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Dakshayani Indices

V.R.Kulli

Department of Mathematics
Gulbarga University, Gulbarga 585106, India
e-mail: vrkulli@gmail.com

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Abstract. We introduce new topological indices, the first and second Dakshayani indices, general Dakshayani index. The second Dakshayani index is a linear combination of the modified first Zagreb index and inverse degree. We initiate a study of these new invariants.

Keywords: Modified first Zagreb index, inverse degree, Dakshayani index, polycyclic aromatic hydrocarbon, benzenoid system.

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*12, 05*C*35

1. Introduction

Let $G = (V(G), E(G))$ be a finite, connected graph. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. The complement $\overline{G}$ of G is the graph with vertex set $V(G)$ in which two vertices are adjacent if they are not adjacent in G. Clearly $d_{\overline{G}}(u) = n-1-d_G(u)$, where n is the number of vertices in G. For other undefined notations and terminology, the readers are referred to [1]. A topological index is a numerical parameter mathematically derived from the graph structure.

In [2], Miličević et al. proposed the modified first Zagreb index, which is defined as

$$^{m}M_1(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)^2}.$$

This index was studied in [3].

The inverse degree is defined as

$$ID(G) = \sum_{u\in V(G)} \frac{1}{d_G(u)}.$$

This index has attracted through a conjecture of Grafitti[4]. The name inverse degree was proposed in [5].

We now introduce the first and second Dakshayani indices, defined as

$$DK_1(G) = \sum_{u\in V(G)} d_{\overline{G}}(u)\frac{1}{d_G(u)}, \tag{1}$$

$$DK_2(G)=\sum_{u\in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)^2}. \tag{2}$$

We continue this generalization and defined the general Dakshayani index of a graph G as

$$DK^a(G)=\sum_{u\in V(G)} d_{\bar{G}}(u)d_G(u)^a \tag{3}$$

where a is a real number.
Clearly, $DK^{-1}(G) = DK_1(G)$, $DK^{-2}(G) = DK_2(G)$.

Recently, many new topological indices were studied, for example, in [6, 7, 8, 9, 10].

In section 2, we obtain exact value of the first and second Dakshayani indices for some standard graphs. In section 3, we determine some basic properties of DK_1 and DK_2. In section 4, the first and second Dakshayani indices and general Dakshayani index of polycyclic aromatic hydrocarbons and jagged rectangle benzenoid systems are computed.

2. Results for some standard graphs

The following are the first and second Dakshayani indices for paths, cycles, complete graphs, bipartite graphs.

Proposition 1. Let P_n be a path with $n \geq 3$ vertices. Then

(i) $DK_1(P_n)=\frac{1}{2}(n-2)(n+1)$. (ii) $DK_2(P_n)=\frac{1}{4}(n-2)(n+5)$.

Proof: Let $G = P_n$. The vertex partition of G is given in Table 1.

$d_G(u) \setminus u \in V(G)$	1	2
$d_{\bar{G}}(u) \setminus u \in V(\bar{G})$	$n-2$	$n-3$
Number of vertices	2	$n-2$

Table 1: Vertex partition of P_n

(i) $$DK_1(P_n)=\sum_{u\in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)}=\frac{(n-2)2}{1}+\frac{(n-3)(n-2)}{2}=\frac{1}{2}(n-2)(n+1).$$

(ii) $$DK_2(P_n)=\sum_{u\in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)^2}=\frac{(n-2)2}{1^2}+\frac{(n-3)(n-2)}{2^2}=\frac{1}{4}(n-2)(n+5).$$

Proposition 2. Let C_n be a cycle with $n \geq 3$ vertices. Then

(i) $DK_1(C_n)=\frac{1}{2}n(n-3)$. (ii) $DK_2(C_n)=\frac{1}{4}n(n-3)$.

Proof: Let $G = C_n$. The degree of each vertex of C_n is 2. Thus the degree each vertex of $\overline{C_n}$ is $(n-3)$. Thus

(i) $$DK_1(C_n)=\sum_{u\in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)}=\frac{(n-3)n}{2}.$$

(ii) $$DK_2(C_n) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)^2} = \frac{(n-3)n}{2^2} = \frac{1}{4}n(n-3).$$

Proposition 3. Let K_n be a complete graph with $n \geq 3$ vertices. Then

(i) $DK_1(K_n) = 0.$ Also $DK_1(\overline{K_n}) = 0.$

(ii) $DK_2(K_n) = 0.$ Also $DK_2(\overline{K_n}) = 0.$

Proposition 4. Let $K_{m,n}$ be a complete bipartite graph with $1 \leq m < n$. Then

(1) $DK_1(K_{m,n}) = \dfrac{n(n-1)}{m} + \dfrac{m(m-1)}{n}.$

(2) $DK_2(K_{m,n}) = \dfrac{n(n-1)}{m^2} + \dfrac{m(m-1)}{n}.$

Proof: Let $G = K_{m,n}$. The vertex partition of G is given in Table 2.

