Communications in Combinatorics and Optimization
Vol. xx, No. x (xxxx), pp. 1-10
https://doi.org/10.22049/cco.2024.29529.2040

CCO
Commun. Comb. Optim.

Research Article

On relations between the modified hyper–Wiener index and some degree–based indices of trees

Ş.B. Bozkurt Altındağ[1,*], I. Milovanović[2,†], E. Milovanović[2,‡]

[1]Department of Mathematics, Faculty of Science, Selçuk University, Konya, Turkey
[*]srf_burcu_bozkurt@hotmail.com

[2]Faculty of Electronic Engineering, University of Niš, Niš, Serbia
[†]igor@elfak.ni.ac.rs
[‡]ema@elfak.ni.ac.rs

Received: 12 March 2024; Accepted: 29 August 2024
Published Online: 7 September 2024

Abstract: Let T be a tree of order n with Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$. The Wiener index of T is defined as $W(T) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}$. The modified hyper–Wiener index of T is stated in terms of $W(T)$ and Laplacian eigenvalues as $WWW(T) = \frac{W(T)^2}{2n} - \frac{n}{2}\sum_{i=1}^{n-1} \frac{1}{\mu_i^2}$. In this study, we present some relations between modified hyper–Wiener index, the first Zagreb index, modified first Zagreb index and inverse degree index of trees when order n and maximal vertex degree of a graph are known.

Keywords: graph, Laplacian eigenvalues, modified hyper–Wiener index.

AMS Subject classification: 05C50, 15A18

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph of order n and size m with the vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Denote by $A(G)$ the $(0, 1)$ −adjacency matrix of G. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$, where $D(G) = \text{diag}(d_1, d_2, \ldots, d_n)$ is the diagonal degree matrix of G [14]. Eigenvalues of $L(G)$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, represent the Laplacian eigenvalues of G [6].

* *Corresponding Author*

© 2024 Azarbaijan Shahid Madani University

In graph theory, a graph invariant is a property of graphs that is preserved by isomorphism [7]. The graph invariants that assume only numerical values are usually referred to as topological indices in chemical graph theory [21]. The Wiener index is a well-known distance-based topological index introduced as structural descriptor for acyclic organic molecules. It was conceived by Harold Wiener in 1947 as [22]

$$W(G) = \sum_{i<j} d_{ij} \,,$$

where d_{ij} is the number of edges in a shortest path between vertices v_i and v_j. The Wiener index is one of the most frequently used molecular shape descriptors. It has found many applications in the modelling of physico-chemical properties of organic molecules. Since many molecular graphs of organic compounds are trees, there are a lot of studies of the properties of the Wiener indices of trees [4]. The hyper–Wiener index [9] and modified hyper–Wiener index are generalization of the concept of Wiener index [20].

The following results connect the Wiener index, modified hyper–Wiener index (quantities defined in terms of distances in a graph) and Laplacian eigenvalues. Namely, for any tree T of order n, the Wiener index can be calculated as [10, 18]:

$$W(T) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} \,,$$

and the modified hyper–Wiener index as [9]

$$WWW(T) = n \sum_{i<j} \frac{1}{\mu_i \mu_j} \,.$$

For any tree T of order n, the following relation between Laplacian eigenvalues, Wiener index and the modified hyper–Wiener index has been obtained in [8]:

$$WWW(T) = \frac{W(T)^2}{2n} - \frac{n}{2} \sum_{i=1}^{n-1} \frac{1}{\mu_i^2}. \tag{1.1}$$

Several lower and upper bounds on $WWW(T)$ can be found in [1].

