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Research Article

Maximizing the Hamming Spectral Radius in Graphs

Zikai Tang[‡], Binlian Li

MOE-LCSM, School of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan, China

Abstract

Let $B(G)$ denote the incidence matrix of a simple connected graph G. The Hamming matrix $H(G)$ of G is defined as the matrix whose entries are the Hamming distances between the binary strings derived from the rows of $B(G)$. The spectral radius of $H(G)$ is called the Hamming spectral radius of G. In this paper, we characterize the graphs that maximize the Hamming spectral radius among connected graphs of a given order under either of the following conditions: (i) exactly one vertex has degree greater than 2; (ii) exactly two vertices have degree greater than 2.

Keywords: incidence matrix; Hamming distance; Hamming matrix; Hamming spectral radius; extremal graphs.

2020 Mathematics Subject Classification: 05C50.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d(v)$ of a vertex v in G is the number of its neighbors. Denote by $A(G)$, $L(G)$, $Q(G)$ and $B(G)$ the adjacency matrix, the Laplacian matrix, the signless Laplacian matrix and the incidence matrix of G, respectively. Let $J_{n\times m}$ be the $n \times m$ matrix with all entries equal to 1. Let $O_{n\times m}$ be the $n \times m$ matrix with all entries equal to 0. If $n = m$, we write J_n and O_n, or simply J and O. Denote by I_n, or simply I, the $n \times n$ identity matrix. Let $M = [m_{ij}]_{n\times n}$ be a real symmetric matrix associated to G. The spectrum Sp_M of the matrix M is the collection of all eigenvalues of M, i.e.,

$$Sp_M := \{\lambda : det(\lambda I - M) = 0\}.$$

In particular, if M is equal to one of the matrices $A(G)$, $L(G)$ and $Q(G)$, then the corresponding eigenvalues (or spectrum) are called A-eigenvalues (or A-spectrum, denoted by $Sp_A(G)$), L-eigenvalues (or L-spectrum, denoted by $Sp_L(G)$) and Q-eigenvalues (or Q-spectrum, denoted by $Sp_Q(G)$), respectively. Throughout this paper, these eigenvalues are denoted by $\lambda_1 \geq \lambda_1 \geq \cdots \geq \lambda_n$, $\mu_1 \geq \mu_1 \geq \cdots \geq \mu_n = 0$ and $q_1 \geq q_2 \geq \cdots \geq q_n$, respectively.

Spectral graph theory is a branch of graph theory with wide-ranging applications in physics, chemistry, operations research, electronics, information theory and network theory. Numerous results concerning the eigenvalues of graph matrices are available in the literature; for instance, see [1, 4–7]. Notation used in this paper can be found in [2].

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[‡]Corresponding author (zikaitang@163.com).
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Let $\mathbb{Z}_2 = \{0, 1\}$ and denote by $(\mathbb{Z}_2, +)$ the additive group, where $+$ denotes addition modulo 2. For any positive integer n, let

$$\mathbb{Z}_2^n = \{(x_1, x_2, \dots, x_n) : x_1, x_2, \dots, x_n \in \mathbb{Z}_2\}.$$

Every element of $\mathbb{Z}_2^n$ is an n-tuple $(x_1, x_2, \dots, x_n)$ written as $x = x_1 x_2 \dots x_n$, where every x_i is either 0 or 1 and it is called a string. Let $x = x_1 x_2 \dots x_n$ and $y = y_1 y_2 \dots y_n$ be the elements of $\mathbb{Z}_2^n$. Then the sum $x \oplus y$ is computed by adding the corresponding components of x and y under addition modulo 2. That is, $x_i + y_i = 0$ if $x_i = y_i$ and $x_i + y_i = 1$ if $x_i \neq y_i$, for $i = 1, 2, \dots, n$.

The Hamming distance $H_d(x, y)$ between the strings $x = x_1 x_2 \dots x_n$ and $y = y_1 y_2 \dots y_n$ is the number of is such that $x_i \neq y_i$, where $i = 1, 2, \dots, n$. Denote by $s(v)$ the row of the incidence matrix corresponding to the vertex v of graph G. It is a string in the set $\mathbb{Z}_2^m$ of all $m-$tuples over the field of order two, where m is the size of G. Recently, Ramane et. al. [11] and Vučićević et. al. [12] introduced the Hamming index $H_B(G)$ and Hamming matrix $H(G)$, which are defined, respectively, as

$$H_B(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} h_{ij}$$

and

$$H(G) = [h_{ij}]_{n \times n}.$$

where $h_{ij} = H_d(s(v_i), s(v_j))$. The spectrum $Sp_H(G)$ of the Hamming matrix $H(G)$ is the collection of all eigenvalues of $H(G)$, i.e.,

$$Sp_H(G) := \{\nu : det(\nu I - H) = 0\} = \{\nu_1, \nu_2, \dots, \nu_n\},$$

where $\nu_1 \geq \nu_2 \geq \cdots \geq \nu_n$. Here, ν_1 is called the Hamming spectral radius of the graph G.

