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On the Eigenvalues of Hamming Matrix and Hamming Energy of a Graph

HARISHCHANDRA S. RAMANE, T. SHIVAPRASAD, AND SHEENA Y. CHOWRI

ABSTRACT. Let G be a graph with n vertices and m edges. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G. The string $s(v_i)$ is the row in the incidence matrix of G corresponding to the vertex v_i, which is an m-tuple in $\mathbb{Z}_2^m$. The Hamming matrix $H(G) = [h_{ij}]$ of a graph G is an $n \times n$ matrix, whose (i, j)-th entry is the Hamming distance between the strings $s(v_i)$ and $s(v_j)$. The Hamming energy $HE(G)$ of a graph G is the sum of the absolute values of the eigenvalues of $H(G)$. Recently the Hamming energy is introduced and obtained bounds for it in terms of the Hamming index and observed its predictive potentiality by correlating the physicochemical properties of molecules. In this paper we give the better bound for Hamming energy in terms of number of vertices and edges. Also obtain the largest eigenvalue of the Hamming matrix of a regular graph. Further obtain explicitly the eigenvalues of the Hamming matrix and Hamming energy of a complete bipartite graph.

1. INTRODUCTION

Let G be a simple undirected graph with n vertices and m edges. Let the vertex set of G be $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set be $E(G) = \{e_1, e_2, \ldots, e_m\}$. If the vertices v_i and v_j are adjacent then we write $v_i \sim v_j$ and if they are not adjacent then we write $v_i \nsim v_j$. The degree of a vertex v_i, denoted by $deg_G(v_i)$, is the number of edges incident to it. If all the vertices have same degree equal to r then the graph is called a regular graph of degree r.

The graph energy $\mathcal{E}(G)$, introduced in 1978 [3], is defined as sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$ of a graph G. That is if $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of $A(G)$, then

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\mu_i|. \tag{1.1}$$

Graph energy has significant applications in chemistry [4, 11]. Several results related to graph energy can be seen in [3, 4, 5, 11, 13, 15].

In literature, several other energies of graphs, particularly, the distance energy [8], Laplacian energy [6], Harary energy [2], Zagreb energy [14], skew energy [1, 10], Seidel energy [7], degree sum energy [17] and minimum second neighborhood degree energy [12] were studied.

Recently, Vučićević, Redžepović and Stojanović [21] introduced the Hamming matrix and Hamming energy of a graph based on the incidence matrix of a graph. They have obtained upper bound for Hamming energy in terms of Hamming index. Also obtained Hamming energy of a complete graph K_n and gave the bound for Hamming energy of cycle. Further they gave bound for the largest eigenvalue of the Hamming matrix of a star. Also they observed that the better predictive potentiality of the Hamming energy with the entropy, heat of vaporization and heat of formulation of octane molecules. In [19], the

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Corresponding author: Harishchandra S. Ramane; hsramane@yahoo.com

sensitivity of Hamming energy on isomers was checked and found that Hamming energy of chemical trees and chemical unicyclic graphs shows high sensitivity compared to graph energy and other eigenvalue-based quantities.

In this paper we give the upper bound for Hamming energy of a graph in terms of number of vertices and edges and lower bound in terms of the determinant of Hamming matrix. Also obtain the largest eigenvalue of the Hamming matrix of a regular graph. Further we give explicitly the eigenvalues of the Hamming matrix and Hamming energy of a complete bipartite graph.

2. PRELIMINARIES

The set $\mathbb{Z}_2 = \{0, 1\}$ is a group under binary operation $+$ with addition modulo 2. Therefore for any positive integer m, $\mathbb{Z}_2^m = \mathbb{Z}_2 \times \mathbb{Z}_2 \times \cdots \times \mathbb{Z}_2$ (m factors) is a group under the operation $+$ defined by

$$(x_1, x_2, \dots, x_m) + (y_1, y_2, \dots, y_m) = (x_1 + y_1, x_2 + y_2, \dots, x_m + y_m),$$

with addition modulo 2.

