The Harary index of digraphs*

Haining Jiang[a], Jixiang Meng[b]†, Yingzhi Tian[b]
[a]School of Mathematical Sciences, Xiamen University
Xiamen, Fujian, 361005, People's Republic of China
[b]College of Mathematics and System Sciences, Xinjiang University
Urumqi, Xinjiang, 830046, People's Republic of China

Abstract: The Harary index is defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph and named in honor of Professor Frank Harary. For a connected graph $G = (V, E)$ with edge connectivity $\lambda(G) \geqslant 2$, and an edge $v_iv_j \in E(G)$, $G - v_iv_j$ is the subgraph formed from G by deleting the edge v_iv_j. Denote the Harary index of G and $G - v_iv_j$ by $H(G)$ and $H(G - v_iv_j)$. Xu and Das [K.X. Xu, K.C. Das, On Harary index of graphs, Dicrete Appl.Math. 159 (2011) 1631-1640] obtained lower and upper bounds on $H(G + v_iv_j) - H(G)$ and characterize the equality cases in those bounds. We find that the equality case in lower bound is not true and we correct it. In this paper, we give lower and upper bounds on $H(G) - H(G - v_iv_j)$, and give some graphs to satisfy the equality cases in these bounds. Furthermore, we extend the Harary index to the directed graphs and get similar conclusions.

Keywords: Graphs; Diameter; Harary index; Directed graphs.

1 Introduction

All graphs (digraphs) considered in this paper are finite and simple (strict). Let $G = (V, E)$ be a graph, where $V(G)$ is the vertex set of G and $E(G)$ is the edge set of G. The degree of a vertex v in a graph G, denoted by $d_G(u)$, is the number of edges of G incident with v, each loop counting as two edges. In particular, if G is a simple graph,$d_G(u)$ is the number of neighbours of v in G. The minimum degree of G is $\delta(G)$=min$\{d_G(u)|u \in V\}$, and the maximum degree of G is $\Delta(G)$=max$\{d_G(u)|u \in V\}$. The

*This research is supported by NSFC (10671165) and NSFCXJ(2010211A06).
†Corresponding author. E-mail addresses: hnjiangsd@163.com (H. Jiang).

distance from a vertex u to a vertex v in G, denoted by $d_G(u, v)$, is the length of a shortest path joining u to v. The *diameter* of G is $D(G) = \max\{d_G(u, v) \mid u, v \in V(G)\}$. An edge set F of a connected graph G is called an edge-cut if $G - F$ is disconnected. The edge connectivity of a graph G, denoted by $\lambda(G)$, is the minimum cardinality over all edge-cuts of G.

Let $X = (V, A)$ be a digraph, where $V(X)$ is the vertex set of X and $A(X)$ is the arc set of X, thus $A(X)$ is a set of ordered pairs (u, v) $\in V \times V$ such that $u \neq v$. The elements of $V(X)$ are called the *vertices* of X and the elements of $A(X)$ are called the *arcs* of X. An arc (u, v) is said to be an *outarc* of u and an *inarc* of v. If u is a vertex of X, then the outdegree of u in X is the number $d_X^+(u)$ of arcs of X originating at u and the indegree of u in X is the number $d_X^-(u)$ of arcs of X terminating at u. The minimum outdegree of X is $\delta^+(X) = min\{d_X^+(u)|u \in V\}$, the minimum indegree of X is $\delta^-(X) = min\{d_X^-(u)|u \in V\}$. we denote by $\delta(X)$ the minimum of $\delta^-(X)$ and $\delta^+(X)$. Respectively, the maximum indegree and outdegree of X are denoted by $\Delta^-(X)$ and $\Delta^-(X)$, and we denote by $\Delta(X)$ the maximum of $\Delta^-(X)$ and $\Delta^+(X)$. The *distance* from vertex u to vertex v in X, denoted by $d_X(u, v)$, is the length of a shortest directed path joining u to v. The vertex u is the tail of this shortest directed path, and the vertex v its head. The *diameter* of X is $D(X) = \max\{d_X(u, v) \mid u, v \in V(X)\}$. Clearly, a directed graph has finite diameter if and only if it is strongly connected. The *reverse digraph* of digraph $X = (V, A)$ is the digraph $X^{(r)} = (V, \{(v, u)|(u, v) \in A\})$. Digraph $X = (V, A)$ is *symmetric* if $A = A^{(r)}$ [1].