The Hamming energy $HE(G)$ of the graph G is defined [12] as

$$HE(G) = \sum_{i=1}^{n} |\nu_i|.$$

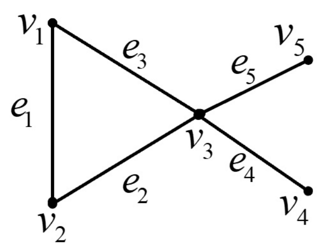

Figure 1.1: The graph G used in Example 1.1.

Example 1.1. *For the graph G shown in Figure 1.1, the incidence matrix $B(G)$ and the Hamming matrix $H(G)$ are given as follows:*

$$B(G) = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \text{ and } H(G) = \begin{pmatrix} 0 & 2 & 4 & 3 & 3 \\ 2 & 0 & 4 & 3 & 3 \\ 4 & 4 & 0 & 3 & 3 \\ 3 & 3 & 3 & 0 & 2 \\ 3 & 3 & 3 & 2 & 0 \end{pmatrix}$$

Hence, the Hamming spectrum of G is $Sp_H(G) = \{12.0780, -2.0000, -2.0000, -3.1742, -4.9038\}$.

In [11], an algorithm was developed to compute the Hamming distance and the Hamming index. In [12], some bounds on the Hamming energy of graphs were derived.

In this paper, we characterize the graphs that maximize the Hamming spectral radius among connected graphs of a given order under either of the following conditions: (i) exactly one vertex has degree greater than 2, (ii) exactly two vertices have degree greater than 2.

2. Preliminaries

In this section, we present several results that will be used in the subsequent section.

Lemma 2.1 (see [11]). *Let G be a graph with n vertices and m edges. Let u and v be any two vertices of G. Let l be the number of those edges that are neither incident to u nor incident to v. Then*

$$H_d(s(v), s(u)) = \begin{cases} m - l - 1 & \text{if } u \sim v; \\ m - l & \text{if } u \nsim v. \end{cases} \tag{1}$$

$$H_d(s(v), s(u)) = \begin{cases} d(u) + d(v) - 2 & \text{if } u \sim v; \\ d(u) + d(v) & \text{if } u \nsim v. \end{cases} \tag{2}$$

Lemma 2.2 (see [10]). *Let M and N be nonnegative irreducible matrices with the same order. If $(N)_{ij} \leq (M)_{ij}$ for each all i and j, then $\rho(N) \leq \rho(M)$ with equality if and only if $M = N$, where $\rho(N)$ and $\rho(M)$ denote the spectral radii of N and M, respectively.*

Lemma 2.3 (see [8]). *Let M be a symmetric matrix and λ_1 be the largest eigenvalue of M. Let x be a non-zero vector, then*

$$\lambda_1 \geq \frac{x^T M x}{x^T x}$$

with equality if and only if $Mx = \lambda_1 x$.

Let $M = (m_{ij})$ be a nonnegative matrix. Let D be a directed graph such that there is a directed arc from vertex i to vertex j if and only if $m_{ij} \neq 0$. This graph is called the directed graph of M and is denoted by $D(M)$. If M is a nonnegative symmetric matrix, then its corresponding directed graph $D(M)$ is an undirected graph. Further details about $D(M)$ can be found in [9].

Lemma 2.4 (see [9]). *Let $A = (a_{ij})$ be the nonnegative matrix with order $n > 1$. Then $D(A)$ is strongly connected if and only if A is irreducible.*

Lemma 2.5. *Let G be a simple connected graph with $n \geq 3$ vertices. Then $H(G)$ is irreducible.*

Proof. By the definition of the Hamming index of G, we have that $h_{ij} > 0$ for $i \neq j$ and $h_{ij} = 0$ for $i = j$. Hence, the directed graph $D(H(G))$ is strongly connected. By Lemma 2.4, the matrix $H(G)$ is irreducible. □

Proposition 2.6. *Let G be a simple connected graph. Let $u, v \in V(G)$ such that $uv \notin E(G)$. Denote by $G' = G + uv$ the graph obtain from G by adding the edge uv. Then, $\nu_1(G') > \nu_1(G)$.*

Proof. By Lemma 2.5, the matrices $H(G)$ and $H(G')$ are irreducible. Let $V(G) = \{u, v\} \cup V_u \cup V_v \cup V_1$, where V_u and V_v are the sets of neighbors of u and v, respectively, whereas $V_1 = V(G) \setminus (\{u, v\} \cup V_u \cup V_v)$.

Let $H(G') = [h'_{ij}]$. By the definition of the Hamming index, we have that

$$h'_{ij} = \begin{cases} h_{ij}+1 & \text{if } v_i = u, v_j \in V_1; \\ h_{ij}+1 & \text{if } v_i = v, v_j \in V_1; \\ h_{ij} & \text{otherwise.} \end{cases}$$

Therefore, from Lemma 2.2, it follows that $\nu_1(G') > \nu_1(G)$. □

Proposition 2.7. *Let G be a simple connected graph with order $n > 3$. Then,*

$$n-1 < \nu_1(G) \le (2n-4)(n-1),$$

where the right equality holds if and only if $G \cong K_n$.

Proof. By Lemma 2.1, we have that $H_d(s(v), s(u)) > 1$ for $u \neq v$ and $H_d(s(v), s(u)) = 0$ for $u = v$. Hence, it follows that $H(G) > J - I$. Let $A(K_n)$ be the adjacency matrix of the complete graph K_n. Then, by Lemma 2.2, we have that $\nu_1(G) > n-1 = \rho(K_n)$.

