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Distance–Based Topological Indices and Double Graph

MUHAMMAD KAMRAN JAMIL•

Abdus Salam School of Mathematical Sciences, GC University, Lahore, Pakistan

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ABSTRACT

Let G be a connected graph, and let $D[G]$ denote the double graph of G. In this paper, we first derive closed-form formulas for some distance based topological indices for $D[G]$ in terms of G. Finally, these formulas are applied for several special kinds of graphs, such as, the complete graph, the path and the cycle.

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1. INTRODUCTION

Topological indices of molecules can be carried out through their molecular graphs. A molecular graph is a collection of points representing the atoms in the molecule and a set of lines representing the covalent bonds. In graph theory, these points and lines are called vertices and edges, respectively. The chemical graph theory is a branch of mathematical chemistry in which topological indices of chemical graphs relates the certain physical, biological or chemical properties of the corresponding molecules.

Many different topological indices have been investigated so far. Most of the useful topological indices are distance based or degree based. The Wiener index, the Harary index and the total eccentricity index are examples of distance based topological indices and the Zagreb indices and Randić [8] index are examples of degree based topological indices.

The Wiener index of a molecular graph is defined as the sum of all distances between different vertices. This topological index was introduced by Wiener [13]. It also

• Corresponding author (Email: m.kamran.sms@gmail.com)
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gave rise to some modifications such as, the hyper-Wiener index and the Tratch-Stankevich-Zefirov index.

Plavšić [7] et. al. and Ivanciuc et. al. [4] independently introduced the Harary index in honor of Frank Harary. The Harary index is obtained from the reciprocal distance matrix and has a number of interesting physical and chemical properties. The Harary index and its related molecular descriptors have shown some success in structure-property correlations [2, 3]. Its modification has also been proposed and their use in combination with other molecular descriptors improves the correlations [10, 11].

In order to improve the interest of the Harary-type indices, many modification were proposed recently. In [1] authors introduced a correction that gives more weight to the contributions of pairs of vertices of high degrees, named as the additively weighted Harary index.

The eccentric connectivity index belongs to the family of distance based topological indices. This quantity has been recently used in several papers on structure-property and structure-activity relationship and its mathematical properties have been investigated [9]. Munarini et. al. [6] define the *double graph* of a simple graph denoted as $D[G]$. The double graph of a simple graph G can be build up taking two distinct copies of the graph G and joining every vertex v in one copy to every vertex w' in the other copy corresponding to a vertex w adjacent to v in the first copy. In this paper we study some distance based topological indices for general double graphs.

2. DEFINITIONS AND PRELIMINARY RESULTS

All the graphs G considered in this paper are finite and simple. For basic definitions and notation see [12]. Let $G(V,E)$ be a simple connected graph where $V(G)$ and $E(G)$ are the set of vertices and set of edges, respectively. By $d_G(v)$ we denote the degree of vertex v in G. The distance between two vertices u and v, in a graph G, is the length of any shortest path connecting u and v and denoted as $d_G(u,v)$. The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G, it is denoted $ecc_G(v)$. By P_n and S_n we denote the path with n vertices and the star graph $k_{1,n-1}$ respectively.

The Wiener index of a given graph G having $V(G)=\{v_1,\ldots,v_n\}$ is defined as the sum of distances between all unordered pairs of vertices of a graph G, i. e.,

$$W(G) = \sum_{1\le i< j\le n} d_G(v_i,v_j).$$

The Harary index of G is defined as the sum of reciprocals of distances between all unordered pairs of vertices of a connected graph:

$$H(G) = \sum_{1\le i\le j\le n} \frac{1}{d_G(v_i,v_j)}.$$

The additively weighted Harary index for G is defined by

$$H_A(G) = \sum_{1 \le i \le j \le n} \frac{d_G(v_i) + d_G(v_j)}{d_G(v_i, v_j)},$$

and multiplicative weighted Harary index for G is defined by

$$H_M(G) = \sum_{1 \le i \le j \le n} \frac{d_G(v_i)\, d(v_j)}{d_G(v_i, v_j)}.$$

The eccentric connectivity index of G is

$$\zeta^c(G) = \sum_{v \in V(G)} d_G(v)\, ecc_G(v),$$

and the total eccentricity of G is defined by

$$\zeta(G) = \sum_{v \in V(G)} ecc_G(v).$$

The *direct product* of two graphs G and H is a graph $G \times H$ with $V(G \times H) = V(G) \times V(H)$ such that (u_1,v_1) is adjacent to (u_2,v_2) in $G \times H$ if and only if $u_1u_2 \in E(G)$ and $v_1v_2 \in E(H)$. By adding a loop to every vertex of K_2 we obtained the graph K_2^s. The double graph of a simple graph G can be expressed as $D[G] = G \times K_2^s$. Since the direct product of a simple graph with any graph is always a simple graph, it follows that the double of a simple graph is still a simple graph. Some of its elementary properties are discussed in [6]. If G has n vertices and m edges then $D[G]$ has $2n$ vertices and $4m$ edges. For illustration see figure1.

