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Research Article

On the Hamming Spectrum and Hamming Energy of Graphs

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Abstract

In this paper, we study the spectrum of the Hamming matrix $H(G)$ of a simple graph G. The Hamming matrix, recently introduced in terms of the Hamming distances between binary strings derived from the incidence matrix, offers an alternative and insightful perspective on spectral and chemical graph theory. We derive upper and lower bounds for the largest and smallest eigenvalues of the Hamming matrix of paths, respectively, as well as closed-form expressions for the Hamming spectrum and Hamming energy of regular graphs (including cycles as a special case), their complements, and their line graphs, with respect to the classical adjacency spectrum. Furthermore, we provide a factorization that relates the characteristic polynomial of the Hamming matrix of a regular graph to that of its complement and its line graph. These results shed new light on how Hamming-based invariants interact with classical spectral quantities.

Keywords: Hamming matrix; graph energy; regular graph; line graph; equitable partition.

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1. Introduction

The study of graph spectra has proven to be an invaluable approach to uncovering the structural properties and dynamics of graphs, with far-reaching applications in chemistry, physics, and computer science. Much attention has been paid to various matrix representations of graphs as a tool for understanding these complex structures.

Let $G = (V(G), E(G))$ be a simple graph with n vertices and m edges, where $V(G) = \{v_1, v_2, \dots, v_n\}$ and $E(G) = \{e_1, e_2, \dots, e_m\}$ are its sets of vertices and edges, respectively. If the vertices v_i and v_j are adjacent, we write $v_i \sim v_j$; otherwise, we write $v_i \nsim v_j$. The edge and its end vertex are said to be incident to each other. With $d_G(v)$ (or $d(v)$ for short) we denote the degree of a vertex v in a graph G, i.e., the number of edges incident to it. A graph is called r-regular if $d(v) = r$ for each vertex v.

The line graph $L(G)$ of a graph G is the graph whose vertices correspond to the edges of G, and two vertices in $L(G)$ are adjacent if and only if the corresponding edges are adjacent, i.e., have exactly one vertex in common.

As usual, we use P_n and C_n to denote the path and the cycle on n vertices, respectively.

With $A = A(G) = (a_{ij})_{n\times n}$ we denote the adjacency matrix of G. Furthermore, $D = D(G) = \mathrm{diag}(d(v_1), \dots, d(v_n))$ is the diagonal matrix of vertex degrees, and $I = I_n$ is the $n \times n$ identity matrix. By $J_{m\times n}$ we denote the $m \times n$ all-one matrix. If $m = n$, we use the notation J_n or J for short when its order is clear from the context.

Recall that the incidence matrix of G is a matrix $B(G) = (b_{ij})_{n\times m}$ in which $b_{ij} = 1$ if the vertex v_i is incident with the edge e_j, and $b_{ij} = 0$, otherwise. Its rows, when interpreted as binary strings, represent the vertices of a graph. Denoting the binary string corresponding to a vertex v by $s(v)$, the authors in the paper [12] introduced the so-called Hamming index of G (H-index for short), denoted by $H_B(G)$, as the sum of Hamming distances between all pairs of strings generated by the incidence matrix of the graph G, i.e.,

$$H_B(G) = \sum_{i<j} H_d(G)(s(v_i), s(v_j)),$$

where $H_d(s(v_i), s(v_j))$ is the standard Hamming distance between v_i and v_j, i.e., the number of coordinates in which they differ.

In the recently published paper [15], the Hamming matrix $H(G) = (h_{ij})_{n\times n}$ of a graph G was introduced, with elements given by

$$h_{ij} = H_d\Big(s(v_i), s(v_j)\Big), \quad i, j = 1, \dots, n. \tag{1}$$

Keeping in mind the definitions of the Hamming index and the Hamming matrix, it is easy to see that $2H_B(G) = \sum_{i,j} h_{ij}$.

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In order to distinguish the eigenvalues of different graph matrices, the eigenvalues of $A(G)$ and $H(G)$ are referred to as A-eigenvalues and H-eigenvalues and they form the A-spectrum and the H-spectrum, respectively. The characteristic polynomials of the H-matrix and the A-matrix are referred to as H-characteristic polynomial and A-characteristic polynomial, respectively.

Since $H(G)$ is a symmetric matrix, the H-eigenvalues are real and let us assume they are denoted by $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ and denote by $Spec(H(G))$ the corresponding H-spectrum.

The graph energy, introduced in 1978 in the seminal paper [3] by I. Gutman, is defined as the sum of the absolute values of the A-eigenvalues of a graph. The concept of graph energy has a chemical origin and a chemical interpretation [4]. Nowadays, the theory of graph energy is a well-developed field of applied mathematics and mathematical chemistry [9, 11]. There are a large number of papers on graph energy and its variants based on different matrices associated with a graph [5, 6].