Before we proceed, let us recall some degree–based indices that are of interest for the present paper. The first Zagreb index is defined by [11]

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \,.$$

The modified first Zagreb index is defined as [19]

$$ {}^{m}M_1(G) = \sum_{i=1}^{n} \frac{1}{d_i^2} \,. $$

The inverse degree index is introduced in [5] as

$$ ID(G) = \sum_{i=1}^{n} \frac{1}{d_i} \,. $$

In this paper, we investigate some relationships between modified hyper–Wiener index, the first Zagreb index, modified first Zagreb index and inverse degree index of trees when order n and maximal vertex degree of a graph are known.

2. Preliminaries and Lemmas

Let α be a real number. The sum of the α-th powers of the Laplacian eigenvalues of graph G closely related with several graph invariants is defined by [23] (see also [2, 3])

$$ s_\alpha\left(G\right) = \sum_{i=1}^{n-1} \mu_i^\alpha . $$

Let us denote by $K_{1,n-1}$ the star graph of order n. We now recall two results from the literature that are of interest for the present paper.

Lemma 1. [13] *Let G be a simple connected graph of order $n \geq 3$ with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$, where $d_{n-2} \geq d_{n-1} + d_n - 1$. If $\alpha < 0$ or $\alpha > 1$, then*

$$ s_\alpha\left(G\right) \geq \left(1 + d_1\right)^\alpha + d_2^\alpha + \cdots + d_{n-2}^\alpha + \left(d_{n-1} + d_n - 1\right)^\alpha \tag{2.1} $$

with equality if and only if $G \cong K_{1,n-1}$.

Lemma 2. [12, 16] *Let $p = (p_i)$, $i = 1, 2, \ldots, n$, be a sequence of non–negative real numbers, and $a = (a_i)$, $i = 1, 2, \ldots, n$, sequence of positive real numbers. Then, for any real r, $r \leq 0$ or $r \geq 1$, holds*

$$ \left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i^r \geq \left(\sum_{i=1}^{n} p_i a_i\right)^r . \tag{2.2} $$

When $0 \leq r \leq 1$, the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = \cdots = a_n$, or $p_{t+1} = \cdots = p_n = 0$ and $a_1 = \cdots = a_t$, for some t , $1 \leq t \leq n-1$.

3. Main Results

In the next theorem we establish a relationship between $WWW(T)$, $W(T)$ and ${}^{m}M_1(T)$, when n and d_1 are known.

Theorem 1. *Let T be a tree of order $n \geq 2$. Then, we have*

$$WWW(T) \leq \frac{n}{2}\left(\frac{W(T)^2 + n^2}{n^2} + \frac{2d_1 + 1}{d_1^2(1+d_1)^2} - {}^{m}M_1(T)\right). \tag{3.1}$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. According to (2.1), for any connected graph G and $\alpha = -2$, the following inequality is valid

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i^2} \geq \frac{1}{(1+d_1)^2} + \sum_{i=2}^{n-2} \frac{1}{d_i^2} + \frac{1}{(d_{n-1} + d_n - 1)^2}, \tag{3.2}$$

with equality if and only if $G \cong K_{1,n-1}$. Let $G \cong T$. Thus $d_n = d_{n-1} = 1$. Then, according to (1.1) and (3.2), we have that

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i^2} = \frac{W(T)^2}{n^2} - \frac{2WWW(T)}{n} \geq 1 + \frac{1}{(1+d_1)^2} + \sum_{i=2}^{n-2} \frac{1}{d_i^2}. \tag{3.3}$$

Since

$$\sum_{i=2}^{n-2} \frac{1}{d_i^2} = {}^{m}M_1(T) - \frac{1}{d_1^2} - 2,$$

from the above and (3.3), we arrive at (3.1).