Since the complete graph K_n can be obtained from any graph G of order n by adding edges, by Lemma 2.6, we have $\nu_1(G) \le \nu_1(K_n) = (2n-4)(n-1)$. □

Lemma 2.8 (see [3]). *Let M be a nonnegative irreducible. Then there is a (unique) positive real number λ_0 with the following properties:*

(i). *There is a real vector $x > 0$ with $Mx = \lambda_0 x$.*

(ii). *λ_0 has geometric and algebraic multiplicity 1.*

(iii). *For each eigenvalue λ of M, it holds that $|\lambda| \le \lambda_0$.*

3. Graphs With Only One Vertex of Degree Greater Than 2

Let $\mathcal{G}_n^{(1)}$ denote the set of graphs of order n in which each graph $G \in \mathcal{G}_n^{(1)}$ has exactly one vertex of degree greater than 2.

Lemma 3.1. *Let $G \in \mathcal{G}_n^{(1)}$ be a graph with the maximum Hamming spectral radius. Let $w \in V(G)$ be the vertex of degree greater than 2. Then, there is at most one vertex of degree 1 in G. Also, if G contains a vertex of degree 1, then it must be adjacent to w.*

Proof. Suppose to the contrary that there are at least two vertices $u, v \in V(G)$ of degree 1. Let $G' = G + uv$ be the graph obtain from G by adding the edge uv. Then, $G' \in \mathcal{G}_n^{(1)}$. By Lemma 2.6, we have that $\nu_1(G') > \nu_1(G)$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(1)}$ has the maximum Hamming spectral radius.

Now, suppose that G contains a vertex v of degree 1 such that v is not adjacent to w. Let $G'' = G + wv$ be the graph obtain from G by adding the edge wv. Then, $G'' \in \mathcal{G}_n^{(1)}$. However, by Lemma 2.6, we have that $\nu_1(G'') > \nu_1(G)$, which is a contradiction to fact that $G \in \mathcal{G}_n^{(1)}$ has the maximum Hamming spectral radius. □

Lemma 3.2. *Let $G \in \mathcal{G}_n^{(1)}$ be a graph with the maximum Hamming spectral radius. Let $w \in V(G)$ be the vertex of degree $d > 2$. Then, G contains no cycle of length more than four.*

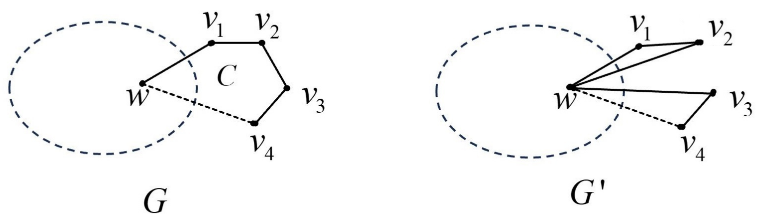

Figure 3.1: Two graphs $G, G' \in \mathcal{G}_n^{(1)}$ used in the proof of Lemma 3.2.

Proof. Suppose to the contrary that G contains a cycle C of length more than four. Let $C = wv_1v_2v_3v_4\dots w$ (see Figure 3.1). Let G' be the graph obtain from G by deleting v_2v_3 and adding wv_2, wv_3 (see Figure 3.1). Then $d_{G'}(w) = d_G(w) + 2$ and $d_{G'}(u) = d_G(u)$ for every other vertex $u \in V(G)$. Let ν_1 and ν_1' be the Hamming spectral radii of the graphs G and G', respectively. Let $V_1 = \{w, v_2, v_3\}$ and $V_2 = V \setminus V_1$. By the definition of the Hamming index, we have that

$$h'_{uv} = \begin{cases} h_{uv} + 2 & \text{if } u = w, v \in V_2; \\ h_{uv} + 2 & \text{if } u = v_2, v = v_3; \\ h_{uv} & \text{otherwise.} \end{cases}$$

Hence, by Lemma 2.2, we have $\nu_1' > \nu_1$, a contradiction to the fact that the graph $G \in \mathcal{G}_n^{(1)}$ has the maximum Hamming spectral radius. □

Lemma 3.3. *Let $G \in \mathcal{G}_n^{(1)}$ be a graph with the maximum Hamming spectral radius. Let $w \in V(G)$ be the vertex of degree $d > 2$. Then, G contains at most one cycle of length four.*

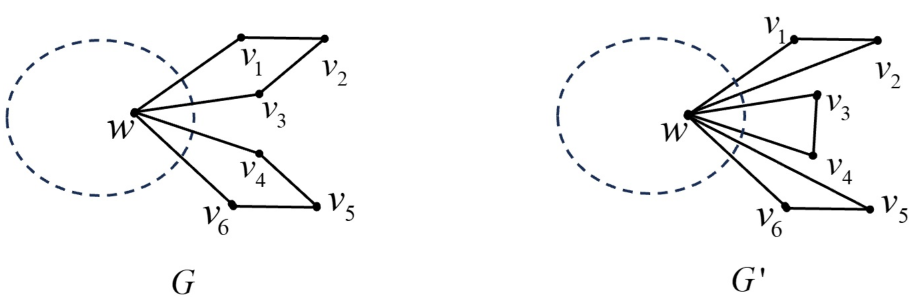

Figure 3.2: Two graphs $G, G' \in \mathcal{G}_n^{(1)}$ used in the proof of Lemma 3.3.

