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Some Bounds for Harary Index of Graphs.

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Abstract— Harary index of graph G is defined as the sum of reciprocal of distance between all pairs of vertices of the graph G and is denoted by $H(G)$. Eccentricity of vertex v in G is the distance to a vertex farthest from v. In this paper we obtain some bounds for $H(G)$ in terms of eccentricities. Further we extend these results to the self-centered graphs and also we have given simple algorithm to find the Harary index of graphs.

Keywords— Diameter, distance, eccentricity, Harary index, radius, self-centered graph..

1 Introduction

THROUGHOUT this paper we have consider only simple and connected graph without loops and multiple edges. Let G be a graph with vertex set $V(G)=\{v_1,v_2,...v_n\}$ and edge set $E(G)$. The *distance* between two vertices u,v of G is denoted by $d(u,v)$ and is defined as the length of the shortest path between u and v in graph G. The *degree* of a vertex v in G is the number of edges incident to it and is denoted by *deg(v)*. The *eccentricity* $e(v)$ of a vertex v is the maximum distance from it to any other vertex,

$$e(v)=\max\{d(u,v)\mid u\in V(G)\}.$$

The *radius* $r(G)$ of a graph G is the minimum eccentricity of the vertices. A shortest $u-v$ path is often called *geodesic*. The *diameter* $d(G)$ of a connected graph G is the length of any longest geodesic. A vertex v is called *central vertex* of G if $e(v)=r(G)$. A graph is said to be self-centered if every vertex is a central vertex. Thus in a *self-centered* graph $r(G)=d(G)$. An eccentric vertex of a vertex v is a vertex farthest from v. An eccentric path $P(v)$ is a path of length $e(v)$ joining v and its eccentric vertex. For a given vertex there may exists more than one eccentric path.

The Harary index of graph G denoted by $H(G)$, has been introduced independently by Plavsic et. al [14] and by Ivanciuc et. al [8] in 1993 for the characterization of molecular graphs. If $v_1,v_2,...v_n$ are the vertices of graph G then the Harary index of G is defined as

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

where $d(v_i,v_j)$ is the distance between vertices v_i and v_j.

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The relation between Harary index and other topological indices of graphs and some properties of Harary index, and so on are reported in [5], [6], [8], [19], [20], [21], [22], [23] and its application in pure graph theory or in mathematical chemistry are reported in literature [1], [2], [9], [10], [11], [12], [13], [14], [16], [17].

The distance number of a vertex v_i of graph G denoted by $d(v_i\mid G)$ is defined as

$$d(v_i\mid G)=\sum_{i=1}^{n}d(v_i,v_j).$$

Therefore ,

$$H(G)=\frac{1}{2}\sum_{i=1}^{n}\frac{1}{d(v_i\mid G)}$$

Inspired by the result of [15], we calculated the Harary index in terms of eccentricities and extended it for self-centered graphs. For graph theoretic terminology readers can refer [3], [4], [7], [18].

2 Main Results

Theorem 2.1 *Let G be a connected graph with n vertices, m edges and $e_i=e(v_i)$, $i=1,2,...n$. Then*

$$H(G)\le\frac{1}{4}\left[n(n-2)+2m+2n\sum_{i=1}^{e_i}\frac{1}{i}-ne_i\right] \qquad (1)$$

Further equality holds if and only if for every v_i of G, if $P(v_i)$ is one of the eccentric path of v_i, then for every $v_j\in V(G)$ which is not on $P(v_i)$, $d(v_i,v_j)\le 2$.

Proof: Let $P(v_i)$ be one of the eccentric path of $v_i\in V(G)$.

Let,

$A_1(v_i)=\{v_j \mid v_j$ is on eccentric path $P(v_i)$ of $v_i\}$,

$A_2(v_i)=\{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,

$A_3(v_i)=\{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.

Clearly, $A_1(v_i)\cup A_2(v_i)\cup A_3(v_i)=V(G)$ and

$|A_1(v_i)|=e_i+1$, $|A_2(v_i)|=deg(v_i)-1$,

$|A_3(v_i)| = n - e_i - deg(v_i)$.