The distance matrix $\mathbf{D}$ of G is an $n \times n$ matrix $(\mathbf{D}_{ij})$, where $\mathbf{D}_{ij}$ is just the distance between the vertices v_i and v_j in G, denoted by $d_G(v_i, v_j)$ [2]. The reciprocal distance matrix $\mathbf{RD}$ of G is an $n \times n$ matrix $(\mathbf{RD}_{ij})$ such that

$$\mathbf{RD}_{ij} = \begin{cases} \frac{1}{\mathbf{D}_{ij}} & \text{if } i \neq j, \\ 0 & \text{if } i = j. \end{cases}$$

Recall the definition of the *Harary index* of G, denoted by $H(G)$,

$$H(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{RD}_{ij}.$$

When G is an undirected graph,

$$H(G) = \sum_{i<j}\mathbf{RD}_{ij}.$$

When X is a directed graph,

$$H(X) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\mathbf{RD}_{ij}.$$

The term $\sum_{i=1}^{n} d_i^2$ is known as the first Zagreb index of G, denoted by $M_1(G)$. The *union* of simple graphs G and H is the graph $G \cup H$ with vertex set $V(G) \cup V(G)$ and edge set $E(G) \cup E(H)$. For terminologies not given here, we refer to [3].

A few years after the two initial publications on *Harary index*, it has been extended to heterosystems [4] and the *hyper − Harary index* was introduced [5]. Its modification has also been proposed [6]. The *Harary index* and related molecular descriptors have shown a modest success in structure-property correlations [7-10], but their use in combination with other molecular descriptors improves the correlations [11].

Theorem 1.1. *([12]) Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter D. If there exist two nonadjacent vertices v_i and v_j in G, then*

$$\frac{1}{2} \leq H(G + v_iv_j) - H(G) \leq (1 - \frac{1}{D}) + \frac{n(n-1) - 2m - 2}{2}(\frac{1}{2} - \frac{1}{D}),$$

With equality on the left hand side if and only if $d_G(v_i) = d_G(v_i) = 1$ and $d_G(v_i, v_j) = 2$ in G, and equality on the right hand side if and only if G is isomorphic to a graph of diameter 2.

Xu and Das characterize the equality case in left bound. We give a graph $K_4 - e$ to explain that this equality case is false. Because there exist two vertices $u, v \in V(K_4 - e)$ such that $d_G(u) = d_G(v) = 2$ *and* $d_G(u, v) = 2$, but $H(G + uv) - H(G) = \frac{1}{2}$.

2 Bounds on $H(G) - H(G - v_iv_j)$ of a graph G

Lemma 2.1. *Let G be a graph with edge connectivity $\lambda(G) \geqslant 2$. Suppose G^*=$G - uv$,where $uv \in E(G)$, then*

$$D(G^*) \leq 2D(G).$$

Proof. Let $D(G^*) = t$. We choose a path in G^* and denote this path $x_0x_1 \cdots x_{t-1}y_0$, We denote $V_i = \{v | d(x_0,\ v) = i,\ v \in V(G)\}$ *for* $i = 1, 2 \cdots t$. We consider two cases in the following proof.

Case 1. If u, v belong to the different $V_i^{'}s$. Without loss of generality, $u \in V_i,\ v \in V_j,\ i \neq j$. We choose $x_{\lceil \frac{i+j}{2} \rceil}$,

$$\begin{aligned} d_{G^*}(x_0,\ y_0) &= d_{G^*}(x_0,\ x_{\lceil \frac{i+j}{2} \rceil}) + d_{G^*}(x_{\lceil \frac{i+j}{2} \rceil},\ y_0) \\ &= d_G(x_0,\ x_{\lceil \frac{i+j}{2} \rceil}) + d_G(x_{\lceil \frac{i+j}{2} \rceil},\ y_0) \\ &\leq D(G) + D(G) \\ &= 2D(G). \end{aligned}$$

Case 2. If u, v belong to the same $V_i^{'}s$. Without loss of generality, $u, v \in V_i$. We choose x_i,

$$\begin{aligned} d_{G^*}(x_0,\ y_0) &= d_{G^*}(x_0,\ x_i) + d_{G^*}(x_i,\ y_0) \\ &= d_G(x_0,\ x_i) + d_G(x_i,\ y_0) \\ &\leq 2D(G). \end{aligned}$$

□

For a graph G with edge connectivity $\lambda(G) \geqslant 2$ and any edge $v_iv_j \in E(G)$ of G. By using the similar method as [12], we give upper and lower bounds on $H(G) - H(G - v_iv_j)$ and obtain some graphs to satisfy the equality cases in these bounds.

