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On the Harary Energy and Harary Estrada Index of a Graph

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Abstract

The main purposes of this paper are to introduce and investigate the Harary energy and Harary Estrada index of a graph. In addition we establish upper and lower bounds for these new energy and index separately.

1 Introduction and Preliminaries

Throughout this paper all graphs will be assumed simple that is without loops, multiple or directed edges. If G is such a graph with n-vertices and m-edges, then G will be called (n, m)-graph.

Let the graph G be connected and let its vertices be labeled by $v_1, v_2, \ldots, v_n$. The Harary matrix ([17]) of a graph G is defined as a square matrix $H = H(G) = \left[\frac{1}{d_{ij}}\right]$, where d_{ij} is the distance (i.e. the length of the shortest path [1]) between the vertices v_i and v_j in G. The eigenvalues of the Harary matrix $H(G)$ are denoted by $\rho_1, \rho_2, \ldots, \rho_n$ and are

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said to be the H-eigenvalues of G. We note that since the Harary matrix is symmetric, its eigenvalues are real and can be ordered as $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. We also note that the lower and upper bounds for the maximum eigenvalue of Harary matrix of a graph G are obtained in detail in [2, 24].

In [16], while the authors proved lower and upper bounds for the distance energy of graphs whose diameter does not exceed two, in the paper [23], Ramane et. al. generalized this result and obtained these lower and upper bounds for the distance energy of arbitrary connected (n,m)-graphs. In the second section of this paper, by considering the papers [13, 14, 16, 23], we will adapt the works on distance energy to introduce and study on Harary energy. We recall that, in [13], the distance energy is defined similar to the graph energy by

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix $A(G)$ of a graph G. In fact the reader can find so many works about $E(G)$ in the literature. Therefore, by considering this, we can define the Harary energy as

$$HE(G) = \sum_{i=1}^{n} |\rho_i| \tag{1}$$

where $\rho_1, \rho_2, \ldots, \rho_n$ are eigenvalues of the Harary matrix.

In Section 3, a new index will be defined, namely *Harary Estrada index* and then will be obtained lower and upper bounds for this new index.

Now let us present the following lemma as the first preliminary result.

Lemma 1.1 *Let G be a connected (n,m)-graph and let $\rho_1, \rho_2, \ldots, \rho_n$ be its H-eigenvalues. Then*

$$\sum_{i=1}^{n} \rho_i = 0$$

and

$$\sum_{i=1}^{n} \rho_i^2 = 2 \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2 . \tag{2}$$

Proof. We clearly have

$$\sum_{i=1}^{n} \rho_i = trace[H(G)] = \sum_{i=1}^{n} \frac{1}{d_{ij}} = 0 .$$

Moreover, for $i = 1, 2, \ldots, n$, the (i,i)-entry of $[H(G)]^2$ is equal to

$$\sum_{j=1}^{n} \frac{1}{d_{ij}} \frac{1}{d_{ji}} = \sum_{j=1}^{n} \left(\frac{1}{d_{ij}}\right)^2 .$$

Hence

$$\sum_{i=1}^{n} \rho_i^2 = trace[H(G)]^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{1}{d_{ij}}\right)^2 = 2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2$$

as required. ■

We also have the following lemma that will be needed for obtaining the bounds of Harary energy (in Section 2) and Harary Estrada index (in Section 3).

Lemma 1.2 *Let G be a (n,m)-graph with diameter less than or equal to 2 and let its eigenvalues be ρ_1, ρ_2, $\ldots$, ρ_n. Then*

$$\sum_{i=1}^{n} \rho_i^2 = \frac{3m}{2} + \frac{n}{4}(n-1) .$$

Proof. In the Harary matrix $H(G)$ of G, there are $2m$ elements equal to unit and $n(n-1) - 2m$ elements equal to $1/2$. Therefore

$$\begin{aligned} \sum_{i=1}^{n} \rho_i^2 = \sum_{i=1}^{n} (H(G)^2)_{ii} &= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{d_{ij}} \frac{1}{d_{ji}} \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \left(\frac{1}{d_{ij}}\right)^2 = (2m)1^2 + (n^2 - n - 2m) \left(\frac{1}{2}\right)^2 \end{aligned}$$

and the lemma follows. ■

2 Bounds for the Harary energy

Let us consider the Harary energy $HE(G)$ as defined in (1).