Recently, in paper [15], the Hamming energy of a graph based on the Hamming matrix was proposed as the sum of the absolute values of H-eigenvalues of a graph, i.e., $HE(G) = \sum_{i=1}^{n} |\lambda_i|$.

In the same paper [15], the authors gave an upper bound for the H-energy in terms of the H-index, as well as the upper bound for the H-energy of the cycle graph. Furthermore, they derived the upper bound for the largest H-eigenvalue of a star graph and analyzed the predictive power of the H-energy by showing that the H-energy of a graph is better correlated with some physicochemical properties of octanes (such as the entropy and the heat of vaporization) compared to the ordinary graph energy.

The same authors investigated, in the paper [13], the discriminative potential of Hamming energy among a set of isomers and showed its high sensitivity in the class of chemical trees and chemical unicyclic graphs with up to 20 vertices, compared to the ordinary graph energy and other eigenvalue-based quantities.

Unlike the adjacency matrix, which reflects local vertex connectivity, the Hamming matrix encodes differences between incidence patterns of vertices and therefore captures structural information of a different type. While the adjacency spectrum has been extensively studied, the H-spectrum represents a comparatively new spectral invariant whose structural properties are not yet fully understood. In particular, the relationship between the H-spectrum and classical spectral parameters remains largely unexplored. Therefore, a systematic investigation of its eigenvalue bounds and structural properties is of independent mathematical interest.

Motivated by these findings, the present paper investigates fundamental spectral properties of the Hamming matrix and derives upper and lower bounds on the largest and smallest H-eigenvalues of a path graph. Furthermore, the H-spectrum and H-energy of regular graphs (and consequently of cycle graphs), as well as of line graphs of regular graphs, are determined. Moreover, we express the H-characteristic polynomial of the complement and the line graph of a regular graph G as a function of the H-characteristic polynomial of G. In addition, relationships between the H-spectrum and conventional spectral invariants derived from the adjacency matrix are presented.

The rest of the paper is organized as follows. In Section 2, we present the necessary preliminaries concerning graph spectra and some known and new results about the H-matrix and the H-index. In Section 2, we present our main theoretical results on the H-spectrum and H-energy, including eigenvalue estimates and comparisons with the A-spectra measures.

2. Preliminaries

In this section we present the basic definitions and concepts that are necessary for our research. In addition, we give the main theorems on which we base our conclusions and assertions.

First, we present the result from [12], which will be used frequently in this paper.

Theorem 2.1 (see [12])**.** *Let u and v be the vertices of a graph G. Then*

$$H_d(G)(s(u), s(v)) = \begin{cases} d(u) + d(v) - 2, & u \sim v, \\ d(u) + d(v), & u \nsim v, \\ 0, & u = v. \end{cases}$$

The Hamming matrix $H(G)$ is a real symmetric non-negative matrix (i.e. a Hermitian matrix) with zeros on the main diagonal, therefore

$$tr(H(G)) = \sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} h_{ii} = 0, \qquad tr(H(G)^2) = tr(H(G)^T H(G)) = \sum_{i,j} h_{ij}^2 = \sum_{i=1}^{n} \lambda_i^2,$$

which will be useful in the further course of our investigation.

It follows from the previous considerations that all statements about Hermitian or non-negative matrices also apply to the matrix $H(G)$.

In the following, we present the definition and the basic properties of irreducible matrices and prove that the Hamming matrices of almost all graphs are irreducible.

Definition 2.1. *The matrix A is called reducible if there is a permutation matrix P such that the matrix $P^{-1}AP$ is of the form $\begin{pmatrix} X & O \\ Y & Z \end{pmatrix}$, where X and Z are square matrices. Otherwise, A is called irreducible.*

Remark 2.1. *By Definition 2.1, matrix $M = (m_{ij})_{n\times n}$ is irreducible if there does not exist partition $\{1, 2, \ldots, n\} = \Delta_1 \cup \Delta_2$, $\Delta_1, \Delta_2 \neq \emptyset$, $\Delta_1 \cap \Delta_2 = \emptyset$, such that $m_{ij} = 0$ for $i \in \Delta_1, j \in \Delta_2$.*

Spectral properties of irreducible non-negative matrices are described in the following theorem.

