Eccentric harmonic index of a graph

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ABSTRACT
In this paper, we introduce the eccentric harmonic index $H_e = H_e(G)$ of a graph $G$, so that it is the sum of the terms $\frac{1}{d(u,v)}$ for the edges $u/v$, where $e$ is the eccentricity of the $i$th vertex of the graph $G$. We compute the exact values of $H_e$ for some standard graphs. Bounds for $H_e$ are established. Relationships between $H_e$ and the eccentric connectivity index $\varepsilon_c(G)$ are derived.

1. Introduction
In this paper, all graphs are assumed to be finite simple connected graphs. A graph $G = (V,E)$ is a simple graph, that is, having no loops, no multiple and directed edges. As usual, we denote $n$ to be the order and $m$ to be the size of the graph $G$. A vertex $v \in V$, the open neighborhood of $v$ in a graph $G$, denoted $N(v)$, is the set of all vertices that are adjacent to $v$ and the closed neighborhood of $v$ is $N[v] = N(v) \cup \{v\}$. The degree of a vertex $v_i$ in $G$ is $d_i = d(v_i) = |N(v_i)|$. A vertex of degree one is called pendant vertex. A graph $G$ is said to be $k$-regular graph if $d(v) = k$ for every $v \in V(G)$. The distance $d(u,v)$ between any two vertices $u$ and $v$ in a graph $G$ is the length of the shortest path connecting them.

The eccentricity of a vertex $v \in V(G)$ is $e(v) = \max\{d(u,v) : u \in V(G)\}$. The radius of $G$ is $r = \min\{e(v) : v \in V(G)\}$ and the diameter of $G$ is $\text{diam}(G) = \max\{e(v) : v \in V(G)\}$. Hence $r(G) \leq e(v) \leq \text{diam}(G)$, for every $v \in V(G)$.

A vertex $v$ in a connected graph $G$ is central vertex if $e(v) = r(G)$, while a vertex $v$ in a connected graph $G$ is peripheral vertex if $e(v) = \text{diam}(G)$. A graph $G$ is called a self-centered graph if $e(v) = r(G) = \text{diam}(G)$ for all $v \in V(G)$. If $G$ is a regular graph with $e(v) = r(G) = \text{diam}(G)$ for all $v \in V(G)$, then $G$ is a regular self-centered graph. We denote the eccentricity of a vertex $v_i$ by $e_i$. As usual we use the characters $T, P_n, C_n, K_{a,b}, K_{1,n-1}, K_n$ for the tree, path, cycle, complete bipartite, star and complete graph, respectively. All the definitions and terminologies about the graph in this paragraph are available in Harary, (1969).

A single number representing a chemical structure, by means of the corresponding molecular graph, is known as topological descriptor. Topological descriptors play a prominent role in mathematical chemistry, particularly in studies of quantitative structure property and quantitative structure activity relationships. Moreover, a topological descriptor is called a topological index if it has a mutual relationship with a molecular property. Thus, since topological indices encode some characteristics of a molecule in a single number, they can be used to study physicochemical properties of chemical compounds (Hernndez-Gmez, Mndez-Bermdez, Rodriguez, & Sigarreata, 2018).

After the seminal work of Wiener (Wiener, 1947), many topological indices have been defined and analyzed. Among all topological indices, probably the most studied is the Randić connectivity index ($R$) (Randić, 1975). Several hundred papers and, at least, two books report studies of $R$ (see, e.g. Gutman & Furtula, 2008; Li & Gutman, 2006 and references therein). Moreover, with the aim of improving the predictive power of $R$, many additional topological descriptors (similar to $R$) have been proposed. In fact, the first and second Zagreb indices, $M_1$ and $M_2$, respectively, can be considered as the main successors of $R$. They are defined as
Both $M_1$ and $M_2$ have recently attracted much interest (see, e.g. Borovičanin & Furtula, 2016; Das, 2020; Das, Gutman, & Furtula, 2011; in particular, they are included in algorithms used to compute topological indices).

Another remarkable topological descriptor is the harmonic index, defined in Fajtlowicz (1987) as

$$H(G) = \sum_{v \in V(G)} \sum_{v \in V(G)} \frac{2}{d_i + d_j}.$$  

This index has attracted a great interest in the last years (see, e.g. Deng, Balachandran, Ayyaswamy, & Venkatakrishnan, 2013; Li & Shi, 2014; Rodriguez & Sigarreta, 2017; Swetha Shetty, Lokesha, & Ranjini, 2015; Wu, Tang, & Deng, 2013; Zhong, 2012). In particular, in Swetha Shetty et al. (2015) it appears relations for the harmonic index of some operations of graphs.