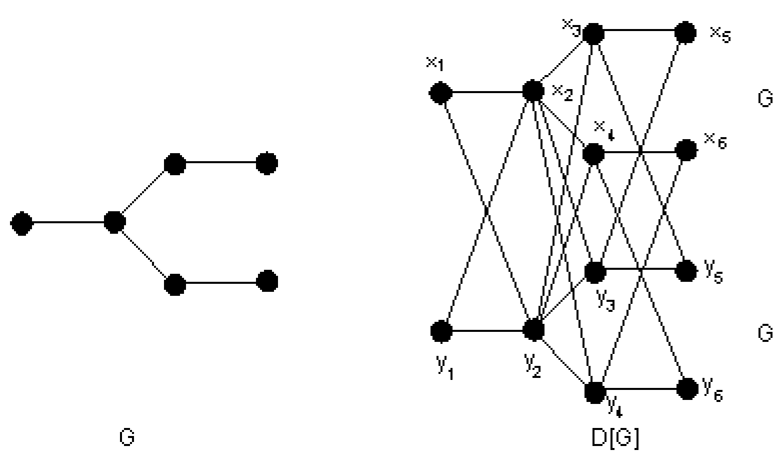

Figure 1 .A graph G and its double graph $D[G]$.

Let $G(V,E)$ be a simple graph and $G'(V', E')$ $'$ be its distinct copy. Let $D[G]$ be the double graph of G and $V(D[G]) = V(G) \cup V(G')$, where $V(G) = \{x_1, x_2, \ldots, x_n\}$ and $V(G') = \{y_1, y_2, \ldots, y_n\}$ and y_i is the corresponding vertex of x_i in $V(G')$.

Lemma 1. *For the above defined double graph* $D[G]$

$$d_{D[G]}(x_i, x_j) = d_G(x_i, x_j) \ ; i, j = 1, \ldots, n.$$

Proof. Clearly, $G \subset D[G]$. Let $\{x_i, \{x_i, x_j\} \subseteq V(G) \subset V(D[G])$ then $d_{D[G]}(x_i, x_j) \leq d_G(x_i, x_j)$. Suppose $l = d_{D[G]}(x_i, x_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ from x_i to x_j is $x_i v_1 v_2 \ldots v_{l-1} x_j$. If $l = 1$ then the property is obvious. Suppose $1 \geq 2$. Since $l < m$, there exists some $v_k \in V(G')$. As v_{k-1} and v_{k+1} are adjacent to v_k, by definition of the double graph, v_{k-1} and v_{k+1} are adjacent to x_k (corresponding vertex of v_k in $V(G)$). Now we have obtained a path $x_i v_1 v_2 \ldots x_k \ldots v_{l-1} x_j$. In this way we can find a path in G of length l, which is a contradiction. It follows that $d_{D[G]}(x_i, x_j) = d_G(x_i, x_j)$. Similarly, $d_{D[G]}(y_i, y_j) = d_G(y_i, y_j)$.

Lemma 2. *For the double graph* $D[G]$

$$d_{D[G]}(x_i, x_j) = d_G(x_i, x_j) \ ; i, j = 1, \ldots, n.$$

Proof. Let $x_i \in V(G)$ and $y_j \in V(G')$. Suppose $l = d_{D[G]}(x_i, y_j) < d_G(x_i, x_j) = m$ and a shortest path in $D[G]$ is $x_i v_1 v_2 \ldots v_{l-1} y_j$. If $l = 1$ the property is true. Let $l \geq 2$. It follows that there exists some $v_k \in V(G')$. Since v_{k-1} and v_{k+1} are adjacent to v_k, by construction v_{k-1} and v_{k+1} are adjacent to x_k (corresponding vertex of v_k in $V(G)$). We have obtained a path $x_i v_1 v_2 \ldots x_k \ldots v_{l-1} y_j$ in $D[G]$, which implies the existence of a path $x_i x_1 x_2 \ldots x_k \ldots x_{l-1} x_j$ in G of length l, a contradiction. If $l = d_{D[G]}(x_i, y_j) > d_G(x_i, x_j) = m$ we get a similar contradiction. Consequently, $d_{D[G]}(x_i, y_j) = d_G(x_i, x_j)$.

The following results are obvious from the construction of the double graph.