$d_G(u) \setminus u \in V(G)$	m	n
$d_{\overline{G}}(u) \setminus u \in V(\overline{G})$	$n-1$	$m-1$
Number of vertices	n	m

Table 2: Vertex partition of $K_{m,n}$

(i) $$DK_1(K_{m,n}) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)} = \frac{(n-1)n}{m} + \frac{(m-1)m}{n}.$$

(ii) $$DK_2(K_{m,n}) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)^2} = \frac{(n-1)n}{m^2} + \frac{(m-1)m}{n^2}.$$

Corollary 4.1. Let $K_{1,n-1}$ be a star with $n \geq 2$ vertices. Then

(i) $DK_1(K_{1,n-1}) = (n-1)(n-2).$ (ii) $DK_2(K_{1,n-1}) = (n-1)(n-2).$

Proposition 5. Let G be an r –regular connected graph with $n \geq 2$ vertices. Then

(i) $DK_1(G) = \dfrac{1}{r}n(n-1-r).$ (ii) $DK_2(G) = \dfrac{1}{r^2}n(n-1-r).$

Proof: The degree of every vertex of an r-regular graph G is r. The degree every vertex of $\overline{G}$ is $n - 1 - r$.

(i) $$DK_1(G) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)} = \frac{(n-1-r)n}{r}.$$

(ii) $$DK_2(G) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)^2} = \frac{(n-1-r)n}{r^2}.$$

A double star $S_{p,\,q}$ is the graph obtained from joining the centers of two stars $K_{1,\ p-1}$ and $K_{1,\ q-1}$ with an edge.

Proposition 6. Let $S_{p,\,q}$ be a double star with $p+q$ vertices. Then

(i) $$DK_1\left(S_{p,q}\right)=\frac{q-1}{p}+\frac{p-1}{q}+\left(p+q-2\right)^2. \tag{4}$$

(ii) $$DK_2\left(S_{p,q}\right)=\frac{q-1}{p^2}+\frac{p-1}{q^2}+\left(p+q-2\right)^2. \tag{5}$$

Proof: Let $G=S_{p,\,q}$. The vertex partition of G is given in Table 3.

$d_G(u) \setminus u \in V(G)$	p	q	1
$d_{\overline{G}}(u) \setminus u \in V(\overline{G})$	$q-1$	$p-1$	$p+q-2$
Number of vertices	1	1	$p+q-2$

Table 3: Vertex partition of $S_{p,\,q}$

(i) $$DK_1\left(S_{p,q}\right)=\sum_{u\in V(G)} d_{\overline{G}}(u)\frac{1}{d_G(u)}=\frac{q-1}{p}+\frac{p-1}{q}+\left(p+q-2\right)^2.$$

(ii) $$DK_2\left(S_{p,q}\right)=\sum_{u\in V(G)} d_{\overline{G}}(u)\frac{1}{d_G(u)^2}=\frac{q-1}{p^2}+\frac{p-1}{q^2}+\left(p+q-2\right)^2.$$

Corollary 6.1. Let $S_{\frac{n}{2},\frac{n}{2}}$ be a double star with n vertices. Then,

(i) $$DK_1\left(S_{\frac{n}{2},\frac{n}{2}}\right)=n^2-4n-\frac{2}{n}+6.$$

(ii) $$DK_2\left(S_{\frac{n}{2},\frac{n}{2}}\right)=n^2-4n+\frac{4}{n}-\frac{8}{n^2}+4.$$

Proof: (i) Put $p=\frac{n}{2},\ q=\frac{n}{2}$ in equation (4), we get the desired result.

(ii) Put $p=\frac{n}{2},\ q=\frac{n}{2}$ in equation (5), we get the desired result.

Proposition 7. Let G be a graph with n vertices. Then (i) $0 \leq DK_1(G)$ and (ii) $0 \leq DK_2(G)$. In (i) and (ii), equality holds if and only if $G=K_n$ or $\overline{K_n}$.

3. Results on Dakshayani indices

In this section, we investigate some mathematical properties of Dakshayani indices.