Now $\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i} \frac{1}{i}$,

$$\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = deg(v_i) - 1$$

$$\sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} \leq \frac{(n - e_i - deg(v_i)}{2} .$$

Therefore,

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)}$$

$$\leq \sum_{i=1}^{e_i} \frac{1}{i} + deg(v_i) - 1 + \frac{(n - e_i - deg(v_i)}{2}$$

$$= \frac{(n + deg(v_i) - 2}{2} + \sum_{i=1}^{e_i} \frac{1}{i} - \frac{e_i}{2} .$$

Therefore,

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)}$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left[\sum_{i=1}^{e_i} \frac{1}{i} + \frac{(n + deg(v_i) - 2}{2} - \frac{e_i}{2} \right]$$

$$= \frac{1}{4} \left[n(n-2) + 2m + 2n \sum_{i=1}^{e_i} \frac{1}{i} - ne_i \right].$$

For equality,

Let G be a graph and $P(v_i)$ be one of the eccentric paths of $v_i \in V(G)$. Let $A_1(v_i)$, $A_2(v_i)$ and $A_3(v_i)$ be the sets as defined in the first part of the proof of this theorem.

Let $d(v_i, v_j) = 2$, where $v_j \in A_3(v_i)$.

Therefore $\sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} = \frac{n - e_i - deg(v_i)}{2}$,

$$\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i} \frac{1}{i}$$

and $\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = deg(v_i) - 1$.

Thus,

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{i=1}^{e_i} \frac{1}{i} + deg(v_i) - 1 + \frac{n - e_i - deg(v_i)}{2}$$

$$= \frac{n + deg(v_i) - 2}{2} + \sum_{i=1}^{e_i} \frac{1}{i} - \frac{e_i}{2} .$$

Hence,

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)}$$

$$= \frac{1}{2} \sum_{i=1}^{n} \left[\sum_{i=1}^{e_i} \frac{1}{i} + \frac{(n + deg(v_i) - 2}{2} - \frac{e_i}{2} \right]$$

$$= \frac{1}{4} \left[n(n-2) + 2m + 2n \sum_{i=1}^{e_i} \frac{1}{i} - ne_i \right]$$

Conversely,

Suppose G is not such graph as defined in the equality part of this theorem. Then there exist at least one vertex $v_j \in A_3(v_i)$ such that $d(v_i, v_j) \geq 3$. Let $A_3(v_i)$ be partitioned into two sets $A_{31}(v_i)$ and $A_{32}(v_i)$, where
$A_{31}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 2\}$
$A_{32}(v_i) = \{v_j \mid v_j$ is not adjacent to v_i, not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 3\}$.
Let $|A_{32}(v_i)| = l \geq 1$. So, $|A_{31}(v_i)| = n - e_i - deg(v_i) - l$.

Therefore, $\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i} \frac{1}{i}$,

$$\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = deg(v_i) - 1,$$

$$\sum_{v_j \in A_{31}(v_i)} \frac{1}{d(v_i, v_j)} = \frac{(n - e_i - deg(v_i) - l)}{2}$$

and $\sum_{v_j \in A_{32}(v_i)} \frac{1}{d(v_i, v_j)} \geq \frac{l}{3}$.

Therefore

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_{31}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_{32}(v_i)} \frac{1}{d(v_i, v_j)}$$

$$\leq \sum_{i=1}^{e_i} \frac{1}{i} + deg(v_i) - 1 + \frac{(n - e_i - deg(v_i) - l)}{2} + \frac{l}{3}$$

$$= \frac{(n - e_i - deg(v_i) - 2)}{2} + \sum_{i=1}^{e_i} \frac{1}{i} - \frac{e_i}{2} - \frac{l}{6} .$$

Thus,

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)}$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left[\sum_{i=1}^{e_i} \frac{1}{i} + \frac{(n - e_i - deg(v_i) - 2)}{2} - \frac{e_i}{2} - \frac{l}{6} \right]$$

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

$$\le \frac{1}{4}\left[n(n-2) + 2m + 2n\sum_{i=1}^{e_i}\frac{1}{i} - ne_i \right]$$

as $l \ge 1$, which is a contradiction. This contradiction proves the result.

□

Corollary 2.2 *Let G be a self-centered graph with n vertices, m edges and radius r = r(G), then*

$$H(G) \le \frac{1}{4}\left[n(n-2) + 2m + 2n\sum_{i=1}^{r}\frac{1}{i} - nr \right].$$

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d(v_i, v_j) \le 2$.