Lemma 3. *We have*

$$d_{D[G]}(x_i, y_i) = 2 \quad ; i = 1, \ldots, n.$$

Lemma 4 . *For the double graph* $D[G]$

$$d_{D[G]}(x_i) = d_{D[G]}(y_i) = 2 d_G(x_i) \qquad ; i = 1, \ldots, n.$$

Lemma 5 . *The eccentricities of the vertices of the double graph* $D[G]$ *are*

$$ecc_{D[G]}(x_i) = ecc_{D[G]}(y_i) = ecc_G(x_i) \ \ if \ \ ecc_G(x_i) \geq 2 \quad ; i = 1, \dots, n$$

$$ecc_{D[G]}(x_i) = ecc_{D[G]}(y_i) = 2 \quad if \quad ecc_G(x_i) = 1 \quad ; i = 1, \dots, n.$$

3. MAIN RESULTS

Theorem 1. *Let* G *be a simple graph with* n *vertices. Then the Wiener index of* $D[G]$ *is given by*

$$W(D[G]) = 4W(G) + 2n.$$

Proof. The Wiener index of $D[G]$ is

$$\begin{aligned} W(D[G]) &= \sum_{1 \leq i < j \leq n} d_{D[G]}(v_i, v_j) \\ &= \sum_{1 \leq i < j \leq n} d_{D[G]}(x_i, x_j) + \sum_{1 \leq i < j \leq n} d_{D[G]}(y_i, y_j) + \sum_{\substack{i, j = 1, \dots, n \\ i = j}} d_{D[G]}(x_i, y_j) + \\ &+ \sum_{i = 1, \dots, n} d_{D[G]}(x_i, y_i). \end{aligned}$$

By Lemmas 1 – 3 we deduce

$$\begin{aligned} W(D[G]) &= \sum_{1 \leq i < j \leq n} d_G(x_i, x_j) + \sum_{1 \leq i < j \leq n} d_G(x_i, x_j) + \sum_{\substack{i, j = 1, \dots, n \\ i = j}} d_G(x_i, x_j) + 2n \\ &= W(G) + W(G) + 2W(G) + 2n \\ &= 4W(G) + 2n. \end{aligned}$$

A well known property of the Wiener index of trees implies the following corollary.

Corollary 1. *Suppose* T_n *is a tree with* n *vertices. Then*

$$W(D[S_n]) \leq W(D[T_n]) \leq W(D[P_n]).$$

Theorem 2. *Let* G *be a simple graph with n vertices. Then the Harary index of* $D[G]$ *is given by*

$$H(D[G]) = 4H(G) + \frac{n}{2}.$$

Proof. The Harary index of $D[G]$ is

$$\begin{aligned} H(D[G]) &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(v_i, v_j)} \\ &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(x_i, x_j)} + \sum_{1 \leq i < j \leq n} \frac{1}{d_{D[G]}(y_i, y_j)} \\ &+ \sum_{\substack{i, j = 1, \dots, n \\ i = j}} \frac{1}{d_{D[G]}(x_i, y_j)} + \sum_{i = 1, \dots, n} \frac{1}{d_{D[G]}(x_i, y_i)} \end{aligned}$$

By Lemmas $1-3$ we have

$$H(D[G]) = \sum_{1\le i<j\le n} \frac{1}{d_G(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{1}{d_G(x_i,x_j)} + \sum_{\substack{i,j=1,\ldots,n\\ i=j}} \frac{1}{d_G(x_i,x_j)} + \frac{n}{2}$$

$$= H(G) + H(G) + 2H(G) + \frac{n}{2}$$

$$= 4H(G) + \frac{n}{2}.$$

Corollary 2. *Let T_n be a tree with n vertices. Then*

$$H(D[P_n]) \le H(D[T_n]) \le H(D[S_n]).$$

Theorem 3. *Let G be a simple graph with m edges. Then the additively weighted Harary index of $D[G]$ is given by*

$$H_A(D[G]) = 8H_A(G) + 4m.$$

Proof. The additively Harary index of $D[G]$ is

$$H_A(D[G]) = \sum_{1\le i<j\le n} \frac{d_{D[G]}(v_i) + d_{D[G]}(v_j)}{d_{D[G]}(v_i,v_j)}$$

$$= \sum_{1\le i<j\le n} \frac{d_{D[G]}(x_i) + d_{D[G]}(x_j)}{d_{D[G]}(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{d_{D[G]}(y_i) + d_{D[G]}(y_j)}{d_{D[G]}(y_i,y_j)}$$