Proposition 8. Let G be a simple connected graph. Then

$DK_1(G)=(n-1)ID(G)-n.$

Proof: Follows from equation (1).

Proposition 9. Let G be a simple connected graph. Then
$n \le (n-1) ID(G)$.

Proof: This follows from propositions 7(i) and 8.

Proposition 10. Let G be a simple connected graph. Then
$DK_2(G) = (n-1)^m M_1(G) - ID(G)$.

Proof: We have

$$DK_2(G) = \sum_{u \in V(G)} d_{\bar{G}}(u) \frac{1}{d_G(u)^2} = \sum_{u \in V(G)} \left[n - 1 - d_G(u)\right] \frac{1}{d_G(u)^2}$$

$$= \sum_{u \in V(G)} \left[(n-1)\frac{1}{d_G(u)^2} - \frac{1}{d_G(u)}\right]$$

Thus $DK_2(G) = (n-1)^m M_1(G) - ID(G)$.

Therefore the second Dakshayani index is a linear combination of the modified first Zagreb index and inverse degree.

Proposition 11. Let G be a simple connected graph. Then

(i) ${}^m M_1(G) = \frac{1}{n-1}\left[DK_2(G) + ID(G)\right]$.

(ii) $ID(G) = (n-1)^m M_1(G) - DK_2(G)$.

Proof: These follow from propositions 7(ii) and 10.

4. Results for some chemical compounds

4.1. Results for polycyclic aromatic hydrocarbons

In this section, we focus on the chemical graph structure of the family of polycyclic aromatic hydrocarbons, denoted by PAH_n. The first three members of the family PAH_n are given in Figure 1.

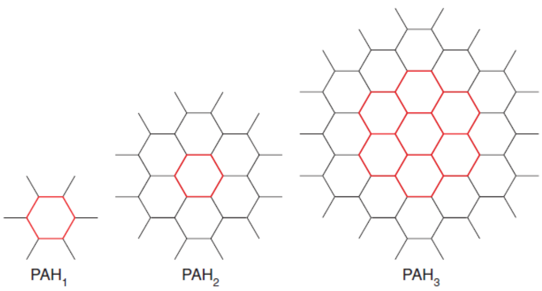

Figure 1:

Let $G=PAH_n$ be the chemical graph in family of polycyclic aromatic hydrocarbons. By calculation, we obtain that G has $6n^2 + 6n$ vertices. There are two types of vertices in G and hence $\bar{G}$ has two types of vertices as given in Table 4.

$d_G(u) \setminus u \in V(G)$	1	3
$d_{\bar{G}}(u) \setminus u \in V(\bar{G})$	$6n^2 + 6n - 2$	$6n^2 + 6n - 4$
Number of vertices	$6n$	$6n^2$

Table 4: Vertex partitions of G and $\bar{G}$.

Theorem 1. The first and second Dakshayani indices of the family of polycyclic aromatic hydrocarbons PAH_n are

(i) $DK_1(PAH_n) = 12n^4 + 48n^3 + 28n^2 - 12n.$

(ii) $DK_2(PAH_n) = 4n^4 + 40n^3 + \frac{100}{3}n^2 - 12n.$

Proof: Let $G = PAH_n$ be the chemical graph in the family of polycyclic aromatic hydrocarbons.

(i) From equation (1) and using Table 1, we deduce

$$DK_1(PAH_n) = \sum_{u \in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)}$$
$$= \left[(6n^2 + 6n - 2)\frac{1}{1}\right]6n + \left[(6n^2 + 6n - 4)\frac{1}{3}\right]6n^2$$
$$= 12n^4 + 48n^3 + 28n^2 - 12n.$$

(ii) From equation (2) and using Table 1, we deduce

$$DK_2(PAH_n) = \sum_{u \in V(G)} d_{\bar{G}}(u)\frac{1}{d_G(u)^2}$$
$$= \left[(6n^2 + 6n - 2)\frac{1}{1^2}\right]6n + \left[(6n^2 + 6n - 4)\frac{1}{3^2}\right]6n^2$$
$$= 4n^4 + 40n^3 + \frac{100}{3}n^2 - 12n.$$