Element of $\mathbb{Z}_2^m$ is an m-tuple $(x_1, x_2, \dots, x_m)$ written as $x = x_1 x_2 \dots x_m$ where every x_i is either 0 or 1 and is called a string. The number of 1 in $x = x_1 x_2 \dots x_m$ is called the weight of x and is denoted by $wt(x)$.

Let $x = x_1 x_2 \dots x_m$ and $y = y_1 y_2 \dots y_m$ be the elements of $\mathbb{Z}_2^m$. Then the sum $x + y$ 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 $x_i \neq y_i$, $i = 1, 2, \dots, m$.

The Hamming distance $H_d(x, y)$ between the strings $x = x_1 x_2 \dots x_m$ and $y = y_1 y_2 \dots y_m$ is the number of is such that $x_i \neq y_i$, $1 \leq i \leq m$. Thus $H_d(x, y) =$ Number of positions in which x and y differ $= wt(x + y)$ [9].

Example 2.1. *If $x = 01001$, $y = 11010$ and $z = 11011$ are the strings, then $H_d(x, y) = 3$ and $H_d(x, z) = 2$.*

The incidence matrix of a graph G is the matrix $B(G) = [b_{ij}]$ of order $n \times m$ in which $b_{ij} = 1$ if the vertex v_i is incident to the edge e_j and $b_{ij} = 0$, otherwise. Denote by $s(v_i)$, the row of the incidence matrix corresponding to the vertex v_i. It is a string in the set $\mathbb{Z}_2^m$ of all m-tuples over the field of order two.

Sum of Hamming distances between all pairs of strings generated by the incidence matrix of a graph G is called the Hamming index of G [16, 18], and is denoted by $H_B(G)$.

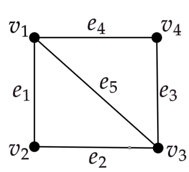

FIGURE 1. Graph

Example 2.2. *For a graph G given in Fig. 1, the incidence matrix is*

$$B(G) = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix}.$$

Therefore $H_d(s(v_1), s(v_2)) = 3$, $H_d(s(v_1), s(v_3)) = 4$, $H_d(s(v_1), s(v_4)) = 3$, $H_d(s(v_2), s(v_3)) = 3$, $H_d(s(v_2), s(v_4)) = 4$ *and* $H_d(s(v_3), s(v_4)) = 3$. *Hence* $H_B(G) = 20$.

The Hamming matrix of a graph G (with respect to its incidence matrix) is a matrix $H(G) = [h_{ij}]$ of order $n \times n$ in which $h_{ij} = H_d(s(v_i), s(v_j))$, where $s(v_i)$ is the string corresponding to the vertex v_i in the incidence matrix of G. $H(G)$ is symmetric matrix with diagonal entries zero. Analogous to graph energy defined in Eq. (1.1), if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of the Hamming matrix $H(G)$ of G, then the Hamming energy of G is defined as [21]

$$HE(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{2.2}$$

Example 2.3. *For a graph G given in Fig. 1, the Hamming matrix is*

$$H(G) = \begin{bmatrix} 0 & 3 & 4 & 3 \\ 3 & 0 & 3 & 4 \\ 4 & 3 & 0 & 3 \\ 3 & 4 & 3 & 0 \end{bmatrix}.$$

The eigenvalues of this matrix are $\lambda_1 = 10$, $\lambda_2 = -2$, $\lambda_3 = -4$ *and* $\lambda_4 = -4$. *Therefore Hamming energy is* $HE(G) = 20$.

We need following results.

Theorem 2.1. [16] *Let* u *and* v *be the vertices of G. Then*

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

Theorem 2.2. [20] *(Geršgorin Theorem) For any matrix* $M = [m_{ij}]$ *of order* $n \times n$ *and any eigenvalue* λ *of* M, *there is an integer* $k \in \mathbb{N} = \{1, 2, \ldots, n\}$ *such that*

$$|\lambda - m_{kk}| \le r_k(M) = \sum_{j \in \mathbb{N} \setminus \{k\}} |m_{kj}|.$$

3. On the Eigenvalues of Hamming Matrix

Theorem 3.3. *If G is a regular graph of degree* r *with* n *vertices, then the maximum eigenvalue of the Hamming matrix of G is* $2r(n-2)$.

