Iranian Journal of Mathematical Chemistry, Vol. 5, Supplement 1, December 2014, pp. s45−s51 **IJMC**

Relation between Wiener, Szeged and detour indices

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ABSTRACT. In theoretical chemistry, molecular structure descriptors are used to compute properties of chemical compounds. Among them Wiener, Szeged and detour indices play significant roles in anticipating chemical phenomena. In the present paper, we study these topological indices with respect to their difference number.

Keywords: Wiener index, Szeged index, detour index.

1. INTRODUCTION

A graph can be represented in an algebraic way, by considering a matrix named, adjacency matrix. This matrix is defined as $A = [a_{ij}]$ where $a_{ij} = 1$, for an adjacent pair v_i and v_j and 0 otherwise. Here $V(G) = \{v_1,v_2, \ldots, v_n\}$ and $E(G)=\{e_1,e_2,\ldots,e_m\}$ are the set of all vertices and edges of G, respectively. If G is given, then A is uniquely determined, and vice versa. The distance matrix $D = [d_{ij}]$ can be defined for G with entries $d_{ii} = 0$ and d_{ij}, $i\neq j$ as the distance between vertices v_i and v_j, see [2,10]. The detour matrix can be defined similarly, with respect to the length of the longest path between vertices. For given vertices $x, y \in V(G)$, $d(x,y)$ and $dd(x,y)$ denote to the lengths of shortest and longest paths between x and y, respectively. The distance and detour matrices were introduced for describing the connectivity in directed graphs. The Wiener and detour indices are defined as follows, respectively:

$$W(G) = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v) \ \ and \ \ DD(G) = \frac{1}{2}\sum_{u,v\in V(G)} dd(u,v).$$

These graph invariant are studied by several authors in recent years [1,3–5,11–16,19–23]. Let $D(u) = \sum_{x\in V(G)} d(u,x)$ and $DD(u) = \sum_{x\in V(G)} d(u,x)$. It is clear that

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Received: February 14, 2014; Accepted: September 11, 2014.

$$W(G)=\frac{1}{2}\sum_{u\in V(G)} D(u) \ and\ DD(G)=\frac{1}{2}\sum_{u\in V(G)} DD(u).$$

For $e=uv\in E(G)$, let $n(u|G)$ and $n(v|G)$ be respectively the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u. The Szeged index of the graph G is defined as [7–9,12]

$$Sz(G)=\sum_{e\in E(G)} n(u\,|\,G)n(v\,|\,G).$$

A well–known result of Klavžar et al. states that $\eta(G)\geq 0$, and by a result of Dobrynin and Gutman $\eta(G) = 0$ if and only if each block of G is complete.

Nadjafi–Arani et al. in [17,18] determined connected graphs whose difference between Szeged and Wiener numbers are n, for $n = 4, 5$. Following their work, Ghorbani et al. in [6] proved that for any integer $n\neq 1,2,4,6$ there is a graph G with $\mu(G)=n$, where $\mu(G)=DD(G)-W(G)$. In other words, they proved the following theorem.

Theorem 1. For any integer $n\geq 7$, there is a graph G where $\mu(G) = n$.

They also showed that for a given integer n, a graph G with $\mu(G) = n$ can't be determined uniquely. The main goal of this paper is to compute the relation between above topological indices.

2. MAIN RESULTS AND DISCUSSIONS

The symmetries of objects can be interpreted by means of group action. Let G be a group and X a nonempty set. An action of G on X is denoted by $(G \mid X)$ and X is called a G-set. It induces a group homomorphism from G into the symmetric group S_X on X, where $gx = x^g$ for all $x\in X$. The orbit of x will be indicated as x^G and defines as the set of all x^g, $g\in G$.

A bijection σ on the vertices of graph G is called an automorphism if for edge $e = uv$ then $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of E. Let $Aut(G) = \{\alpha\colon V\to V,\ \alpha \text{ is bijection}\}$, then $Aut(G)$ under the composition of mappings forms a group. We say $Aut(G)$ acts transitively on V if for any vertices u and v in V there is $\alpha\in Aut(G)$ such that $\alpha(u)=v$. Similarly, the edge transitive graph can be defined.

