BULLETIN OF THE INTERNATIONAL MATHEMATICAL VIRTUAL INSTITUTE
ISSN (p) 2303-4874, ISSN (o) 2303-4955
www.imvibl.org /JOURNALS/BULLETIN
Bull. Int. Math. Virtual Inst., **14**(2)(2024), 249–254
DOI: 10.7251/BIMVI2402249C

Former
BULLETIN OF THE SOCIETY OF MATHEMATICIANS BANJA LUKA
ISSN 0354-5792 (o), ISSN 1986-521X (p)

GENERALIZED ZAGREB INDEX OF GRAPH OPERATIONS

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Abstract. Let G be a simple connected graph with the edge set $E(G)$. For arbitrary real numbers r and s, the generalized Zagreb index of a graph G is defined as

$$M_{r,s}(G) = \sum_{uv\in E(G)} [d(u)^r d(v)^s + d(v)^r d(u)^s],$$

where $d(u)$ is the degree of a vertex u in G. In this paper, we establish the relationship between generalized Zagreb index of a graph and its line graph. In addition, we show that the general TEMO-type regularity holds for the generalized Zagreb index.

1. Introduction

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $d_G(u)$ and $N_G(u)$ denote the degree and the set of neighbors of u in G. The minimum degree and maximum degree of G are denoted by $\delta(G)$ and $\Delta(G)$. Let $I_G(u) = \{uu_i : uu_i \in E(G), u_i \in N_G(u)\}$. If there is no confusion, we simply denote the above notation as $d(u)$, $N(u)$, $I(u)$, δ, Δ. The cycle with n vertices is denoted by C_n. The line graph $L(G)$ is a graph whose vertices are the edges of G, with two of vertices being adjacent if the corresponding edges are adjacent in G. Clearly, $L(C_n) \cong C_n$. The line graph of a graph is currently the most common type of graph operation.

In 1947, Wiener discovered that certain physical properties of various paraffin species are correlated with the Wiener index (the sum of distances between all unordered pairs of vertices) of the tree determined by the carbon atoms of the

2020 *Mathematics Subject Classification.* Primary 05C09; Secondary 05C76; 05C92.
Key words and phrases. Generalized Zagreb index, Line graph, TEMO problem.
Communicated by Dusko Bogdanic.

corresponding molecules. Since then, a class of graph invariants known today as topological indices are being increasingly realized by chemists and others to be powerful tools in the description of chemical phenomena. Especially, the first Zagreb index, the second Zagreb index and Randić index are the most important topological index. The first and second Zagreb indices [**13**, **14**] are vertex-degree-based topological indices defined as

$$M_1(G) = \sum_{u \in V(G)} d^2(u) = \sum_{uv \in E(G)} (d(u) + d(v))$$

and

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

In 1975, Randić [**20**] introduced branching index (referred to as Randić index) as a suitable measure of the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. This index is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

Bollobás and Erdős [**2**] generalized Randić index by replacing $-1/2$ with any real number α, and obtained

$$R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^\alpha.$$

In 2011, Azari and Ironmanesh [**1**] further generalized the above topological indices, and proposed

$$M_{r,s}(G) = \sum_{uv \in E(G)} [d(u)^r d(v)^s + d(v)^r d(u)^s]$$

under the name generalized Zagreb index, where r and s are real numbers. Clearly,

$$M_{0,1}(G) = M_{1,0}(G) = M_1(G), \quad M_{1,1}(G) = 2M_2(G),$$
$$M_{-1/2,-1/2}(G) = 2R(G), \qquad M_{\alpha,\alpha}(G) = 2R_\alpha(G).$$

There are two interesting graph operations in mathematical chemistry. One is the relationship between the topological indices of graphs and their line graphs, the other is TEMO (topological effect on molecular orbitals) problem. Scholars have conducted extensive research on these two types of graph operations, see [3-12, 15-18, 22-26]. In particular, Qi and Lin [**19**] recently generalized TEMO problem, and proposed the general TEMO-type regularity problem (GTEMO problem for short). Let k be a positive even number, F and H be arbitrary vertex-disjoint connected graphs with $V(F) = \{u_1, u_2, \ldots, u_n\}$ and $V(H) = \{v_1, v_2, \ldots, v_n\}$. Then G_1 is the graph obtained from F and H by connecting u_i with v_i for $i = 1, 2, \ldots, k$. The graph G_2 is obtained analogously, by connecting u_i with v_{i+1} and v_i with u_{i+1} for $i = 1, 2, \ldots, k$, see Figure 1. The general TEMO-type regularity problem is whether it is possible to strictly determine the size of the topological indices corresponding to graphs G_1 and G_2 for $d(u_i) \neq d(u_{i+1})$ and $d(v_i) \neq d(v_{i+1})$, $i = 1, 3, 5, \cdots, k-1$.