Theorem 2.1 *If G is a connected (n,m)-graph, then*

$$\sqrt{2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2} \le HE(G) \le \sqrt{2n \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2} . \tag{3}$$

Proof. In the Cauchy–Schwartz inequality

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^2\right) \left(\sum_{i=1}^{n} b_i^2\right)$$

if we choose $a_i = 1$ and $b_i = |\rho_i|$, then we get

$$\left(\sum_{i=1}^{n} |\rho_i|\right)^2 \leq n \sum_{i=1}^{n} \rho_i^2$$

from which

$$HE(G)^2 \leq 2n \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2 .$$

Therefore this gives the upper bound for $HE(G)$.

Now for the lower bound of $HE(G)$, we can easily obtain the inequality

$$HE(G)^2 = \left(\sum_{i=1}^{n} |\rho_i|\right)^2 \geq \sum_{i=1}^{n} |\rho_i|^2 = 2 \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2$$

which gives directly the required lower bound.

We should note that the *second proof for the upper bound* can be given as follows:

Consider the sum

$$S = \sum_{i=1}^{n} \sum_{j=1}^{n} (|\rho_i| - |\rho_j|)^2 .$$

By a direct calculation, we obtain

$$S = 2n \sum_{i=1}^{n} |\rho_i|^2 - 2 \left(\sum_{i=1}^{n} |\rho_i| \sum_{j=1}^{n} |\rho_j|\right) .$$

It follows from (2) and the definition of $HE(G)$ that

$$S = 4n \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2 - 2HE(G)^2 .$$

Since $S \geq 0$, we have $HE(G) \leq \sqrt{2n \sum_{1 \leq i < j \leq n} (1/d_{ij})^2}$. Hence the result. ■

Corollary 2.2 *If G is a connected (n,m)-graph, then $HE(G) \leq n\sqrt{n-1}$.*

Proof. Since $d_{ij} \geq 1$ for $i \neq j$ and there are $n(n-1)/2$ pairs of vertices in G, by the upper bound of Theorem 2.1, we get

$$HE(G) \leq \sqrt{2n \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2} \leq \sqrt{2n \frac{n(n-1)}{2}} = n\sqrt{n-1} .$$

■

In [15, Theorem 1, Theorem 2], as a generalization, Gutman et. al. showed lower and upper bounds for an energy-like quantity, E_X say, and defined this by

$$E_X = \sum_{i=1}^{n} |x_i - \overline{x}|$$

where $x_1, x_2, \ldots, x_n$ are real numbers, and $\overline{x}$ is their arithmetic mean. Clearly, *graph energy, Laplacian energy* and *distance energy* are the special cases of E_X. In the following result, as another special case of E_X, we state and prove a lower and an upper bound for the Harary energy $HE(G)$.

Theorem 2.3 *Let G be a connected (n,m)-graph and let Δ be the absolute value of the determinant of the Harary matrix $H(G)$. Then*

$$\sqrt{2\sum_{1\le i<j\le n}\left(\frac{1}{d_{ij}}\right)^2 + n(n-1)\Delta^{2/n}} \le HE(G) \le \sqrt{2n\sum_{1\le i<j\le n}\left(\frac{1}{d_{ij}}\right)^2}\ .$$

Proof. In the light of Theorem 2.1, if we show the validity of the lower bound, then this will finish the proof. We note that a lower bound for the graph energy is analogously deduced in [20].