Proof. For self-centered graph each vertex has same eccentricity equal to the radius r, that is, $e_i = e(v_i) = r$, $i = 1, 2, \ldots, n$. Therefore from Eq. (1)

$$H(G) \le \frac{1}{4}\left[n(n-2) + 2m + 2\sum_{i=1}^{n}\sum_{i=1}^{r}\frac{1}{i} - \sum_{i=1}^{n} r \right]$$

$$= \frac{1}{4}\left[n(n-2) + 2m + 2n\sum_{i=1}^{r}\frac{1}{i} - nr \right]$$

The proof of the equality part is similar to the proof of equality part of Theorem 2.1.

□

Theorem 2.3 *Let G be a connected graph with n vertices and $e_i = e(v_i)$, i = 1, 2, …, n, then*

$$H(G) \le \frac{1}{2}\left[n(n-1) + n\sum_{i=1}^{e_i}\frac{1}{i} - ne_i \right]. \qquad (2)$$

Equality holds if and only if for every vertex v_i of G, if $P(v_i)$ is is one of the eccentric path of v_i, then for every $v_j \in V(G)$ which is not on $P(v_i)$, $d(v_i, v_j) = 1$.

Proof: Let $e_i = e(v_i)$, $i = 1, 2, \ldots, n$ and $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$.

Let $B_1(v_i) = \{v_j \mid v_j$ is on eccentric path $P(v_i)$ of $v_i\}$,
$B_2(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of $v_i\}$.

Clearly $B_1(v_i) \cup B_2(v_i) = V(G)$ and
$|B_1(v_i)| = e_i + 1$, $|B_2(v_i)| = n - e_i - 1$.

Now $$\sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i}\frac{1}{i},$$

$$\sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \le (n - e_i - 1),$$

Therefore

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n}\frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)}$$

$$\le \sum_{i=1}^{e_i}\frac{1}{i} + n - e_i - 1.$$

Therefore

$$H(G) = \frac{1}{2}\sum_{i=1}^{n}\frac{1}{d(v_i \mid G)}$$

$$\le \frac{1}{2}\sum_{i=1}^{n}\left[\sum_{i=1}^{e_i}\frac{1}{i} + (n - e_i - 1) \right]$$

$$= \frac{1}{2}\left[n(n-1) + n\sum_{i=1}^{e_i}\frac{1}{i} - ne_i \right].$$

For equality,

Let G be a graph and $P(v_i)$ be one of the eccentric paths of $v_i \in V(G)$. Let $B_1(v_i)$ and $B_2(v_i)$ be the sets as defined in the first part of the proof of this theorem.

Let $d(v_i, v_j) = 1$, where $v_j \in B_2(v_i)$.

Therefore $$\sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} = n - e_i - 1,$$

and $$\sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i}\frac{1}{i}.$$

Therefore

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n}\frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{i=1}^{e_i}\frac{1}{i} + n - e_i - 1.$$

Therefore

$$H(G) = \frac{1}{2}\sum_{i=1}^{n}\frac{1}{d(v_i \mid G)}$$

$$= \frac{1}{2}\sum_{i=1}^{n}\left[\sum_{i=1}^{e_i}\frac{1}{i} + (n - e_i - 1) \right]$$

$$= \frac{1}{2}\left[n(n-1) + n\sum_{i=1}^{e_i}\frac{1}{i} - ne_i \right].$$

Conversely,

Suppose G is not such graph as defined in the equality part of this theorem. Then there exist at least one vertex $v_j \in B_2(v_i)$ such that $d(v_i, v_j) \ge 2$. Let $B_2(v_i)$ be

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partitioned into two sets $B_{21}(v_i)$ and $B_{22}(v_i)$, where

$B_{21}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) = 1\}$

$B_{22}(v_i) = \{v_j \mid v_j$ is not on the eccentric path $P(v_i)$ of v_i and $d(v_i, v_j) \geq 2\}$.

Let $|B_{22}(v_i)| = l \geq 1$

Therefore $|B_{21}(v_i)| = n - e_i - 1 - l$.

