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Degree Distance of Some Planar Graphs

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Abstract - A novel graph invariant: degree distance index was introduced by Andrey A. Dobrynin and Amide A. Kochetova [3] and at the same time by Gutman as true Schultz index [4]. In this paper we establish explicit formulae to calculate the degree distance of some planar graphs.

Index terms— Degree distance, planar graph, tree graph, regular graph, star graph.

I. INTRODUCTION

Topological indices are numbers associated with molecular graphs for the purpose of allowing quantitative structure-activity/property/toxicity relationships. Wiener index is the best known topological index introduced by Harry Wiener to study the boiling points of alkane molecules. By now there exist a lot of different types of such indices (based either on the vertex adjacency relationship or on the topological distances) which capture different aspects of the molecular graphs associated with the molecules under study. For a graph $G=(V,E)$ the degree distance of G is defined as $DD(G)=\sum_{\{u,v\}\subseteq V(G)}\left(\deg_G(u)+\deg_G(v)\right)d_G(u,v)$ where $\deg_G(u)$ is the degree of the vertex u in G and $d_G(u,v)$ is the shortest distance between u and v. Klein et al. [5] showed that if G is a tree on n vertices then $DD(G)=4W(G)-n(n-1)$ where $W(G)=\sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$ is the Wiener index of the graph G. Thus the study of the degree distance for trees is equivalent to the study of the Wiener index. But the degree distance of a graph is a more sensitive invariant than the Wiener index.

In this paper we compute the degree distance of some planar and tree graphs. In Section II, we introduce multi-star graph $K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$ [2] and calculate its degree distance, in Section III, we calculate the degree distance of planar graphs $Pl_n\,(n\geq 5)$ and $P_m\times C_n\,(m\geq 2, n\geq 3)$ and in Section IV, We introduce the graph operation $\hat{e}$ and compute the degree distance of $\left(P_{m_1}\times C_{n_1}\right)\hat{e}\left(P_{m_2}\times C_{n_2}\right)$.

II. MULTI-STAR GRAPH $K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$

In this section we give the construction of multi-star graph and calculate its degree distance.

2.1 Construction

Starting from the star graph $K_{1,n}$ with vertices $\{v_0, v_1, v_2, \ldots, v_n\}$ introduce an edge to each of the pendant vertices $v_1, v_2, \ldots, v_n$ to get the resulting graph $K_{1,n,n}$ with vertices $\{v_0, v_1, \ldots, v_n, v_{(n+1)}, \ldots, v_{2n}\}$, again introduce an edge to each of the pendant vertices $v_{(n+1)}, \ldots, v_{2n}$, to get the graph $K_{1,n,n,n}$. Repeating this procedure $(m-1)$ times the resulting graph $K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$ with,

$(mn+1)$ vertices

$\{v_0, v_1, v_2, \ldots, v_n, v_{(n+1)} \ldots, v_{2n}, v_{(2n+1)}, \ldots, v_{3n}, \ldots, v_{((m-1)n+1)}, \ldots, v_{mn}\}$ and mn edges is obtained as shown in Fig. 1.

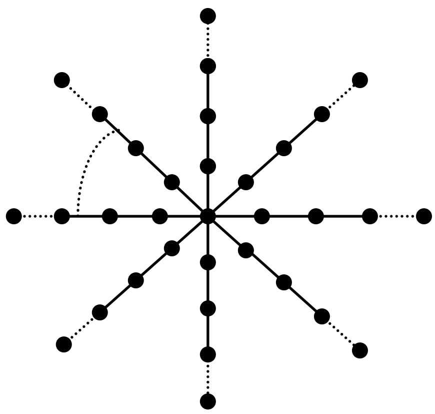

Fig. 1. Multi-star graph $K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$.

Result 2.2: Degree distance of the Multi-star graph $K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$ is

$$DD\left(K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}\right)=\frac{nm}{3}\left[6m^2n-4m^2+3mn+1\right]$$

Proof: Let the $(mn+1)$ vertices of the multi-star graph

$K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}$ be $\{v_0, v_1, v_2, \ldots, v_n, v_{(n+1)}, \ldots, v_{2n}, \ldots, v_{((m-1)n+1)}, \ldots, v_{mn}\}$