By the definition of Harary energy given in (1) and Equation (2), we have

$$\begin{aligned}
HE(G)^2 &= \left(\sum_{i=1}^{n}|\rho_i|\right)^2 = \sum_{i=1}^{n}|\rho_i|^2 + 2\sum_{1\le i<j\le n}|\rho_i||\rho_j| \\
&= 2\sum_{1\le i<j\le n}\left(\frac{1}{d_{ij}}\right)^2 + 2\sum_{1\le i<j\le n}|\rho_i||\rho_j| \\
&= 2\sum_{1\le i<j\le n}\left(\frac{1}{d_{ij}}\right)^2 + \sum_{i\ne j}|\rho_i||\rho_j|\ . \qquad (4)
\end{aligned}$$

Since, for nonnegative numbers, the arithmetic mean is not smaller than the geometric mean, we then have

$$\begin{aligned}
\frac{1}{n(n-1)}\sum_{i\ne j}|\rho_i||\rho_j| &\ge \left(\prod_{i\ne j}|\rho_i||\rho_j|\right)^{1/n(n-1)} = \left(\prod_{i=1}^{n}|\rho_i|^{2(n-1)}\right)^{1/n(n-1)} \\
&= \prod_{i=1}^{n}|\rho_i|^{2/n} = \Delta^{2/n}\ . \qquad (5)
\end{aligned}$$

After that, by combining Equations (4) and (5), we obtain the required lower bound, as required. ■

By using Equation (2), Lemma 1.2 and Theorem 2.3, we obtain the following corollary of Theorem 2.3.

Corollary 2.4 *Let G be a (n,m)-graph with diameter less than or equal to 2 and let Δ be the absolute value of the determinant of its Harary matrix. Then*

$$\sqrt{\frac{3m}{2}+\frac{n}{4}(n-1)+n(n-1)\Delta^{2/n}} \leq HE(G) \leq \sqrt{n\left(\frac{3m}{2}+\frac{n}{4}(n-1)\right)}\,.$$

Theorem 2.5 *If G is a connected (n,m)-graph, then*

$$\begin{aligned} HE(G) &\leq \frac{2}{n}\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2 \\ &+ \sqrt{(n-1)\left[2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2-\left(\frac{2}{n}\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2\right)^2\right]}\,. \qquad (6)\end{aligned}$$

Proof. As it seen in the literature (see, for instance, [18, 19]), the standard procedure can be applied to obtain such upper bounds. So the proof can be done as in the following.

By applying the Cauchy–Schwartz inequality to the two $(n-1)$ vectors $(1,1,\ldots,1)$ and $(|\rho_1|,|\rho_2|,\ldots,|\rho_n|)$, we have

$$\begin{aligned} \left(\sum_{i=2}^{n}|\rho_i|\right)^2 &\leq (n-1)\left(\sum_{i=2}^{n}\rho_i^2\right) \\ (HE(G)-\rho_1)^2 &\leq (n-1)\left(2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2-\rho_1^2\right) \\ HE(G) &\leq \rho_1+\sqrt{(n-1)\left(2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2-\rho_1^2\right)}\,. \end{aligned}$$

Now let us define a function

$$f(x)=x+\sqrt{(n-1)\left(2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2-x^2\right)}\,.$$

In fact, by keeping in mind $\rho_1\geq 1$, we set $\rho_1=x$. Using

$$\sum_{i=2}^{n}\rho_i^2=2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2$$

we get that

$$x^2 = \rho_1^2 \le 2 \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2 .$$

In other words,

$$x \le \sqrt{2 \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2} .$$

Meanwhile $f'(x) = 0$ implies that

$$x = \sqrt{\frac{2}{n} \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2} .$$

Therefore f is a decreasing function in the interval

$$\sqrt{\frac{2}{n} \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2} \le x \le 2\sqrt{\sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2}$$

and

$$\sqrt{\frac{2}{n} \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2} \le \frac{2}{n} \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2 \le \rho_1 .$$

Hence

$$f(\rho_1) \le f\left(\frac{2}{n} \sum_{1\le i<j\le n} \left(\frac{1}{d_{ij}}\right)^2\right)$$

and so the inequality in (6) holds. ■

By Equation (2), Lemma 1.2 and Theorem 2.5, one can obtain the following consequence result on Harary energy $HE(G)$.