Sharma et al. introduced the eccentric connectivity index of a graph (Sharma, Goswami, & Madan, 1997), where they defined it for a graph with $n$ vertices and $m$ edges, as

$$\xi^c = \xi^c(G) = \sum_{v \in V(G)} e_v = \sum_{v \in V(G)} d_v.$$  

In analogy with the harmonic index and its applications, we introduce the eccentric harmonic index as an eccentric version of the harmonic index. Also, the relation between the eccentric harmonic index and the eccentric connectivity index motivates us to study the eccentric connectivity index and its applications in another way.

### 2. Eccentric harmonic index of a graph

In this section, we define the eccentric harmonic index $H_e(G)$ of a graph $G$. The eccentric harmonic index of some well-known graphs are computed. The starting is with the definition of $H_e(G)$ which is explained in the following definition.

**Definition 2.1.** Let $G$ be a graph with $n$ vertices and $m$ edges. Then the eccentric harmonic index $H_e(G)$ of $G$ is defined as

$$H_e(G) = \sum_{v \in V(G)} \frac{2}{d_i + e_j}.$$  

**Theorem 2.2.** Let $G$ be a self-centered graph of order $n$ and size $m$. Then

$$H_e(G) = \frac{m}{\text{diam}(G)}.$$  

**Proof.** Let $G$ be a self-centered graph of order $n$ and size $m$. Then

$$H_e(G) = \sum_{v \in V(G)} \frac{2}{d_i + e_j}.$$  

**Corollary 2.3.** For the cycle $C_n$, the eccentric harmonic index is

$$H_e(C_n) = \left\{ \begin{array}{ll} 2, & \text{if } n \text{ is even} \\ \frac{2n}{n-1}, & \text{if } n \text{ is odd} \end{array} \right.$$  

**Proof.** Let $G = C_n$ and assume $n$ is even. It is clear that $C_n$ is a self-centered graph with $\text{diam}(G) = \frac{n}{2}$. Thus, by Theorem 2.2

$$H_e(C_n) = \frac{m}{\frac{n}{2}} = \frac{2m}{n}.$$  

But, $m = n$, so

$$H_e(C_n) = 2.$$  

Let $n$ be odd. Then $\text{diam}(G) = \frac{n-1}{2}$. Thus, by Theorem 2.2

$$H_e(C_n) = \frac{m}{\frac{n-1}{2}} = \frac{2m}{n-1}.$$  

Since $m = n$, then

$$H_e(C_n) = \frac{2n}{n-1}.$$  

**Example 2.4.** The following are two examples of $H_e(G)$ for a self-centered graphs.

1. The complete graph $K_n$ is a self-centered graph with $\text{diam}(K_n) = 1$. Thus, by Theorem 2.2

$$H_e(K_n) = \frac{m}{\frac{n(n-1)}{2}}.$$  

2. The complete bipartite graph $K_{ab}$ is a self-centered graph with $\text{diam}(K_{ab}) = 2$. Thus, by Theorem 2.2

$$H_e(K_{ab}) = \frac{m}{\frac{ab}{2}}.$$  

**Theorem 2.5.** Let $P_n$ be a path of order $n$, $n \geq 2$. Then

$$H_e(P_n) = \left\{ \begin{array}{ll} \frac{1}{n} + \frac{n-2}{2} + \frac{1}{i=2}, & \text{if } n \text{ is even} \\ \frac{2}{n-1} + \frac{1}{i=2}, & \text{if } n \text{ is odd} \end{array} \right.$$  