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Then, $DD\left(K_{1,\underbrace{n,n,\ldots,n}_{m\text{ times}}}\right)$

$$=\sum_{i<j}\left(\deg(v_i)+\deg(v_j)\right)d(v_i,v_j)$$

$$=\left[n(n+2)\left(1+2+\ldots+(m-1)\right)+n(n+1)m\right]+$$

$$\left[4\left(2\times1+2\times2+\ldots+2\times(m-1)\right)\left((n-1)+(n-2)+\ldots+1\right)\right]+$$

$$\begin{bmatrix}4n(n-1)\left(2\times1+1+2\times1+2+\ldots+2\times1+(m-2)\right)+\\4n(n-1)\left(2\times2+1+2\times2+2+\ldots+2\times2+(m-3)\right)+\\\ldots+4n(n-1)\left(2\times(m-2)+1\right)\end{bmatrix}+$$

$$\left[3n(n-1)\left(2\times1+(m-1)+2\times2+(m-2)+\ldots+2\times(m-1)+1\right)\right]+$$

$$\left[4n\left(1+2+\ldots+(m-2)\right)+4n\left(1+2+\ldots+(m-3)\right)+\ldots+4n(1)\right]+$$

$$\left[3n\left((m-1)+(m-2)+\ldots+2+1\right)\right]+\left[2\times2m\times\left((n-1)+\ldots+1\right)\right]$$

$$=\frac{nm}{3}\left(6m^2n-4m^2+3mn+1\right)$$

III. PLANAR GRAPHS

In this section we compute the degree distance of planar graph with maximal edges [1], $Pl_n\,(n\geq5)$ (Fig. 2) and structured web graph $P_m\times C_n\,(m\geq2,n\geq3)$ (Fig. 3).

Result 3.1: *Degree distance of* $Pl_n\,(n\geq5)$ *graph is*
$DD(Pl_n)=10n^2-48n+68$

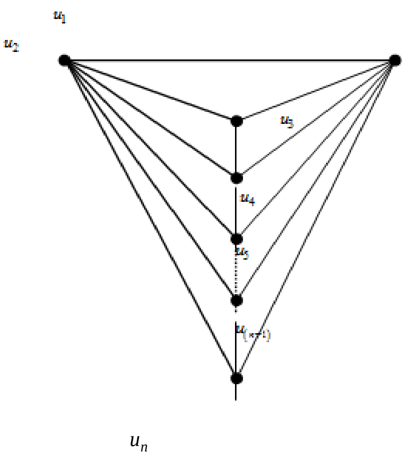

Fig. 2. $Pl_n\,(n\geq5)$ graph.

Proof: Let the n vertices of the $Pl_n\,(n\geq5)$ graph be $\{u_1,u_2,\ldots,u_n\}$. Then the degree distance of Pl_n is $DD(Pl_n)=\sum_{i<j}\left(\deg(u_i)+\deg(u_j)\right)d(u_i,u_j)$. Note that

$\deg_G(u_1)=\deg_G(u_2)=n-1;\deg_G(u_3)=\deg_G(u_n)=3;$

$\deg_G(u_4)=\ldots=\deg\left(u_{(n-1)}\right)=4;d_G(u_1,u_j)=1,\ j=2,\ldots,n;$

$d_G(u_2,u_j)=1,\ j=1,\ldots,n,\ j\neq2;d_G(u_j,u_{j+1})=1,\ j=3,\ldots,n-1;$

$d(u_i,u_j)=2;i=3,4,\ldots,(n-2);(i+2)\leq j\leq n$.

$$DD(Pl_n)$$

$$=\left[n(n-1)+2(3)+4(n-4)\right]+\left[(n-2)(n-1)+2(3)+4(n-4)\right]$$

$$+\left[3\left(1+\underbrace{2+2+\ldots+2}_{(n-4)}\right)+4\left(1+\underbrace{2+2+\ldots+2}_{(n-5)}\right)+2(3)\right]$$

$$+\left[4\left(1+\underbrace{2+2+\ldots+2}_{(n-5)}\right)+4\left(1+\underbrace{2+2+\ldots+2}_{(n-6)}\right)+2(3)\right]$$

$$+\left[4\left(1+\underbrace{2+2+\ldots+2}_{(n-6)}\right)+4\left(1+\underbrace{2+2+\ldots+2}_{(n-7)}\right)+2(3)\right]$$

$$+\left[4(1+2+2)+4(1+2)+2(3)\right]+\left[4(1+2)+4(1)+2(3)\right]+4(1)+3(1)$$

$$=10n^2-48n+68$$

Result 3.2: Degree distance of structured web 3-regular graph $P_m\times C_n\,(m\geq2,n\geq3)$ is

$$DD(P_m\times C_n)=\begin{cases}\frac{3}{4}m^2n\left(n^2-1\right)+mn^2\left(m^2-1\right) & \text{when n is odd}\\\frac{3}{4}n^3m^2+mn^2\left(m^2-1\right) & \text{when n is even}\end{cases}$$