Proof. Since G is a regular graph of degree r, by Theorem 2.1

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

Hence in each row of $H(G)$, we have r times $(2r-2)$ and $n-1-r$ times $2r$. Therefore $r_i(H(G)) = r(2r-2) + (n-1-r)2r = 2r(n-2)$ for all $i = 1, 2, \ldots, n$.

Let $\mathbf{u} = [1, 1, \ldots, 1]^T$ be the column vector. Then

$$H(G)\mathbf{u} = 2r(n-2)\mathbf{u}.$$

Hence $2r(n-2)$ is the eigenvalue of $H(G)$.

By Theorem 2.2, if λ is the eigenvalue of $H(G)$ then $|\lambda| \le r_i(H(G)) = 2r(n-2)$. Hence maximum eigenvalue of $H(G)$ is $2r(n-2)$. □

In [21], bound for maximum eigenvalue of the Hamming matrix of a star $S_n = K_{1,n-1}$ is given. Here we obtain the eigenvalues of the Hamming matrix of complete bipartite graph $K_{p,q}$, wher $p, q \ge 1$ are the integers.

Theorem 3.4. *If $K_{p,q}$ is the complete bipartite graph, then the characteristic polynomial of $H(K_{p,q})$ is*

$$(\lambda+2p)^{q-1}(\lambda+2q)^{p-1}[\lambda^2-(4pq-2p-2q)\lambda-pq(p-q)^2].$$

Proof. Let V_1 and V_2 be the partite sets of the vertex set of $K_{p,q}$, where $|V_1|=p$ and $|V_2|=q$. By Theorem 2.1 the Hamming distance in $K_{p,q}$ is

$$H_d(s(u),s(v))=\begin{cases} p+q-2 & \text{if } u\in V_1 \text{ and } v\in V_2 \text{ or vice versa}\\ 2q & \text{if } u,v\in V_1\\ 2p & \text{if } u,v\in V_2.\end{cases}$$

Therefore the Hamming matrix of $K_{p,q}$ is in the form

$$\begin{bmatrix} 2qJ_{p\times p}-2qI_p & (p+q-2)J_{p\times q}\\ (p+q-2)J_{q\times p} & 2pJ_{q\times q}-2pI_q\end{bmatrix}, \tag{3.3}$$

where J is a matrix whose all entries are equal to 1 and I is the identity matrix.

Let $X=p+q-2$, $Y=\lambda+2q$, $Z=\lambda+2p$, $P=2(p-1)q$ and $Q=2(q-1)p$. The characteristic polynomial of the matrix (3.3) is

$$\begin{vmatrix} \lambda & -2q & \cdots & -2q & -X & -X & \cdots & -X\\ -2q & \lambda & \cdots & -2q & -X & -X & \cdots & -X\\ \vdots & & \vdots & & & & \vdots & \\ -2q & -2q & \cdots & \lambda & -X & -X & \cdots & -X\\ -X & -X & \cdots & -X & \lambda & -2p & \cdots & -2p\\ -X & -X & \cdots & -X & -2p & \lambda & \cdots & -2p\\ \vdots & & \vdots & & & & \vdots & \\ -X & -X & \cdots & -X & -2p & -2p & \cdots & \lambda \end{vmatrix}. \tag{3.4}$$

Substracting first row from rows $2,3,\ldots,p$ and substracting $(p+1)$-th row from rows $p+2,p+3,\ldots,p+q$ in (3.4) we get

$$\begin{vmatrix} \lambda & -2q & \cdots & -2q & -X & -X & \cdots & -X\\ -Y & Y & \cdots & 0 & 0 & 0 & \cdots & 0\\ \vdots & & \vdots & & & & \vdots & \\ -Y & 0 & \cdots & Y & 0 & 0 & \cdots & 0\\ -X & -X & \cdots & -X & \lambda & -2p & \cdots & -2p\\ 0 & 0 & \cdots & 0 & -Z & Z & \cdots & 0\\ \vdots & & \vdots & & & & \vdots & \\ 0 & 0 & \cdots & 0 & -Z & 0 & \cdots & Z \end{vmatrix}. \tag{3.5}$$

