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Research Article

Bounds for some distance-based and degree-distance-based topological indices

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Abstract

In this paper, lower and upper bounds for the Wiener, hyper-Wiener, and Harary indices of simple connected non-trivial graphs are derived. Inequalities involving some degree-distance-based and distance-based topological indices are also obtained.

Keywords: distance in graphs; topological indices; vertex degrees.

2020 Mathematics Subject Classification: 05C09.

1. Introduction

Graph theory is one of the fast growing areas of mathematics that found applications in many scientific fields. This paper is concerned with some special graph invariants which are known as topological indices in chemical graph theory [11]. The primary purpose of the topological indices in chemical graph theory is to predict physico-chemical properties of chemical compounds. There are many topological indices in literature; for example, see the articles [6–8, 10, 18], survey [23], and the references cited therein.

Let G be a graph on n vertices and m edges. Its vertex set and edge set are denoted by $V(G)$ and $E(G)$, respectively. The distance between two vertices u and v of G is denoted by $d_G(u,v)$ and is defined as the length of a shortest u-v path in G [5]. The eccentricity $\varepsilon(i)$ of a vertex $i \in V(G)$ is defined as the distance between i and a vertex farthest from it, that is $\varepsilon(i) = \max\{d_G(i,j) : j \in V(G)\}$. The maximum value of $\varepsilon(i)$ over all vertices of G is called the diameter of G and is denoted by d, that is $d = \max\{\varepsilon(i) : i \in V(G)\}$.

The oldest topological index is the Wiener index, which is defined [3, 21] for a graph G as

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d_G(u,v).$$

The hyper-Wiener index is one of the well-known variants of the Wiener index. The hyper-Wiener index of a graph G is defined [16] as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d_G(u,v) + d_G(u,v)^2).$$

The Harary index is another well-studied variant of the Wiener index. The Harary index of a graph G is defined [15, 20, 22] as

$$H(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d_G(u,v)}.$$

All the above-mentioned three indices are distance-based topological indices. We are also concerned in this paper with the degree-distance-based topological indices. One of such indices is the degree distance index, which is defined [2, 4, 14] as

$$DD(G) = \frac{1}{2} \sum_{u,v \in V(G)} (d(u) + d(v)) d_G(u,v),$$

where $d(u)$ and $d(v)$ are the degrees of the vertices u and v, respectively. The Schultz index (also known as the Gutman index) is another degree-distance-based topological index, which is defined [1] for a graph G as

$$S_c^*(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u) d(v) d_G(u,v).$$

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The reciprocal degree distance index is also a degree-distance-based topological index, which is defined [13] as

$$RDD(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{d(u) + d(v)}{d_G(u,v)}.$$

The first goal of this paper is to obtain upper and lower bounds for the Wiener, hyper-Wiener, and Harary indices of simple connected non-trivial graphs. Obtaining inequalities involving the above-mentioned distance-based and degree-distance-based topological indices is the second goal of this paper.

2. Lemmas

In this section, two existing lemmas are stated. Both of these results are crucial in proving the main results of this paper.

Lemma 2.1 (see [19]). *For $1 \leq i \leq n$, if x_i and y_i are non-negative real numbers, then*

$$\sum_{i=1}^{n} (x_i)^2 \sum_{i=1}^{n} (y_i)^2 - \left(\sum_{i=1}^{n} x_i y_i \right)^2 \leq \frac{n^2}{4} (M_1 M_2 - m_1 m_2)^2,$$

where $M_1 = \max_{1 \leq i \leq n} \{x_i\}$, $M_2 = \max_{1 \leq i \leq n} \{y_i\}, m_1 = \min_{1 \leq i \leq n} \{x_i\}$, and $m_2 = \min_{1 \leq i \leq n} \{y_i\}$.

Lemma 2.2 (see [17]). *Let $a_1, a_2, \ldots, a_n, b_1, b_2, \ldots, b_n$ be real numbers such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$ for $i = 1, 2, \ldots, n$. The following inequality holds*

$$\left| \frac{1}{n} \sum_{i=1}^{n} a_i b_i - \left(\frac{1}{n} \sum_{i=1}^{n} a_i \right) \left(\frac{1}{n} \sum_{i=1}^{n} b_i \right) \right| \leq \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \left(1 - \frac{1}{n} \left\lfloor \frac{n}{2} \right\rfloor \right) (A - a)(B - b).$$

3. Upper and lower bounds for $W(G)$, $WW(G)$, and $H(G)$

Theorem 3.1. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$n^2 - n - m \leq W(G) \leq \binom{n}{2} (d - 1) + k$$

where k is the number of pairs of vertices having distance d in G.