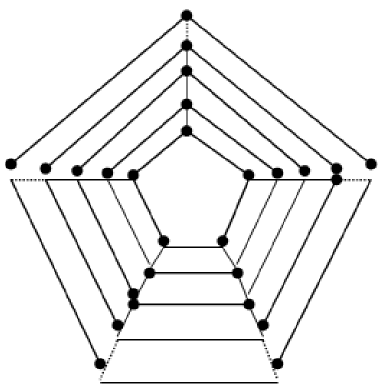

Fig. 3. $P_m\times C_5$ graph.

Proof: Case (i) when n is *odd*.
$DD(P_m\times C_n)=\sum_{i<j}\left(\deg(u_i)+\deg(u_j)\right)d(u_i,u_j)$

$$DD(P_m \times C_n) =$$
$$\left[\frac{1}{2}\left(6\times 2\left(1+2+...+\left(\frac{n-1}{2}\right)\right)\right)\times mn\right]+$$
$$\left[\begin{array}{l} 12n\left(\frac{m(m-1)}{2}\left(\frac{n-1}{2}\right)+(m-1)\frac{(n^2-1)}{8}\right)+ \\ 12n\left(\frac{(m-2)(m-1)}{2}\left(\frac{n-1}{2}\right)+(m-2)\frac{(n^2-1)}{8}\right)+ \\ ...+12n\left(\frac{1\times 2}{2}\left(\frac{n-1}{2}\right)+(1)\frac{(n^2-1)}{8}\right) \end{array}\right]$$
$$+\left[6\left(n+2n+...+(m-1)n\right)+6\left(n+2n+...+(m-2)n\right)+...+6(n)\right]$$
$$=\frac{3}{4}m^2n\left(n^2-1\right)+mn^2\left(m^2-1\right)$$

Case (ii) when n is *even*.

$$DD(P_m \times C_n)$$
$$=\sum_{i<j}\left(\deg(u_i)+\deg(u_j)\right)d(u_i,u_j)$$
$$=\left[\frac{1}{2}\left(6\left(2\left(1+2+...+\left(\frac{n}{2}-1\right)\right)+\frac{n}{2}\right)\right)\times mn\right]+$$
$$\left[6n\left(2\left(\frac{n}{2}-1\right)^{m}C_2+\left(\frac{n}{2}-1\right)\left(\frac{n}{2}\right)(m-1)+\frac{n}{2}(m-1)+{}^{m}C_2\right)\right]+$$
$$\left[6n\left(2\left(\frac{n}{2}-1\right)^{(m-1)}C_2+\left(\frac{n}{2}-1\right)\left(\frac{n}{2}\right)(m-2)+\frac{n}{2}(m-2)+{}^{(m-1)}C_2\right)\right]$$
$$+...+\left[6n\left(2\left(\frac{n}{2}-1\right)^{2}C_2+\left(\frac{n}{2}-1\right)\left(\frac{n}{2}\right)(1)+\frac{n}{2}(1)+{}^{2}C_2\right)\right]+mn\left(m^2-1\right)$$
$$=\frac{3}{4}n^3m^2+mn^2\left(m^2-1\right)$$

IV. NEW GRAPH OPERATION $\hat{e}$

In this section we introduce new graph operation $\hat{e}$ and establish the degree distance of $\left(P_{m_1}\times C_{n_1}\right)\hat{e}\left(P_{m_2}\times C_{n_2}\right)$.

Definition 4.1: $G_1\hat{e}G_2$ is a connected graph obtained from G_1 and G_2 by introducing an edge e between an arbitrary vertex of G_1 and an arbitrary vertex of G_2.

If $G_1(p_1,q_1)$ has p_1 vertices and q_1 edges and $G_2(p_2,q_2)$ has p_2 vertices and q_2 edges then $G_1\hat{e}G_2$ will have (p_1+p_2) vertices and (q_1+q_2+1) edges. If $G_1=P_{m_1}\times C_{n_1}$ and $G_2=P_{m_2}\times C_{n_2}$ an interesting graph structure $G=G_1\hat{e}G_2$ (example shown in Fig. 4) is obtained by using the new graph operation defined above and we prove the following result.

