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The connectivity and the Harary index of a graph[☆]

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ABSTRACT

The Harary index of a graph is defined as the sum of reciprocals of distances between all pairs of vertices of the graph. In this paper we provide an upper bound of the Harary index in terms of the vertex or edge connectivity of a graph. We characterize the unique graph with the maximum Harary index among all graphs with a given number of cut vertices or vertex connectivity or edge connectivity. In addition we also characterize the extremal graphs with the second maximum Harary index among all graphs with given vertex connectivity.

1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The *distance* between two vertices u and v of G, denoted by $d_G(u, v)$, is defined as the minimum length of the paths between u and v in G. The Harary index of a graph G, denoted by $H(G)$, has been introduced independently by Plavšić et al. [9] and by Ivanciuc et al. [7] in 1993 for the characterization of molecular graphs. It has been named in honor of Professor Frank Harary on the occasion of his 70th birthday. The *Harary index* $H(G)$ is defined as the sum of reciprocals of distances between all pairs of vertices of the graph G, i.e.

$$H(G) = \sum_{u,v \in V(G)} \frac{1}{d_G(u, v)}.$$

Mathematical properties and applications of the Harary index are reported in [2,3,5,8,16]. Note that in any disconnected graph G, the distance is infinite between any two vertices from two distinct components. Therefore its reciprocal can be viewed as 0. Thus, we can define validly the Harary index of disconnected graph G as follows:

$$H(G) = \sum_{i=1}^{k} H(G_i),$$

where $G_1, G_2, \ldots, G_k$ are the components of G.

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Another distance-based topological index of a graph G is the Wiener index, denoted by $W(G)$. As an oldest topological index, the *Wiener index* of a graph G, first introduced by Wiener [10] in 1947, was defined as

$$W(G) = \sum_{u,v \in V(G)} d_G(u, v).$$

The motivation for introduction of the Harary index was pragmatic—the aim was to design a distance index differing from the Wiener index in that the contributions to it from the distant atoms in a molecule should be much smaller than from near atoms, since in many instances the distant atoms influence each other much less than near atoms.

Let $\gamma(G, k)$ be the number of vertex pairs of the graph G that are at distance k. Then

$$H(G) = \sum_{k \geq 1} \frac{1}{k} \gamma(G, k). \tag{1.1}$$

It will be convenient to determine the exact value by Eq. (1.1) for some graphs with the simple structure (e.g. the graphs with small diameter), but in general it is very difficult to give the exact value of $\gamma(G, k)$. So it is very useful to provide upper or lower bounds for the Harary index; see e.g. [1,5,16]. In addition, the extremal Harary index of a given class of graphs has also been studied extensively; see e.g. [4,6,14,12,11,13,15].

In this paper we provide an upper bound of the Harary index in terms of the vertex or edge connectivity of a graph. We characterize the unique graph with the maximum Harary index among all graphs with a given number of cut vertices or vertex connectivity or edge connectivity. In addition we also characterize the extremal graphs with the second maximum Harary index among all graphs with given vertex connectivity.

2. Main results

In Section 2.1 we determine the unique graph with the maximum Harary index among all graphs with a given number of cut vertices. We find that the optimal graph is surely connected with vertex or edge connectivity 1. In Section 2.2 we consider a general problem, that is, determining the graph(s) with the maximum Harary index among all graphs with fixed vertex or edge connectivity. By these results we provide an upper bound of the Harary index of a graph in terms of the vertex or edge connectivity.

We introduce some notions used in this paper. Let G be a graph. For a vertex $v \in V(G)$, denote by $N_G(v)$ the neighborhood of v in G and by $d_G(v) = |N_G(v)|$ the degree of v in G. A vertex of G is called *pendent* if it has degree 1, and the edge incident with a pendent vertex is a *pendent edge*. A *pendent path* at v in a graph G is a path in which no vertex other than v is incident with any edge of G outside the path, where the degree of v is at least three. A *cut vertex* of a graph is a vertex whose removal increases the number of components of the graph. A *block* of a connected graph is defined to be a maximum connected subgraph without cut vertices. The *vertex connectivity* (respectively, *edge connectivity*) of a graph is the minimum number of vertices (respectively, minimum number of edges) whose deletion yields the resulting graph disconnected or a singleton.

For a subset $W \subset V(G)$, let $G - W$ be the subgraph of G obtained by deleting the vertices of W together with the edges incident with them. Similarly, for a subset $E_1 \subset E(G)$, denote by $G - E_1$ the subgraph of G obtained by deleting the edges of E_1. For an edge set $E_2 \not\subseteq E(G)$, if two endpoints of any edge in E_2 belong to $V(G)$, then we denote by $G + E_2$ the graph obtained from G by adding the edges of E_2. Denote by $P_n = \mathrm{P}v_1v_2 \cdots v_n$ a path on vertices $v_1, v_2, \ldots, v_n$ with edges v_iv_{i+1} for $i = 1, 2, \ldots, n-1$, and denote by K_n a complete graph on n vertices.

2.1. Maximum Harary index with a given number of cut vertices

Lemma 2.1 (*[12]*). *Let G be a graph with $u, v \in V(G)$. If $uv \notin E(G)$, then $H(G) < H(G + uv)$. If $uv \in E(G)$, then $H(G) > H(G - uv)$.*

Lemma 2.2. *Let G_1, G_2, P_s be pairwise vertex-disjoint connected graphs, where G_1 contains an edge uv such that $N_{G_1}(u) \setminus \{v\} = N_{G_1}(v) \setminus \{u\} = \{w_1, w_2, \ldots, w_k\}$ $(k \geq 1)$, G_2 contains a shortest path $\mathrm{P}x_1 \cdots x_t$ from x_1 to x_t, $P_s = \mathrm{P}z_1z_2 \ldots z_s$, and $t \geq s + 2$. Let G be obtained from G_1 by identifying u with x_1 of G_2 and identifying v with z_1 of P_s, and let $G' = G - \{vw_1, vw_2, \ldots, vw_k\} + \{x_2w_1, x_2w_2, \ldots, x_2w_k\}$. Then*

$$H(G) < H(G'),$$

where the graphs G and G' are shown in Fig. 2.1.

Proof. Let P be the path of G obtained by connecting the paths $\mathrm{P}x_1x_2 \cdots x_t$, $\mathrm{P}uv$ and $\mathrm{P}z_1z_2 \cdots z_s$, where $u = x_1$ and $v = z_1$. Partition the vertex set of G as

$$V(G) = (V(G_1)\backslash\{u, v\}) \cup (V(G_2)\backslash\{x_i : i = 1, 2, \ldots, t\}) \cup V(P) =: S_1 \cup S_2 \cup S_3.$$

From G to G', the distance between any two vertices in each S_i is unchanged for $i = 1, 2, 3$; the distance from any vertex of S_1 to any of S_2 is not increased; the distance from any vertex of S_1 to any of z_i $(i = 1, 2, \ldots, s)$ of S_3 is increased by 1, and to any of x_i $(i = 2, 3, \ldots, t)$ is decreased by 1, and to the vertex u is unchanged; the distance from any vertex of S_2 and any of S_3 is unchanged.