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On Hamiltonian properties of bipartite graphs and several topological indices

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Abstract. For a connected graph H, the first Zagreb index $M_1(H)$ is equal to the sum of squares of the degrees of the vertices of H. The reciprocal degree distance of H, denoted by $\mathrm{RDD}(H)$, is defined as

$$\mathrm{RDD}(H) = \sum_{x \neq y} \frac{\deg_H(x) + \deg_H(y)}{\mathrm{dist}_H(x, y)},$$

where $\deg_H(x)$ is the degree of the vertex x in H and $\mathrm{dist}_H(x, y)$ denotes the distance between two vertices x and y in H. The forgotten topological index $F(H)$ of H is the sum of cubes of all its vertex degrees. In this paper, we give a best possible lower bound on $M_1(H)$, $\mathrm{RDD}(H)$ or $F(H)$ to ensure that a bipartite graph H is Hamiltonian.

1. Introduction

We study simple, undirected, connected and finite graphs throughout this paper. Let H be a graph with vertex set $V(H) = \{v_1, v_2, \ldots, v_p\}$, i.e., $p = |V(H)|$. For a vertex $v_s \in V(H)$, the degree $\deg_H(v_s)$ $(= d_s)$ of v_s is the number of edges incident with v_s in H. Let $\mathrm{dist}_H(v_s, v_t)$ be the length of any shortest path in H connecting v_s and v_t. Denote by $(d_1, d_2, \ldots, d_p)$ the *degree sequence* of H with $d_1 \leq d_2 \leq \cdots \leq d_p$. We delete the footnote H from the symbols in the following context if there is no ambiguity.

A cycle of length $|V(H)|$ is called a *Hamiltonian cycle* of H. If H contains a Hamiltonian cycle, then H is *Hamiltonian*. We refer the reader to [8] for undefined notation and terminologies.

The first (M_1) and second (M_2) Zagreb indices of a graph H, which introduced by Gutman and Trinajstić in [14], are defined respectively as:

$$M_1(H) = \sum_{x \in V(H)} \deg(x)^2 \quad \text{and} \quad M_2(H) = \sum_{xy \in E(H)} \deg(x)\deg(y).$$

The *reciprocal degree distance* $\mathrm{RDD}(H)$ of H, which was first independently introduced in [2, 16], is defined as

$$\mathrm{RDD}(H) = \sum_{x \neq y} \frac{\deg(x) + \deg(y)}{\mathrm{dist}_H(x, y)}.$$

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Denote $\widehat{D}_H(v_i) = \Sigma_{v_j \in V(H)\setminus\{v_i\}} \frac{1}{\mathrm{dist}_H(v_j,v_i)}$. Then one can transform RDD(H) into

$$\mathrm{RDD}(H) = \sum_{v_i \in V(H)} \deg(v_i)\widehat{D}_H(v_i).$$

According to the definition of $\widehat{D}_H(v_i)$, for a bipartite graph H of order $2p$ with $p \geq 2$ vertices in each part, we get

$$\widehat{D}_H(v_i) \leq \deg(v_i) + \frac{1}{2}\Big(p-1\Big) + \frac{1}{3}\Big(p - \deg(v_i)\Big). \tag{1}$$

The *forgotten topological index*, which denoted by $F(H)$ and first introduced in [12], is defined as:

$$F(H) = \sum_{x \in V(H)} \deg(x)^3.$$

For historical background and mathematical properties of $M_1(H)$, $M_2(H)$,RDD(H) and $F(H)$, one can refer to [1, 9, 13, 17, 24–26].

A popular research topic in graph theory is the study of whether a given graph has some important property (such as Hamiltonicity or traceability). It shows that [18] determining whether a graph has a Hamiltonian cycle is NP-complete. Although there are some literatures [7, 11, 15, 19–23, 27] using the bounds of topological indices or spectral conditions to determine the structure of graphs, there are still few results related to them. Recently, based on the first Zagreb index or reciprocal degree distance, the κ-connectivity, β-deficiency [4, 6], Hamiltonian-connectedness [3] and $\hbar$-Hamiltonicity, $\hbar$-path-coverability and $\hbar$-edge-Hamiltonicity [5] of graphs have been discussed. By employing the Wiener index, some vulnerability parameters (such as integrity, toughness, tenacity and binding number) of graphs have been studied [28]. However, It is not clear whether a bipartite graph is Hamiltonian by using the above topological indices.

In this paper, we have partially solved the problems above, that is to say, we provide a best possible lower bound on $M_1(H)$, RDD(H) or $F(H)$ to ensure that a bipartite graph H is Hamiltonian.

In Section 2, we give a necessary lemma. The results and their proofs will be presented in the last section.