Lemma 2. Suppose G is a graph, A_1, A_2, ….,A_t are the orbits of $Aut(G)$ under its natural action on $V(G)$ and $x,y\in A_i$, $1\leq i\leq t$. Then $D(x)=D(y)$ and $DD(x)=DD(y)$. In particular, if G is vertex-transitive then for every pair (u,v) of vertices $D(u) = D(v)$ *and* $DD(u)=DD(v)$.

Proof. It is easy to see that if vertices u and v are in the same orbit, then there is an automorphism φ such that $\varphi(u)=v$. Thus

$$D(v)=\textstyle\sum_{y\in V(G)} d(v,y)=\sum_{w\in V(G)} d(\varphi(u),\varphi(w))=\sum_{w\in V(G)} d(u,w)=D(u),$$

$$DD(v)=\textstyle\sum_{y\in V(G)} dd(v,y)=\sum_{w\in V(G)} dd(\varphi(u),\varphi(w))=\sum_{w\in V(G)} dd(u,w)=DD(u).$$

If G be a vertex-transitive graph then $D(u) = D(v)$ *and* $DD(u)=DD(v)$, $u,v\in V(G)$. This completes the proof.

Theorem 3. If G is vertex-transitive, then for every vertex u in G we have

$$W(G)=\frac{|V|}{2}D(u) \text{ and } DD(G)=\frac{|V|}{2}DD(u).$$

Proof. By using Lemma 2, one can verify that

$$W(G)=\frac{1}{2}\sum_{x,y\in V(G)}d(x,y)=\frac{1}{2}\sum_{x\in V(G)}\sum_{y\in V(G)}d(x,y)=\frac{1}{2}\sum_{x\in V(G)}D(y)=\frac{|V|}{2}D(y).$$

Similarly the second part can be resulted from Lemma 2.

Lemma 4. Suppose G is a graph, E_1, E_2, ….,E_t are the orbits of $Aut(G)$ under its natural action on $E(G)$ and $e=uv\in E_i$, $1\le i\le t$. Then $n(u|G)=n(v|G)$. In particular, if G is edge-transitive then for every edge e=uv, $n(u|G)=n(v|G)$.

Theorem 5. If G is edge-transitive then for every edge e=uv, we have

$$Sz(G)=|E|n(u|G)n(v|G).$$

Proof. Apply Lemma 4.

Suppose now $\eta(G)=Sz(G)-W(G)$ and $\kappa(G)=DD(G)-Sz(G)$, then

$$\kappa(G)=\mu(G)-\eta(G).$$

Example 1. Consider the square H depicted in Figure 1. It is well-known fact that H is both vertex and edge-transitive. The distance and detour matrices of H are as follows:

$D(G)$	v_1	v_2	v_3	v_4
v_1	0	1	2	1
v_2	1	0	1	2
v_3	2	1	0	1
v_4	1	2	1	0

$DD(G)$	v_1	v_2	v_3	v_4
v_1	0	3	2	3
v_2	3	0	3	2
v_3	2	3	0	3
v_4	3	2	3	0

Hence, by Theorems 3,5 one can deduce that

$$W(H)=\frac{4}{2}\times4=8,\ DD(G)=\frac{4}{2}\times8=16,\ Sz(G)=4\times4=16 \text{ and } \mu(H)=8.$$

In general, for a cycle on n vertices, we have the following theorem.

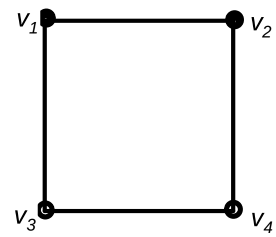

Figure 1. A labeled square.

Theorem 6. For the cycle C_n on n vertices, we have

$$\kappa(C_n)=\begin{cases}\dfrac{n^2(n-4)}{8} & 2\mid n\\[2ex] \dfrac{n(n^2-1)}{8} & 2\nmid n\end{cases}.$$

Proof. Since C_n is both vertex and edge-transitive, by a direct computation, we have

- n is even, $DD(u)=2(n-1)+2(n-2)+\ldots+1(n-n/2) = (5n^2-4n)/4$.
- n is odd, $DD(u)=2(n-1)+2(n-2)+\ldots+2(n-1)/2 = (5n^2-7n)/4$.