Theorem 2.2. *Let G be a graph with edge connectivity $\lambda(G) \geqslant 2$ with n vertices, m edges and diameter D. Then for any edge $v_iv_j \in E(G)$, we have*

$$\frac{1}{2} \leq H(G) - H(G - v_iv_j) \leq (1 - \frac{1}{2D}) + \frac{n(n-1) - 2m}{2}(\frac{1}{2} - \frac{1}{2D}). \quad (1)$$

Proof. Denote by $d_{G^*}(v_r,\ v_s)$ the distance of two vertices v_r and v_s in $G^* = G - v_iv_j$. We have

$$\begin{aligned} H(G) - H(G - v_iv_j) &= \sum_{1 \leq r < s \leq n} (\frac{1}{d_G(v_r,\ v_s)} - \frac{1}{d_{G^*}(v_r,\ v_s)}) \\ &= (\frac{1}{d_G(v_i,\ v_j)} - \frac{1}{d_{G^*}(v_i,\ v_j)}) \\ &\quad + \sum_{\substack{1 \leq r < s \leq n \\ (r,\ s) \neq (i,\ j)}} (\frac{1}{d_G(v_r,\ v_s)} - \frac{1}{d_{G^*}(v_r,\ v_s)}). \quad (2) \end{aligned}$$

Since $d_G(v_i,\ v_j)$=1 and $d_{G^*}(v_i,\ v_j) \geq 2$,
$d_G(v_r,\ v_s) \leq d_{G^*}(v_r,\ v_s)$ for $\{r,\ s\} \neq \{i,\ j\}$, we have

$$\frac{1}{d_G(v_i,\ v_j)} - \frac{1}{d_{G^*}(v_i,\ v_j)} \geq \frac{1}{2},$$

and

$$\frac{1}{d_G(v_r,\ v_s)} - \frac{1}{d_{G^*}(v_r,\ v_s)} \geq 0.$$

From (2), we get the lower bound in (1).

By Lemma 2.1, we get $d_{G^*}(v_i,\ v_j) \leq 2D$, then

$$\frac{1}{d_G(v_i,\ v_j)} - \frac{1}{d_{G^*}(v_i,\ v_j)} \leq 1 - \frac{1}{2D},$$

and

$$\frac{1}{d_G(v_r,\ v_s)} - \frac{1}{d_{G^*}(v_r,\ v_s)} \leq \frac{1}{2} - \frac{1}{2D}\ for \{r,\ s\} \neq \{i,\ j\}\ and\ d_G(v_r,\ v_s) \geq 2.$$

We get the upper bound in (1)

$$\begin{aligned} H(G) - H(G - v_iv_j) &\leq (1 - \frac{1}{2D}) + [\binom{n}{2} - (m-1) - 1](\frac{1}{2} - \frac{1}{2D}) \\ &= (1 - \frac{1}{2D}) + \frac{n(n-1) - 2m}{2}(\frac{1}{2} - \frac{1}{2D}). \end{aligned}$$

□

We can describe graphs to satisfied the equality cases in the left bound. We need G be a chordal graph with edge connectivity $\lambda(G) \geqslant 2$. Arbitrarily delete any edge e=v_iv_j, $d_{G^*}(v_i,\ v_i) = 2$, then any edge in a triangle. But if exist two of maximal cliques have a common vertex, such graphs do not satisfy the equality cases in the left bound. Let $e_1 = v_iv_j$, $e_2 = v_jv_k$. If e_i belong to maximal cliques V_i, (i=1,2). $V_i \cap V_j = v_j$. Then $d_G(v_i,\ v_k) = 2$. But if we delete e_1, $d_G(v_i,\ v_k) > 2$. For example, let K_5 be the graph with vertex set v_1, v_2, v_3, v_4, v_5. We construct G from K_5 by adding two vertices v_6 and v_7, such that v_6 is adjacent to v_2 and v_3, and v_7 is adjacent to v_4 and v_5. Then $H(G) - H(G - v_1v_4) = \frac{1}{2}$.

We know that the complete graph K_n satisfies the equality in the right hand side of (1).

Theorem 2.3. *Let G be a triangle-free and quadrangle-free graph with edge connectivity $\lambda(G) \geqslant 2$, n vertices, m edges, diameter D and the maximum degree $\Delta(G)$. Then for any edge $v_iv_j \in E(G)$,*

$$\frac{3}{4} \leq H(G) - H(G - v_iv_j) \leq (1 - \frac{1}{2D})$$

$$+\frac{n(n-1) - M_1(G) + 4\Delta(G) - 4}{2}(\frac{1}{2} - \frac{1}{2D}). \quad (3)$$