$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{d_{D[G]}(x_i) + d_{D[G]}(y_j)}{d_{D[G]}(x_i,y_j)} + \sum_{i=1,\ldots,n} \frac{d_{D[G]}(x_i) + d_{D[G]}(y_i)}{d_{D[G]}(x_i,y_i)}.$$

by Lemmas $1-4$ the last expression is equal to

$$\sum_{1\le i<j\le n} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)}$$

$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{2d_G(x_i) + 2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{x_i\in V(G)} \frac{2d_G(x_i) + 2d_G(x_i)}{2}$$

$$= 2H_A(G) + 2H_A(G) + 4H_A(G) + 2\sum_{x_i\in V(G)} d_G(x_i)$$

$$= 8H_A(G) + 4m.$$

Corollary 3. *Suppose T_n and U_n be tree and unicyclic graphs, respectively, with n vertices. Then*

$$H_A(D[T_n]) = 8H_A(T_n) + 4(n-1).$$
$$H_A(D[U_n]) = 8H_A(U_n) + 4n.$$

Corollary 4 . *Suppose T_n is a tree with n vertices. Then*

$$H_A(D[P_n]) \le H_A(D[T_n]) \le H_A(D[S_n]).$$

Theorem 4. *Let G be a simple graph. The multiplicative weighted Harary index of $D[G]$ is given by*

$$H_M(D[G]) = 16H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2.$$

Proof. The multiplicative Harary index of $D[G]$ is

$$H_M(D[G]) = \sum_{1\le i<j\le n} \frac{d_{D[G]}(v_i)\,d_{D[G]}(v_j)}{d_{D[G]}(v_i,v_j)}$$
$$= \sum_{1\le i<j\le n} \frac{d_{D[G]}(x_i)\,d_{D[G]}(x_j)}{d_{D[G]}(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{d_{D[G]}(y_i)\,d_{D[G]}(y_j)}{d_{D[G]}(y_i,y_j)}$$
$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{d_{D[G]}(x_i)\,d_{D[G]}(y_j)}{d_{D[G]}(x_i,y_j)} + \sum_{i=1,\ldots,n} \frac{d_{D[G]}(x_i)\,d_{D[G]}(y_i)}{d_{D[G]}(x_i,y_i)}.$$

By Lemmas 1 − 4 this expression equals

$$\sum_{1\le i<j\le n} \frac{2d_G(x_i)2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{1\le i<j\le n} \frac{2d_G(x_i)2d_G(x_j)}{d_G(x_i,x_j)}$$
$$+ \sum_{\substack{i,j=1,\ldots,n\\ i\ne j}} \frac{2d_G(x_i)2d_G(x_j)}{d_G(x_i,x_j)} + \sum_{x_i \in V(G)} \frac{2d_G(x_i)2d_G(x_i)}{2}$$
$$= 4H_M(G) + 4H_M(G) + 8H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2$$
$$= 16H_M(G) + 2\sum_{x_i \in V(G)} d_G(x_i)^2.$$

Corollary 5 . *Suppose P_n , S_n ,C_n and K_n be the path, star cyclic and complete graphs with n vertices. Then*

$$H_M(D[P_n]) = 16H_M(P_n) + 8n - 12$$
$$H_M(D[S_n]) = 16H_M(S_n) + 2n(n-1)$$
$$H_M(D[C_n]) = 16H_M(C_n) + 8n$$
$$H_M(D[K_n]) = 16H_M(K_n) + 2n(n-1)^2.$$

Theorem 5. *Suppose G is a graph of order n, having k vertices v such that* $ecc(v)=1$ (*or equivalently,* $d_G(v)=n-1$). *The eccentric connectivity index of* $D[G]$ *is given by*

$$\zeta^c(D[G]) = 4\zeta^c(G) + 4k(n-1).$$

Proof.

$$\zeta^c(D[G]) = \sum_{i=1}^{n} d_{D[G]}(x_i)\, ecc_{D[G]}(x_i) + \sum_{i=1}^{n} d_{D[G]}(y_i)\, ecc_{D[G]}(y_i).$$

By Lemmas 4 and 5 we have

Theorem 6. *Let G be a simple graph having k vertices with* $ecc_G(v) = 1$. *The total eccentricity index of* $D[G]$ *is given by*

$$\zeta(D[G]) = 2\zeta(G) + 2k.$$

Proof.

$$\zeta(D[G]) = \sum_{i=1}^{n} ecc_{D[G]}(x_i) + \sum_{i=1}^{n} ecc_{D[G]}(y_i).$$

By Lemma 5, we have

$$\zeta(D[G]) = 2\left(\sum_{iecc_G(x_i)\geq 2} ecc_G(x_i) + \sum_{iecc_G(x_i)=1} 2 \right) = 2\zeta(G) + 2k.$$

Corollary 6. *For the star and the complete graph we have:*

$$\zeta(D[S_n]) = 2\zeta(S_n) + 2;$$
$$\zeta(D[K_n]) = 2\zeta(K_n) + 2n.$$

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