Hence, by using Theorems 3,5 one can prove that for any vertex u of C_n,

$$DD(C_n)=\begin{cases}\dfrac{n^2(3n-4)}{8} & 2\mid n\\[2ex] \dfrac{n(3n^2-4n+1)}{8} & 2\nmid n\end{cases},\quad Sz(C_n)=\begin{cases}\dfrac{n^3}{4} & 2\mid n\\[2ex] \dfrac{n(n-1)^2}{4} & 2\nmid n\end{cases}.$$

This completes the proof.

Theorem 7. Suppose G is both vertex and edge-transitive r-regular graph, then

$$DD(G)-Sz(G)=\frac{|V|}{2}[DD(u)-r\times n(u\mid G)n(v\mid G)].$$

Proof. According to Theorems 3,5 for every edge $e=uv$ we have

$$DD(G)-Sz(G)=\frac{|V|}{2}DD(u)-|E|\,n(u\mid G)n(v\mid G)=\frac{|V|}{2}DD(u)-\frac{r\,|V|}{2}n(u\mid G)n(v\mid G)$$
$$=\frac{|V|}{2}[DD(u)-r\times n(u\mid G)n(v\mid G)].$$

It is clear that if T is a tree, then $W(T)=DD(T)=\mathrm{Sz}(T)$ and so $\kappa(G)=0$. Further, $\kappa(G)=\mu(G)$ if and only if all blocks of G are complete. In other words, if G is a graph whose blocks are complete, then $\kappa(G)\notin\{1,2,4,6\}$. Hence, it is natural to ask about values of $\kappa(G)$?

Let *r, s* ≥ 0, denoted by $U_n^{r,s}$ means a complete graph on *n* vertices with *r* and *s* pendent vertices added to *a* and *b*, respectively, see Figure 2. In the following, we determine this value for graph $U_n^{r,s}$.

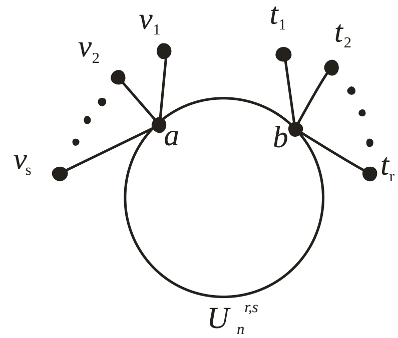

Figure 2. Graph $U_n^{r,s}$.

Theorem 8.

$$\kappa(U_n^{s,r}) = \frac{n^3 - 3n^2 + 6n - 6}{2} + n^2(s+r) - 2r(n+s) - sn(r+3) - n + 2.$$

Proof. Let *Q* be the clique of *G*, by using group action, we have to consider five types of vertices:

- **Case 1**, $e=v_1a$ by Figure 2, one can see that
$$n(v_1 | G)n(a | G) = n + s + r - 1.$$
There are *s*+*r* edges of this type and so the contribution of these edges is $(s+r)(n+s+r-1)$.
- **Case 2**, $e=ab$ by Figure 2, one can see that
$$n(a | G)n(b | G) = (s+1)(r+1).$$
- **Case 3**, $e=x_1a$ where $x_1 \in Q$. By Figure 2, one can see that
$$n(x_1 | G)n(a | G) = s + 1.$$
There are *n*-2 edges of this type and so the contribution of these edges is $(n-2)(s+1)$.
- **Case 4**, $e=x_1b$ where $x_1 \in Q$. By Figure 2, one can see that
$$n(x_1 | G)n(b | G) = r + 1.$$
There are *n*-2 edges of this type and so the contribution of these edges is $(n-2)(r+1)$.
- **Case 5**, $e=x_ix_j$ where $i \neq j$ and $x_i, x_j \in Q$. By Figure 2, one can see that
$$n(x_i | G)n(x_j | G) = 1.$$
There are $(n-2)(n-3)/2$ edges of this type and so the contribution of these edges is $(n-2)(n-3)/2$.

It follows that

$$DD(U_n^{s,r}) = \frac{n(n-1)^2}{2} + (s+r)(n^2-n+1) + s(s-1) + r(r-1) + sr(n+1)$$

and

$$SZ(U_n^{s,r}) = (n+r+s-1)(s+r) + (s+1)(n+r-1) + (n-2)(r+1+\frac{n-3}{2}).$$

Thus,

$$DD(U_n^{s,r}) - Sz(U_n^{r,s}) = \frac{n^3-3n^2+6n-6}{2} + n^2(s+r) - 2r(n+s) - sn(r+3) - n + 2$$

and the proof is comple.

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