Corollary 2.6 *Let G be a connected (n,m)-graph with diameter less than or equal to* 2. *Then*

$$HE(G) \le \frac{1}{n}\left[\frac{3m}{2} + \frac{n}{4}(n-1)\right] + \sqrt{(n-1)\left\{\frac{3m}{2} + \frac{n}{4}(n-1) - \left[\frac{1}{n}\left(\frac{3m}{2} + \frac{n}{4}(n-1)\right)\right]^2\right\}}.$$

3 Harary Estrada index of graphs

As a new direction for the studying on indexes and their bounds, we will introduce and investigate Harary Estrada index and its bounds. Moreover we will obtain upper bounds for the Harary Estrada index involving the Harary energy of graphs. Hence this section will be devoted in two subsections.

We first recall that the Estrada index of a graph G is defined by

$$EE = EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of the adjacency matrix $A(G)$ of G (see [7, 8, 9, 10, 11, 12]). Denoting by $M_k = M_k(G)$ to the k-th moment of the graph G, we get

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k$$

and recalling the power-series expansion of e^x, we have

$$EE = \sum_{k=0}^{\infty} \frac{M_k}{k!} \ . \tag{7}$$

It is well known that ([10]) $M_k(G)$ is equal to the number of closed walks of length k of the graph G. In fact Estrada index of graphs has an important role in Chemistry and Physics and there exists a vast literature that studies this special index. In addition to the Estrada's papers depicted above, we may also refer [5, 6] to the reader for detail information such as lower and upper bounds for EE in terms of the number of vertices and edges, and some inequalities between EE and the energy of G.

Our second reminder will be about *Harary index* $H_e(G)$ for a graph G. In fact the Harary index of a graph G on n vertices was first defined by Plavšic et al. ([22]) as

$$H_e(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (H(G))_{ij} = \sum_{1 \leq i < j \leq n} (H(G))_{ij} \tag{8}$$

where

$$(H(G))_{ij} = \begin{cases} \dfrac{1}{d_{ij}} & \text{if} \quad i \neq j \\ 0 & \text{if} \quad i = j \end{cases}$$

(see also [3, 4, 25]). We should note that some authors include the leading factor of 1/2 (e.g., [21, 22]) others omit it (e.g., [4, pp. 111, 112]). We also note that Harary index also plays an important role in the molecular) chemistry and, in [3, 25], it has been recently given a well organized introduction and references about Harary index, and, additionally, depicted some connections and bounds on the Harary index.

3.1 Bounds for the Harary Estrada index

In this subsection we will mainly introduce the Harary Estrada index of a graph G, and also present upper and lower bounds for it.

Definition 3.1 *If G is an (n,m)-graph, then the Harary Estrada index of G, denoted by $HEE(G)$, is equal to*

$$HEE = HEE(G) = \sum_{i=1}^{n} e^{\rho_i} \tag{9}$$

where $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ are the H-eigenvalues of G.

Let

$$N_k = \sum_{i=1}^{n} (\rho_i)^k \ .$$

Then

$$HEE(G) = \sum_{k=0}^{\infty} \frac{N_k}{k!} \ . \tag{10}$$

The main result of this section is the following.

Theorem 3.2 *Let G be a connected (n,m)-graph with diameter less than or equal to 2. Then the Harary Estrada index is bounded as*

$$\sqrt{n^2 + 2\left(\frac{3m}{2} + \frac{n(n-1)}{4}\right)} \leq HEE(G) \leq n - 1 + e^{\sqrt{\frac{3m}{2}+\frac{n(n-1)}{4}}} \ . \tag{11}$$

Equality holds in both sides if and only if $G \simeq K_1$.