Theorem 2.2 (see [2]). *Let M be an irreducible symmetric matrix with non-negative entries. Then the largest eigenvalue λ_1 of M is simple, with a corresponding eigenvector whose entries are all positive (known as the Perron vector). Moreover, $|\lambda| \leqslant \lambda_1$ for all eigenvalues λ of M.*

Theorem 2.3 (see [2]). *Let A be a real symmetric matrix with eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. Given a partition $\{1, 2, \ldots, n\} = \Delta_1 \cup \Delta_2 \cup \cdots \cup \Delta_m$, with $|\Delta_i| = n_i > 0$, $\sum\limits_{i=1}^{m} n_i = n$, consider the corresponding blocking $A = (A_{ij})$ such that A_{ij} is a $n_i \times n_j$ block. Let e_{ij} be the sum of the entries in A_{ij} and set $B = (e_{ij}/n_i)$ (e_{ij}/n_i is the average row sum in A_{ij}). Then the spectrum of B is contained in the segment $[\lambda_n, \lambda_1]$.*

Theorem 2.4 (see [2]). *Let A be any non-negative symmetric matrix partitioned into blocks as in Theorem 2.3. Let the blocks A_{ij} have constant row sums b_{ij} and $B = (b_{ij})$. Then the spectrum of B is contained in the spectrum of A (taking into account the multiplicities of the eigenvalues). Furthermore, the largest eigenvalue (index) of B is equal to the largest eigenvalue of A.*

Remark 2.2. *The matrix B defined in Theorem 2.3 is called the quotient matrix of A. In the case of constant row sums of A_{ij} for each pair i and j, B is called equitable quotient matrix of A, and the corresponding partition of the matrix A into blocks A_{ij} is called equitable partition.*

Taking into account Theorem 2.1, if we denote $d(v_i) = d_i$, $i = 1, 2, \ldots, n$, the elements of the Hamming matrix $H(G) = (h_{ij})$ of a graph G can be written as

$$h_{ij} = \begin{cases} d_i + d_j - 2\chi_{ij}, & i \neq j, \\ 0, & i = j, \end{cases} \tag{2}$$

where

$$\chi_{ij} = \begin{cases} 1, & v_i \sim v_j, \\ 0, & v_i \nsim v_j. \end{cases} \tag{3}$$

According to the above notation, $h_{ij} = 0\,(i \neq j)$ if and only if $d_i + d_j - 2\chi_{ij} = 0$, i.e.

- if $v_i \sim v_j$, then $d_i = d_j = 1$;
- if $v_i \nsim v_j$, then $d_i = d_j = 0$.

It is now easy to conclude that the matrix $H(G)$ is only reducible if $G \cong nK_1$ or $G \cong K_2$. In all other cases, including disconnected graphs, since the elements of the matrix $H(G)$ are obtained from vertex degrees “globally”, off-diagonal elements of this matrix, corresponding to vertices from different connected components will be positive, which means that the matrix $H(G)$ is irreducible. Consequently, except in these trivial cases, the theory of non-negative irreducible matrices can be applied for the matrix $H(G)$.

Theorem 2.5 (see [1]). *The increase of any element of a non-negative matrix A does not decrease the largest eigenvalue. The largest eigenvalue increases strictly if A is an irreducible matrix.*

Furthermore, for our research we need an estimate of the largest eigenvalue of the Hamming matrix of a graph in terms of the graph’s Hamming index.

Theorem 2.6 (see [15]). *Let G be a graph with n vertices and let $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ be eigenvalues of the Hamming matrix $H(G)$. If $H_B(G)$ is the Hamming index of the graph G, then $\lambda_1 \geqslant \frac{2H_B(G)}{n}$.*

Finally, recall that the first Zagreb index $M_1(G)$ of a graph G, introduced in [7, 8], is defined as $M_1(G) = \sum_{i=1}^{n} d_i^2$ and is widely studied in the literature (e.g., see the paper [10]).

3. Main Results

In the paper [12], the authors have determined the H-index of some classes of graphs (e.g., regular graphs, complete bipartite graphs). In the following theorem, we generalize this result by providing a closed-form expression for the H-index of an arbitrary graph as a function of the number of vertices and the number of edges. In addition, we determine $tr(H(G)^2)$ and thus improve the result of [15], where the upper bound for this quantity was given.

Theorem 3.1. *Let G be a graph on n vertices and m edges and $H = H(G)$ its Hamming matrix. Then,*

(a) $H_B(G) = \sum\limits_{i<j} h_{ij} = 2(n-2)m$;

(b) $tr(H^2) = \sum\limits_{i,j} h_{ij}^2 = 2(n-6)M_1 + 8m(m+1)$, where $M_1 = M_1(G)$ is the first Zagreb index of G.