Proof. Suppose to the contrary that G contains two cycles of length four. Let $wv_1v_2v_3$ and $wv_4v_5v_6$ be two cycles of length four in G (see Figure 3.2). Let G' be the graph obtain from G by deleting two edges v_2v_3, v_4v_5 and adding three edges v_3v_4, wv_2, wv_5 (see Figure 3.1). Then, $d_{G'}(w) = d_G(w) + 2$ and $d_{G'}(u) = d_G(u)$ for every other vertex $u \in V(G)$. Let ν_1 and ν_1' be the Hamming spectral radii of the graphs G and G', respectively. By Proposition 2.7, we have that $\nu_1 > n - 1$ and $\nu_1' > n - 1$. By Lemma 2.8, there is a vector $x > 0$ with $H(G)x = \nu_1 x$ and $|x| = 1$. Let $x = (x_0, x_1, x_2, x_3, x_4, \dots, x_n)^T$ with corresponding vertices in the set $\{w, v_1, v_2, v_3, v_4, \dots, v_{n-1}\}$. By symmetry, we have that $x_1 = x_3 = x_4 = x_6$ and $x_2 = x_5$. By the characteristic equations for the vertices v_1, v_2, we have that

$$\begin{cases} dx_0 + 2x_2 + 4x_3 + a = \nu_1 x_1, \\ (d+2)x_0 + 2x_1 + 2x_3 + a = \nu_1 x_2, \end{cases}$$

and hence, $2x_0 = (\nu_1 - 2)(x_2 - x_1) > 0$. Therefore, $x_2 > x_1 > 0$.

On the other hand, by the definition of the Hamming index, we have that

$$H(G') - H(G) = \begin{pmatrix} A_1 & A_2 \\ A_2^T & O_{(n-7)\times(n-7)} \end{pmatrix},$$

where

$$A_1 = \begin{array}{c} \begin{array}{ccccccc} w & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 \end{array} \\ \begin{pmatrix} 0 & 2 & 0 & 2 & 2 & 0 & 2 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & -2 & 0 & 0 \\ 2 & 0 & 0 & -2 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \quad \text{and } A_2 = \begin{pmatrix} 2J_{1\times(n-7)} \\ O_{6\times(n-7)} \end{pmatrix}.$$

Since $x_5 = x_2 > x_1 = x_3 = x_4 = x_6$ and $x_i > 0$ for any $i = 0, 1, 2, \ldots, n-1$, we have that

$$\begin{aligned} x^T(H(G') - H(G))x &= 2x_0\left(x_1 + x_3 + x_4 + x_6 + \sum_{i=7}^{n-1} x_i\right) + 2x_0x_1 + 2x_3x_2 + 2x_3(x_0 + x_2 - x_4) \\ &\quad + 2x_4(x_0 - x_3 + x_5) + 2x_5x_4 + 2x_6x_0 + 2x_0\sum_{i=7}^{n-1} x_i \\ &= 16x_0x_1 + 8x_1x_2 - 4x_1^2 + 4x_0\sum_{i=7}^{n-1} x_i > 0. \end{aligned}$$

Therefore, by Lemma 2.3, we have $\nu_1 < \nu_1'$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(1)}$ has the maximum Hamming spectral radius. □

Theorem 3.4. *Let $G \in \mathcal{G}_n^{(1)}$ be a graph and $w \in V(G)$ be the vertex of degree $d > 2$.*

(i). *If $n > 4$ is even, then $\nu_1(G) \le \nu_1(G_1)$, where the equality holds if and only if $G \cong G_1$ (see Figure 3.3).*

(ii). *If $n > 5$ is odd, then $\nu_1(G) \le \nu_1(G_3)$, where the equality holds if and only if $G \cong G_3$ (see Figure 3.3).*

Proof. Let $G \in \mathcal{G}_n^{(1)}$ be a graph with the maximum Hamming spectral radius. Let $w \in V(G)$ be the vertex of degree $d > 2$. From Lemmas 3.1, 3.2 and 3.3, it follows that $G \in \mathcal{G}_n^{(1)}$ must be isomorphic to either G_1 or G_2 (depicted in Figure 3.3) when n is even, and $G \in \mathcal{G}_n^{(1)}$ is isomorphic to either G_3 or G_4 (shown in Figure 3.3) when n is odd.

