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Two upper bounds on the weighted Harary indices

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Abstract

The paper is concerned with the weighted Harary indices, namely the multiplicatively weighted Harary index H_M and the additively weighted Harary index H_A. For a simple connected graph G with n vertices, m edges and k cut edges, sharp upper bounds on $H_M(G)$ and $H_A(G)$ are derived and the corresponding extremal graphs are characterized. From one of the established bounds, a main result of the paper [X. Li, J. B. Liu, On the reciprocal degree distance of graphs with cut vertices or cut edges, *Ars Combin.* **130** (2017) 303–318] follows instantly.

Keywords: weighted Harary indices; multiplicatively weighted Harary index; additively weighted Harary index; reciprocal degree distance; cut edge.

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1. Introduction

All graphs considered in this note are simple and finite. Those notations and terminologies from graph theory, which are not defined here can be found in the books [5, 17].

In 1993, Plavšić *et al.* [26] and Ivanciuc *et al.* [19] independently introduced the following graph invariant within the study of molecular modeling:

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u,v)}\,,$$

where $d(u,v)$ is the distance (that is, the length of any shortest path) between the vertices u,v of a non-trivial connected graph G and d_u denotes the degree of u. The authors of [26] named H as the Harary index in honor of Professor Frank Harary. The same quantity also appeared in papers dealing with various generalizations of Zagreb indices, such as, e.g., [24]. Some time ago, Alizadeh *et al.* [2] proposed the following two variants of H:

$$H_M(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_u d_v}{d(u,v)} \quad \text{and} \quad H_A(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{d_u + d_v}{d(u,v)}\,.$$

The graph invariants H_M and H_A were referred [2] as the *multiplicatively weighted Harary index* and the *additively weighted Harary index*, respectively. The invariant H_A was also put forward independently by Hua and Zhang [18], under the name *reciprocal degree distance*. Details about the mathematical properties of all the above mentioned graph invariants can be found in the book [28], papers [21–23] and related references listed therein.

The motivation for introducing and studying Harary index and its generalizations came from mathematical chemistry. The Harary index belongs to a class of distance-based topological indices (or molecular descriptors, as they are also known in QSAR/QSPR studies). Its introduction was an attempt to find an index that will correspond to the intuitive feeling that molecular properties should be influenced more by contributions of pairs of close atoms than by the contributions of the pairs of more distant ones. However, as the performance of Harary index in QSAR/QSPR studies was not very impressive, weightings were introduced in order to value more the contributions of pairs of vertices of high degrees.

Besides in the mathematical chemistry, Harary indices also appear in the study of complex networks. A normalization of $H(G)$ obtained by dividing it by $n(n-1)$ (where n denotes the number of vertices of G) is called the efficiency of G [20]; the reciprocal value of efficiency is called the performance of G [25]. Efficiency and performance provide also a way of expressing and quantifying the small-world property of a given network. As a rule, the strength of interactions between nodes in a network is not correctly described by their topological distances only. Hence, it was

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necessary to introduce also the weighted versions of efficiency and performance. Such weightings can be useful also as measures of centrality with respect to the information flow [9].

An edge e of a connected graph G is said to be a cut edge if $G - e$ is a disconnected graph. Denote by $K_{n-k}^{(k)}$ the graph obtained from the complete graph K_{n-k} (on $n-k$ vertices) by attaching k pedant vertices to one of the vertices of K_{n-k}.

Li and Liu [21] derived a sharp upper bound on the graph invariant $H_A(G)$ in terms of order n and number of cut edges k of a non-trivial connected G, and proved that this bound is attained if and if only if $G \cong K_{n-k}^{(k)}$. Motivated by this result, a similar sharp upper bound for the multiplicatively weighted Harary index H_M is established in this paper. Also, the aforementioned bound obtained by Li and Liu [21] for H_A is improved here - this new improved bound depends on the order n, size m and number of cut edges k of G, and it is also attained only by the graph $K_{n-k}^{(k)}$.

2. Main result

Let H be a subgraph of a graph G. Denote by $N_H(v)$ the set of all those vertices of G which are adjacent to v in H. The fact that an edge e of an n-vertex connected graph G is a cut edge if and only if e does not lie on any cycle of G, implies that the number of cut edges in G cannot be equal to $n-2$.