2. Preliminaries

In this section, a useful lemma will be given. Firstly, we define the graph H_k^* as follows: a graph whose set of vertices is $X \cup Y \cup Z \cup W$ with X, Y, Z, W pairwise disjoint such that $|X| = |Z| = k$, and $|Y| = |W| = p - k$, and whose edges join each vertex $u \in X \cup Y$ to each vertex $v \in Z \cup W$ except when $u \in X$ and $v \in W$.

Especially, when $k = p - 1$, we denote the graph H_k^* by H^*.

Lemma 2.1. [10] *Let H be a bipartite graph with vertices $u_1, u_2, \ldots, u_p$ and $v_1, v_2, \ldots, v_p$ such that $p \geq 2$, $d(u_1) \leq d(u_2) \leq \cdots \leq d(u_p)$, $d(v_1) \leq d(v_2) \leq \cdots \leq d(v_p)$ and*

$$d(u_k) \leq k < p \Rightarrow d(v_{p-k}) \geq p - k + 1.$$

Then H is either Hamiltonian or $H \cong H_k^*$.

3. Results

Now, we present a best possible lower bound on $M_1(H)$, RDD(H) or $F(H)$ to ensure that a bipartite graph H is Hamiltonian.

Theorem 3.1. *Let H be a bipartite graph of order $2p$ with $p \geq 2$ vertices in each part and $\delta(H) \geq k \geq 1$. If*

$$M_1(H) \geq 2p^3 - 3p^2 + 3p,$$

then H is Hamiltonian if and only if $H \ncong H^*$.

Proof. Sufficiency. Suppose that H is not Hamiltonian, and without loss of generality, let $V(H) = \{u_1, u_2, \ldots, u_p; v_1, v_2, \ldots, v_p\}$. Then by Lemma 2.1, and note that H cannot be isomorphic to H_i^* and H_j^* at the same time if $i \neq j$, there exists an integer t with $t < p$ such that $d(u_t) \leq t$ and $d(v_{p-t}) \leq p - t$. Thus we have

$$\begin{aligned} M_1(H) &= \sum_{j=1}^{p} d_j^2 \\ &\leq tt^2 + (p-t)p^2 + (p-t)(p-t)^2 + tp^2 \\ &= 3pt^2 - 3p^2 t + 2p^3. \end{aligned}$$

Define

$$f(x) = 3px^2 - 3p^2 x = 3px(x - p)$$

with $1 \leq k \leq x \leq p - 1$. Then we get

$$f'(x) = 6px - 3p^2, \text{ and } f''(x) = 6p > 0, \text{ as } p \geq 2.$$

Hence $f(x)$ is strictly convex up for $k \leq x \leq p-1$. Note that $f(1) = f(p-1)$. Since $k \geq 1$, we have $f(x) \leq f(p-1)$ for $k \leq x \leq p - 1$. By direct calculation, we obtain

$$f(p - 1) = -3p^2 + 3p.$$

Thus

$$M_1(H) \leq 2p^3 - 3p^2 + 3p.$$

In combination with the conditions of the theorem, the above inequality is true if and only if we take an equal sign, i.e.,

$$M_1(H) = 2p^3 - 3p^2 + 3p.$$

This implies that $H \cong H^*$, contrary to the assumption. Hence H is Hamiltonian.

Conversely, suppose that $H \cong H^*$. Then one can check that H is not Hamiltonian. □

Theorem 3.2. *Let H be a bipartite graph of order $2p$ with $p \geq 2$ vertices in each part and $\delta(H) \geq k \geq 1$. If*

$$RDD(H) \geq 3p^3 - \frac{14}{3}p^2 + \frac{14}{3}p - 1,$$

then H is Hamiltonian if and only if $H \ncong H^*$.

Proof. Sufficiency. Suppose that H is not Hamiltonian, and lets say $V(H) = \{u_1, u_2, \ldots, u_p; v_1, v_2, \ldots, v_p\}$. Therefore according to Lemma 2.1, and notice that H cannot be isomorphic to H_i^* and H_j^* at the same time if $i \neq j$, there exists an integer t with $t < p$ such that $d(u_t) \leq t$ and $d(v_{p-t}) \leq p - t$. Therefore by the definition of RDD and inequality (1), we have

$$\begin{aligned} \mathrm{RDD}(H) &= \sum_{v_j \in V(H)} \deg(v_j)\widehat{D}_H(v_j) \\ &\leq \sum_{v_j \in V(H)} \deg(v_j)\Big(\deg(v_j) + \frac{1}{2}\big(p-1\big) + \frac{1}{3}\big(p - \deg(v_j)\big)\Big) \\ &= \frac{1}{6}\Big((5p-3)\sum_{v_j \in V(H)} \deg(v_j) + 4\sum_{v_j \in V(H)} \deg(v_j)^2\Big) \\ &\leq \frac{1}{6}(5p-3)\Big(tt + (p-t)p + (p-t)(p-t) + tp\Big) \\ &\quad + \frac{4}{6}\Big(tt^2 + (p-t)p^2 + (p-t)(p-t)^2 + tp^2\Big) \\ &= \frac{1}{3}\Big((11p-3)t^2 - (11p^2 - 3p)t\Big) + 3p^3 - p^2. \end{aligned}$$