If $n > 4$ is even, then we have that $d_{G_1}(w) = d = n-1$ and $d_{G_2}(w) = d-1 = n-2$. Let ν_1 and ν_1' be the Hamming spectral radii of the graphs G_1 and G_2, respectively. By Proposition 2.7, we have that $\nu_1 > n-1$ and $\nu_1' > n-1$. By Lemma 2.8, there is a vector $x > 0$ with $H(G_2)x = \nu_1'x$ and $|x| = 1$. Let $x = (x_0, x_1, x_2, x_3, x_4, \ldots, x_n)^T$ with corresponding vertices in $\{w, v_1, v_2, v_3, v_4, \ldots, v_{n-1}\}$. By symmetry, we have that $x_1 = x_3$ and $x_i = a$ for $4 \le i \le n-1$. By the characteristic equations for vertices w, v_1, v_2, v_4, we have that

$$\begin{cases} x_1(d-1) + x_2(d+1) + x_3(d-1) + a(d-1)(n-4) = \nu_1'x_0, \\ x_0(d-1) + 2x_2 + 4x_3 + 4a(n-4) = \nu_1'x_1, \\ x_0(d+1) + 2x_1 + 2x_3 + 4a(n-4) = \nu_1'x_2, \\ x_0(d-1) + 4x_1 + 4x_2 + 4x_3 + 2a + 4a(n-6) = \nu_1'a. \end{cases}$$

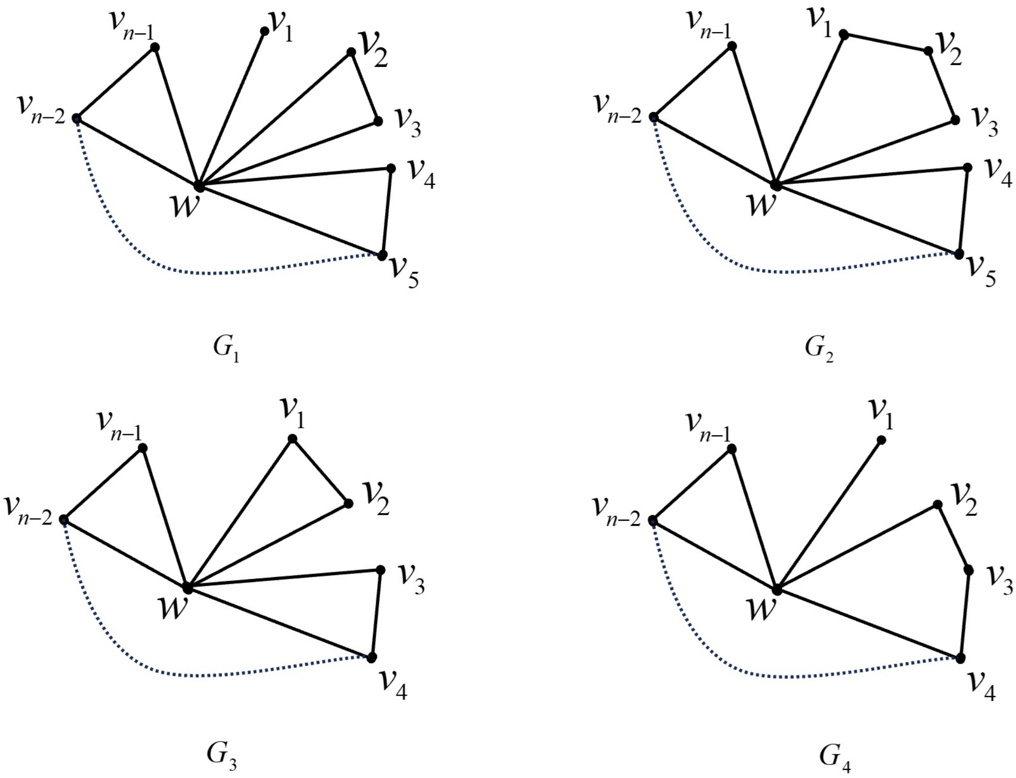

Figure 3.3: Four graphs used in the proof of Theorem 3.4.

Consequently, we obtain

$$\begin{cases} x_2(d-1)+x_3(d-5)+a(d-5)(n-4)=(\nu_1'+d-1)(x_0-x_1)>0,\\ x_1(d-1)+x_3(d-5)+a(d-5)(n-4)=(\nu_1'+d+1)(x_0-x_2)>0,\\ 2(x_0-x_2)=\nu_1'(x_2-x_1),\\ 2(x_2-x_1)=(\nu_1'+6)(a-x_1). \end{cases}$$

Hence, $x_0-x_1>0$, $x_0-x_2>0$, $x_2-x_1>0$ and $a>x_1$. By the definition of the Hamming index, we have that

$$H(G_1)-H(G_2)=\begin{pmatrix} A_1 & A_2 \\ A_2^T & O_{(n-4)\times(n-4)} \end{pmatrix},$$

where

$$A_1=\begin{array}{c} \begin{array}{cccc} w & v_1 & v_2 & v_3 \end{array} \\ \begin{pmatrix} 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix} \end{array}$$

and

$$A_2=\begin{pmatrix} J_{1\times(n-4)} \\ -J_{1\times(n-4)} \\ O_{2\times(n-4)} \end{pmatrix}.$$

Since $x_0 - x_1 > 0$, $x_0 - x_2 > 0$, $x_2 - x_1 > 0$ and $2(x_2 - x_1) = (\nu_1' + 6)(a - x_1)$, we have that

$$\begin{aligned} x^T(H(G_1) - H(G_2))x &= (-x_2 + x_3 + a(n-4))x_0 + (x_2 - x_3 - a(n-4))x_1 \\ &\quad + (-x_0 + x_1)x_2 + (x_0 - x_1)x_3 + a(x_0 - x_1)(n-4) \\ &= 2(x_1 - x_2)(x_0 - x_1) + 2a(x_0 - x_1)(n-4) \\ &= 2(x_0 - x_1)\left(a(n-4) - \frac{2}{\nu_1' + 6}(a - x_1)\right) \\ &= \frac{2(x_0 - x_1)}{\nu_1' + 6}\Big(a(n-4)(\nu_1' + 6) - 2(a - x_1)\Big). \end{aligned}$$

Since $n > 4$ and $\nu_1' > n_1$, we have that $(n-4)(\nu_1' + 6) - 2 > 0$. Hence, $x^T(H(G_1) - H(G_2))x > 0$. Now, from Lemma 2.3, it follows that $\nu_1 > \nu_1'$.