Adding columns $2,3,\ldots,p$ to the first column and adding columns $p+2,p+3,\ldots,p+q$ to the $(p+1)$-th column in (3.5) we get

$$(3.6)\qquad \begin{vmatrix} \lambda-P & -2q & \cdots & -2q & -qX & -X & \cdots & -X \\ 0 & Y & \cdots & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & \vdots & & & & \vdots & \\ 0 & 0 & \cdots & Y & 0 & 0 & \cdots & 0 \\ -pX & -X & \cdots & -X & \lambda-Q & -2p & \cdots & -2p \\ 0 & 0 & \cdots & 0 & 0 & Z & \cdots & 0 \\ \vdots & & \vdots & & & & \vdots & \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & Z \end{vmatrix}.$$

It reducess to following in which the determinant is of order $(p+1)$.

$$\begin{aligned} & Z^{q-1}\begin{vmatrix} \lambda-P & -2q & \cdots & -2q & -qX \\ 0 & Y & \cdots & 0 & 0 \\ \vdots & & \vdots & & \\ 0 & 0 & \cdots & Y & 0 \\ -pX & -X & \cdots & -X & \lambda-Q \end{vmatrix} \\ = \ & Z^{q-1}\left[(\lambda-P)Y^{p-1}(\lambda-Q)-pqX^2Y^{p-1}\right] \\ = \ & Z^{q-1}Y^{p-1}\left[(\lambda-P)(\lambda-Q)-pqX^2\right] \\ = \ & (\lambda+2p)^{q-1}(\lambda+2q)^{p-1}[\lambda^2-(4pq-2p-2q)\lambda-pq(p-q)^2]. \end{aligned}$$

□

Corollary 3.1. *The eigenvalues of the Hamming matrix of the complete bipartite graph $K_{p,q}$ are $-2p$ ($q-1$ times), $-2q$ ($p-1$ times) and $(2pq-p-q)\pm\sqrt{(2pq-p-q)^2+pq(p-q)^2}$.*

Lemma 3.1. *If $\lambda_1,\lambda_2,\ldots,\lambda_n$ are the eigenvalues of the Hamming matrix $H(G)$ of a graph G, then*

$$\sum_{i=1}^{n}\lambda_i=0 \quad \text{and} \quad \sum_{i=1}^{n}\lambda_i^2=2\sum_{1\le i<j\le n}[H_d(s(v_i),s(v_j))]^2.$$

Proof. Sum of eigenvalues is the trace of a matrix. Hence

$$\sum_{i=1}^{n}\lambda_i=\text{Trace}(H(G))=0.$$

For second result,

$$\begin{aligned}\sum_{i=1}^{n}\lambda_i^2 &= \text{Trace}(H(G)^2)=\sum_{i=1}^{n}\sum_{j=1}^{n}[H_d(s(v_i),s(v_j))]^2 \\ &= 2\sum_{1\le i<j\le n}[H_d(s(v_i),s(v_j))]^2.\end{aligned}$$

□

4. Bounds for Hamming Energy

In [21] it is proved that for a graph G with n vertices,

$$HE(G)\le 2\sqrt{n}H_B(G). \tag{4.7}$$

In the following theorem we give the lower bound for Hamming energy analogous to the McClelland bound for graph energy [3, 13].