Result 4.2: Degree distance of $G=\left(P_{m_1}\times C_{n_1}\right)\hat{e}\left(P_{m_2}\times C_{n_2}\right)$ is

$$DD(G)=DD(G_1)+DD(G_2)+(6n_2+2)D_{G_1}(u_1,u)$$
$$+(6n_1+2)D_{G_2}(v_1,v)+n_1+n_2+6n_1n_2$$

Where,

$$D_{G_1}(u_1,u)=\sum_{u\neq u_1\in V(G_1)}d_{G_1}(u_1,u)=\begin{cases}\frac{n_1^2m_1}{4}+n_1\left({}^{m_1}C_2\right) & \text{when } n_1 \text{ is even}\\ \frac{(n_1^2-1)m_1}{4}+n_1\left({}^{m_1}C_2\right) & \text{when } n_1 \text{ is odd}\end{cases}$$

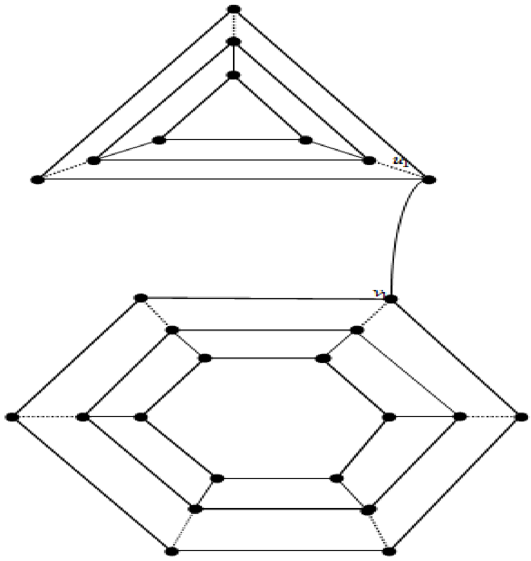

Fig. 4. Graph $\left(P_{m_1}\times C_3\right)\hat{e}\left(P_{m_2}\times C_6\right)$.

$$D_{G_2}(v_1,v)=\sum_{v\neq v_1\in V(G_2)}d_{G_2}(v_1,v)=\begin{cases}\frac{n_2^2m_2}{4}+n_2\left({}^{m_2}C_2\right) & \text{when } n_2 \text{ is even}\\ \frac{(n_2^2-1)m_2}{4}+n_2\left({}^{m_2}C_2\right) & \text{when } n_2 \text{ is odd}\end{cases}$$

Proof: Let an edge be introduced between the arbitrary vertex u_1 of G_1 and the arbitrary vertex v_1 of G_2, then the degree distance of $G=G_1\hat{e}G_2=\left(P_{m_1}\times C_{n_1}\right)\hat{e}\left(P_{m_2}\times C_{n_2}\right)$ is given by

$$DD(G)$$
$$=\sum_{i<j}\left(\deg_{G_1}(u_i)+\deg_{G_1}(u_j)\right)d_{G_1}(u_i,u_j)$$
$$+\sum_{i<j}\left(\deg_{G_2}(v_i)+\deg_{G_2}(v_j)\right)d_{G_2}(v_i,v_j)$$
$$+\sum_{i=1}^{m_1n_1}\sum_{j=1}^{m_2n_2}\left(\deg_{G_1}(u_i)+\deg_{G_2}(v_j)\right)d_G(u_i,v_j)$$
$$=DD(G_1)+\sum_{u\neq u_1\in V(G_1)}d_{G_1}(u,u_1)+DD(G_2)+\sum_{v\neq v_1\in V(G_2)}d_{G_2}(v,v_1)$$
$$+\sum_{i=1}^{m_1n_1}\sum_{j=1}^{m_2n_2}\left(\deg_{G_1}(u_i)+\deg_{G_2}(v_j)\right)\left[d_{G_1}(u_i,u_1)+1+d_{G_2}(v_1,v_j)\right]$$
$$=DD(G_1)+\sum_{u\neq u_1\in V(G_1)}d_{G_1}(u_1,u)+DD(G_2)+\sum_{v\neq v_1\in V(G_2)}d_{G_2}(v_1,v)$$
$$+6n_2\sum_{u\neq u_1\in V(G_1)}d_{G_1}(u_1,u)+6n_2n_1$$
$$+\sum_{u\neq u_1\in V(G_1)}d_{G_1}(u_1,u)+(n_1-1)+2+(n_2-1)$$
$$+6n_1\sum_{v\neq v_1\in V(G_2)}d_{G_2}(v_1,v)+\sum_{v\neq v_1\in V(G_2)}d_{G_2}(v_1,v)$$
$$DD(G)=DD(G_1)+DD(G_2)++(6n_2+2)D_{G_1}(u_1,u)$$
$$+(6n_1+2)D_{G_2}(v_1,v)+n_1+n_2+6n_1n_2$$