If $n > 5$ is odd, then we have that $d_{G_3}(w) = d = n - 1$ and $d_{G_4}(w) = d - 1 = n - 2$. Let ν_1 and ν_1' be the Hamming spectral radii of the graphs G_3 and G_4, respectively. By Proposition 2.7, we have that $\nu_1 > n - 1$ and $\nu_1' > n - 1$. By Lemma 2.8, there is a vector $x > 0$ with $H(G_4)x = \nu_1' x$ and $|x| = 1$. Let $x = (x_0, x_1, x_2, x_3, x_4, \ldots, x_n)^T$ with corresponding vertices in $\{w, v_1, v_2, v_3, v_4, \ldots, v_{n-1}\}$. By symmetry, we have that $x_2 = x_4$ and $x_i = a$ for $5 \le i \le n - 1$. By the characteristic equations for vertices w, v_1, v_2, v_3, v_5, we have that

$$\begin{cases} x_1(d-2) + x_2(d-1) + x_3(d+1) + x_4(d-1) + a(d-1)(n-5) = \nu_1' x_0, \\ x_0(d-2) + 3x_2 + 3x_3 + 3x_4 + 3a(n-5) = \nu_1' x_1, \\ x_0(d-1) + 3x_1 + 2x_3 + 4x_4 + 4a(n-5) = \nu_1' x_2, \\ x_0(d+1) + 3x_1 + 2x_2 + 2x_4 + 4a(n-5) = \nu_1' x_3, \\ x_0(d-1) + 3x_1 + 4x_2 + 4x_3 + 4x_4 + 2a + 4a(n-7) = \nu_1' a. \end{cases}$$

By the above system of equations, we have that

$$x_0(d-4) + 5x_3 + 5x_4 + 3a(n-5) = \nu_1'(x_1 + x_2 - x_3) > 0,$$

and therefore, $x_1 + x_2 - x_3 > 0$. By the definition of the Hamming index, we have that

$$H(G_1) - H(G_2) = \begin{pmatrix} A_1 & A_2 \\ A_2^T & O_{(n-5)\times(n-5)} \end{pmatrix},$$

where

$$A_1 = \begin{array}{c} \begin{array}{ccccc} w & v_1 & v_2 & v_3 & v_4 \end{array} \\ \begin{pmatrix} 0 & 2 & 1 & -1 & 1 \\ 2 & 0 & -1 & 1 & 1 \\ 1 & -1 & 0 & 2 & 0 \\ -1 & 1 & 2 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

and

$$A_2 = \begin{pmatrix} J_{1\times(n-5)} \\ J_{1\times(n-5)} \\ O_{3\times(n-5)} \end{pmatrix}.$$

Since $x > 0$ and $x_1 + x_2 - x_3 > 0$, we have that

$$\begin{aligned} x^T(H(G_1) - H(G_2))x &= x_0(2x_1 + x_2 - x_3 + x_4 + a(n-5)) + x_1(2x_0 - x_2 + x_3 + x_4 + a(n-5)) \\ &\quad + x_2(x_0 - x_1 + 2x_3) + x_3(-x_0 + x_1 + 2x_2) + x_4(x_0 + x_1) + a(x_0 + x_1)(n-5) \\ &= x_0(2x_1 + 2x_2 - x_3) + x_1(2x_0 + x_3) + x_2(x_0 - x_1 + 2x_3) + x_3(-x_0 + x_1 + 2x_2) \\ &\quad + x_2(x_0 + x_1) + 2a(x_0 + x_1)(n-5) \\ &= 4x_0x_1 + 4x_0x_2 - 2x_0x_3 + 2x_1x_3 + 4x_2x_3 + 2a(x_0 + x_1)(n-5) \\ &> 2x_0(x_1 + x_2 - x_3) > 0. \end{aligned}$$

Hence, $x^T(H(G_3) - H(G_4))x > 0$. Therefore, from Lemma 2.3, it follows that $\nu_1 > \nu_1'$. □

4. Graph With Exactly Two Vertices of Degree Greater Than 2

Let $\mathcal{G}_n^{(2)}$ denote the set of graphs of order n in which each graph $G \in \mathcal{G}_n^{(1)}$ has exactly two vertices of degree greater than 2.

Lemma 4.1. *Let $G \in \mathcal{G}_n^{(2)}$ be a graph with the maximum Hamming spectral radius. Let $w_1, w_2 \in V(G)$ be the vertices of degree greater than 2. Then, $w_1w_2 \in E(G)$ and G contains no pendant vertex.*

Proof. Suppose to the contrary that w_1 and w_2 are not adjacent. Let $G' = G + w_1w_2$ be the graph obtained from G by adding the edge w_1w_2. Then $G' \in \mathcal{G}_n^{(2)}$. By Lemma 2.6, we have that $\nu_1(G') > \nu_1(G)$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(2)}$ has the maximum Hamming spectral radius.