Proof. (a) $H_B(G) = \sum\limits_{i<j} h_{ij} = \sum\limits_{i<j}(d_i + d_j - 2\chi_{ij}) = \sum\limits_{i<j}(d_i+d_j) - 2\sum\limits_{i<j}\chi_{ij}$. As $\sum\limits_{i<j}\chi_{ij} = m$, and

$$\begin{aligned}\sum_{i<j}(d_i+d_j) &= \frac{1}{2}\sum_{i\neq j}(d_i+d_j)\\ &= \frac{1}{2}\Big((d_1+d_2)+\cdots+(d_1+d_n)+(d_2+d_1)+\cdots+(d_2+d_n)+\cdots+(d_n+d_1)+\cdots+(d_n+d_{n-1})\Big)\\ &= \frac{1}{2}\left(2(n-1)\sum_{i=1}^{n} d_i\right) = 2(n-1)m,\end{aligned}$$

the statement holds.

(b) Recall that $h_{ii} = 0$ and $H^T = H$.

$$\begin{aligned} tr(H^2) &= \sum_{i,j} h_{ij}^2 = \sum_{i\neq j} h_{ij}^2 = \sum_{i\neq j}(d_i+d_j-2\chi_{ij})^2 = \sum_{i\neq j}\left(d_i^2+d_j^2+4\chi_{ij}^2+2d_id_j-4(d_i+d_j)\chi_{ij}\right)\\ &= \sum_{i\neq j}(d_i^2+d_j^2) + 4\sum_{i\neq j}\chi_{ij} + 2\sum_{i\neq j} d_id_j - 4\sum_{v_i\sim v_j}(d_i+d_j).\end{aligned}$$

We used the fact that $\chi_{ij}^2 = \chi_{ij}$. As $\sum\limits_{i\neq j}(d_i^2+d_j^2) = 2(n-1)\sum\limits_{i=1}^{n} d_i^2 = 2(n-1)M_1$, $\sum\limits_{v_i\sim v_j}(d_i+d_j) = 2\sum\limits_{i=1}^{n} d_i^2 = 2M_1$ and

$$\begin{aligned}\sum_{i\neq j} d_id_j &= d_1\left(d_2+\cdots+d_n\right) + d_2\left(d_1+\cdots+d_n\right)+\cdots+d_n\left(d_1+\cdots+d_{n-1}\right)\\ &= \sum_{i=1}^{n} d_i(2m-d_i) = 2m\sum_{i=1}^{n} d_i - \sum_{i=1}^{n} d_i^2 = 4m^2 - M_1,\end{aligned}$$

so, the statement holds. □

Theorem 3.2. *Let $G \neq K_n$ be a graph with $n > 2$ vertices and $u, v \in V(G)$ any two non-adjacent vertices. For a graph $G' = G + uv$ it holds $\lambda_1(G) < \lambda_1(G')$.*

Proof. Let $H' = (h'_{ij})_{n\times n}$ be the Hamming matrix of G' and let $H = (h_{ij})_{n\times n}$ be the Hamming matrix of G. Then $h'_{uv} = (d(u)+1) + (d(v)+1) - 2 = d(u) + d(v) = h_{uv}$. Furthermore, $h'_{uw} = h_{uw} + 1$ and $h'_{vw} = h_{vw} + 1$, for $w \neq u, v$.

If $G \neq nK_1$, the statement holds by Theorem 2.5. If $G = nK_1$, then $\lambda_1(G) = 0$. Furthermore, $G' = K_2 \cup (n-2)K_1$, and by Theorems 2.6 and 3.1 we have $\lambda_1(G') \geqslant \frac{4(n-2)}{n} > 0$, so that the statement is valid. □

Corollary 3.1. *(a) $\lambda_1(P_n) < \lambda_1(C_n)$;*

(b) $\lambda_1(G) < \lambda_1(K_n)$ for an arbitrary graph G on n vertices, $G \neq K_n$.

In the sequel, we will use the following observation.

Remark 3.1. *The all-one matrix $J = J_n$ has eigenvalues: n (with the corresponding eigenvector $\mathbf{1} = (\underbrace{1, 1, \ldots, 1}_{n})^T$) and 0 with multiplicity $n-1$ (with corresponding eigenvectors orthogonal to the eigenvector $\mathbf{1}$).*

Taking into account the relations (2) and (3), we can express the matrix $H = H(G)$ as

$$H = M - 2A, \tag{4}$$

where $M = D(J-I) + (J-I)D$, $D = \operatorname{diag}(d_1, d_2, \dots, d_n)$ is the diagonal matrix of vertex degrees and $A = A(G)$ is the adjacency matrix of G. From the definition of M, it follows that $m_{ij} = d_i + d_j$ for $i \neq j$, while $m_{ii} = 0$.