Therefore $\displaystyle\sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i} \frac{1}{i}$,

$$\sum_{v_j \in B_{21}(v_i)} \frac{1}{d(v_i, v_j)} = n - e_i - 1 - l \text{ and } \sum_{v_j \in B_{22}(v_i)} \frac{1}{d(v_i, v_j)} \geq \frac{l}{2}.$$

Therefore

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{21}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{22}(v_i)} \frac{1}{d(v_i, v_j)}$$

$$\leq \sum_{i=1}^{e_i} \frac{1}{i} + (n - e_i - 1 - \frac{l}{2}).$$

Therefore

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)}$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left[\sum_{i=1}^{e_i} \frac{1}{i} + (n - e_i - 1 - \frac{l}{2}) \right]$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left[n(n-1) \sum_{i=1}^{n} \frac{1}{2} + n \sum_{i=1}^{e_i} \frac{1}{i} - ne_i \right] \text{ as } l \geq 1.$$

$$\leq \frac{1}{2} \sum_{i=1}^{n} \left[n(n-1) - \frac{n}{2} + n \sum_{i=1}^{e_i} \frac{1}{i} - ne_i \right].$$

This is a contradiction. Hence the proof.

□

If G is a self-centered graph then $e_i = e(v_i) = r(G)$ for all $i = 1, 2, \ldots, n$. Substituting this in Eq. (2) we get following corollary.

Corollary 2.4: *Let G be a self-centered graph with n vertices and radius r = r(G), then* $H(G) \leq \frac{1}{2} \left[n(n-1) + n \sum_{i=1}^{e_i} \frac{1}{i} - nr \right]$.

Equality holds if and only if for every vertex v_i of a self-centered graph G, if $P(v_i)$ is one of the eccentric path of v_i then for every $v_j \in V(G)$ which is not on the eccentric path $P(v_i)$, $d(v_i, v_j) = 1$.

Theorem 2.5 *Let G be a connected graph with n vertices, m edges and diam(G) = d. Let $e_i = e(v_i)$, i = 1, 2, … , n, then*

$$H(G) \geq \frac{1}{2d} \left[n^2 - ne_i + 2m(d-1) - nd \left(1 - \sum_{i=1}^{e_i} \frac{1}{i} \right) \right]. \quad (3)$$

Equality holds if and only if diam(G) ≤ 2.

Proof: Let $P(v_i)$ be one of the eccentric path of $v_i \in V(G)$.

Let $A_1(v_i) = \{v_j \mid v_j$ is on the eccentric path $P(v_i)$ of $v_i\}$,

$A_2(v_i) = \{v_j \mid v_j$ is adjacent to v_i and which is not on the eccentric path $P(v_i)$ of $v_i\}$,

$A_3(v_i) = \{v_j \mid v_j$ is not adjacent to v_i and not on the eccentric path $P(v_i)$ of $v_i\}$.

Clearly $A_1(v_i) \cup A_2(v_i) \cup A_3(v_i) = V(G)$ and $|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = deg(v_i) - 1$, $|A_3(v_i)| = n - e_i - deg(v_i)$.

Now $\displaystyle\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{e_i} \frac{1}{i}$,

$$\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = deg(v_i) - 1$$

$$\sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} \geq \frac{(n - e_i - deg(v_i))}{d}.$$

Therefore

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)}$$

$$\geq \sum_{i=1}^{e_i} \frac{1}{i} + deg(v_i) - 1 + \frac{(n - e_i - deg(v_i))}{d}$$

$$= \left[n - e_i + deg(v_i)(d-1) - d \left(1 - \sum_{i=1}^{e_i} \frac{1}{i} \right) \right].$$

Therefore

$$H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)}$$

$$\geq \frac{1}{2d} \sum_{i=1}^{n} \left[n - e_i + deg(v_i)(d-1) - d \left(1 - \sum_{i=1}^{e_i} \frac{1}{i} \right) \right]$$

$$= \frac{1}{2d} \left[n^2 - ne_i + 2m(d-1) - nd \left(1 - \sum_{i=1}^{e_i} \frac{1}{i} \right) \right].$$

since $\displaystyle\sum_{i=1}^{n} deg(v_i) = 2m$.

For equality,

Let $diam(G) \leq 2$.

Case 1: If $diam(G) = 1$ then $G = K_n$. Therefore $A_3(v_i) = \Phi$ and $e_i = e(v_i) = 1$, $i = 1, 2, \dots, n$.

