

NEW BOUNDS FOR THE HARARY ENERGY AND HARARY ESTRADA INDEX OF GRAPHS

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The harary index is defined as the sum of reciprocal distances between all pairs of vertices in a nontrivial connected graph. In this paper, we establish upper and lower bounds for the harary energy and harary Estrada index in terms of graph invariants such as the number of vertices, the number degree sequence and spectral radius.

1. INTRODUCTION

Let G be a simple, undirected, connected graph with n vertices and m edges. Let the vertices of G be labeled as v_1, v_2, \dots, v_n . The *adjacency matrix* of a graph G is the square matrix $A = A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if v_i is adjacent to v_j and $a_{ij} = 0$, otherwise. The *eigenvalues* of $A(G)$ are the adjacency eigenvalues of G , they are labeled as $\lambda_1, \lambda_2, \dots, \lambda_n$. These form the adjacency spectrum of G [3]. Thus

$$\det A = \prod_{i=1}^n \lambda_i.$$

The *rank* matrix of A is the maximal number of linearly independent column vectors in A . The *distance* between the vertices v_i and v_j , denoted by d_{ij} , is the length of the shortest path joining v_i and v_j . The harary matrix [13] of a graph G is a square matrix $H = [H_{ij}]$ of order n , where

$$h_{ij} = \begin{cases} \frac{1}{d_{ij}} & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases}$$

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The eigenvalues of $\mathbf{H}(G)$ labeled as $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ are said to be the harary eigenvalues or *H-eigenvalues* of G and their collection is called harary spectrum or *H-spectrum* of G . harary matrix (also called as reciprocal distance matrix [22]) of a graph was introduced by Ivanciuc et al. In [13] which has in use the study of molecules in *QSPR* (quantitative structure property relationship) models [13]. Two non-isomorphic graphs are said to be *H-cospectral* if they have same *H-spectra*. The results on *H-eigenvalues* of a graph are obtained in [2, 4, 7, 12, 26]. The details about ordinary graph *energy* can be found in [23]. Bounds for the harary energy of a graph are reported in [1, 2, 8].

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present bounds on the harary energy. In Section 4, we present bounds on the harary Estrada index.

2. PRELIMINARIES AND KNOWN RESULTS

In this section, we shall list some previously known results that will be needed in the next sections. Recall that [8] for a graph with harary eigenvalues $\rho_1, \rho_2, \dots, \rho_n$, $N_k = \text{tr}(\mathbf{H}^k) = \sum_{i=1}^n (\rho_i)^k$.

$$\begin{aligned} (1) \quad & N_0 = n, \\ (2) \quad & N_1 = \text{tr}(\mathbf{H}) = 0, \\ (3) \quad & N_2 = \text{tr}(\mathbf{H}^2) = 2\kappa. \end{aligned}$$

Where

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

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

Lemma 1. *Let G be a graph with n vertices and harary matrix \mathbf{H} . Then*

$$\begin{aligned} (4) \quad N_3 = \text{tr}(\mathbf{H}^3) &= 2 \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right). \\ (5) \quad N_4 = \text{tr}(\mathbf{H}^4) &= \sum_{i=1}^n \left(\sum_{j=1}^n \frac{1}{(d_{ij})^2} \right)^2 + \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right)^2. \end{aligned}$$

Proof. By definition, the diagonal elements and for $i = 1, 2, \dots, n$, the (i, i) -entry of $[\mathbf{H}(G)]^2$ is equal to

$$(\mathbf{H}^2)_{ij} = \sum_{j=1}^n \mathbf{H}_{ij} \mathbf{H}_{ji} = \sum_{j=1}^n (\mathbf{H}_{ij})^2 = \sum_{j=1}^n (\mathbf{H}_{ij})^2 = \sum_{j=1}^n \frac{1}{(d_{ij})^2}.$$

Hence

$$(\mathbf{H}^2)_{ij} = \sum_{j=1}^n \mathbf{H}_{ij} \mathbf{H}_{ji} = \mathbf{H}_{ii} \mathbf{H}_{ij} + \mathbf{H}_{ij} \mathbf{H}_{jj} + \sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \mathbf{H}_{ik} \mathbf{H}_{kj} = \frac{1}{(d_{ij})} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right).$$

Since the diagonal elements of \mathbf{H}^3 are

$$(\mathbf{H}^3)_{ii} = \sum_{j=1}^n \mathbf{H}_{ij} (\mathbf{H}^2)_{jk} = \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})} (\mathbf{H}^2)_{ij} = \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right)$$

we obtain

$$\text{tr}(\mathbf{H}^3) = \sum_{i=1}^n \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right) = 2 \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right).$$