**Proof.** Let $P_n$ be a path with vertex set $\{v_1, v_2, \ldots, v_n\}$, $n \geq 2$ and assume that $n$ is odd.
Then, for \( n = 3, \)
\[
\frac{H_e(P_3)}{2} = \frac{1}{2(1) + 1} = \frac{2}{3}.
\]
Assume that it is true for \( n = k, \) \( k \) is odd, i.e.
\[
\frac{H_e(P_k)}{2} = 2^{\frac{k-1}{2}} \frac{1}{2(1) + 1},
\]
where \( r \) is the radius of \( G. \)
For \( n = k + 2, \) the radius is \( r = \frac{k + 2 - 1}{2} = \frac{k + 1}{2}, \) so
\[
\frac{H_e(P_{k+2})}{2} = 2^{\frac{k-2}{2}} \frac{1}{2(1) + 1} \frac{1}{(k + 2) - 2 + (k + 2) - 1} + \frac{1}{(k + 2) - 2 + (k + 2) - 1}
\]
\[= 2^{\frac{k-2}{2}} \frac{1}{2(1) + 1} \frac{1}{(k + 2) - 2 + (k + 2) - 1}
\]
\[= 2^{\frac{k-2}{2}} \frac{1}{2(1) + 1}.
\]
Thus, we show the part when \( n \) is odd. For the part, when \( n \) is even, the proof is similar with a little difference for the \( \frac{n}{2}, \frac{n}{2} + 1 \) vertices; which are the central vertices of the path with eccentricities \( \frac{n}{2}, \frac{n}{2}. \)
By putting this term, which equals to \( \frac{1}{\frac{n}{2} + 1} = \frac{1}{n} \) outside the summation, then the result follows.

### 3. Bounds for eccentric harmonic index of a graph

In this section, we derive upper and lower bounds for \( H_e(G) \) of a graph \( G. \) Relations between \( H_e(G) \) and the eccentric connectivity index \( \xi_e(G) \) are established.

**Theorem 3.1.** Let \( G \) be a graph of order \( n \) and size \( m. \) Then
\[
\frac{m}{\text{diam}(G)} \leq H_e(G) \leq \frac{m}{r},
\]
with equality holds if and only if \( G \) is a self-centered graph.

**Proof.** Let \( G \) be a graph of order \( n \) and size \( m. \) Then, for \( v, v_j \in E \)
\[
2r \leq e_i + e_j \leq 2\text{diam}(G).
\]
So,
\[
\frac{1}{2\text{diam}(G)} \leq \frac{1}{e_i + e_j} \leq \frac{1}{2r}.
\]
By taking the summation over the edges of the graph, we get
\[
\frac{m}{2\text{diam}(G)} \leq H_e(G) \leq \frac{m}{2r}.
\]
Hence the result follows.

To show the equality, it is clear that the equality holds if and only if \( e_i + e_j = 2r = 2\text{diam}(G), \) which holds if and only if \( G \) is a self-centered graph.

**Theorem 3.2.** Let \( G \) be a graph with \( n \) vertices and \( m \) edges. Then
\[
H_e(G) \geq m(1 - \ln (\text{diam}(G))),
\]
with equality holds if and only if \( G \) is a complete graph.

**Proof.** Let \( G \) be a graph of order \( n \) and size \( m. \) Assume the function \( f(x) = x - \ln x - 1. \) Easy calculations gives \( f(x) \geq 0. \)

Hence, for \( v, v_j \in E \)
\[
\frac{2}{e_i + e_j} - \ln \left( \frac{2}{e_i + e_j} \right) - 1 \geq 0.
\]
So,
\[
\frac{2}{e_i + e_j} \geq 1 + \ln \left( \frac{2}{e_i + e_j} \right).
\]
By taking the summation over the edges of the graph, we get
\[
H_e(G) \geq m + \sum_{v, v_j \in E} \ln \left( \frac{2}{e_i + e_j} \right)
\]
\[= m + \ln \left( \prod_{v, v_j \in E} \frac{2}{e_i + e_j} \right)
\]
\[\geq m + \ln \left( \frac{1}{(\text{diam}(G))^m} \right)
\]
\[= m - m \ln (\text{diam}(G)).
\]
Hence,
\[
H_e(G) \geq m(1 - \ln (\text{diam}(G))).
\]

To show the equality, let \( f(x) = 0, \) then \( x = 1. \) So \( \frac{2}{e_i + e_j} = 1, v, v_j \in E. \) Hence \( e_i + e_j = 2, \) which holds if and only if \( e_i = e_j = 1 \) for all \( i, j = 1, \ldots, n. \) Thus \( G \) is complete.

**Theorem 3.3.** Let \( G \) be a graph with \( n \) vertices \( n \geq 2 \) and \( m \) edges. Then
\[
H_e(G) \geq 2m - \frac{\xi_e(G)}{2}
\]
with equality holds if and only if \( G \) is a complete graph.