Therefore

$$H(G) = \frac{1}{2}\left[n^2 - n(1) + 2m(d-1) - nd\left(1 - \sum_{i=1}^{e_i}\frac{1}{i}\right)\right] = \frac{n(n-1)}{2}.$$

Case 2: If $diam(G) = 2$, then for $v_j \in A_3(v_i)$, $d(v_i, v_j) = 2$.

Therefore, $\sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} = \frac{(n - e_i - deg(v_i))}{2}$.

Hence $H(G) = \frac{1}{2d}\left[n^2 - ne_i + 2m(d-1) - nd\left(1 - \sum_{i=1}^{e_i}\frac{1}{i}\right)\right]$

$$= \frac{1}{4}\left[n(n-2) - ne_i + 2m + 2n\sum_{i=1}^{e_i}\frac{1}{i}\right].$$

Conversely,

$$\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n}\frac{1}{d(v_i, v_j)}$$

$$= \sum_{v_j \in A_1(v_i)}\frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)}\frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_3(v_i)}\frac{1}{d(v_i, v_j)} \qquad (4)$$

The first summation of Eq. (4) contains the Harary distance between v_i and the vertices on its eccentric path $P(v_i)$. Second summation of Eq. (4) contains the distance between v_i and its neighbor which are not on the eccentric path $P(v_i)$. The third summation of Eq. (4) contains the distance between v_i and a vertex which is neither adjacent to v_i nor on the eccentric path $P(v_i)$. Hence the equality in Eq. (4) holds if and only if $d = diam(G) \le 2$. It is true for all $v_i \in V(G)$. Hence $diam(G) \le 2$.

□

Corollary 2.6: *Let G be a self-centered graph with n vertices and radius r = r(G), then*

$$H(G) \ge \frac{1}{2r}\left[n(n-2r) + 2m(r-1) - nr\left(1 - \sum_{i=1}^{r}\frac{1}{i}\right)\right]. \qquad (5)$$

Equality holds if and only if diam(G) ≤ 2.

Proof: Proof follows by substituting $e_i = e(v_i) = r$, $i = 1, 2, \dots, n$ in Eq. (3).

□

ALGORITHM

Adjacency matrix A(G) of graph G is defined as, the rows and columns of $A(G)$ are indexed by $V(G)$. If $i \ne j$ then the (i, j)- entry of $A(G)$ is 0 for vertices i and j non-adjacent, and the (i, j)- entry is 1 for i and j adjacent. The (i, i)- entry 0f $A(G)$ is 0 for i=1, 2, …, n.

Input: Adjacency matrix of *G*.

a) Here we propose a simple algorithm to find Harary index of graphs with $diam(G) \le 2$.

Step1: Declare the order of adjacency matrix of graph G.
Step 2: Consider, for each $(ij)^{th}$ entry

$$a[i][j] = 1 \to S[i][j] = 1,$$

and

$$a[i][j] = 0 \to S[i][j] = \frac{1}{2}.$$

Step 4: Corresponding to each i^{th} row the string $S(u_i)$ is

$$S(u_i) = \sum_{a[i][j]=1} S(a[i][j]) + \sum_{a[i][j]=0} S(a[i][j]) - \frac{1}{2}.$$

Step 5: Find the Harary index of graph G as

$$H(G) = \frac{1}{2}\sum_{i=1}^{n} S(u_i).$$

Output: Harary index of graph *G* with $diam(G) \le 2$.

b) Here we have given a simple algorithm to find upper bounds for Harary index of graphs.

Input: Adjacency matrix of *G*.

Step1: Declare the order of adjacency matrix of graph G.
Step 2: Consider for each $(ij)^{th}$ entry

$$a[i][j] = 1 \to S[i][j] = 1,$$

and

$$a[i][j] = 0 \to S[i][j] < \frac{1}{2}.$$

Step 4: Corresponding to each i^{th} row the string $S(u_i)$ is

$$S(u_i) < \sum_{a[i][j]=1} S(a[i][j]) + \sum_{a[i][j]=0} S(a[i][j]) - \frac{1}{2}.$$

Step 5: Find the Harary index of graph G as

$$H(G) < \frac{1}{2}\sum_{i=1}^{n} S(u_i).$$

Output: Bound for the Harary index of graph *G*.

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