We now calculate $\text{tr}(\mathbf{H}^4)$. Because $\text{tr}(\mathbf{H}^4) = \|\mathbf{H}^2\|_F^2$, where $\|\mathbf{H}^2\|_F^2$ denotes the *Frobenius norm* of \mathbf{H}^2 , we obtain

$$\begin{aligned} \text{tr}(\mathbf{H}^4) &= \sum_{i,j=1}^n |(\mathbf{H}^2)_{ii}|^2 = \sum_{j=1}^n |(\mathbf{H}^2)_{ii}|^2 + \sum_{1 \leq i < j \leq n} |(\mathbf{H}^2)_{ij}|^2 \\ &= \sum_{i=1}^n \left(\sum_{j=1}^n \frac{1}{(d_{ij})^2} \right)^2 + \sum_{1 \leq i < j \leq n} \frac{1}{(d_{ij})^2} \left(\sum_{\substack{1 \leq i < k \leq n \\ 1 \leq k < j \leq n}} \frac{1}{(d_{ik})(d_{kj})} \right)^2. \end{aligned}$$

□

For any square matrix A we denote by $\rho_1(A)$ its spectral radius $\rho_1(A) = \max\{|\lambda| : \lambda \text{ is an eigenvalue for } A\}$. We obtain lower bounds for ρ_1 .

Lemma 2. [24] Let A be a real matrix with $r = \text{rank}(A) \geq 2$. If $\text{tr}(A^2) \geq \frac{(\text{tr}(A))^2}{r}$, then

$$\rho(A) \geq \frac{|\text{tr}(A)|}{r} + \sqrt{\frac{[\text{tr}(A^2) - (\frac{1}{r})(\text{tr}(A))^2]}{(r(r-1))}}.$$

Lemma 3. [25] If x_1, x_2, \dots, x_n are real numbers such that

$$x_n \leq x_{n-1} \leq \dots \leq x_2 \leq x_1,$$

then

$$\frac{\sum_{i=1}^n x_i}{n} + \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^n \left(x_i - \frac{\sum_{i=1}^n x_i}{n} \right)^2} \leq x_1.$$

Lemma 4. [25] *Let y_1, y_2, \dots, y_n are real numbers and k is any positive integer, then*

$$\left(\frac{\sum_{i=1}^n y_i^{2k}}{n} + \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^n \left(y_i - \frac{\sum_{i=1}^n y_i^{2k}}{n} \right)^2} \right)^{\frac{1}{2k}} \leq \max_i |y_i|.$$

By equations (2), (3) and Lemma 2, we can obtain follow lemma.

Lemma 5. *Let G be a graph with n vertices, $r = \text{rank}(\mathbf{H}) \geq 2$ and $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ be its eigenvalues of the harary matrix \mathbf{H} .*

If $\text{tr}(\mathbf{H}^2) \geq \frac{(\text{tr}(\mathbf{H}))^2}{r}$, then

$$\rho_1 \geq \sqrt{\frac{2\kappa}{r(r-1)}}.$$

Now equations (2), (3) and Lemma 3, we can obtain follow lemma.

Lemma 6. *Let G be a graph with n vertices and $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ be its eigenvalues of the harary matrix \mathbf{H} . Then*

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n(n-1)}}.$$

By equations (2), (3), (5) and Lemma 4 (for $k=1$), we can obtain follow lemma.

Lemma 7. *Let G be a graph with n vertices and $\rho_1 \geq \rho_2 \geq \dots \geq \rho_n$ be its eigenvalues of the harary matrix \mathbf{H} . Then*

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n}} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)}.$$

Lemma 8. *Let G be a graph of order n . Then*

$$\text{HE}(G) \leq \sqrt{2n\kappa}.$$

Proof. By Cauchy-Schwarz inequality, for real numbers a_i and b_i , we have

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

assuming, $a_i = 1$, $b_i = |\rho_i|$ and equation (3), we have

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

Therefore

$$HE(G) \leq \sqrt{2n\kappa}.$$

□

3. BOUNDS FOR THE HARARY ENERGY OF GRAPHS

In this section, we obtain bounds for the harary energy in terms of number of vertices, determinant of the adjacency matrix and *distance* between the vertices of graph G .

The *energy* of the graph G is defined as:

$$(6) \quad E = E(G) = \sum_{i=1}^n |\lambda_i|.$$

Where $\lambda_i, i = 1, 2, \dots, n$, are the *eigenvalues* of graph G .

This concept was introduced by *I. Gutman* and is intensively studied in *chemistry*, since it can be used to approximate the total π -*electron* energy of a *molecule* (see, e.g. [10, 11]). Since then, numerous other bounds for energy were found (see, e.g. [9, 17, 18, 19]).

