



Some inequalities for the exponential Zagreb indices

Mahdieh Azari

Department of Mathematics, Kazerun Branch, Islamic Azad University, P. O. Box: 73135-168, Kazerun, Iran

Farzaneh Falahati-Nezhad¹

Department of Mathematics, Safadasht Branch, Islamic Azad University, Tehran, Iran

Nasrin Dehgardi

Department of Mathematics and Computer Science, Sirjan University of Technology, Sirjan, Iran

Abstract

The first and second Zagreb indices are among the best-known and most thoroughly investigated vertex-degree-based topological indices in mathematical chemistry. The exponential of these two invariants were proposed by Rada (MATCH Commun. Math. Comput. Chem. 82(1) 29–41) in 2019. In this paper, we present some inequalities for the exponential Zagreb indices of some classical graph products which connect them to the exponential Zagreb indices of their building blocks.

Keywords: Topological indices, Graph products, Vertex degree, Lower bound.

AMS Mathematical Subject Classification [2010]: 05C07, 05C76.

1 Introduction

Let \mathcal{G} be a nontrivial simple connected graph with vertex set $V_{\mathcal{G}}$ and edge set $E_{\mathcal{G}}$. We denote by $n_{\mathcal{G}} = |V_{\mathcal{G}}|$ and $m_{\mathcal{G}} = |E_{\mathcal{G}}|$ the order and size of \mathcal{G} , respectively. For a vertex $a \in V_{\mathcal{G}}$, the degree $d_{\mathcal{G}}(a)$ is the number of all vertices of \mathcal{G} adjacent with a . If $d_{\mathcal{G}}(a) = d_{\mathcal{G}}(b)$ for each $a, b \in V_{\mathcal{G}}$, then \mathcal{G} is called a *regular* graph. We denote by $\delta_{\mathcal{G}}$, the minimum degree \mathcal{G} .

Topological indices are real numbers related to the molecular graph of a chemical structure which are invariant under graph isomorphism. They are applied in predicting the physico-chemical properties of chemical structures and considered as helpful tools in QSPR/QSAR investigations (see, for example, [5]).

The *first and second Zagreb indices* are among the foremost and well-investigated vertex-degree-based topological indices. These indices were proposed by Gutman *et al.* [6, 8] in 1970s and formulated for a graph \mathcal{G} as

$$M_1(\mathcal{G}) = \sum_{a \in V(\mathcal{G})} d_{\mathcal{G}}^2(a) \quad \text{and} \quad M_2(\mathcal{G}) = \sum_{aa' \in E(\mathcal{G})} d_{\mathcal{G}}(a)d_{\mathcal{G}}(a').$$

The readers interested in more information on the theory, applications and variants of Zagreb indices can be referred to the survey [7] and the references cited therein.

¹Speaker

In 2019, Rada [10] put forward the *exponential* of a vertex-degree-based invariant. In particular, the *exponential of Zagreb indices* are defined as

$$e^{M_1}(\mathcal{G}) = \sum_{a \in V(\mathcal{G})} e^{d_{\mathcal{G}}^2(a)} \quad \text{and} \quad e^{M_2}(\mathcal{G}) = \sum_{aa' \in E(\mathcal{G})} e^{d_{\mathcal{G}}(a)d_{\mathcal{G}}(a')}.$$

For more information on the exponential Zagreb indices, see [3, 4, 11].

In this paper, we give lower bounds on the exponential first and second Zagreb indices of some classical graph products such as join, corona product, Cartesian product and composition in terms of the exponential Zagreb indices and some parameters of their components. We refer the interested readers to [1, 2, 9] for more information on topological indices of graph operations.

2 Main results

In this section, the exponential Zagreb indices are studied for certain graph products. The factors of each graph product are assumed to be simple connected graphs \mathcal{G} and \mathcal{H} . We start with the join operation.

2.1 Join

Definition 2.1. The *join* $\mathcal{G} \nabla \mathcal{H}$ is the graph union $\mathcal{G} \cup \mathcal{H}$ together with all the edges joining $V_{\mathcal{G}}$ and $V_{\mathcal{H}}$.

Obviously, $n_{\mathcal{G} \nabla \mathcal{H}} = n_{\mathcal{G}} + n_{\mathcal{H}}$ and $m_{\mathcal{G} \nabla \mathcal{H}} = m_{\mathcal{G}} + m_{\mathcal{H}} + n_{\mathcal{G}}n_{\mathcal{H}}$.

