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

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

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 $d(v_i | G)$ is defined as $d(v_i | G) = \sum_{i=1}^{n} d(v_i, v_j)$.

Therefore, $H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i | G)}$.

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

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

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 $P(v_i)$, $d(v_i, v_j) \leq 2$.

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

Let,

$A_1(v_i) = \{v_i \mid v_j \in P(v_i) \}$,

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

$A_3(v_i) = \{v_i \mid v_j \text{ is not adjacent to } v_i \}$ 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 $|A_1(v_i)| = e_i + 1$, $|A_2(v_i)| = \deg(v_i) - 1$,

where $d(v_i, v_j)$ is the distance between vertices $v_i$ and $v_j$.
Now \( \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{\ell'} \),
\[
\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = \deg(v_i) - 1
\]
\[
\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} \leq \frac{n - e_i - \deg(v_i)}{2}.
\]
Therefore, 
\[
\frac{1}{d(v_i | G)} = \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)}
\]
\[
\leq \frac{n - e_i - \deg(v_i)}{2} + \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)}.
\]
Hence, 
\[
H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i | G)}
\]
\[
= \frac{1}{2} \sum_{i=1}^{n} \left[ \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)} + (n - e_i - \deg(v_i)) \right]
\]
\[
= \frac{1}{4} \left[ n(n-2) + 2m + 2n \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)} \right] - \frac{1}{i}.
\]
Conversely, 
\[
\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = \deg(v_i) - 1
\]
\[
\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \frac{n - e_i - \deg(v_i) - \ell}{2}.
\]
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 
\[
\sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} = \frac{n - e_i - \deg(v_i)}{2},
\]
\[
\sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} = \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)}
\]
and 
\[
\sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} = \deg(v_i) - 1.
\]
Thus, 
\[
\frac{1}{d(v_i | G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)}
\]
\[
= \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)}
\]
\[
= \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)} + \frac{n - e_i - \deg(v_i)}{2} + \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)}.
\]
Thus, 
\[
H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i | G)}
\]
\[
\leq \frac{1}{2} \sum_{i=1}^{n} \left[ \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)} + (n - e_i - \deg(v_i)) - \frac{l}{6} \right]
\]
\[
= \frac{1}{2} \sum_{i=1}^{n} \left[ \sum_{i=1}^{\ell'} \frac{1}{d(v_i, v_j)} + (n - e_i - \deg(v_i) - \ell) - \frac{l}{6} \right].
\]
\[
\frac{1}{4} \left[ n(n-2) + 2m + 2n \sum_{i=1}^{n} \left( \frac{1}{e_i} - \frac{n}{3} \right) \right] \\
\leq \frac{1}{4} \left[ n(n-2) + 2m + 2n \sum_{i=1}^{n} \left( \frac{1}{e_i} - ne_i \right) \right]
\]
as \(l \geq 1\), 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

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

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 \(P(v_i)\), \(d(v_i, v_j) \leq 2\).

**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)

\[
H(G) \leq \frac{1}{4} \left[ n(n-1) + n \sum_{i=1}^{r} \left( \frac{1}{e_i} - n \right) \right].
\]
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 \(e_i = e(v_i), i = 1, 2, \ldots, n\), then

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

Equality holds if and only if for every vertex \(v_i\) 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 \(P(v_i)\), \(d(v_i, v_j) = 1\).

**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 \(B_1(v_i) = \{v_j \mid v_j \in P(v_i)\}\)

\(B_2(v_i) = \{v_j \mid v_j \notin P(v_i)\}\)

Clearly \(B_1(v_i) \cup B_2(v_i) = V(G)\) and

\(|B_1(v_i)| = e_i + 1, \quad |B_2(v_i)| = n - e_i - 1.\)

Now

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

\[
\sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \leq (n - e_i - 1).\]

Therefore

\[
\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)} = \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \leq \sum_{i=1}^{e_i} \frac{1}{i} + n - e_i - 1.
\]

Therefore

\[
H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)} = \frac{1}{2} \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \leq \frac{1}{2} \sum_{i=1}^{e_i} \frac{1}{i} + n - e_i - 1.
\]

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 \(v_i \in B_2(v_i)\).

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

\[
\frac{1}{d(v_i \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)} = \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \leq \sum_{i=1}^{e_i} \frac{1}{i} + n - e_i - 1.
\]

Therefore

\[
H(G) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{d(v_i \mid G)} = \frac{1}{2} \sum_{v_j \in B_1(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_2(v_i)} \frac{1}{d(v_i, v_j)} \leq \frac{1}{2} \sum_{i=1}^{e_i} \frac{1}{i} + n - e_i - 1.
\]

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 \(d(v_i, v_j) \geq 2\). Let \(B_2(v_i)\) be
partitioned into two sets \(B_{21}(v_i)\) and \(B_{22}(v_i)\), where
\[
B_{21}(v_i) = \{ v_j \mid v_j \text{ is not on the eccentric path } P(v_i) \text{ of } v_i \text{ and } d(v_i, v_j) = 1 \}
\]
\[
B_{22}(v_i) = \{ v_j \mid v_j \text{ is not on the eccentric path } P(v_i) \text{ of } v_i \text{ and } d(v_i, v_j) \geq 2 \}.
\]
Let \(|B_{22}(v_i)| = l \geq 1\).

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

\[
\sum_{v_j \in B_{21}(v_i)} \frac{1}{d(v_i, v_j)} = \frac{1}{l}
\]

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

Therefore
\[
\frac{1}{d(v_i \mid G)} = \frac{1}{n} \sum_{j=1}^{n} \frac{1}{d(v_i, v_j)} = \sum_{v_j \in B_{1}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{2}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{22}(v_i)} \frac{1}{d(v_i, v_j)} \leq \sum_{i=1}^{e_i} i + (n - e_i - 1 - l) + \frac{l}{2}.
\]

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 \(H(G) \leq \frac{1}{2} n(n - 1) + n \sum_{i=1}^{e_i} \frac{1}{i} - nr\).