Suppose that there is a pendant vertex u in G. Let $d(w_1, u) < d(w_2, u)$. Let $G'' = G + w_2u$ be the graph obtained from G by adding the edge w_2u. Then $G'' \in \mathcal{G}_n^{(2)}$. By Lemma 2.6, we have that $\nu_1(G'') > \nu_1(G)$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(2)}$ has the maximum Hamming spectral radius. □

Lemma 4.2. *Let $G \in \mathcal{G}_n^{(2)}$ be a graph with the maximum Hamming spectral radius. Let $w_1, w_2 \in V(G)$ be the vertices of degree greater than 2. Then, there is no cycle of the form $C = w_2v_1v_2 \ldots w_2$ in G.*

Proof. Suppose to the contrary that there is a cycle $C = w_2v_1v_2 \ldots w_2$ in G. Let G' be the graph obtained from G by deleting the edge v_1v_2 and adding the two edges w_1v_1, w_1v_2 (see Figure 4.1). Then, $d_{G'}(w_1) = d_G(w_1) + 2$ and $d_{G'}(u) = d_G(u)$ for every other vertex $u \in V(G)$.

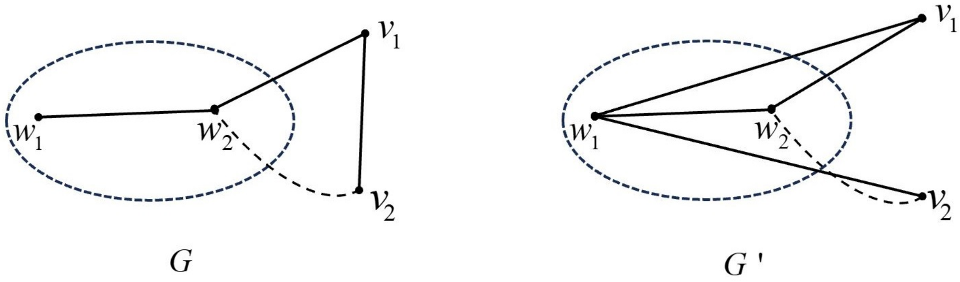

Figure 4.1: Two graphs used in the proof of Lemma 4.2.

Let $V_1 = \{w_1, w_2, v_1, v_2\}$ and $V_2 = V \setminus V_1$. By the definition of the Hamming index, we have that

$$h'_{uv} = \begin{cases} h_{uv} + 2 & \text{if } u = w_1, v = w_2; \\ h_{uv} + 2 & \text{if } u = v_1, v = v_2; \\ h_{uv} + 2 & \text{if } u = w_1, v \in V_2; \\ h_{uv} & \text{otherwise.} \end{cases}$$

Therefore, from Lemma 2.2, it follows that $\nu_1(G') > \nu_1(G)$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(2)}$ has the maximum Hamming spectral radius. □

Lemma 4.3. *Let $G \in \mathcal{G}_n^{(2)}$ be a graph with the maximum Hamming spectral radius. Let $w_1, w_2 \in V(G)$ be the vertices of degree greater than 2. Then, G contains no cycle of the form $C = w_1v_1v_2 \dots w_2w_1$ of length more than four.*

Proof. Suppose to the contrary that there is a cycle $C = w_1v_1v_2 \dots w_2w_1$ with a length of more than four in G. Let G' be the graph obtained from G by deleting the two edges v_1v_2, v_2v_3, and adding the four edges $w_1v_2, w_1v_3, w_2v_1, w_2v_2$ (see Figure 4.2). Then, $d_{G'}(w_1) = d_G(w_1) + 2$ and $d_{G'}(w_2) = d_G(w_2) + 2$ and $d_{G'}(u) = d_G(u)$ for every other vertex $u \in V(G)$.

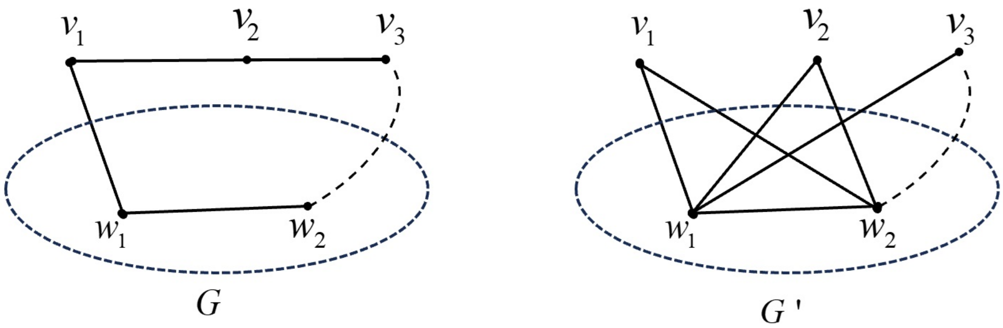

Figure 4.2: Two graphs used in the proof of Lemma 4.3.