Lemma 2.1. *If a connected graph G has the maximal size among all n–vertex graphs with k cut edges, namely $e_1, e_2, \cdots, e_k$, then $G - \{e_1, e_2, \cdots, e_k\} \cong K_{n-k} \cup kK_1$.*

Proof. If $G - \{e_1, e_2, \cdots, e_k\}$ contains a component C which is not complete then adding an edge in C (and hence in G) results in a contradiction. Clearly, $G - \{e_1, e_2, \cdots, e_k\}$ does not contain any component isomorphic to K_2 (for otherwise G contains more than k cut edges, a contradiction). Now, contrarily, suppose that C' and C'' are two (distinct) non-trivial components of $G - \{e_1, e_2, \cdots, e_k\}$. Suppose that the vertices $u \in V(C')$ and $v \in V(C'')$ are incident with cut edge(s) in G. Let $N_{C''}(v) = \{v_1, v_2, \cdots, v_r\}$. Let G' be the graph obtained from G by removing the edges $vv_1, vv_2, \cdots, vv_r$ and adding the edges $uv_1, uv_2, \cdots, uv_r, wv_1$, where $w \in N_{C'}(u)$. Certainly, the graph G' has k cut edges but it has size greater than that of G, which contradicts the definition of G.

□

The following corollary is a direct consequence of Lemma 2.1.

Corollary 2.1. *If G is an n–vertex connected graph with m edges and k cut edges, namely $e_1, e_2, \cdots, e_k$, then*

$$m \leq \frac{(n-k)(n-k-1)}{2} + k\,,$$

with equality if and only if $G - \{e_1, e_2, \cdots, e_k\} \cong K_{n-k} \cup kK_1$.

The *first Zagreb index*, introduced in [15], and the *second Zagreb index*, introduced in [16], for a graph G can be defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv is the edge connecting the vertices $u, v \in V(G)$. The *first Zagreb coindex* and *second Zagreb coindex* of a graph G, defined as

$$\overline{M}_1(G) = \sum_{uv \notin E(G); u \neq v} (d_u + d_v)$$

and

$$\overline{M}_2(G) = \sum_{uv \notin E(G); u \neq v} (d_u d_v)\,,$$

were introduced in [12] in order to quantify the contributions of pairs of non-adjacent vertices to the additively and multiplicatively weighted versions, respectively, of the Wiener index of G.

The relations between Zagreb indices and Zagreb coindices (implicit in Das and Gutman [10] and established explicitly by Ashrafi *et al.* [3]), given in the following lemma, play an important role in proving the main result of this paper.

Lemma 2.2. [3, 10] *If G is an n-vertex graph with m edges then*

$$\overline{M}_1(G) = 2m(n-1) - M_1(G) \tag{1}$$

and

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G). \tag{2}$$

Clearly, mathematical properties of the (first and second) Zagreb indices and coindices are closely interlinked, because of the identities (1) and (2). Details about the mathematical properties of the invariants M_1, M_2 (and hence their implications for $\overline{M}_1$, $\overline{M}_2$) can be found in the recent surveys [1, 6, 7]. For more on Zagreb coindices, in particular for their extremal properties, see [4].

The next three lemmas are also crucial for proving the main result.

Lemma 2.3. [8, 14, 27] *If G is an n–vertex connected graph with k cut edges then*

$$M_1(G) \leq (n-k-1)^3 + (n-1)^2 + k,$$

with equality if and only if $G \cong K_{n-k}^{(k)}$.

Lemma 2.4. [13] *If G is an n–vertex tree then*

$$2M_2(G) - M_1(G) \leq (n-2)(n-1)\,,$$

with equality if and only if G has diameter at most 3.

If we assume that the graph G_1 considered in Lemma 1 and Lemma 2 of [8] is not a tree then these two lemmas also hold for the graph invariant $2M_2 - M_1$. Furthermore, it can be easily checked that Proposition 1 and Lemma 3 (that is, Lemma 2.2 of [11]) of [8], are also true for the invariant $2M_2 - M_1$. Consequently, proof of the next result is fully analogous to that of Theorem 1 of [8] and hence omitted.

Lemma 2.5. *If G is an n–vertex connected graph with k cut edges such that $0 \leq k \leq n-3$, then*

$$2M_2(G) - M_1(G) \leq (n-k-3)(n-k-1)^3 + (n-1)\Big(2(n-k-1)^2 + 2k - n + 1\Big) - k\,,$$

with equality if and only if $G \cong K_{n-k}^{(k)}$.

Now, the main result can be easily proved.

Theorem 2.1. *If G is an n-vertex connected graph with m edges and k cut edges then*

$$H_A(G) \leq m(n-1) + \frac{1}{2}\Big((n-k-1)^3 + (n-1)^2 + k\Big)$$

and

$$H_M(G) \leq m^2 + \frac{1}{4}\bigg((n-k-3)(n-k-1)^3 + (n-1)\Big(2(n-k-1)^2 + 2k - n + 1\Big) - k\bigg),$$

where the equality sign in either of the above two inequalities holds if and only if $G \cong K_{n-k}^{(k)}$.