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 \(\text{diam}(G) = d\). Let \(e_i = e(v_i)\), \(i = 1, 2, \ldots, n\), then

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

Equality holds if and only if \(\text{diam}(G) \leq 2\).

**Proof:** Let \(P(v_i)\) be one of the eccentric path of \(v_i \in V(G)\). Let \(A_1(v_i) = \{ v_j \mid v_i \text{ is on the eccentric path } P(v_i) \text{ of } v_i \}\), \(A_2(v_i) = \{ v_j \mid v_i \text{ is adjacent to } v_j \text{ and which is not on the eccentric path } P(v_i) \text{ of } v_i \}\), \(A_3(v_i) = \{ v_j \mid v_i \text{ is not adjacent to } v_j \text{ and not on the eccentric path } P(v_i) \text{ of } v_i \}\).

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

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

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

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

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

\[
= \frac{1}{2} \left[ \sum_{i=1}^{e_i} i + \sum_{v_j \in B_{1}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{2}(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in B_{22}(v_i)} \frac{1}{d(v_i, v_j)} \right] \geq \sum_{i=1}^{e_i} i + \deg(v_i) - 1 + \frac{(n - e_i - \deg(v_i))}{d} = \left[ n - e_i + \deg(v_i)(d-1) - d \left(1 - \sum_{i=1}^{e_i} \frac{1}{i}\right) \right].
\]

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

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

since \(\sum_{i=1}^{n} \deg(v_i) = 2m\).
Case 1: If \( \text{diam}(G) = 1 \) then \( G = K_n \). Therefore \( A_3(v_i) = \emptyset \) and \( e_i = e(v_i) = 1, i = 1, 2, \ldots, n. \)

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

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

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

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

Conversely,
\[
\frac{1}{d(v_j \mid G)} = \sum_{j=1}^{n} \frac{1}{d(v_j, v_j)} = \sum_{v_j \in A_3(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_2(v_i)} \frac{1}{d(v_i, v_j)} + \sum_{v_j \in A_1(v_i)} \frac{1}{d(v_i, v_j)} \quad (4)
\]

The first summation of Eq. (4) contains the Harary distance between \( v_1 \) and the vertices on its eccentric path \( P(v_1) \). Second summation of Eq. (4) contains the distance between \( v_1 \) and its neighbor which are not on the eccentric path \( P(v_1) \). The third summation of Eq. (4) contains the distance between \( v_1 \) and a vertex which is neither adjacent to \( v_1 \) nor on the eccentric path \( P(v_1) \). Hence the equality in Eq. (4) holds if and only if \( d = \text{diam}(G) \leq 2 \). It is true for all \( v_i \in V(G) \). Hence \( \text{diam}(G) \leq 2 \).

**Corollary 2.6:** Let \( G \) be a self-centered graph with \( n \) vertices and radius \( r = r(G) \), then
\[
H(G) \geq \frac{1}{2r} \left[ n(n-2r) + 2m(r-1) - nr \left( 1 - \sum_{i=1}^{r} \frac{1}{i} \right) \right]. \quad (5)
\]

Equality holds if and only if \( \text{diam}(G) \leq 2 \).

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

\[
\text{ALGORITHM}
\]

Adjacency matrix \( A(G) \) of graph \( G \) is defined as, the rows and columns of \( A(G) \) are indexed by \( V(G) \). If \( i \neq j \) 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 of \( A(G) \) is 0 for \( i = 1, 2, \ldots, n \).

**Input:** Adjacency matrix of \( G \).

\begin{itemize}
  \item a) Here we propose a simple algorithm to find Harary index of graphs with \( \text{diam}(G) \leq 2 \).
  \begin{itemize}
    \item Step 1: Declare the order of adjacency matrix of graph \( G \).
    \item Step 2: Consider, for each \((ij)^{th}\) entry
      \[ a[i][j] = 1 \rightarrow S[i][j] = 1, \]
      \[ a[i][j] = 0 \rightarrow S[i][j] = \frac{1}{2}, \]
  \end{itemize}
  \item Step 4: Corresponding to each \((i)\)th row the string \( S(u_i) \) is
    \[ S(u_i) = \sum_{a[i][j]=1} S(a[i][j]) + \sum_{a[i][j]=0} S(a[i][j]) - \frac{1}{2}. \]
  \item Step 5: Find the Harary index of graph \( G \) as
    \[ H(G) = \frac{1}{2} \sum_{i=1}^{n} S(u_i). \]
  \end{itemize}

  \begin{itemize}
    \item b) Here we have given a simple algorithm to find upper bounds for Harary index of graphs.
    \begin{itemize}
      \item Step 1: Declare the order of adjacency matrix of graph \( G \).
      \item Step 2: Consider, for each \((ij)^{th}\) entry
        \[ a[i][j] = 1 \rightarrow S[i][j] = 1, \]
        \[ a[i][j] = 0 \rightarrow S[i][j] < \frac{1}{2}. \]
      \item Step 4: Corresponding to each \((i)\)th row the string \( S(u_i) \) is
        \[ S(u_i) < \sum_{a[i][j]=1} S(a[i][j]) + \sum_{a[i][j]=0} S(a[i][j]) - \frac{1}{2}. \]
      \item Step 5: Find the Harary index of graph \( G \) as
        \[ H(G) < \frac{1}{2} \sum_{i=1}^{n} S(u_i). \]
    \end{itemize}
  \end{itemize}

\textbf{Output:} Bound for the Harary index of graph \( G \).

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