Let $V_1 = \{w_1, w_2, v_1, v_2, v_3\}$ and $V_2 = V \setminus V_1$. By the definition of the Hamming index, we have that

$$h'_{uv} = \begin{cases} h_{uv} + 4 & \text{if } u = w_1, v = w_2; \\ h_{uv} + 2 & \text{if } u = v_1, v = v_2; \\ h_{uv} + 2 & \text{if } u = v_2, v = v_3; \\ h_{uv} + 2 & \text{if } u = w_1, v \in V_2; \\ h_{uv} + 2 & \text{if } u = w_2, v \in V_2; \\ h_{uv} & \text{otherwise.} \end{cases}$$

By Lemma 2.2, we have $\nu_1(G') > \nu_1(G)$, which is a contradiction to the fact that $G \in \mathcal{G}_n^{(2)}$ has the maximum Hamming spectral radius. □

The join $G_1 \vee G_2$ of two graphs G_1 and G_2 is the graph consisting of all the vertices and edges of both graphs G_1 and G_2 together with all possible edges between their vertex sets. Let $G_0 = K_2 \vee (n-2)K_1$, then $G_0 \in \mathcal{G}_n^{(2)}$.

Theorem 4.4. *If $G \in \mathcal{G}_n^{(2)}$, then $\nu_1(G) \leq \nu_1(G_0)$, where the equality holds if and only if $G \cong G_0$.*

Proof. Let $G \in \mathcal{G}_n^{(2)}$ be a graph with the maximum Hamming spectral radius. Let $w_1, w_2 \in V(G)$ be the vertices of degree greater than 2. Suppose that there is a cycle $C = w_1v_1v_2w_2w_1$. By Lemma 4.1 and 4.2 and 4.3, we have that $d_G(w_1) = d_G(w_2) = d$. Let G' be the graph obtained from G by deleting the edge v_1v_2 and adding the two edges w_1v_2, w_2v_1 (see Figure 4.3). Then, $d_{G'}(w_1) = d_G(w_1) + 1$ and $d_{G'}(w_2) = d_G(w_2) + 1$ and $d_{G'}(u) = d_G(u)$ for every other vertex $u \in V(G)$. By Lemma 2.8, there is a vector $x > 0$ with $H(G)x = \nu_1 x$ and $|x| = 1$. Let $x = (x_1, x_2, x_3, x_4, \dots, x_n)^T$ with corresponding vertices in $\{w_1, w_2, v_1, v_2, \dots, v_{n-2}\}$. By symmetry, we have that $x_1 = x_2$ and $x_3 = x_4$.

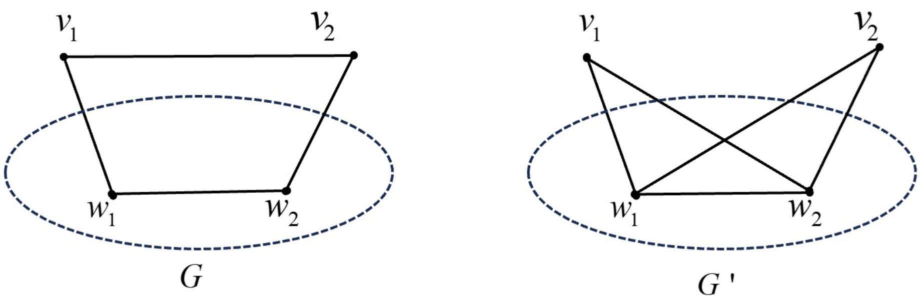

Figure 4.3: Two graphs used in the proof of Theorem 4.4.

By the definition of the Hamming index, we have that

$$H(G') - H(G) = \begin{pmatrix} A_1 & A_2 \\ A_2^T & O_{(n-4)\times(n-4)} \end{pmatrix},$$

where

$$A_1 = \begin{array}{c} \begin{array}{cccc} w_1 & w_2 & v_1 & v_2 \end{array} \\ \begin{pmatrix} 0 & 2 & 1 & -1 \\ 2 & 0 & 0 & 1 \\ 1 & 0 & 0 & 2 \\ -1 & 1 & 2 & 0 \end{pmatrix} \end{array}$$

and

$$A_2 = \begin{pmatrix} J_{1\times(n-4)} \\ J_{1\times(n-4)} \\ O_{2\times(n-4)} \end{pmatrix}.$$

Since $x > 0$, $x_1 = x_2$ and $x_3 = x_4$, we have that

$$\begin{aligned} x^T(H(G') - H(G))x &= x_1\left(2x_2 + x_3 - x_4 + \sum_{i=5}^{n} x_i\right) + x_2\left(2x_1 + x_4 + \sum_{i=5}^{n} x_i\right) + x_3(x_1 + 2x_4) \\ &\quad + x_4(-x_1 + x_2 + 2x_3) + (x_1 + x_2)\sum_{i=5}^{n} x_i \\ &= 4x_1x_2 + x_2x_4 + x_3(x_1 + 2x_4) + 2x_4x_3 + 2(x_1 + x_2)\sum_{i=5}^{n} x_i \\ &= 4x_1^2 + 2x_1x_3 + 4x_3^2 + 4x_1\sum_{i=5}^{n} x_i > 0. \end{aligned}$$

Therefore, $x^T(H(G') - H(G))x > 0$. Hence, by Lemma 2.3, we have $\nu_1(G') > \nu_1(G)$. Consequently, from Lemmas 4.1, 4.2 and 4.3, the required conclusion follows. □

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