Proof. From the definition of the invariant H_A, it follows that

$$\begin{aligned} H_A(G) &= \sum_{uv \in E(G)} \frac{d_u + d_v}{d(u,v)} + \sum_{uv \notin E(G);\, u \neq v} \frac{d_u + d_v}{d(u,v)} \\ &\leq M_1(G) + \frac{\overline{M}_1(G)}{2}, \end{aligned} \tag{3}$$

with equality if and only if distance between every two distinct non–adjacent vertices of G is 2. Similarly, it holds that

$$H_M(G) \leq M_2(G) + \frac{\overline{M}_2(G)}{2}, \tag{4}$$

with equality if and only if distance between every two distinct non–adjacent vertices of G is 2.

By using Lemmas 2.2 and 2.3, one has

$$M_1(G) + \frac{\overline{M}_1(G)}{2} = m(n-1) + \frac{M_1(G)}{2}$$

$$\leq \quad m(n-1)+\frac{1}{2}\Big((n-k-1)^3+(n-1)^2+k\Big), \tag{5}$$

with equality if and only if $G \cong K_{n-k}^{(k)}$. Similarly, by using Lemmas 2.2, 2.4 and 2.5, we get

$$\begin{aligned} M_2(G)+\frac{\overline{M}_2(G)}{2} &= m^2+\frac{M_2(G)}{2}-\frac{M_1(G)}{4} \\ &\leq \begin{cases} m^2+\frac{(n-2)(n-1)}{4}\,, & \text{if } k=n-1, \\ m^2+\frac{\phi(n,k)}{4}\,, & \text{otherwise.} \end{cases} \end{aligned} \tag{6}$$

with equality if and only if G is isomorphic to the

$$\begin{cases} \text{graph having diameter at most } 3\,, & \text{if } k=n-1, \\ K_{n-k}^{(k)}\,, & \text{otherwise.} \end{cases}$$

where

$$\phi(n,k)=(n-k-3)(n-k-1)^3+(n-1)[2(n-k-1)^2+2k-n+1]-k.$$

Since the distance between every two distinct non–adjacent vertices of $K_{n-k}^{(k)}$ is 2 and it has diameter at most 2, from Equations (3), (5) and Equations (4), (6), the desired result follows. $\square$

If $k=0$ (or $k=n-1$), then from Theorem 2.1 it follows that the complete graph K_n (the star graph S_n, respectively) is the only graph with maximal H_M and H_A values among all n-vertex connected graphs (trees, respectively).

Remark 2.1. *The fact that the function f, defined by $f(m)=m(n-1)+\frac{1}{2}[(n-k-1)^3+(n-1)^2+k]$, $1 \leq n-1 \leq m \leq \frac{(n-k)(n-k-1)}{2}+k$, is strictly increasing implies that $f(m) \leq f\left(\frac{(n-k)(n-k-1)}{2}+k\right)$, from which it follows that*

$$m(n-1)+\frac{1}{2}\left((n-k-1)^3+(n-1)^2+k\right) \leq n^3-\left(\frac{5}{2}k+2\right)n^2+\left(2k^2+\frac{11}{2}k+1\right)n-\left(\frac{1}{2}k^3+2k^2+\frac{5}{2}k\right),$$

with equality if and only if $m=\frac{(n-k)(n-k-1)}{2}+k$.

From Corollary 2.1, Theorem 2.1 and Remark 2.1, the next result follows.

Corollary 2.2. [21] *If G is an n-vertex connected graph with k cut edges, then*

$$H_A(G) \leq n^3-\left(\frac{5}{2}k+2\right)n^2+\left(2k^2+\frac{11}{2}k+1\right)n-\left(\frac{1}{2}k^3+2k^2+\frac{5}{2}k\right),$$

with equality if and only if $G \cong K_{n-k}^{(k)}$.

From Remark 2.1, it is clear that if G is an n-vertex graph with k cut edges such that the size of G is different from $\frac{(n-k)(n-k-1)}{2}+k$ then the upper bound on H_A given in Theorem 2.1 is always better than the one mentioned in Corollary 2.2.

The next corollary is also a direct consequence of Theorem 2.1.

Corollary 2.3. *If G is an n-vertex connected graph with k cut edges, then*

$$\begin{aligned} H_M(G) \quad \leq \quad & \left(\frac{(n-k)(n-k-1)}{2}+k\right)^2 \\ & +\frac{1}{4}\left((n-k-3)(n-k-1)^3+(n-1)[2(n-k-1)^2+2k-n+1]-k\right), \end{aligned}$$

with equality if and only if $G \cong K_{n-k}^{(k)}$.

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