Proof. Note that $d_G(u,v) = 1$ for $uv \in E(G)$ and $d_G(u,v) \geq 2$ for $uv \notin E(G)$. Thus, the lower bound is obtained as

$$\left(\binom{n}{2} - m \right) 2 + m = n^2 - n - m \leq W(G).$$

Since $d_G(u,v) \leq d$ for every pair of vertices $u, v \in V(G)$ and k is the number of pairs of vertices having distance d in G, the upper bound is derived as

$$W(G) \leq \left(\binom{n}{2} - k \right) (d - 1) + kd = \binom{n}{2} (d - 1) + k.$$

□

Theorem 3.2. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$3n(n-1) - 4m \leq WW(G) \leq \binom{n}{2} d(d-1) + 2kd$$

where k is the number of pairs of vertices having distance d in G.

Proof. Note that $d_G(u,v) = 1$ for $uv \in E(G)$ and $d_G(u,v) \geq 2$ for $uv \notin E(G)$. Thus, the lower bound is obtained as

$$2m + \left(\binom{n}{2} - m \right) 6 = 3n(n-1) - 4m \leq WW(G).$$

Since $d_G(u,v) \leq d$ for every pair of vertices $u, v \in V(G)$ and k is the number of pairs of vertices having distance d in G, the upper bound is derived as

$$WW(G) \leq \left(\binom{n}{2} - k \right) d(d-1) + kd(d+1) = \binom{n}{2} d(d-1) + 2kd.$$

□

Theorem 3.3. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$\left(\binom{n}{2}-k\right)\left(\frac{1}{d-1}\right)+\frac{k}{d}\leq H(G)\leq\frac{1}{2}\left(\binom{n}{2}+m\right)$$

where k is the number of pairs of vertices having distance d in G.

Proof. Since $\frac{1}{d_G(u,v)}\geq\frac{1}{d}$ for every pair of vertices $u,v\in V(G)$ and k is the number of pairs of vertices having distance d in G, the lower bound is derived as

$$\left(\binom{n}{2}-k\right)\left(\frac{1}{d-1}\right)+\frac{k}{d}\leq H(G).$$

Note that $\frac{1}{d_G(u,v)}=1$ for $uv\in E(G)$ and $\frac{1}{d_G(u,v)}\leq\frac{1}{2}$ for $uv\notin E(G)$. Thus, the upper bound is obtained as

$$H(G)\leq\frac{1}{2}\left(\binom{n}{2}-m\right)+m\cdot 1=\frac{1}{2}\left(\binom{n}{2}+m\right).$$

□

4. Inequalities involving some distance-based and degree-distance-based indices

Theorem 4.1. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$\left|DD(G)-\frac{4m}{n}W(G)\right|\leq 2\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)(d-1).$$

Proof. We know that the inequality $1\leq d_G(u_i,v_i)\leq d$ holds for every pair of distinct vertices $u_i,v_i\in V(G)$. Also, for every $w_i\in V(G)$, it holds that $\delta\leq d(w_i)\leq\Delta$. Moreover, the number of elements of the set $\big\{\{u_i,v_i\}:\ u_i,v_i\in V(G)\big\}$ is equal to $n(n-1)/2$. If we take $a_i=d(u_i)+d(v_i)$ and $b_i=\frac{d_G(u_i,v_i)}{2}$ in Lemma 2.2, we get

$$\left|\frac{2}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\frac{(d(u_i)+d(v_i))d(u_i,v_i)}{2}-\left(\frac{2}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\big(d(u_i)+d(v_i)\big)\right)\left(\frac{2}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\frac{d_G(u_i,v_i)}{2}\right)\right|$$

$$\leq\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)2(\Delta-\delta)\left(\frac{d}{2}-\frac{1}{2}\right).$$

Since

$$\sum_{i=1}^{n(n-1)/2}\big(d(u_i)+d(v_i)\big)=\sum_{u_iv_i\in E(G)}\big(d(u_i)+d(v_i)\big)+\sum_{u_iv_i\notin E(G)}\big(d(u_i)+d(v_i)\big)=2m(n-1),\quad\text{see [12]},$$

by using the definitions of $DD(G)$ and $W(G)$, one has

$$\left|\frac{1}{n(n-1)}DD(G)-\frac{4m}{n^2(n-1)}W(G)\right|\leq\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)(d-1),$$

which is equivalent to

$$\left|DD(G)-\frac{4m}{n}W(G)\right|\leq 2\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)(d-1).$$

□

Theorem 4.2. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$\Big(4m^2+(n-2)M_1(G)\Big)\Big(\frac{1}{2}WW(G)-\frac{1}{4}W(G)\Big)-\frac{1}{4}\big(DD(G)\big)^2\leq\left(\frac{n(n-1)}{4}\right)^2(\Delta d-\delta)^2.$$

Proof. Let u_i,v_i be an arbitrary pair of distinct vertices of G. In Lemma 2.1, if one takes $x_i=d(u_i)+d(v_i)$ and $y_i=\frac{d_G(u_i,v_i)}{2}$, then

$$\sum_{i=1}^{n(n-1)/2}(d(u_i)+d(v_i))^2\sum_{i=1}^{n(n-1)/2}\left(\frac{d_G(u_i,v_i)}{2}\right)^2-\left(\sum_{i=1}^{n(n-1)/2}\frac{(d(u_i)+d(v_i))d_G(u_i,v_i)}{2}\right)^2\leq\left(\frac{n(n-1)}{4}\right)^2\left(2\Delta\cdot\frac{d}{2}-2\delta\cdot\frac{1}{2}\right)^2.$$