Proof. Since G is a triangle-free and quadrangle-free graph, then $d_{G^*}(v_i, v_j) \geq 4$ and $\frac{1}{d_G(v_i, v_j)} - \frac{1}{d_{G^*}(v_i, v_j)} \geq \frac{3}{4}$. From (2), we get the lower bound in (3). Again since the number of vertex pairs in G^* at distance 1 is $m - 1$ and the number of vertex pairs in G^* at distance 2 is

$$\sum_{k=1}^{n} \binom{d_G(v_k)}{2} - (d_G(v_i) + d_G(v_j) - 2) = \frac{1}{2}M_1(G) - m - (d_G(v_i) + d_G(v_j) - 2),$$

then

$$\begin{aligned} &\binom{n}{2} - (m-1) - 1 - [\frac{1}{2}M_1(G) - m - (d_G(v_i) + d_G(v_j) - 2)] \\ \leq\ &\binom{n}{2} - m - \frac{1}{2}M_1(G) + m + \Delta(G) + \Delta(G) - 2 \\ =\ &\binom{n}{2} - m - \frac{1}{2}M_1(G) + m + 2\Delta(G) - 2. \end{aligned}$$

From (2), we get the right hand side of (3). □

3 Bounds on $H(X + v_iv_j) - H(X)$ of a digraph X

Theorem 3.1. *Let X be a strongly connected digraph with n vertices, m arcs, and diameter D. If there exist two nonadjacent vertices v_i and v_j, then*

$$\frac{1}{2} \leq H(X + v_iv_j) - H(X) \leq (1 - \frac{1}{D}) + (n^2 - n - m - 1)(\frac{1}{2} - \frac{1}{D}). \quad (4)$$

with equality on the right hand side if and only if X is isomorphic to a digraph of diameter 2.

Proof. Denote by $d_{X^\diamond}(v_r,\ v_s)$ the distance of two vertices v_r and v_s in $X+(v_i,v_j)$.

$$\begin{aligned} H(X+v_iv_j)-H(X) &= \sum_{1\le r,\ s\le n}\left(\frac{1}{d_{X^\diamond}(v_r,\ v_s)}-\frac{1}{d_X(v_r,\ v_s)}\right) \\ &= \left(\frac{1}{d_{X^\diamond}(v_i,\ v_j)}-\frac{1}{d_X(v_i,\ v_j)}\right) \\ &\quad + \sum_{\substack{1\le r,\ s\le n \\ (r,\ s)\neq(i,\ j)}}\left(\frac{1}{d_{X^\diamond}(v_r,\ v_s)}-\frac{1}{d_X(v_r,\ v_s)}\right). \qquad (5)\end{aligned}$$

Since

$$\frac{1}{d_{X^\diamond}(v_i,\ v_j)}-\frac{1}{d_X(v_i,\ v_j)}\ge\frac{1}{2}$$

and

$$d_{X^\diamond}(v_r,\ v_s)\le d_X(v_r,\ v_s)\ for\ (r,\ s)\neq(i,\ j),$$

from(5), we get the lower bound in (4).

Again since

$$\frac{1}{d_{X^\diamond}(v_i,\ v_j)}-\frac{1}{d_X(v_i,\ v_j)}\le 1-\frac{1}{D}$$

and

$$\frac{1}{d_{X^\diamond}(v_r,\ v_s)}-\frac{1}{d_X(v_r,\ v_s)}\le\frac{1}{2}-\frac{1}{D}\ for\ (r,\ s)\neq(i,\ j)\ and\ d_X(v_r,\ v_s)\ge 2,$$

there are $2\binom{n}{2}$ vertex pairs (at lest 1) in X. The number of vertex pairs in X at distance 1 is m. From (5), we get the right hand side of (4).

Now suppose that the right hand side equality holds in (4). Then

$$\frac{1}{d_{X^\diamond}(v_i,\ v_j)}-\frac{1}{d_X(v_i,\ v_j)}=1-\frac{1}{D}$$

and

$$\frac{1}{d_{X^\diamond}(v_r,\ v_s)}-\frac{1}{d_X(v_r,\ v_s)}=\frac{1}{2}-\frac{1}{D}\ for\ (r,\ s)\neq(i,\ j)\ and\ d_X(v_r,\ v_s)\ge 2,$$

that is, $d_G(v_i,v_j)=D$. By contradiction we show that X is isomorphic to a digraph of diameter 2. For this we assume that X is a graph of diameter

3 or more. Then there exists a vertex v_t adjacent to the vertex v_j such that $d_G(v_i,\ v_t) = D-1$. Then

$$\frac{1}{d_{X^\diamond}(v_i,\ v_t)} - \frac{1}{d_X(v_i,\ v_t)} \leq \frac{1}{2} - \frac{1}{D-1} < \frac{1}{2} - \frac{1}{D},$$

a contradiction. Hence X is isomorphic to a digraph of diameter 2.