Denote by $\nu_1(M) \geqslant \nu_2(M) \geqslant \cdots \geqslant \nu_n(M)$ the eigenvalues of the matrix M and by $\mu_1(-2A) \geqslant \mu_2(-2A) \geqslant \cdots \geqslant \mu_n(-2A)$ the eigenvalues of the matrix $-2A$. In addition, let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of the matrix H.

Since H, M, and $-2A$ are real symmetric matrices, we may apply Weyl's inequalities (see, for example, [2])

$$\lambda_i(H) \leqslant \nu_j(M) + \mu_{i-j+1}(-2A),\ 1 \leqslant j \leqslant i \leqslant n;$$

$$\lambda_i(H) \geqslant \nu_j(M) + \mu_{i-j+n}(-2A),\ 1 \leqslant i \leqslant j \leqslant n.$$

As $\mu_k(-2A) = -2\mu_{n+1-k}(A),\ 1 \leqslant k \leqslant n$, we can estimate $\lambda_i(H)$ using $\nu_j(M)$ and $\mu_k(A)$. For example, we obtain

$$\lambda_1(H) \leqslant \nu_1(M) - 2\mu_n(A), \tag{5}$$

$$\lambda_n(H) \geqslant \nu_n(M) - 2\mu_1(A). \tag{6}$$

In the following, we will apply these inequalities to the path P_n.

First, we denote by $\|X\|_* = \sum_{i=1}^{n} |\theta_i(X)|$ the nuclear norm (also called trace norm or Schatten 1-norm) of the real symmetric $n \times n$ matrix X, where $\theta_i(X)$, $i = 1, 2, \dots, n$, are the eigenvalues of the matrix X. If we apply the triangle inequality $\|X + Y\|_* \leqslant \|X\|_* + \|Y\|_*$ to the matrix $H = M + (-2A)$, we obtain the following inequality between the H-energy and the ordinary A-energy of $G : HE(G) = \|X\|_* = \|M - 2A\|_* \leqslant \|M\|_* + 2\|A\|_* = \|M\|_* + 2E(G)$. This inequality can be further refined for specific classes of graphs, such as the path graph P_n, or under additional structural conditions.

Let us assume that $\Delta = \max_{1 \leqslant i \leqslant n} d_i$. For the matrix $M = (m_{ij})_{n \times n}$ we have $\|M\|_* = \sum_{i=1}^{n} |\nu_i(M)|$, and according to the Gershgorin theorem (see [14]), each eigenvalue $\nu(M)$ belongs to at least one Gershgorin disc $D(m_{ii}, R_i)$, where $R_i = \sum_{j \neq i} |m_{ij}|$. Since $m_{ii} = 0, i = 1, 2, \dots, n$, it holds that $|\nu_i(M)| \leqslant \max\limits_{1 \leqslant i \leqslant n} R_i = \max\limits_{i} \sum\limits_{j \neq i} |m_{ij}|$.

Having in mind that the off-diagonal elements of the matrix M have the form $d_i + d_j$, $i \neq j$, we obtain

$$\|M\|_* = \sum_{i=1}^{n} |\nu_i(M)| \leqslant n \max_i \sum_{j \neq i} |m_{ij}| \leqslant 2n(n-1)\Delta,$$

which implies $HE(G) \leqslant 2n(n-1)\Delta + 2E(G)$.

For certain classes of graphs, one can establish sharper inequalities that relate the H-energy to the ordinary energy of a graph. For example, in the case of the path graph P_n, the eigenvalues of the matrix M can be determined explicitly, which makes such refined comparisons possible. If $V(P_n) = \{v_1, v_2, \dots, v_n\}$, $n \geqslant 4$, with $d_1 = d_n = 1$, we partition $V(P_n)$ into two classes $X = \{v_1, v_n\}$ and $Y = \{v_2, \dots, v_{n-1}\}$. With respect to this partition, the matrix M can be written in block form as

$$M = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}.$$

Here, M_{11} is a 2×2 matrix corresponding to the vertices in X, and

$$M_{11} = \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} = 2(J_2 - I_2).$$

The block M_{12} is the $2 \times (n-2)$ matrix whose (i,j)-entry equals $d_i + d_j$ for $v_i \in X$ and $v_j \in Y$, which yields $M_{12} = 3J_{2\times(n-2)}$. Similarly, $M_{21} = M_{12}^T$ and $M_{22} = 4(J_{n-2} - I_{n-2})$.

The partition of matrix M into blocks in the described way is equitable with the quotient matrix given by

$$B = \begin{bmatrix} 2 & 3(n-2) \\ 6 & 4(n-3) \end{bmatrix}.$$

According to Theorem 2.4, the spectrum of B is contained in the spectrum of M, and their indices (maximum eigenvalues) coincide.