Proof. *Lower bound:* Directly from Equation (9), we get

$$HEE^2(G) = \sum_{i=1}^{n} e^{2\rho_i} + 2 \sum_{1\leq i<j\leq n} e^{\rho_i} e^{\rho_j} \ . \tag{12}$$

By the Arithmetic-Geometric Mean Inequality, shortly $AGMI$ say, we also get

$$\begin{aligned} 2 \sum_{1\leq i<j\leq n} e^{\rho_i} e^{\rho_j} &\geq n(n-1) \left(\prod_{1\leq i<j\leq n} e^{\rho_i} e^{\rho_j} \right)^{\frac{2}{n(n-1)}} \\ &= n(n-1) \left[\left(\prod_{i=1}^{n} e^{\rho_i} \right)^{n-1} \right]^{\frac{2}{n(n-1)}} \\ &= n(n-1)(e^{N_1})^{\frac{2}{n}} \\ &= n(n-1) \ . \end{aligned} \tag{13}$$

By means of a power-series expansion and $N_0 = n$; $N_1 = 0$ and $N_2 = 2 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2$, we clearly obtain

$$\sum_{i=1}^{n} e^{2\rho_i} = \sum_{i=1}^{n} \sum_{k \ge 0} \frac{(2\rho_i)^k}{k!} = n + 4 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2 + \sum_{i=1}^{n} \sum_{k \ge 3} \frac{(2\rho_i)^k}{k!} \; .$$

Since we require a lower bound as good as possible, it looks reasonable to replace $\sum_{k \ge 3} \frac{(2\rho_i)^k}{k!}$ by $4 \sum_{k \ge 3} \frac{(\rho_i)^k}{k!}$. Furthermore we use a multiplier $t \in [0, 4]$ instead of $4 = 2^2$, so as to arrive at

$$\begin{aligned}
\sum_{i=1}^{n} e^{2\rho_i} &\ge n + 4 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2 + t \sum_{i=1}^{n} \sum_{k \ge 3} \frac{(\rho_i)^k}{k!} \\
&= n + 4 \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2 - tn - t \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2 + t \sum_{i=1}^{n} \sum_{k \ge 0} \frac{(\rho_i)^k}{k!} \\
&= n(1 - t) + (4 - t) \sum_{1 \le i < j \le n} \left(\frac{1}{d_{ij}}\right)^2 + t \cdot HEE(G) \; .
\end{aligned}$$

By Lemma 1.2, we have

$$\sum_{i=1}^{n} e^{2\rho_i} \ge n(1 - t) + (4 - t) \frac{1}{2} \left(\frac{3m}{2} + \frac{n(n-1)}{4}\right) + t \cdot HEE(G) \; . \tag{14}$$

Also, by substituting (13) and (14) back into (12), and then solving for $HEE(G)$, we get

$$HEE(G) \ge \frac{t}{2} + \sqrt{\left(n - \frac{t}{2}\right)^2 + (4 - t) \frac{1}{2} \left(\frac{3m}{2} + \frac{n(n-1)}{4}\right)} \; .$$

Now, for $n \ge 2$ and $m \ge 1$, it is easy to see that the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4 - x) \frac{1}{2} \left(\frac{3m}{2} + \frac{n(n-1)}{4}\right)}$$

monotonically increases in the interval $[0, 4]$. As a result, the best lower bound for $HEE(G)$ is attained for $t = 0$. This gives us the first part of the theorem.

Upper bound. Starting from the following inequality, we get

$$\begin{aligned}
HEE(G) &= n + \sum_{i=1}^{n} \sum_{k \ge 1} \frac{(\rho_i)^k}{k!} \\
&= n + \sum_{i=1}^{n} \sum_{k \ge 1} \frac{|\rho_i|^k}{k!} \\
&= n + \sum_{k \ge 1} \frac{1}{k!} \sum_{i=1}^{n} (\rho_i^2)^{\frac{k}{2}}
\end{aligned}$$

and then

$$\begin{aligned}
n+\sum_{k\geq 1}\frac{1}{k!}\sum_{i=1}^{n}(\rho_i^2)^{\frac{k}{2}} &\leq n+\sum_{k\geq 1}\frac{1}{k!}\left[\sum_{i=1}^{n}(\rho_i^2)\right]^{\frac{k}{2}}\\
&= n+\sum_{k\geq 1}\frac{1}{k!}\left[2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2\right]^{\frac{k}{2}}\\
&= n-1+\sum_{k\geq 0}\frac{\left(\sqrt{2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2}\right)^k}{k!}\\
&= n-1+e^{\sqrt{2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2}}.
\end{aligned}$$

By Lemma 1.2, we obtain

$$HEE(G)\leq n-1+e^{\sqrt{\frac{3m}{2}+\frac{n(n-1)}{4}}}.$$

Hence we get the right-hand side of the inequality given in (11).