Theorem 2.2. *The following inequalities hold.*

$$\begin{aligned} e^{M_1}(\mathcal{G} \nabla \mathcal{H}) &\geq e^{2n_{\mathcal{H}}\delta_{\mathcal{G}}+n_{\mathcal{H}}^2} e^{M_1}(\mathcal{G}) + e^{2n_{\mathcal{G}}\delta_{\mathcal{H}}+n_{\mathcal{G}}^2} e^{M_1}(\mathcal{H}), \\ e^{M_2}(\mathcal{G} \nabla \mathcal{H}) &\geq e^{2n_{\mathcal{H}}\delta_{\mathcal{G}}+n_{\mathcal{H}}^2} e^{M_2}(\mathcal{G}) + e^{2n_{\mathcal{G}}\delta_{\mathcal{H}}+n_{\mathcal{G}}^2} e^{M_2}(\mathcal{H}) + n_{\mathcal{G}}n_{\mathcal{H}} e^{(\delta_{\mathcal{G}}+n_{\mathcal{H}})(\delta_{\mathcal{H}}+n_{\mathcal{G}})}. \end{aligned}$$

The equality holds in both cases if and only if \mathcal{G} and \mathcal{H} are regular graphs.

2.2 Corona product

Definition 2.3. The *corona product* $\mathcal{G} \circ \mathcal{H}$ is the graph obtained by a copy of \mathcal{G} and $n_{\mathcal{G}}$ copies of \mathcal{H} and joining the i th vertex of \mathcal{G} to each vertex in the i th copy of \mathcal{H} for each $1 \leq i \leq n_{\mathcal{G}}$.

Obviously, $n_{\mathcal{G} \circ \mathcal{H}} = n_{\mathcal{G}} + n_{\mathcal{G}}n_{\mathcal{H}}$ and $m_{\mathcal{G} \circ \mathcal{H}} = m_{\mathcal{G}} + n_{\mathcal{G}}m_{\mathcal{H}} + n_{\mathcal{G}}n_{\mathcal{H}}$.

Theorem 2.4. *The following inequalities hold.*

$$\begin{aligned} e^{M_1}(\mathcal{G} \circ \mathcal{H}) &\geq e^{2n_{\mathcal{H}}\delta_{\mathcal{G}}+n_{\mathcal{H}}^2} e^{M_1}(\mathcal{G}) + n_{\mathcal{G}} e^{2\delta_{\mathcal{H}}+1} e^{M_1}(\mathcal{H}), \\ e^{M_2}(\mathcal{G} \circ \mathcal{H}) &\geq e^{2n_{\mathcal{H}}\delta_{\mathcal{G}}+n_{\mathcal{H}}^2} e^{M_2}(\mathcal{G}) + n_{\mathcal{G}} e^{2\delta_{\mathcal{H}}+1} e^{M_2}(\mathcal{H}) + n_{\mathcal{G}}n_{\mathcal{H}} e^{(\delta_{\mathcal{G}}+n_{\mathcal{H}})(\delta_{\mathcal{H}}+1)}. \end{aligned}$$

The equality holds in both cases if and only if \mathcal{G} and \mathcal{H} are regular graphs.

2.3 Cartesian product

Definition 2.5. The *Cartesian product* $\mathcal{G}\square\mathcal{H}$ is a graph with vertex set $V_{\mathcal{G}\square\mathcal{H}} = V_{\mathcal{G}} \times V_{\mathcal{H}}$ and $(a, b)(a', b') \in E_{\mathcal{G}\square\mathcal{H}}$ if and only if $(a = a' \text{ and } bb' \in E_{\mathcal{H}})$ or $(b = b' \text{ and } aa' \in E_{\mathcal{G}})$.

Obviously, $n_{\mathcal{G}\square\mathcal{H}} = n_{\mathcal{G}}n_{\mathcal{H}}$ and $m_{\mathcal{G}\square\mathcal{H}} = n_{\mathcal{G}}m_{\mathcal{H}} + n_{\mathcal{H}}m_{\mathcal{G}}$.

Theorem 2.6. *The following inequalities hold.*

$$\begin{aligned} e^{M_1}(\mathcal{G}\square\mathcal{H}) &\geq e^{2\delta_{\mathcal{G}}\delta_{\mathcal{H}}} e^{M_1}(\mathcal{G}) e^{M_1}(\mathcal{H}), \\ e^{M_2}(\mathcal{G}\square\mathcal{H}) &\geq e^{2\delta_{\mathcal{G}}\delta_{\mathcal{H}}} (e^{M_1}(\mathcal{H})e^{M_2}(\mathcal{G}) + e^{M_1}(\mathcal{G})e^{M_2}(\mathcal{H})). \end{aligned}$$

The equality holds in both cases if and only if \mathcal{G} and \mathcal{H} are regular graphs.