We can obtain the H-spectrum of B as solutions of the characteristic equation $det(B - \nu I) = 0$, from which we obtain

$$\nu = 2n - 5 \pm \sqrt{(2n-5)^2 + 10n - 12} = 2n - 5 \pm \sqrt{4n^2 - 10n + 13}.$$

We obtain the remaining eigenvalues of M from the blocks M_{11} and M_{22}, taking into account Remark 3.1.

The matrix $M_{11} = 2(J_2 - I_2)$ has eigenvalues 2 and -2, with eigenvectors $(1,1)^T$ and $(1,-1)^T$, respectively. Since the partition $\{X, Y\}$ is equitable, the eigenvalues of the quotient matrix correspond to eigenvalues of M associated with eigenvectors that are constant on each partition class. The vector $(1,1)^T$ is constant on X, and therefore belongs to the invariant subspace associated with the quotient matrix. Hence, the corresponding eigenvalue is represented through the spectrum of B. In contrast, the eigenvector $(1,-1)^T$ is orthogonal to the constant vectors on X, and therefore, the eigenvalue -2 does not arise from the quotient matrix. Extending this vector by zeros on Y, we obtain the eigenvector $(1,\underbrace{0,\ldots,0}_{n-2},-1)^T$ of M corresponding to the eigenvalue -2.

The matrix $M_{22}=4(J_{n-2}-I_{n-2})$ has a simple eigenvalue $4(n-3)$ (with constant eigenvector $\mathbf{1}=(\underbrace{1,1,\ldots,1}_{n-2})^T$) and -4 of multiplicity $n-3$. To confirm that -4 is also the eigenvalue of M of multiplicity $n-3$, we construct the set of $n-3$ linearly independent eigenvectors $v^{(i)}\in\mathbf{R}^n$, $i=1,2,\ldots,n-3$, corresponding to the eigenvalue -4.

Let $\{e_1,\ldots,e_{n-2}\}$ be the standard orthonormal basis of $\mathbf{R}^{n-2}$ and $w^{(i)}=e_i-e_{i+1}$, $i=1,2,\ldots,n-3$. The vectors $v^{(i)}=(0,w^{(i)},0)^T$ are linearly independent and it holds that $Mv^{(i)}=-4v^{(i)}$, $i=1,2,\ldots,n-3$. Thus,

$$Spec(M)=\{2n-5\pm\sqrt{4n^2-10n+13},-2,\underbrace{-4,-4,\ldots,-4}_{n-3}\}$$

and $\|M\|_*=\sum_{i=1}^n|\nu_i(M)|=2\left(2n-5+\sqrt{4n^2-10n+13}\right)$. Consequently, $HE(P_n)\leqslant 2\left(2n-5+\sqrt{4n^2-10n+13}\right)+2E(P_n)$, from which we obtain, using the A-spectrum of P_n (see e.g. [2]), the following

$$HE(P_n)\leqslant 2\left(2n-5+\sqrt{4n^2-10n+13}+2\sum_{k=1}^{n}\left|\cos\frac{\pi k}{n+1}\right|\right).$$

Also, from the inequality (5), we obtain $\lambda_1(P_n)\leqslant 2n-5+\sqrt{4n^2-10n+13}+4\cos\frac{\pi}{n+1}$. As $2n-5-\sqrt{4n^2-10n+13}>-4$ for $n>2$, from the inequality (6) we get $\lambda_n(P_n)\geqslant -4-4\cos\frac{\pi}{n+1}$.

Theorem 3.3. *Let G be a connected r-regular graph with n vertices. Then the H-spectrum of the graph G is given by $Spec(H(G))=\{2r(n-2),-2(r+\mu_i),i=2,3,\ldots,n\}$, where $\{\mu_i\,|\,i=2,3,\ldots,n\}$ are the A-eigenvalues of G. Furthermore, it holds $HE(G)=4r(n-2)$.*

Proof. Let $H(G)=(h_{ij})_{n\times n}$ be the H-matrix of r-regular graph G. Then,

$$h_{ij}=\begin{cases}2r-2, & v_i\sim v_j,\\ 2r, & v_i\not\sim v_j,\\ 0, & i=j,\end{cases}$$

which implies that $H(G)=2r(J-I)-2A(G)$.
Since G is r-regular, the adjacency matrix $A(G)$ has the maximum eigenvalue (index) $\mu_1=r$, with the corresponding eigenvector $\mathbf{1}=(1,1,\ldots,1)^T$. Denote by $S=\{\mu_i\,|\,i=2,3,\ldots,n\}$ the set of remaining eigenvalues of the matrix $A(G)$ (the corresponding eigenvectors of these eigenvalues are orthogonal to the eigenvector $\mathbf{1}$). By Remark 3.1, we obtain

$$H(G)\cdot\mathbf{1} \quad=\quad (2r(J-I)-2A(G))\cdot\mathbf{1}=(2r(n-1)-2r)\cdot\mathbf{1}=2r(n-2)\cdot\mathbf{1},$$

which implies that $\lambda_1(G)=2r(n-2)$.