Equality in (3.3), and consequently in (3.1), holds if and only if $T \cong K_{1,n-1}$. □

Corollary 1. *Let T be a tree of order $n \geq 4$. Then*

$$WWW(T) \leq \frac{n}{2}\left[\frac{W(T)^2 - n^2}{n^2} - \frac{1}{(1+d_1)^2} - \sqrt{\frac{\left(ID(T) - 2 - \frac{1}{d_1}\right)^3}{2(n-2) - d_1}}\right].$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. In [15] it was proven that

$$^{m}M_1(T) \geq 2 + \frac{1}{d_1^2} + \sqrt{\frac{\left(ID(T) - 2 - \frac{1}{d_1}\right)^3}{2(n-2) - d_1}}\,,$$

with equality if and only if $T \cong P_n$, or $T \cong K_{1,n-1}$. From the above and inequality (3.1), the required result is obtained. □

Corollary 2. *Let T be a tree of order $n \geq 4$. Then*

$$WWW(T) \leq \frac{n}{2}\left[\frac{W(T)^2 - n^2}{n^2} - \frac{1}{(1+d_1)^2} - \frac{(n-3)^3}{(2(n-2)-d_1)^2}\right].$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. In [15] it was proven that

$$^{m}M_1(T) \geq 2 + \frac{1}{d_1^2} + \frac{(n-3)^3}{(2(n-2)-d_1)^2}\,,$$

with equality if and only if $T \cong P_n$, or $T \cong K_{1,n-1}$. From the above and inequality (3.1), we get the required result. □

Corollary 3. *Let T be a tree of order $n \geq 4$. Then*

$$WWW(T) \leq \frac{n}{2}\left[\frac{W(T)^2 - n^2}{n^2} - \frac{1}{(1+d_1)^2} - \frac{(n-3)^2}{M_1(T) - 2 - d_1^2}\right].$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. According to the inequality between arithmetic and harmonic means (see e.g. [17]), the following is valid

$$\sum_{i=2}^{n-2}\frac{1}{d_i^2}\sum_{i=2}^{n-2} d_i^2 \geq (n-3)^2\,,$$

that is

$$\sum_{i=2}^{n-2}\frac{1}{d_i^2} \geq \frac{(n-3)^2}{M_1(T) - d_1^2 - 2}\,.$$

From the above and inequality (3.3), we obtain that

$$\frac{W(T)^2}{n^2} - \frac{2WWW(T)}{n} \geq 1 + \frac{1}{(1+d_1)^2} + \frac{(n-3)^2}{M_1(T) - d_1^2 - 2}\,,$$

from which we obtain the required result. □

Theorem 2. *Let T, $T \ncong P_n$, be a tree of order $n \geq 4$. Then we have*

$$WWW(T) \leq \frac{n}{2}\left[\frac{W(T)^2-n^2}{n^2} - \frac{1}{(1+d_1)^2} - \right. \\ \left. - \frac{1}{d_1}\left(ID(T)-2-\frac{1}{d_1}+\frac{(d_1(ID(T)-2)-n+2)^2}{(n-2)(d_1-2)}\right)\right]. \tag{3.4}$$

Equality holds if and only if $T \cong K_{1,n-1}$.

Proof. The inequality (2.2) can be considered as

$$\left(\sum_{i=2}^{n-2} p_i\right)^{r-1} \sum_{i=2}^{n-2} p_i a_i^r \geq \left(\sum_{i=2}^{n-2} p_i a_i\right)^r. \tag{3.5}$$

For $r=2$, $p_i = \frac{d_1-d_i}{d_i^2}$, $a_i = d_i$, $i=2,3,\ldots,n-2$, the above inequality becomes

$$\sum_{i=2}^{n-2} \frac{d_1-d_i}{d_i^2} \sum_{i=2}^{n-2}(d_1-d_i) \geq \left(\sum_{i=2}^{n-2} \frac{d_1-d_i}{d_i}\right)^2. \tag{3.6}$$