2.4 Composition

Definition 2.7. The *composition* $\mathcal{G}[\mathcal{H}]$ is a graph with vertex set $V_{\mathcal{G}[\mathcal{H}]} = V_{\mathcal{G}} \times V_{\mathcal{H}}$ and $(a, b)(a', b') \in E_{\mathcal{G}[\mathcal{H}]}$ if and only if $aa' \in E_{\mathcal{G}}$ or $(a = a' \text{ and } bb' \in E_{\mathcal{H}})$.

Obviously, $n_{\mathcal{G}[\mathcal{H}]} = n_{\mathcal{G}}n_{\mathcal{H}}$ and $m_{\mathcal{G}[\mathcal{H}]} = m_{\mathcal{G}}n_{\mathcal{H}}^2 + n_{\mathcal{G}}m_{\mathcal{H}}$.

Theorem 2.8. *The following inequalities hold.*

$$\begin{aligned} e^{M_1}(\mathcal{G}[\mathcal{H}]) &\geq n_{\mathcal{G}} e^{n_{\mathcal{H}}^2\delta_{\mathcal{G}}^2+2n_{\mathcal{H}}\delta_{\mathcal{G}}\delta_{\mathcal{H}}} e^{M_1}(\mathcal{H}), \\ e^{M_2}(\mathcal{G}[\mathcal{H}]) &\geq n_{\mathcal{H}}^2 m_{\mathcal{G}} e^{n_{\mathcal{H}}^2\delta_{\mathcal{G}}^2+2n_{\mathcal{H}}\delta_{\mathcal{G}}\delta_{\mathcal{H}}+\delta_{\mathcal{H}}^2} + n_{\mathcal{G}} e^{n_{\mathcal{H}}^2\delta_{\mathcal{G}}^2+2n_{\mathcal{H}}\delta_{\mathcal{G}}\delta_{\mathcal{H}}} e^{M_2}(\mathcal{H}). \end{aligned}$$

The equality holds in both cases if and only if \mathcal{G} and \mathcal{H} are regular graphs.

References

- [1] M. Azari, *On the Zagreb and eccentricity coindices of graph products*, Iran. J. Math. Sci. Inf., 18(1) (2023), pp. 165–178.
- [2] M. Azari and N. Dehgardi, *Measuring peripherality extent in chemical graphs via graph operations*, Int. J. Quantum. Chem., 122 (2022), # e26835.
- [3] S. Balachandran and T. Vetrík, *Exponential second Zagreb index of chemical trees*, Trans. Comb., 10(2) (2021), pp. 97–106.
- [4] R. Cruz, J. D. Monsalve and J. Rada, *The balanced double star has maximum exponential second Zagreb index*, J. Comb. Optim., 41 (2021), pp. 544–552.
- [5] M. V. Diudea, *QSPR/QSAR Studies by Molecular Descriptors*, Nova Science, Huntingdon, New York, USA, 2000.
- [6] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals, Total π -electron energy of alternant hydrocarbons*, Chem. Phys. Lett., 17 (1972), pp. 535–538.
- [7] I. Gutman, E. Milovanović and E. Milovanović, *Beyond the Zagreb indices*, AKCE Int. J. Graphs Comb., 17(1) (2020), pp. 74–85.

-
- [8] I. Gutman, B. Rušćić, N. Trinajstić and C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys., 62 (1975), pp. 3399–3405.
- [9] M. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, *The first and second Zagreb indices of some graph operations*, Discrete Appl. Math., 157 (2009), pp. 804–811.
- [10] J. Rada, *Exponential vertex-degree-based topological indices and discrimination*, MATCH Commun. Math. Comput. Chem., 82(1) (2019), 29–41.
- [11] M. Zeng and H. Deng, *An open problem on the exponential of the second Zagreb index*, MATCH Commun. Math. Comput. Chem., 85 (2021), pp. 367–373.

e-mail: mahdie.azari@gmail.com, mahdieh.azari@iau.ac.ir

e-mail: farzanehfalahati_n@yahoo.com

e-mail: n.dehgardi@sirjantech.ac.ir