We define

$$g(x) = (11p-3)x^2 - (11p^2 - 3p)x = (11p-3)x(x-p)$$

with $1 \leq k \leq x \leq p-1$. Then we get

$$g'(x) = 2(11p-3)x - 11p^2 + 3p, \text{ and } g''(x) = 2(11p-3) > 0, \text{ as } p \geq 2,$$

which implies that $g(x)$ is convex up on $k \leq x \leq p-1$. One can see that $g(1) = g(p-1)$. Since $k \geq 1$, we have $g(x) \leq g(p-1)$. Note that

$$g(p-1) = -11p^2 + 14p - 3.$$

Hence

$$\mathrm{RDD}(H) \leq \frac{1}{3}\Big(-11p^2 + 14p - 3\Big) + 3p^3 - p^2 = 3p^3 - \frac{14}{3}p^2 + \frac{14}{3}p - 1.$$

In combination with the conditions of the theorem, the above inequality holds if and only if the equation holds, i.e.,

$$\mathrm{RDD}(H) = \frac{1}{3}\Big(-11p^2 + 14p - 3\Big) + 3p^3 - p^2 = 3p^3 - \frac{14}{3}p^2 + \frac{14}{3}p - 1.$$

This implies that $H \cong H^*$, contrary to the assumption. Hence H is Hamiltonian.

Conversely, suppose that $H \cong H^*$. Then one can check that H is not Hamiltonian. □

Theorem 3.3. *Let H be a bipartite graph of order $2p$ with $p \geq 2$ vertices in each part and $\delta(H) \geq k \geq 1$. If*

$$F(H) \geq 2(p^4 - 2p^3 + 3p^2 - 2p + 1),$$

then H is Hamiltonian if and only if $H \ncong H^*$.

Proof. Sufficiency. Suppose that H is not Hamiltonian, and denote $V(H) = \{u_1, u_2, \ldots, u_p; v_1, v_2, \ldots, v_p\}$. So by using Lemma 2.1, and paying attention to a fact that H cannot be isomorphic to H_i^* and H_j^* at the same time if $i \neq j$, there exists an integer t with $t < p$ such that $d(u_t) \leq t$ and $d(v_{p-t}) \leq p - t$. So by the definition of the forgotten topological index, we get

$$\begin{aligned} F(H) &= \sum_{j=1}^{p} d_j^3 \\ &\leq tt^3 + (p-t)p^3 + (p-t)(p-t)^3 + tp^3 \\ &= 2\Big(t^4 - 2pt^3 + 3p^2t^2 - 2p^3t\Big) + 2p^4. \end{aligned}$$

Considering the following function

$$h(x) = x^4 - 2px^3 + 3p^2x^2 - 2p^3x = x(x-p)(x^2 - px + 2p^2)$$

with $1 \le k \le x \le p-1$. Note that $x^2 - px + 2p^2 > 0$ for any $x \in [k, p-1]$.
Claim 1 : $h(x)$ is convex up for $k \le x \le p-1$.

Proof. By taking the first and second derivatives of $h(x)$, we have

$$h'(x) = 4x^3 - 6px^2 + 6p^2x - 2p^3, \text{ and } h''(x) = 6(2x^2 - 2px + p^2).$$

Then the discriminant of the equation $h''(x) = 0$ is $\gamma(p) = -4p^2 < 0$. So $h''(x) > 0$, and Claim 1 is proven. □

By Claim 1, and notice that x is an integer, one can see that the maximum value of $h(x)$ can only be $h(k)$ or $h(p-1)$. Since $h(1) = h(p-1)$, and $k \ge 1$, we have $h(x) \le h(p-1)$ for $k \le x \le p-1$. Thus

$$F(H) \le 2(p^4 - 2p^3 + 3p^2 - 2p + 1).$$

In combination with the conditions of the theorem, the above inequality is true if and only if we take an equal sign, i.e.,

$$F(H) = 2(p^4 - 2p^3 + 3p^2 - 2p + 1).$$

This implies that $H \cong H^*$, contrary to the assumption. Hence H is Hamiltonian.
Conversely, suppose that $H \cong H^*$. Then one can check that H is not Hamiltonian. □

Data availability

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