In this paper, we obtain the following two theorems:

THEOREM 1.1. *Let G be a connected graph with n vertices and $\delta(G) \geqslant 2$. The following results hold.*

(i) *If $r \geqslant 0$ and $s \geqslant 0$, then $2M_{r,s}(G) \leqslant M_{r,s}(L(G))$;*

(ii) *If $r < 0$ and $s < 0$, then $2M_{r,s}(G) > M_{r,s}(L(G))$.*

THEOREM 1.2. *Let F and H be arbitrary vertex-disjoint connected graphs with $V(F) = \{u_1, u_2, \cdots, u_n\}$ and $V(H) = \{v_1, v_2, \cdots, v_n\}$, shown in Figure 1. If $d(u_i) \neq d(u_{i+1})$ and $d(v_i) \neq d(v_{i+1})$ for even k and $i = 1, 3, 5, \cdots, k-1$, then*

(i) *$M_{r,s}(G_1) > M_{r,s}(G_2)$ for $rs > 0$;*

(ii) *$M_{r,s}(G_1) < M_{r,s}(G_2)$ for $rs < 0$.*

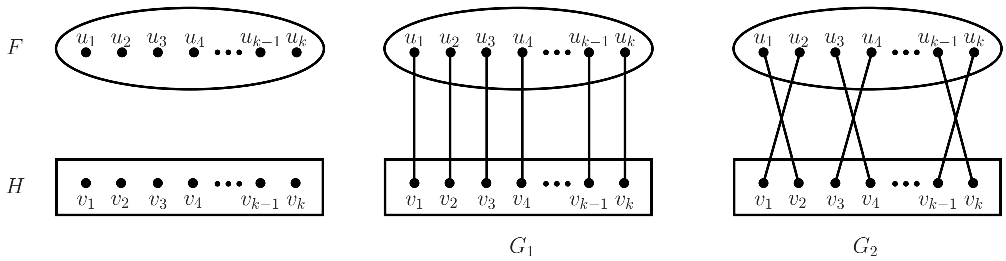

Figure 1. The structure of the graphs G_1 and G_2 and the labeling of their vertices.

2. The proof of Theorems 1.1 and 1.2

LEMMA 2.1. *For a vertex u of a connected graph G with nvertices and $\delta(G) \geqslant 2$. The following results hold.*

(i) *If $r \geqslant 0$ and $s \geqslant 0$, then*

$$\sum_{v \in N(u)} [d^r(u)d^s(v) + d^r(v)d^s(u)] \leqslant \sum_{e,f \in I(u)} [d_L^r(e)d_L^s(f) + d_L^r(f)d_L^s(e)]$$

with equality if and only if $G \cong C_n$.

(ii) *If $r < 0$ and $s < 0$, then*

$$\sum_{v \in N(u)} [d^r(u)d^s(v) + d^r(v)d^s(u)] \geqslant \sum_{e,f \in I(u)} [d_L^r(e)d_L^s(f) + d_L^r(f)d_L^s(e)]$$

with equality if and only if $G \cong C_n$.

PROOF. Let $d(u) = t$ and $N(u) = \{u_1, u_2, \cdots, u_t\}$. For convenience, $e_j = uu_j$ for j satisfying $1 \leqslant j \leqslant t$ and $d_{L(G)}(e)$ is simply denoted by $d_L(e)$ for any $e \in E(G)$. Assume that $d(u_1) \leqslant d(u_2) \leqslant \cdots \leqslant d(u_t)$. Since $t \geqslant 2$, $r \geqslant 0$ and $s \geqslant 0$, for any $j \in \{2, \cdots, t\}$, we have

$$\begin{aligned} d_L^r(e_1)d_L^s(e_j) + d_L^r(e_j)d_L^s(e_1) &= (d(u) + d(u_1) - 2)^r(d(u) + d(u_j) - 2)^s + (d(u) \\ &\quad + d(u_j) - 2)^r(d(u) + d(u_1) - 2)^s \\ &\geqslant d^r(u)d^s(u_j) + d^r(u_j)d^s(u) \end{aligned}$$

and

$$\begin{aligned} d_L^r(e_{t-1})d_L^s(e_t)+d_L^r(e_t)d_L^s(e_{t-1}) &= (d(u)+d(u_{t-1})-2)^r(d(u)+d(u_t)-2)^s \\ &\quad +(d(u)+d(u_t)-2)^r(d(u)+d(u_{t-1})-2)^s \\ &\geqslant d^r(u)d^s(u_1)+d^r(u_1)d^s(u). \end{aligned}$$