For any eigenvector $x_i\neq\mathbf{0}$ of $A(G)$ orthogonal to $\mathbf{1}$ (corresponding to the eigenvalue μ_i), we have

$$H(G)\cdot x_i \quad=\quad (2r(J-I)-2A(G))\cdot x_i=(2r(-1)-2\mu_i)\cdot x_i=-2(r+\mu_i)\cdot x_i,$$

thus, $\lambda_i(G)=-2(r+\mu_i)$, $i=2,3,\ldots,n$.

As $HE(G)=\sum_{i=1}^n|\lambda_i|=2r(n-2)+2\sum\limits_{i=2}^{n}|r+\mu_i|$, and by Theorem 2.2 it holds $|\mu_i|\leqslant r$, i.e. $r+\mu_i\geqslant 0$, we get

$$HE(G) \quad=\quad 2r(n-2)+2\sum_{i=2}^{n}(r+\mu_i)=2r(n-2)+2\sum_{i=2}^{n}r+2\left(\sum_{i=1}^{n}\mu_i-r\right)=4r(n-2).$$

□

It is known (see, e.g., [2]) that the A-eigenvalues of the n-cycle C_n are $2\cos\frac{2k\pi}{n}$, $k=0,1,2,\ldots,n-1$, so we get the following result.

Corollary 3.2. *$Spec(H(C_n))=\{4n-8\}\cup\{-4-4\cos\frac{2k\pi}{n}\,|\,k=1,2,\ldots,n-1\}$ and $HE(C_n)=8(n-2)$.*

Remark 3.2. *The result given in Corollary 3.2 improves the result from [15], where it was proved that $HE(C_n)\leqslant 4n(n-2)$.*

Theorem 3.4. *Let $P(G,\lambda)$ be the H-characteristic polynomial of the r-regular graph G on n vertices. Then the H-characteristic polynomial of its complement $\overline{G}$ can be expressed as*

$$P(\overline{G},\lambda)=(-1)^n\,\frac{\lambda-2(n-2-r)(n-1)-2r}{\lambda+2(n-2)(r+1)}\,P(G,-2(n-2)-\lambda).$$

Proof. If G is an r-regular graph on n vertices, its complement $\overline{G}$ is an $(n-1-r)$-regular graph, i.e.

$$H(\overline{G})=2(n-1-r)(J-I)-2A(\overline{G}),$$

where $A(\overline{G})=J-I-A(G)$ is the adjacency matrix of $\overline{G}$, which implies $H(\overline{G})=2(n-2-r)(J-I)+2A(G)$. Let $S=\{r,\mu_2,\dots,\mu_n\}$ be the A-spectrum of G. Then, using a similar approach as in the proof of Theorem 3.3, we conclude that the H-spectrum of $\overline{G}$ is $\{2(n-2-r)(n-1)+2r\}\cup\{-2(n-2-r-\mu_i)\,|\,i=2,3,\dots,n\}$. It holds that $\lambda_1(G)+\lambda_1(\overline{G})=2r(n-2)+2(n-2-r)(n-1)+2r=2(n-1)(n-2)$ and $\lambda_i(G)+\lambda_i(\overline{G})=-2(r+\mu_i)-2(n-2-r-\mu_i)=-2(n-2)$ for $i=2,3,\dots,n$. Set $\overline{\lambda_i}=\lambda_i(\overline{G})$. Then, we have

$$P(\overline{G},\lambda)=(\lambda-\overline{\lambda_1})\cdot\prod_{i=2}^{n}(\lambda-\overline{\lambda_i})=(\lambda-2(n-2-r)(n-1)-2r)\cdot\prod_{i=2}^{n}(\lambda-\overline{\lambda_i}).$$