Conversely, one can see easily that the left hand side equality holds in (4) for $d_G(v_i)^+ \geq 1$, $d_G(v_j)^+ \geq 1$, $d_G(v_i,v_j) = 2$, $d_G(v_i)^- = 0$, $d_G(v_j)^+ = 0$ and equality on the right hand side if and only if X is isomorphic to a digraph of diameter 2. □

Theorem 3.2. *Let X be a strongly connected digraph with n vertices, m arcs, diameter D, the maximum degree $\Delta(X)$, and the minimum degree $\delta(X)$. Its underlying graph is triangle- and quadrangle-free. If there exist two nonadjacent vertices v_i and v_j, then*

$$\frac{1}{2} \leq H(X + v_iv_j) - H(X) \leq (1 - \frac{1}{D}) + (n(n-1-\delta^2(X)$$
$$+\Delta(X)) - m)(\frac{1}{2} - \frac{1}{D}). \quad (6)$$

with equality on the right hand side if and only if X is isomorphic to a digraph of diameter 2.

Proof. The proof of left hand side of (6) is same as Theorem 3.1.

The number of vertex pairs at distance 2 which simultaneously belongs to $X + v_iv_j$ and X is

$$\sum_{i=1}^{n}(d_X^+(v_i)d_X^-(v_i) - \varepsilon_i) - \varepsilon,$$

where

$$\varepsilon = \begin{cases} 1 & \text{if } d_G(v_i,\ v_j) = 2, \\ 0 & \text{if } d_G(v_i,\ v_j) > 2. \end{cases}$$

and ε_i is the number of directed cycles of length 2 that contain v_i. Then

$$2\binom{n}{2} - m - 1 - (\sum_{i=1}^{n}(d_X^+(v_i)d_X^-(v_i) - \varepsilon_i) - \varepsilon)$$

$$= 2\binom{n}{2} - m - 1 - \sum_{i=1}^{n}(d_X^+(v_i)d_X^-(v_i) + \sum_{i=1}^{n}\varepsilon_i + \varepsilon$$

$$
\begin{aligned}
&\leq 2\binom{n}{2} - m - 1 - n\delta^2(X) + n\Delta(X) + 1 \\
&= n(n - 1 - \delta^2(X) + \Delta(X)) - m.
\end{aligned}
$$

Moreover, the equality holds in right hand side if and only if X is isomorphic to a digraph of diameter 2. □

References

[1] R. Tindell, Connectivity of cayley graphs, in: D.Z. Du, D.F. Hsu (Eds.), Combinatorial Network Theory. 41-64.

[2] B. Zhou, X. Cai, On the Harary index, J.Math.Chem. 44 (2008) 611-618.

[3] J.A. Bondy, U.S.R. Murty, Graph Theory with Applications, North-Holland, New York, 1976.

[4] O. Ivanciuc, T. Ivanciuc, A.T. Balaban, Design of topological indices. Part 10. Parameters based on electronegativity and vovalent radius for the computation of molecular graph descriptors for hetero-atom-containing molecules. J. Chem.Inf.Comput. Sci. 38, 395-401 (1998).

[5] M.V. Diudea, Indices of reciprocal properties or Harary indices. J.Chem. Inf.Comput. Sci. 37, 292-299 (1997).

[6] B. Lučić, A. Miličević, S. Nikolić, N. Trinajstić, Harary index-twelve years later. Croat. Chem. Acta 75, 847-868 (2002).

[7] R. Todeschini, V. Consonni, Handbook of Molecular Descriptors (Wiley-VCH, Weinheim, 2000).

[8] Z. Mihalić, N. Trinajstić, A graph-theoretical approach to structure-property relationships. J. Chem. Educ. 69, 701-712 (1992).

[9] O. Ivanciuc, QSAR comparative study of Wiener descriptors for weighted molecular graphs. J. Chem. Inf. Comput. Sci. 40, 1412-1422 (2000).

[10] B. Lučić, I. Lukovits, S. Nikolić, N. Trinajstić, Distance-related indexes in the quantitative structure-property relationship modeling. J. Chem. Inf. Comput. Sci. 41, 527-535 (2001).

[11] N. Trinajstić, S. Nikolić, S.C. Basak, I. Lukovits, Distance indices and their hyper-counterparts: Inter-correlation and use in the structure-property modeling. SAR QSAR Environ. Res. 12, 31-54 (2001).

[12] K.X. Xu, K.C. Das, On Harary index of graphs, Dicrete Appl.Math. 159 (2011) 1631-1640.