Theorem 2. The general Dakshayani index of the family of polycyclic aromatic hydrocarbons PAH_n is

$$DK^a(PAH_n) = 6n(6n^2 + 6n - 2) + 6 \times 3^a n^2 (6n^2 + 6n - 4)$$

Proof: Let $G = PAH_n$. By using equation (3) and Table 1, we obtain

$$DK^a(PAH_n) = \sum_{u \in V(G)} d_{\bar{G}}(u) d_G(u)^a$$
$$= \left[(6n^2 + 6n - 2)1^a\right]6n + \left[(6n^2 + 6n - 4)3^a\right]6n^2$$
$$= (6n^2 + 6n - 2)6n + 3^a(6n^2 + 6n - 4)6n^2.$$

4.2. Results for Benzenoid systems

In this section, we focus on the chemical graph structure of a jagged rectangle benzenoid system, denoted by $B_{m,n}$ for all $m, n \in N$. Three chemical graphs of jagged rectangle benzenoid systems are presented in Figure 2.

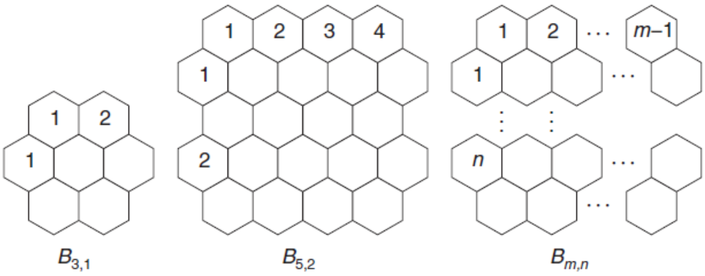

Figure 2:

Let G=$B_{m,n}$ be the graph in the family of a jagged rectangle benzenoid system. By calculation, we obtain that G has $4mn + 4m + 2n - 2$ vertices. The graph G has two types of vertices and hence $\overline{G}$ has two types of vertices as given in Table 5.

$d_G(u) \setminus u \in V(G)$	2	3
$d_{\overline{G}}(u) \setminus u \in V(\overline{G})$	$4mn + 4m + 2n - 3$	$4mn + 4m + 2n - 4$
Number of vertices	$2m + 4n + 2$	$4mn + 2m - 2n - 4$

Table 5: Vertex partitions of G and $\overline{G}$.

Theorem 3. The first and second Dakshayani indices of the family of jagged benzenoid systems $B_{m,n}$ are

(i) $DK_1(B_{m,n}) = \frac{16}{3}m^2n^2 + 12m^2n + 8mn^2 + 2mn + \frac{20}{3}m^2 - 7m + \frac{8}{3}n^2 - 4n + \frac{7}{3}$

(ii) $DK_2(B_{m,n}) = \frac{16}{9}m^2n^2 + \frac{42}{9}m^2n + 4mn^2 + 3mn + \frac{26}{9}m^2 - \frac{13}{6}m + \frac{14}{9}n^2 - 2n + \frac{5}{18}$.

Proof: Let $G = B_{m,n}$.

(i) From equation (1) and using Table 2, we derive

$$DK_1(B_{m,n}) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)}$$

$$= \left[(4mn + 4m + 2n - 3)\frac{1}{2}\right](2m + 4n + 2)$$

$$+ \left[(4mn + 4m + 2n - 4)\frac{1}{3}\right](4mn + 2m - 2n - 4)$$

$$= \frac{16}{3}m^2n^2 + 12m^2n + 8mn^2 + 2mn + \frac{20}{3}m^2 - 7m + \frac{8}{3}n^2 - 4n + \frac{7}{3}$$

(ii) From equation (2) and using Table 2, we derive

$$DK_2(B_{m,n}) = \sum_{u \in V(G)} d_{\overline{G}}(u) \frac{1}{d_G(u)^2}$$

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

$$+\left[(4mn+4m+2n-4)\frac{1}{3^2}\right](4mn+2m-2n-4)$$
$$=\frac{16}{9}m^2n^2+\frac{42}{9}m^2n+4mn^2+3mn+\frac{26}{9}m^2-\frac{13}{6}m+\frac{14}{9}n^2-2n+\frac{5}{18}.$$

Theorem 4. The general Dakshayani index of the family of jagged rectangle benzenoid systems $B_{m,n}$ is

$$DK^a\left(B_{m,n}\right)=2^a(4mn+4m+2n-3)(2m+4n-2)$$
$$+3^a(4mn+4m+2n-4)(4mn+2m-2n-4).$$

Proof: Let $G = B_{m,n}$. By using equation (3) and Table 2, we deduce

$$DK^a\left(B_{m,n}\right)=2^a(4mn+4m+2n-3)(2m+4n-2)$$
$$+3^a(4mn+4m+2n-4)(4mn+2m-2n-4).$$

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