**Proof.** Let \( G \) be a graph of order \( n, n \geq 2 \) and size \( m. \) Assume the function \( f(x) = x + \frac{1}{x} - 2. \) Easy calculations gives \( f(x) \geq 0. \)

Thus, for \( v, v_j \in E \)
\[
\frac{2}{e_i + e_j} + \frac{1}{2} - 2 \geq 0.
\]
By taking the summation over the edges of the graph \( G, \) we get
By Cauchy-Schwarz inequality we obtain,

\[ H_e(G) + \frac{\xi_c(G)}{2} - \sum_{v \neq w \in E} 2 \geq 0. \]

Hence,

\[ H_e(G) \geq 2m - \frac{\xi_c(G)}{2}. \]

To show the equality, let \( f(X) = 0 \), then \( x = 1 \). The rest of the proof is similar to that in Theorem 3.2.

**Theorem 3.4.** Let \( G \) be a graph with \( n \geq 2 \) vertices and \( m \) edges. Then

\[ H_e(G) \leq H_e(K_n). \]

**Proof.** Let \( G \) be a graph of order \( n \), \( n \geq 2 \) and size \( m \). Then for \( v, w \in E \)

\[ \frac{2}{e_i + e_j} \leq 1. \]

By taking the summation over the edges, we get

\[ H_e(G) \leq m \]

with equality holds if and only if \( G = K_n \). Thus

\[ H_e(G) \leq m = H_e(K_n). \]

**Theorem 3.5.** Let \( G \) be a graph with \( n \geq 2 \) vertices and \( m \) edges. Then

\[ H_e(G) \leq \frac{2m^2}{\xi_c(G)} \tag{3.1} \]

The bound is sharp and the self-centered graph satisfies it.

**Proof.** Let \( G \) be a graph of order \( n \geq 2 \), and size \( m \). By Cauchy-Schwarz inequality we obtain,

\[
\left( \sum_{v, w \in E} \frac{2}{e_i + e_j} \sqrt{\frac{e_i + e_j}{2}} \right)^2 \leq \sum_{v, w \in E} \left( \frac{e_i + e_j}{2} \right)^2 \sum_{v, w \in E} \left( \frac{2}{e_i + e_j} \right)^2. \tag{3.2}
\]

Thus, 3.2 becomes

\[ m^2 \leq \sum_{v, w \in E} \frac{e_i + e_j}{2} \sum_{v, w \in E} \frac{2}{e_i + e_j} \}

\[ = \frac{1}{2} \xi_c(G)H_e(G). \]

Hence,

\[ H_e(G) \geq \frac{2m^2}{\xi_c(G)}. \]

To show that the inequality is sharp, let \( G \) be a self-centered graph with \( \text{diam}(G) = r \). Then

\[ H_e(G)\xi_c(G) = \sum_{v, w \in E} \frac{2}{e_i + e_j} \sum_{v, w \in E} e_i + e_j \]

\[ = \sum_{v, w \in E} \frac{2}{2r} \sum_{v, w \in E} 2r \]

\[ = \frac{1}{r} m2rm \]

\[ = 2m^2. \]

On the other hand, let

\[ H_e(G)\xi_c(G) = m^2. \tag{3.3} \]

Also we have

\[ \frac{r}{\text{diam}(G)} m^2 \leq H_e(G) \frac{\xi_c(G)}{2} \leq \frac{\text{diam}(G)m^2}{r} \tag{3.4} \]

and 3.4 is sharp if and only if \( r = \text{diam}(G) \). Thus, by using 3.3 the result follows.

In case of \( G \) is a tree of order \( n \) and size \( m \), we find that the maximum eccentric harmonic index holds for the star. The following theorem explains this.

**Theorem 3.6.** Let \( T \) be a tree with \( n \) vertices and \( m \) edges. Then

\[ H_e(T) \geq \frac{2}{3} m \]

with equality holds if and only if \( T = S_{1,n-1} \)

**Proof.** Let \( T \) be a tree of order \( n \) and size \( m \). Then we assume the following cases.

**Case 1.** There exist \( v_i \in V(T) \) such that \( d(v_i) = n - 1 \), then \( T = S_{1,n-1} \) and hence \( e_i = 1, e_j = 2 \) for all \( j = 1, 2, \ldots, i-1, i+1, \ldots, n \). Thus

\[ H_e(T) = H_e(S_{1,n-1}) = \sum_{v, w \in E} \frac{2}{e_i + e_j} = \frac{2}{3} m. \]

**Case 2.** There is no such \( v_i \) with \( d(v_i) = n - 1 \), then \( e_i \geq 2 \) for all \( i = 1, 2, \ldots, n \). So, \( e_i + e_j \geq 4 \) for all \( v, w \in E \).

Hence,

\[ H_e(T) \leq \frac{1}{2} m < \frac{2}{3} m. \]

\[ \square \]

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