In addition to the above progress, it is clear that Equality (11) holds if and only if the graph G has all zero H-eigenvalues. Since G is a connected graph, this only happens when $G\simeq K_1$.

Hence the result. ■

In the following, we present another lower bound for the Harary Estrada index $HEE(G)$.

In [24], Zhou et al. gave the following lower bound for $\rho_1(G)$ in terms of the sum of i-th row of Harary matrix $H(G)$ and for n.

Lemma 3.3 **[24]** *Let G be a connected graph with $n\geq 2$ vertices. Then*

$$\sqrt{\frac{\sum_{i=1}^{n}H_i^2}{n}}\leq \rho_1(G)$$

where H_i is the sum of the i-th row of $H(G)$.

Equality holds if and only if $H_1=H_2=\cdots=H_n$.

Now we obtain the lower bound on the Harary Estrada index of graph G as follows.

Theorem 3.4 *Let G be a connected (n,m)-graph with $n \geq 2$. Then we have*

$$HEE(G) \geq e^{\sqrt{\frac{\sum_{i=1}^{n} H_i^2}{n}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{\sum_{i=1}^{n} H_i^2}{n}}}} \,. \tag{15}$$

Proof. If G is equal to null graph N_n, then for each $1 \leq i \leq n$, $H_i = 0$ and $\rho_1 = \rho_2 = \cdots = \rho_n = 0$. Then $HEE(G) = n$, and equality holds in Equation (15). When $HEE(G) = n$, by *AGMI*, one can see easily that $\rho_1 = \rho_2 = \cdots = \rho_n = 0$ and hence $G = N_n$. Otherwise, $G \neq N_n$ and hence $\rho_1 > 0$. Now,

$$\begin{aligned} HEE(G) &= e^{\rho_1} + e^{\rho_2} + \cdots + e^{\rho_n} \\ &\geq e^{\rho_1} + (n-1)\left(\prod_{i=2}^{n} e^{\rho_1}\right)^{\frac{1}{n-1}}, \quad \text{by } AGMI \qquad (16) \\ &\geq e^{\rho_1} + (n-1)\left(e^{-\rho_1}\right)^{\frac{1}{n-1}}, \quad \text{as } \sum_{i=1}^{n} \rho_i = 0 \,. \qquad (17) \end{aligned}$$

Now let us consider a function

$$f(x) = e^x + \frac{n-1}{e^{\frac{x}{n-1}}}, \qquad \text{for } x > 0 \,.$$

We have

$$f'(x) = e^x - e^{-\frac{x}{n-1}}, \qquad \text{for } x > 0 \,.$$

Therefore f is an increasing function for $x > 0$. From (16), we get

$$HEE(G) \geq e^{\sqrt{\frac{\sum_{i=1}^{n} H_i^2}{n}}} + \frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{\sum_{i=1}^{n} H_i^2}{n}}}} \quad \text{by Lemma 3.3.} \tag{18}$$

This completes of the proof of (15).

Now suppose that equality holds in (15). Then equality holds throughout (16) - (18). From equality in (16) and by *AGMI*, we obtain $\rho_2 = \rho_3 = \cdots = \rho_n = 0$. Since $\rho_1 > 0$ and $\sum_{i=1}^{n} \rho_i = 0$, we must have $\rho_2 < 0$. Thus G is a connected graph. From equality in (18), we have $\rho_1 = H_1 = H_2 = \cdots = H_n$. Since $\rho_2 = \rho_3 = \cdots = \rho_n = 0$ and $\rho_1 = H_i$, by Lemma 3.3, G is a complete graph K_n.

Conversely, one can easily see that the equality holds in (15) for the complete graph K_n.