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To find $D_{G_1}(u_1,u)$ when n_1 is even,

$$\begin{aligned}
&D_{G_1}(u_1,u)\\
&=\sum_{u\neq u_1\in V(G_1)} d_{G_1}(u_1,u)\\
&=\left[2\left(1+2+\ldots+\left(\frac{n_1}{2}-1\right)\right)+\frac{n_1}{2}\right]\\
&\quad+\left[2\left((1+1)+(2+1)+\ldots+\left(\left(\frac{n_1}{2}-1\right)+1\right)\right)+\left(\frac{n_1}{2}+1\right)\right]+1\\
&\quad+\left[2\left((1+2)+(2+2)+\ldots+\left(\left(\frac{n_1}{2}-1\right)+2\right)\right)+\left(\frac{n_1}{2}+2\right)\right]+2+\ldots\\
&\quad+\left[2\left((1+(m-1))+\ldots+\left(\left(\frac{n_1}{2}-1\right)+(m_1-1)\right)\right)+\left(\frac{n_1}{2}+(m_1-1)\right)\right]\\
&\quad+(m_1-1)\\
&=\frac{n_1m_1(m_1-1)}{2}+\frac{m_1n_1^2}{4}
\end{aligned}$$

Similarly,

$$\begin{aligned}
D_{G_2}(v_1,v)&=\sum_{v\neq v_1\in V(G_2)} d_{G_2}(v_1,v)\\
&=\frac{n_2m_2(m_2-1)}{2}+\frac{m_2n_2^2}{4} \text{ when } n_2 \text{ is even}
\end{aligned}$$

To find $D_{G_1}(u_1,u)$ when n_1 is odd,

$$D_{G_1}(u_1,u)=\sum_{u\neq u_1\in V(G_1)} d_{G_1}(u_1,u)$$

$$\begin{aligned}
&D_{G_1}(u_1,u)\\
&=\left[2\left(1+2+\ldots+\left(\frac{n_1-1}{2}\right)\right)\right]\\
&\quad+\left[2\left((1+1)+(2+1)+\ldots+\left(\left(\frac{n_1-1}{2}\right)+1\right)\right)\right]+1\\
&\quad+\left[2\left((1+2)+(2+2)+\ldots+\left(\left(\frac{n_1-1}{2}\right)+2\right)\right)\right]+2\\
&\quad+\ldots+\left[2\left((1+(m-1))+\ldots+\left(\left(\frac{n_1-1}{2}\right)+(m_1-1)\right)\right)\right]+(m_1-1)\\
&=\frac{n_1m_1(m_1-1)}{2}+\frac{m_1(n_1^2-1)}{4}
\end{aligned}$$

Similarly,

$$\begin{aligned}
D_{G_2}(v_1,v)&=\sum_{v\neq v_1\in V(G_2)} d_{G_2}(v_1,v)\\
&=\frac{n_2m_2(m_2-1)}{2}+\frac{m_2(n_2^2-1)}{4} \text{ when } n_2 \text{ is odd}
\end{aligned}$$

Using Result 3.2,

$$DD(G_1)=DD(P_{m_1}\times C_{n_1})=\begin{cases}\frac{3}{4}m_1^2n_1(n_1^2-1)+m_1n_1^2(m_1^2-1) & \text{when } n_1 \text{ is odd}\\ \frac{3}{4}n_1^3m_1^2+m_1n_1^2(m_1^2-1) & \text{when } n_1 \text{ is even}\end{cases}$$

$$DD(G_2)=DD(P_{m_2}\times C_{n_2})=\begin{cases}\frac{3}{4}m_2^2n_2(n_2^2-1)+m_2n_2^2(m_2^2-1) & \text{when } n_2 \text{ is odd}\\ \frac{3}{4}n_2^3m_2^2+m_2n_2^2(m_2^2-1) & \text{when } n_2 \text{ is even}\end{cases}$$

V. CONCLUSIONS

In this paper we have computed the degree distance index of some planar graphs. Nevertheless, there are still many classes of interesting and chemically relevant graphs not covered by our approach. So it would be interesting to find explicit formulae for computing the degree distance and other topological indices for various classes of chemical graphs.

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