The above equation holds if and only if the degrees of all vertices are 2, that is, $G \cong C_n$. Similarly, conclusion (ii) holds. This completes the proof. □

The proof of Theorem 1.1 If $r \geqslant 0$ and $s \geqslant 0$, for each $u \in V(G)$ with $\delta \geqslant 2$, by Lemma 2.1, we have

$$\begin{aligned} M_{r,s}(G) &= \sum_{uv\in E(G)} [d^r(u)d^s(v)+d^r(v)d^s(u)] \\ &= \frac{1}{2}\sum_{u\in V(G)}\sum_{v\in N(u)} [d^r(u)d^s(v)+d^r(v)d^s(u)] \\ &\leqslant \frac{1}{2}\sum_{u\in V(G)}\sum_{e,f\in I(u)} [d_L^r(e)d_L^s(f)+d_L^r(f)d_L^s(e)] \\ &= \frac{1}{2}M_{r,s}(L(G)). \end{aligned}$$

Similarly, conclusion (ii) holds. This completes the proof.

The proof of Theorem 1.2 According to the construction of G_1 and G_2, we have

$$\begin{aligned} & M_{r,s}(G_1)-M_{r,s}(G_2) \\ = \ & (d^r(u_1)d^s(v_1)+d^r(v_1)d^s(u_1))+(d^r(u_2)d^s(v_2)+d^r(v_2)d^s(u_2))+\cdots+ \\ & (d^r(u_{k-1})d^s(v_{k-1})+d^r(v_{k-1})d^s(u_{k-1}))+(d^r(u_k)d^s(v_k)+d^r(v_k)d^s(u_k))- \\ & (d^r(u_1)d^s(v_2)+d^r(v_2)d^s(u_1))-(d^r(u_2)d^s(v_1)+d^r(v_1)d^s(u_2))-\cdots- \\ & (d^r(u_{k-1})d^s(v_k)+d^r(v_k)d^s(u_{k-1}))-(d^r(u_k)d^s(v_{k-1})+d^r(v_{k-1})d^s(u_k)) \\ = \ & d^r(u_1)(d^s(v_1)-d^s(v_2))+d^s(u_1)(d^r(v_1)-d^r(v_2))+d^r(u_2)(d^s(v_2)-d^s(v_1))+ \\ & d^s(u_2)(d^r(v_2)-d^r(v_1))+\cdots+d^r(u_{k-1})(d^s(v_{k-1})-d^s(v_k))+ \\ & d^s(u_{k-1})(d^r(v_{k-1})-d^r(v_k))+d^r(u_k)(d^s(v_k)-d^s(v_{k-1}))+d^s(u_k)(d^r(v_k)-d^r(v_{k-1})) \\ = \ & (d^r(u_1)-d^r(u_2))(d^s(v_1)-d^s(v_2))+(d^s(u_1)-d^s(u_2))(d^r(v_1)-d^r(v_2))+\cdots+ \\ & (d^r(u_{k-1})-d^r(u_k))(d^s(v_{k-1})-d^s(v_k))+(d^s(u_{k-1})-d^s(u_k))(d^r(v_{k-1})-d^r(v_k)) \\ = & \sum_{i=1,3,\cdots,k-1} [(d^r(u_i)-d^r(u_{i+1}))(d^s(v_i)-d^s(v_{i+1}))+(d^s(u_i)-d^s(u_{i+1}))(d^r(v_i)-d^r(v_{i+1}))]. \end{aligned}$$

If $d(u_i) \neq d(u_{i+1})$ and $d(v_i) \neq d(v_{i+1})$ for even k and $i = 1, 3, 5, \cdots, k-1$, then we have $(d^r(u_i)-d^r(u_{i+1}))(d^s(v_i)-d^s(v_{i+1})) > 0$ and $(d^s(u_i)-d^s(u_{i+1}))(d^r(v_i)-d^r(v_{i+1})) > 0$ for $rs > 0$, that is, $M_{r,s}(G_1)-M_{r,s}(G_2) > 0$ for $rs > 0$. Conversely, $(d^r(u_i)-d^r(u_{i+1}))(d^s(v_i)-d^s(v_{i+1})) < 0$ and $(d^s(u_i)-d^s(u_{i+1}))(d^r(v_i)-d^r(v_{i+1})) < 0$ for $rs < 0$ and $i = 1, 3, \cdots, k-1$, that is, $M_{r,s}(G_1)-M_{r,s}(G_2) < 0$ for $rs < 0$. This completes the proof.

