on $n$ vertices. Then

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

Theorem

Let $G$ be a connected graph on $n$ vertices. Then

$W_e(G) \leq \frac{4}{5^5} n^5 + O(n^4)$. 
Estimate the ratio $W(L^i(G))/W(G)$, where $L^i(G)$ stands for an *iterated line graph*, defined inductively as

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

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

**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* $\frac{W_e(G)}{W(G)} = \frac{n-2}{2(n-1)}$. 
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THANK YOU