Note that

$$\sum_{i=2}^{n-2} \frac{d_1-d_i}{d_i^2} = d_1 \sum_{i=2}^{n-2} \frac{1}{d_i^2} - \sum_{i=2}^{n-2} \frac{1}{d_i} = d_1 \sum_{i=2}^{n-2} \frac{1}{d_i^2} - \left(ID(T)-2-\frac{1}{d_1}\right),$$

$$\sum_{i=2}^{n-2}(d_1-d_i) = d_1(n-3)-(2(n-1)-d_1-2) = (n-2)(d_1-2),$$

$$\sum_{i=2}^{n-2} \frac{d_1-d_i}{d_i} = d_1\left(ID(T)-2-\frac{1}{d_1}\right)-(n-3) = d_1(ID(T)-2)-n+2,$$

From the above arguments and (3.6), we obtain

$$\left(d_1 \sum_{i=2}^{n-2} \frac{1}{d_i^2} - (ID(T)-2-\frac{1}{d_1})\right)(n-2)(d_1-2) \geq (d_1(ID(T)-2)-n+2)^2.$$

Since $n \geq 4$ and $d_1 \neq 2$, from the above inequality we have that

$$\sum_{i=2}^{n-2} \frac{1}{d_i^2} \geq \frac{1}{d_1}\left(ID(T)-2-\frac{1}{d_1}+\frac{(d_1(ID(T)-2)-n+2)^2}{(n-2)(d_1-2)}\right).$$

Now, from the above and inequality (3.3) we obtain

$$\frac{W(T)^2}{n^2}-\frac{2WWW(T)}{n}\geq 1+\frac{1}{(1+d_1)^2}+\frac{1}{d_1}\left(ID(T)-2-\frac{1}{d_1}+\frac{(d_1(ID(T)-2)-n+2)^2}{(n-2)(d_1-2)}\right),$$

from which we arrive at (3.4).

Equality in (3.6) holds if and only if $d_2=d_3=\cdots=d_{n-2}$, or $d_1=d_2=\cdots=d_t\geq d_{t+1}=\cdots=d_{n-2}$, for some t, $1\leq t\leq n-3$. Equality in (3.3) holds if and only if $T\cong K_{1,n-1}$. This implies that equality in (3.4) holds if and only if $T\cong K_{1,n-1}$. □

In the next theorem we establish a relationship between $WWW(T)$, $M_1(T)$ and $ID(T)$, when n and d_1 are known.

Theorem 3. *Let T, $T\ncong P_n$, be a tree of order $n\geq 4$. Then*

$$\begin{aligned}WWW(T)\leq \frac{n}{2}\Bigg[&\frac{W(T)^2-n^2}{n^2}-\frac{1}{(1+d_1)^2}-\frac{n-3}{d_1^2}-\\&-\frac{(d_1^2(ID(T)-2)-2(n-2))^2}{d_1^2(d_1^2(n-2)-M_1(T)+2)}\Bigg].\end{aligned}\tag{3.7}$$

Equality holds if and only if $T\cong K_{1,n-1}$.

Proof. For $r=2$, $p_i=\frac{d_1^2-d_i^2}{d_i^2}$, $a_i=d_i$, $i=2,3,\ldots,n-2$, the inequality (3.5) becomes

$$\sum_{i=2}^{n-2}\frac{d_1^2-d_i^2}{d_i^2}\sum_{i=2}^{n-2}(d_1^2-d_i^2)\geq\left(\sum_{i=2}^{n-2}\frac{d_1^2-d_i^2}{d_i}\right)^2.\tag{3.8}$$

Since

$$\begin{aligned}\sum_{i=2}^{n-2}\frac{d_1^2-d_i^2}{d_i^2}&=d_1^2\sum_{i=2}^{n-2}\frac{1}{d_i^2}-n+3,\\ \sum_{i=2}^{n-2}(d_1^2-d_i^2)&=d_1^2(n-2)-M_1(T)+2,\\ \sum_{i=2}^{n-2}\frac{d_1^2-d_i^2}{d_i}&=d_1^2\sum_{i=2}^{n-2}\frac{1}{d_i}-\sum_{i=2}^{n-2}d_i=d_1^2\left(ID(T)-2\right)-2(n-2).\end{aligned}$$