Hence the result. ■

We can present the following two consequences of the above result.

Corollary 3.5 *Let G be a connected (n,m)-graph with diameter less than or equal to* 2. *Then*

$$e^{\sqrt{\frac{1}{n}\left(\frac{3m}{2}+\frac{n}{4}(n-1)\right)}}+\frac{n-1}{e^{\frac{1}{n-1}\sqrt{\frac{1}{n}\left(\frac{3m}{2}+\frac{n}{4}(n-1)\right)}}}\leq HEE(G)\ .$$

Proof. Since

$$\sum_{i=1}^{n}H_i^2\geq 2\sum_{1\leq i<j\leq n}\left(\frac{1}{d_{ij}}\right)^2$$

the result is obvious from Lemma 1.2. ■

The following corollary states a lower bound for the Harary Estrada index involving Harary index.

Corollary 3.6 *Let G be a connected graph with $n\geq 2$ vertices. Then*

$$e^{\frac{2H_e(G)}{n}}+\frac{n-1}{e^{\frac{2H_e(G)}{n(n-1)}}}\leq HEE(G)$$

where $H_e(G)$ denotes the Harary index of graph G, as defined in (8). *Moreover, in the above, equality holds if and only if $H_1=H_2=\cdots=H_n$.*

Proof. By Theorem 3.4 and using Cauchy–Schwartz inequality, we have

$$\sqrt{\frac{\sum_{i=1}^{n}H_i^2}{n}}\geq\frac{\sum_{i=1}^{n}H_i}{n}=\frac{2H_e(G)}{n}$$

with the equality holds if and only if $H_1=H_2=\cdots=H_n$. ■

3.2 An upper bound for the Harary Estrada index involving the Harary energy

In the following result, the main aim is to show that there exist two upper bounds for the Harary Estrada index $HEE(G)$ where G is a connected graph of diameter not greater than 2.

Theorem 3.7 *Let G be as above. Then*

$$HEE(G)-HE(G)\leq n-1-\sqrt{\frac{3m}{2}+\frac{n(n-1)}{4}}+e^{\sqrt{\frac{3m}{2}+\frac{n(n-1)}{4}}}\tag{19}$$

and

$$HEE(G) \leq n - 1 + e^{HE(G)} \ . \tag{20}$$

Equality holds in (19) *or* (20) *if and only if* $G \simeq K_1$.

Proof. By considering the proof of Theorem 3.2, we have

$$HEE(G) = n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{(\rho_i)^k}{k!} \leq n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{|\rho_i|^k}{k!}.$$

Moreover, by considering Harary energy defined in (1), we get

$$HEE(G) \leq n + HE(G) + \sum_{i=1}^{n} \sum_{k \geq 2} \frac{|\rho_i|^k}{k!}$$

which leads to (as in Theorem 3.2)

$$\begin{aligned} HEE(G) - HE(G) &\leq n + \sum_{i=1}^{n} \sum_{k \geq 2} \frac{|\rho_i|^k}{k!} \\ &\leq n - 1 - \sqrt{2 \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2} + e^{\sqrt{2 \sum_{1 \leq i < j \leq n} \left(\frac{1}{d_{ij}}\right)^2}} \ . \end{aligned} \tag{21}$$

Hence we obtain Equation (19).

Another approximation to connect $HEE(G)$ and $HE(G)$ can be seen as follows:

$$\begin{aligned} HEE(G) &\leq n + \sum_{i=1}^{n} \sum_{k \geq 1} \frac{|\rho_i|^k}{k!} \\ &\leq n + \sum_{k \geq 1} \frac{1}{k!} \left(\sum_{i=1}^{n} |\rho_i|^k \right) \\ &= n + \sum_{k \geq 1} \frac{(HE(G))^k}{k!} \\ &= n - 1 + \sum_{k \geq 0} \frac{(HE(G))^k}{k!} \end{aligned}$$

which implies

$$HEE(G) \leq n - 1 + e^{HE(G)}$$

as depicted in (20).

Moreover the equality holds in (19) or (20) if and only if $G \simeq K_1$. ■

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