The harary energy of a (molecular) graph G was introduced by Güngör et al. [8] as follows:

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

where $\rho_1, \rho_2, \dots, \rho_n$ are eigenvalues of the harary matrix. We start by proving some lower bounds for this energy of graphs.

Theorem 1. *Let G be a graph of order n with m edges such that $2m \geq n$. Then*

$$HE(G) \geq \sqrt{\frac{2\kappa}{n(n-1)}} + (n-1) \left(\frac{|\det H|}{\sqrt{\frac{2\kappa}{n(n-1)}}} \right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic-geometric* mean inequality, we have

$$\begin{aligned} HE(G) &= \rho_1 + \sum_{i=2}^n |\rho_i| \geq \rho_1 + (n-1) \left(\prod_{i=2}^n |\rho_i| \right)^{\frac{1}{(n-1)}} \\ &= \rho_1 + (n-1) \left(\frac{|\det H|}{\rho_1} \right)^{\frac{1}{(n-1)}}. \end{aligned}$$

Now we consider the function

$$f(x) = x + (n-1) \left(\frac{|\det H|}{x} \right)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geq \left(|\det H|\right)^{\frac{1}{n(n-1)}}$. As well known from Lemma 6,

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n(n-1)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n(n-1)}} \geq \frac{HE(G)}{n(n-1)} = \frac{\sum_{i=1}^n |\rho_i|}{n(n-1)} \geq \left(|\det H|\right)^{\frac{1}{n(n-1)}}.$$

Therefore

$$HE(G) \geq \sqrt{\frac{2\kappa}{n(n-1)}} + (n-1) \left(\frac{|\det H|}{\sqrt{\frac{2\kappa}{n(n-1)}}}\right)^{\frac{1}{(n-1)}}.$$

□

Theorem 2. *Let G be a graph of order n with m edges such that $2m \geq n$. Then*

$$HE(G) \geq \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n}\right)}} + (n-1) \left(\frac{|\det H|}{\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n}\right)}}}\right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic-geometric* mean inequality, we have

$$\begin{aligned} HE(G) &= \rho_1 + \sum_{i=2}^n |\rho_i| \geq \rho_1 + (n-1) \left(\prod_{i=2}^n |\rho_i|\right)^{\frac{1}{(n-1)}} \\ &= \rho_1 + (n-1) \left(\frac{|\det H|}{\rho_1}\right)^{\frac{1}{(n-1)}}. \end{aligned}$$

Now we consider the function

$$f(x) = x + (n-1) \left(\frac{|\det H|}{x}\right)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geq \left(|\det H|\right)^{\frac{1}{n}}$. As well known from Lemma 7, for $k = 1$

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n}\right)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\begin{aligned} \rho_1 &\geq \sqrt{\frac{2\kappa}{n}} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)} \geq \sqrt{\frac{2\kappa}{n}} \\ &\geq \frac{HE(G)}{n} \geq \left(|det\mathbf{H}| \right)^{\frac{1}{n}}. \end{aligned}$$

Therefore

$$\begin{aligned} HE(G) &\geq \sqrt{\frac{2\kappa}{n}} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)} \\ &\quad + (n-1) \left(\frac{|det\mathbf{H}|}{\sqrt{\frac{2\kappa}{n}} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)}} \right)^{\frac{1}{(n-1)}}. \end{aligned}$$

□

Theorem 3. *Let G be a graph of order n with m edges such that $2m \geq n$ and $rank(\mathbf{H}) = r \geq 2$. Then*

$$HE(G) \geq \sqrt{\frac{2\kappa}{r(r-1)}} + (n-1) \left(\frac{|det\mathbf{H}|}{\sqrt{\frac{2\kappa}{r(r-1)}}} \right)^{\frac{1}{(n-1)}}.$$

Proof. Starting with the *arithmetic-geometric* mean inequality, we have

$$\begin{aligned} HE(G) &= \rho_1 + \sum_{i=2}^n |\rho_i| \geq \rho_1 + (n-1) \left(\prod_{i=2}^n |\rho_i| \right)^{\frac{1}{(n-1)}} \\ &= \rho_1 + (n-1) \left(\frac{|det\mathbf{H}|}{\rho_1} \right)^{\frac{1}{(n-1)}}. \end{aligned}$$

Now we consider the function

$$f(x) = x + (n-1) \left(\frac{|det\mathbf{H}|}{x} \right)^{\frac{1}{(n-1)}}.$$

Note that f is increasing for $x \geq \left(|det\mathbf{H}| \right)^{\frac{1}{n(n-1)}}$. As well known from Lemma 5,

$$\rho_1 \geq \sqrt{\frac{2\kappa}{r(r-1)}}.$$

Moreover, by Lemma 8 and the *arithmetic geometric* mean inequality, we have

$$\rho_1 \geq \sqrt{\frac{2\kappa}{r(r-1)}} \geq \frac{HE(G)}{r(r-1)} = \frac{\sum_{i=1}^n |\rho_i|}{r(r-1)} \geq \frac{\sum_{i=1}^n |\rho_i|}{n(n-1)} \geq \left(|\det H| \right)^{\frac{1}{n(n-1)}}.$$