Note that

$$\sum_{i=1}^{n(n-1)/2}(d(u_i)+d(v_i))^2=\sum_{u_iv_i\in E(G)}(d(u_i)+d(v_i))^2+\sum_{u_iv_i\notin E(G)}(d(u_i)+d(v_i))^2,$$

which is equal to $4m^2+(n-2)M_1(G)$ (see [9]), where $M_1(G)=\sum_{u_iv_i\in E(G)}(d(u_i)+d(v_i))$. Thus, by using the definitions of $W(G)$, $WW(G)$, and $DD(G)$, one has

$$\left(4m^2+(n-2)M_1(G)\right)\left(\frac{1}{2}WW(G)-\frac{1}{4}W(G)\right)-\frac{1}{4}\big(DD(G)\big)^2\leq\left(\frac{n(n-1)}{4}\right)^2(\Delta d-\delta)^2.$$

□

Theorem 4.3. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$WW(G)\leq\frac{1}{2}W(G)+\frac{1}{2\sum_{i=1}^{n(n-1)/2}\big(d(u_i)d(v_i)\big)^2}\left((S_c^*(G))^2+\left(\frac{n(n-1)}{4}\right)^2\left(\Delta^2d-\delta^2\right)^2\right).$$

Proof. Let u_i,v_i be an arbitrary pair of distinct vertices of G. By taking $x_i=d(u_i)d(v_i)$ and $y_i=d_G(u_i,v_i)$ in Lemma 2.1, one gets

$$\sum_{i=1}^{n(n-1)/2}\big(d(u_i)d(v_i)\big)^2\sum_{i=1}^{n(n-1)/2}\big(d_G(u_i,v_i)\big)^2-\left(\sum_{i=1}^{n(n-1)/2}d(u_i)d(v_i)d_G(u_i,v_i)\right)^2\leq\left(\frac{n(n-1)}{4}\right)^2\left(\Delta^2d-\delta^2\right)^2.$$

Using the definitions of $W(G)$, $WW(G)$, and $S_c^*(G)$, one has

$$\big(2WW(G)-W(G)\big)\sum_{i=1}^{n(n-1)/2}\big(d(u_i)d(v_i)\big)^2-(S_c^*(G))^2\leq\left(\frac{n(n-1)}{4}\right)^2\left(\Delta^2d-\delta^2\right)^2,$$

which implies that

$$WW(G)\leq\frac{1}{2}W(G)+\frac{1}{2\sum_{i=1}^{n(n-1)/2}\big(d(u_i)d(v_i)\big)^2}\left((S_c^*(G))^2+\left(\frac{n(n-1)}{4}\right)^2\left(\Delta^2d-\delta^2\right)^2\right).$$

□

Theorem 4.4. *If G is a simple connected non-trivial graph with order n, size m, and diameter d, then*

$$\left|RDD(G)-\frac{4m}{n}H(G)\right|\leq2\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)\left(1-\frac{1}{d}\right),$$

Proof. Let u_i,v_i be an arbitrary pair of distinct vertices of G. In Lemma 2.2, by taking $a_i=d(u_i)+d(v_i)$ and $b_i=\frac{1}{2d_G(u_i,v_i)}$, one arrives at

$$\left|\frac{1}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\frac{d(u_i)+d(v_i)}{d_G(u_i,v_i)}-\left(\frac{2}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\big(d(u_i)+d(v_i)\big)\right)\left(\frac{1}{n(n-1)}\sum_{i=1}^{n(n-1)/2}\frac{1}{d_G(u_i,v_i)}\right)\right|$$

$$\leq\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(2\Delta-2\delta)\left(\frac{1}{2}-\frac{1}{2d}\right).$$

Since

$$\sum_{i=1}^{n(n-1)/2}\big(d(u_i)+d(v_i)\big)=\sum_{u_iv_i\in E(G)}\big(d(u_i)+d(v_i)\big)+\sum_{u_iv_i\notin E(G)}\big(d(u_i)+d(v_i)\big)=2m(n-1),\quad\text{see [12]},$$

by using the definitions of $RDD(G)$ and $H(G)$, one has

$$\left|\frac{1}{n(n-1)}RDD(G)-\frac{4m}{n^2(n-1)}H(G)\right|\leq\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)\left(1-\frac{1}{d}\right),$$

which is equivalent to

$$\left|RDD(G)-\frac{4m}{n}H(G)\right|\leq2\left\lfloor\frac{n(n-1)}{4}\right\rfloor\left(1-\frac{2}{n(n-1)}\left\lfloor\frac{n(n-1)}{4}\right\rfloor\right)(\Delta-\delta)\left(1-\frac{1}{d}\right).$$

□

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