Since

$$\begin{aligned}P(G,-2(n-2)-\lambda)&=(-2(n-2)-\lambda-\lambda_1)\cdot\prod_{i=2}^{n}(-2(n-2)-\lambda-\lambda_i)=-(2(n-2)+\lambda+\lambda_1)\cdot\prod_{i=2}^{n}(\overline{\lambda_i}-\lambda)\\&=(-1)^n(2(n-2)(r+1)+\lambda)\cdot\prod_{i=2}^{n}(\lambda-\overline{\lambda_i}),\end{aligned}$$

we obtain the required relation. □

The relations between the spectrum of different matrices associated with a graph and the spectrum of its line graph are well known, especially in the case of regular graphs. We will establish such a relation for the H-spectrum of r-regular graphs. If G is an r-regular graph with n vertices, then $L(G)$ is a $(2r-2)$-regular graph with $m=\frac{1}{2}nr$ vertices. Let $H(L(G))=(h_{ef})_{m\times m}$ be the H-matrix of $L(G)$, where

$$h_{ef}=\begin{cases}4r-6, & e\sim f,\\ 4r-4, & e\not\sim f,\\ 0, & e=f.\end{cases}$$

Then, $H(L(G))=(4r-4)(J-I)-2A(L(G))$, where $A(L(G))$ is the adjacency matrix of $L(G)$ with the spectrum $\{\theta_1=2r-2,\theta_2,\dots,\theta_m\}$.

Analogous to the proof of Theorem 3.3, we obtain the H-spectrum of $L(G)$ as

$$Spec(H(L(G)))=\{(4r-4)(m-2)\}\cup\{-(4r-4+2\theta_i)\,|\,i=2,3,\dots,m\}.$$

It is known that for an r-regular graph G ($r\geqslant 2$) with adjacency spectrum $\{\mu_1=r,\mu_2,\dots,\mu_n\}$, the eigenvalues of $A(L(G))$ are given by $\theta_i=\mu_i+r-2$, $i=1,2,\dots,n$, and additionally the eigenvalue -2 with multiplicity $m-n$. Thus,

$$Spec(H(L(G)))=\{(4r-4)(m-2)\}\cup\{-2(3r-4+\mu_i)\,|\,i=2,3,\dots,n\}\cup\{\underbrace{-4(r-2),-4(r-2),\dots,-4(r-2)}_{m-n}\},$$

so, we have

$$HE(L(G))=4(r-1)(m-2)+4(m-n)(r-2)+2\sum_{i=2}^{n}|3r+\mu_i-4|.$$

As $3r+\mu_i-4\geqslant 2r-4\geqslant 0$, it holds that $|3r+\mu_i-4|=3r+\mu_i-4$, which implies

$$\begin{aligned}HE(L(G))&=4(r-1)(m-2)+4(m-n)(r-2)+2(n-1)(3r-4)+2\sum_{i=2}^{n}\mu_i\\&=4(r-1)(m-2)+4(m-n)(r-2)+2(n-1)(3r-4)-2r=2r(4m+n-8)-4(3m-4).\end{aligned}$$

In the sequel, we show that the H-characteristic polynomial of $L(G)$ can be expressed by the H-characteristic polynomial of G.

Theorem 3.5. *Let $P(G,\lambda)$ be the H-characteristic polynomial of the r-regular graph G on n vertices. Then the H-characteristic polynomial of the line graph $L(G)$ of the graph G can be expressed as*

$$P(L(G),\lambda)=\frac{(\lambda-4(r-1)(m-2))(\lambda+4r-8)^{m-n}}{\lambda-2r(n-4)-8}\,P(G,\lambda+4r-8).$$

Proof. If $Spec(A(G))=\{r,\mu_2,\dots,\mu_n\}$, then $Spec(H(G))=\{2r(n-2)\}\cup\{-2(r+\mu_i)\mid i=2,3,\dots,n\}$ and

$$Spec(H(L(G)))=\{4(r-1)(m-2)\}\cup\{-2(3r+\mu_i-4)\mid i=2,3,\dots,n\}\cup\{\underbrace{-4(r-2),-4(r-2),\dots,-4(r-2)}_{m-n}\}.$$

Thus, if the H-eigenvalues of G and $L(G)$ are denoted by ${\lambda_i}^G$ and ${\lambda_i}^{L(G)}$, respectively, then ${\lambda_i}^{L(G)}={\lambda_i}^G-4r+8$, for $i=2,3,\dots,n$, and the following applies:

$$P(G,\lambda+4r-8)=(\lambda+4r-8-2r(n-2))\cdot\prod_{i=2}^{n}\left(\lambda+4r-8-\lambda_i^G\right)=(\lambda-2r(n-4)-8)\cdot\prod_{i=2}^{n}\left(\lambda-\lambda_i^{L(G)}\right) \quad (7)$$

and

$$P(L(G),\lambda)=(\lambda-4(r-1)(m-2))(\lambda+4r-8)^{m-n}\cdot\prod_{i=2}^{n}\left(\lambda-\lambda_i^{L(G)}\right). \quad (8)$$

From relations (7) and (8), we obtain the desired result. □

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