From the above identities and inequality (3.8) we obtain that

$$\left(d_1^2\sum_{i=2}^{n-2}\frac{1}{d_i^2}-n+3\right)(d_1^2(n-2)-M_1(T)+2)\geq(d_1^2(ID(T)-2)-2(n-2))^2.$$

Since $T \ncong P_n$ then $d_1^2(n-2) - M_1(T) + 2 \neq 0$. Therefore we have that

$$\sum_{i=2}^{n-2} \frac{1}{d_i^2} \geq \frac{n-3}{d_1^2} + \frac{(d_1^2(ID(T)-2) - 2(n-2))^2}{d_1^2(d_1^2(n-2) - M_1(T) + 2)}, .$$

From the above and (3.3) we obtain that

$$\frac{W(T)^2}{n^2} - \frac{2WWW(T)}{n} \geq 1 + \frac{1}{(1+d_1)^2} + \frac{n-3}{d_1^2} + \frac{(d_1^2(ID(T)-2) - 2(n-2))^2}{d_1^2(d_1^2(n-2) - M_1(T) + 2)},$$

from which the inequality (3.7) follows.
Equality in (3.8) holds if and only if $d_2 = d_3 = \cdots = d_{n-2}$, or $d_1 = d_2 = \cdots = d_t \geq d_{t+1} = \cdots = d_{n-2}$, for some t, $1 \leq t \leq n-3$. Equality in (3.3) holds if and only if $T \cong K_{1,n-1}$. Then the equality in (3.7) holds if and only if $T \cong K_{1,n-1}$. □

By a similar procedure as in case of Theorems 2 and 3, the following results can be proven.

Theorem 4. *Let T be a tree of order $n \geq 5$. If $T \cong K_{1,n-1}$, then*

$$WWW(T) = \frac{(n-1)^4 - n^2(n-2) - 1}{2n}.$$

If $T \ncong K_{1,n-1}$ and $T \ncong P_n$, then

$$\begin{aligned} WWW(T) \; < \; & \frac{n}{2}\left[\frac{W(T)^2 - n^2}{n^2} - \frac{1}{(1+d_1)^2} - \right. \\ & \left. - \frac{1}{d_2}\left(ID(T) - \frac{1}{d_1} - 2 + \frac{\left(d_2\left(ID(T) - 2 - \frac{1}{d_1}\right) - n + 3\right)^2}{d_2(n-3) + d_1 - 2(n-2)}\right)\right]. \end{aligned}$$

Theorem 5. *Let T be a tree, $T \ncong K_{1,n-1}$ and $T \ncong P_n$, of order $n \geq 5$. Then we have*

$$\begin{aligned} WWW(T) \; < \; & \frac{n}{2}\left[\frac{W(T)^2 - n^2}{n^2} - \frac{1}{(1+d_1)^2} - \frac{n-3}{d_2^2} - \right. \\ & \left. - \frac{\left(d_2^2\left(ID(T) - \frac{1}{d_1} - 2\right) - (2(n-2) - d_1)\right)^2}{d_2^2(d_2^2(n-3) - M_1(T) + d_1^2 + 2)}\right]. \end{aligned}$$

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

References

[1] Ş.B.B. Altındağ, I.Ž. Milovanović, E.I. Milovanović, and M.M. Matejić, *Modified hyper-Wiener index of trees*, Discrete Appl. Math. **334** (2023), 101–109. https://doi.org/10.1016/j.dam.2023.03.005.

[2] X. Chen and J. Qian, *Bounding the sum of powers of the Laplacian eigenvalues of graphs*, Appl. Math. J. Chin. Univ. **26** (2011), no. 2, 142–150. https://doi.org/10.1007/s11766-011-2732-4.

[3] K.C. Das, K. Xu, and M. Liu, *On sum of powers of the Laplacian eigenvalues of graphs*, Linear Algebra Appl. **439** (2013), no. 11, 3561–3575. https://doi.org/10.1016/j.laa.2013.09.036.