Therefore

$$HE(G) \geq \sqrt{\frac{2\kappa}{r(r-1)}} + (n-1) \left(\frac{|\det H|}{\sqrt{\frac{2\kappa}{r(r-1)}}} \right)^{\frac{1}{(n-1)}}.$$

□

4. BOUNDS FOR THE HARARY ESTRADA INDEX OF GRAPHS

In this section, we obtain lower bounds for the harary Estrada index in terms of number of vertices and *distance* between the vertices of graph G . The Estrada index of a graph G is defined by

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

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

$$EE = \sum_{i=1}^{\infty} \frac{M_k(G)}{k!}.$$

In fact *Estrada index* of graphs has an important role in *Chemistry* and *Physics* and there exists a vast *litarature* that studies this special index. In addition to the Estrada's papers depicted above, we may also refer[5, 6, 14, 15, 16, 20, 21] to the reader for detail informations 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 . The harary Estrada index of G , was introduced in [8] as follows:

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

We begin this section with theorem as follows:

Theorem 4. Let G be a graph of order $n \geq 2$. Then

$$HEE(G) \geq e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)}}.$$

Proof. By definition of harary Estrada index, we have

$$\begin{aligned} HEE(G) &= e^{\rho_1} + e^{\rho_2} + \dots + e^{\rho_n} \\ &\geq e^{\rho_1} + (n-1) \left(\prod_{i=2}^n \right)^{\frac{1}{n-1}} \\ &\geq e^{\rho_1} + (n-1) e^{\frac{\sum_{i=2}^n \rho_i}{n-1}} \\ (7) \quad &= e^{\rho_1} + (n-1) e^{\frac{-\rho_1}{n-1}}. \end{aligned}$$

Now let us consider a function

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

Therefore f is an increasing function for $x > 0$. By Lemma 6, we have

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n(n-1)}}.$$

From Inequality (7), we get

$$HEE(G) \geq e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n(n-1)}}\right)}}.$$

□

Theorem 5. Let G be a graph of order $n \geq 2$ and $r = \text{rank}(A) \geq 2$. Then

$$HEE(G) \geq e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)}}.$$

Proof. By definition of harary Estrada index, we hav

$$\begin{aligned} HEE(G) &= e^{\rho_1} + e^{\rho_2} + \dots + e^{\rho_n} \\ &\geq e^{\rho_1} + (n-1) \left(\prod_{i=2}^n \right)^{\frac{1}{n-1}} \\ &\geq e^{\rho_1} + (n-1) e^{\frac{\sum_{i=2}^n \rho_i}{n-1}} \\ (8) \quad &= e^{\rho_1} + (n-1) e^{\frac{-\rho_1}{n-1}}. \end{aligned}$$

Now let us consider a function

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

Therefore f is an increasing function for $x > 0$. By Lemma 5, we have

$$\rho_1 \geq \sqrt{\frac{2\kappa}{r(r-1)}}.$$

From Inequality (8), we get

$$HEE(G) \geq e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{r(r-1)}}\right)}}.$$

□

Theorem 6. *Let G be a graph of order $n \geq 2$. Then*

$$HEE(G) \geq e^{\left(\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}\right)} + \frac{n-1}{e^{\left(\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}\right)}}.$$

Proof. By definition of harary Estrada index, we hav

$$\begin{aligned} HEE(G) &= e^{\rho_1} + e^{\rho_2} + \dots + e^{\rho_n} \\ &\geq e^{\rho_1} + (n-1) \left(\prod_{i=2}^n \right)^{\frac{1}{n-1}} \\ &\geq e^{\rho_1} + (n-1) e^{\frac{\sum_{i=2}^n \rho_i}{n-1}} \\ (9) \qquad &= e^{\rho_1} + (n-1) e^{\frac{-\rho_1}{n-1}}. \end{aligned}$$

Now let us consider a function

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

Therefore f is an increasing function for $x > 0$. By Lemma 7, we have

$$\rho_1 \geq \sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)}\left(N_4 - \frac{4\kappa}{n}\right)}}.$$

From Inequality (9), we get

$$\begin{aligned} HEE(G) \geq e & \left(\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)}} \right) \\ & + \frac{n-1}{e \left(\sqrt{\frac{2\kappa}{n} + \sqrt{\frac{1}{n(n-1)} \left(N_4 - \frac{4\kappa}{n} \right)}} \right)}. \end{aligned}$$

□

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