References

1. M. Azari and A. Ironmanesh, Generalized Zagreb index of graphs. *Studia Universitatis Babes-Bolyai. Chemia*, **56** (2011), 59–70.
2. B. Bollobás and P. Erdős, Graphs of extremal weights. *Ars Comb.*, **50** (1998), 225–233.
3. F. Buckley, Mean distance of line graphs. *Congr. Numer.*, **32** (1981), 153–162.
4. N. Cohen, D. Dimitrov, R. Krakovski, R. Škrekovski, and V. Vukašinović, On Wiener index of graphs and their line graphs. *MATCH Commun. Math. Comput.Chem.*, **64** (2010), 683–698.
5. W. Carballosa, A. Granados, D. Pestana, A. Portilla, and J. M. Sigarreta, Relations between some topological indices and the line graph. *J. Math. Chem.*, **58** (2020), 632–646.
6. W. Carballosa, D. Pestana, J. M. Sigarreta, and E. Tourís, Relations between the general sum connectivity index and the line graph. *J. Math. Chem.*, **58** (2020), 2273–2290.
7. S. Cheng and B. Wu, The first general Zagreb index of graphs and their line graphs. *J. Appl. Math. Comput.*, **70** (2024), 1937–1951.
8. I. Gutman, TEMO theorem for Sombor index. *Open J. Discrete Appl. Math.*, **5** (2022), 25–28.
9. A. Graovac, I. Gutman, and O. E. Polansky, An interlacing theorem in simple molecular-orbital theory. *J. Chem. Soc. Faraday Trans.*, **81** (1985), 1543–1553.
10. I. Gutman, A. Graovac, and O. E. Polansky, On the theory of S- and T-isomers. *Chem. Phys. Lett.*, **116** (1985), 206–209.
11. I. Gutman, A. Graovac, and O. E. Polansky, Spectral properties of some structurally related graphs. *Discrete Appl. Math.*, **19** (1988), 195–203.
12. I. Gutman and L. Pavlović, More on distance of line graphs. *Graph Theory Notes N. Y.*, **33** (1997), 14–18.
13. I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes. *J. Chem. Phys.*, **62** (1975), 3399–3405.
14. I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chem. Phys. Lett.*, **17** (1972), 535–538.
15. H. Liu and Y. Huang, Sharp bounds on the symmetric division deg index of graphs and line graphs. *Comput. Appl. Math.*, **42** (2023), 285.
16. G. Li and M. Zhang, Sharp bounds on the arithmetic-geometric index of graphs and line graphs. *Discrete Appl. Math.*, **318** (2022), 47–60.
17. O. E. Polansky, Topological effects displayed in absorption and photoelectron spectra. *J. Mol. Struct.*, **113** (1984), 281–298.
18. O. E. Polansky and M. Zander, Topological effect on MO energies. *J. Mol. Struct.*, **84** (1982), 361–385.
19. F. Qi and Z. Lin, TEMO-type regularity for topological indices. *Bull. Int. Math. Virtual Inst.*, **13** (2023), 511–515.
20. M. Randić, On characterization of molecular branching. *J. Am. Chem. Soc.*, **97** (1975), 6609–6615.
21. H. Wiener, Structural determination of paraffin boiling points. *J. Am. Chem. Soc.*, **69** (1947), 17–20.
22. B. Wu, Wiener index of line graphs. *MATCH Commun. Math. Comput. Chem.*, **64** (2010), 699–706.
23. J. Wang, Z. Lin, and S. Zhang, TEMO-type regularity for two general degree-based topological indices. *Bull. Int. Math. Virtual Inst.*, **12** (2022), 401–407.
24. T. Wang, B. Wu, and T. Wang, Harmonic index of a line graph. *Discrete Appl. Math.*, **325** (2023), 284–296.
25. J. Zhang, B. Wu, Randić index of a line graph. *Axioms*, **11** (2022), 210.
26. Z. Zou and L. Zhong, A lower bound on the modified Randić index of line graphs. *Discrete Appl. Math.*, **345** (2024), 136–140.

Received by editors 26.7.2024; Revised version 28.10.2024; Available online 30.11.2024.

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