[4] A.A. Dobrynin, R. Entringer, and I. Gutman, *Wiener index of trees: theory and applications*, Acta Appl. Math. **66** (2001), no. 3, 211–249. https://doi.org/10.1023/A:1010767517079.

[5] S. Fajtlowicz, *On conjectures of Graffiti II*, Congr. Numer. **60** (1987), 187–197.

[6] R. Grone and R. Merris, *The Laplacian spectrum of a graph II*, SIAM J. Discrete Math. **7** (1994), no. 2, 221–229. https://doi.org/10.1137/S0895480191222653.

[7] J.L. Gross, J. Yellen, and M. Anderson, *Graph Theory and Its Applications*, CRC Press, New York, 2018.

[8] I. Gutman, *Hyper-Wiener index and Laplacian spectrum*, J. Serb. Chem. Soc. **68** (2003), no. 12, 949–952.

[9] I. Gutman, B. Furtula, and J. Belić, *Note of the hyper-Wiener index*, J. Serb. Chem. Soc. **68** (2003), no. 12, 943–948. http://dx.doi.org/10.2298/JSC0312943G.

[10] I. Gutman, S.L. Lee, C.H. Chu, and Y.L. Luo, *Chemical applications of the Laplacian spectrum of molecular graphs: studies of the Wiener number*, Indian J. Chem. **33A** (1994), no. 7, 603–608.

[11] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total $\pi-$ electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538. https://doi.org/10.1016/0009-2614(72)85099-1.

[12] J.L.W.V. Jensen, *Sur les fonctions convexes et les inégalités entre les valeurs moyennes*, Acta math. **30** (1906), no. 1, 175–193. https://doi.org/10.1007/BF02418571.

[13] M. Liu and B. Liu, *A note on sum of powers of the Laplacian eigenvalues of graphs*, Appl. Math. Lett. **24** (2011), no. 3, 249–252. https://doi.org/10.1016/j.aml.2010.09.013.

[14] R. Merris, *Laplacian matrices of graphs: A survey*, Linear Algebra Appl. **197–198** (1994), 143–176. https://doi.org/10.1016/0024-3795(94)90486-3.

[15] I.Ž Milovanović, E.I. Milovanović, M. Matejić, and A. Ali, *Some new bounds on*

the modified first Zagreb index, Commun. Comb. Optim. **8** (2023), no. 1, 13–21. https://doi.org/10.22049/cco.2021.27159.1205.

[16] D.S. Mitrinović, J. Pečarić, and A.M. Fink, *Classical and New Inequalities in Analysis*, Kluwer Academic Publishers, Dordrecht, 1993.

[17] D.S. Mitrinović and P.M. Vasić, *Analytic Inequalities*, Springer Verlag, Berlin–Heidelberg–New York, 1970.

[18] B. Mohar, D. Babić, and N. Trinajstić, *A novel definition of the Wiener index for trees*, J. Chem. Inf. Comput. **33** (1993), no. 1, 153–154. https://doi.org/10.1021/ci00011a023.

[19] S. Nikolić, G. Kovačević, A. Miličević, and N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003), no. 2, 113–124.

[20] M. Randić, *Novel molecular descriptor for structure–property studies*, Chem. Phys. Lett. **211** (1993), no. 4-5, 478–483. https://doi.org/10.1016/0009-2614(93)87094-J.

[21] S. Wagner and H. Wang, *Introduction to Chemical Graph Theory*, CRC Press, Boca Raton, 2018.

[22] H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc. **69** (1947), no. 1, 17–20. https://doi.org/10.1021/ja01193a005.

[23] B. Zhou, *On sum of powers of the Laplacian eigenvalues of graphs*, Linear Algebra Appl. **429** (2008), no. 8-9, 2239–2246.