Theorem 4.5. *Let G be a graph with n vertices and $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G. Then*

$$HE(G) \geq \sqrt{2 \sum_{1 \leq i < j \leq n} [H_d(s(v_i), s(v_j))]^2 + n(n-1)|\det(H(G))|^{2/n}}.$$

Proof. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $H(G)$. Then

$$\begin{aligned}(HE(G))^2 &= \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \\ &= \sum_{i=1}^{n} |\lambda_i|^2 + 2 \sum_{1 \leq i < j \leq n} |\lambda_i||\lambda_j| \\ &= 2 \sum_{1 \leq i < j \leq n} [H_d(s(v_i), s(v_j))]^2 + \sum_{i \neq j} |\lambda_i||\lambda_j|. \qquad (4.8)\end{aligned}$$

Since the Arithmetic Mean is not smaller than Geometric Mean, we have

$$\begin{aligned}\frac{1}{n(n-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| &\geq \left(\prod_{i \neq j} |\lambda_i||\lambda_j|\right)^{1/n(n-1)} \\ &= \left(\prod_{i=1}^{n} |\lambda_i|^{2(n-1)}\right)^{1/n(n-1)} \\ &= \left(\prod_{i=1}^{n} |\lambda_i|\right)^{2/n} \\ &= |\det(H(G))|^{2/n}. \qquad (4.9)\end{aligned}$$

By Eqs. (4.8) and (4.9), the result follows. □

In the following theorem we give improved bound than Eq. (4.7).

Theorem 4.6. *Let G be a graph with n vertices and m edges. Then*

$$HE(G) \leq 4m(n-2).$$

Proof. By Theorem 2.1

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

Let $v_1, v_2, \ldots, v_n$ be the vertices of G and let $deg_G(v_i) = d_i$, $i = 1, 2, \ldots, n$.

Without loss of generality suppose the vertex v_1 is adjacent to the vertices $v_2, v_3, \ldots, v_{d_1+1}$ and it is not adjacent to the vertices $v_{d_1+2}, v_{d_1+3}, \ldots, v_n$. Then the entries in the row of $H(G)$ corresponding to the vertex v_1 are

$$0, d_1 + d_2 - 2, d_1 + d_3 - 2, \ldots, d_1 + d_{d_1+1} - 2, d_1 + d_{d_1+2}, d_1 + d_{d_1+3}, \ldots, d_1 + d_n.$$

Therefore

$$
\begin{aligned}
r_1(H(G)) &= \sum_{i=2}^{d_1+1}(d_1+d_i-2)+\sum_{i=d_1+2}^{n}(d_1+d_i)\\
&= \sum_{i=2}^{n} d_1+\sum_{i=2}^{n} d_i-\sum_{i=2}^{d_1+1} 2\\
&= (n-1)d_1+(2m-d_1)-2d_1 \quad \text{since } \sum_{i=1}^{n} d_i=2m\\
&= 2m+(n-4)d_1.
\end{aligned}
$$

Thus in general $r_i(H(G)) = 2m + (n-4)d_i$ for $i = 1, 2, \ldots, n$.
By Theorem 2.2, $|\lambda| \leq r_i(H(G))$, $i = 1, 2, \ldots, n$. Hence

$$
\begin{aligned}
HE(G) &= \sum_{i=1}^{n}|\lambda_i|\\
&\leq \sum_{i=1}^{n} r_i(H(G))\\
&= \sum_{i=1}^{n}[2m+(n-4)d_i]\\
&= 2mn+(n-4)2m \quad \text{since } \sum_{i=1}^{n} d_i=2m\\
&= 4m(n-2).
\end{aligned}
$$

□

Corollary 4.2. *If G is a regular graph of degree r on n vertices, then*

$$HE(G) \leq 2nr(n-2).$$

Corollary 4.3. [21] *For a cycle C_n on n vertices, $HE(C_n) \leq 4n(n-2)$.*

Following theorem follows from the Corollary 3.1 and Eq. (2.2).

Theorem 4.7. *For a complete bipartite graph $K_{p,q}$,*

$$HE(K_{p,q}) = 4pq - 2p - 2q + 2\sqrt{(2pq-p-q)^2 + pq(p-q)^2}.$$

Corollary 4.4. *For a star $S_n = K_{1,n-1}$, $HE(S_n) = 2(n-2)(1+\sqrt{n})$.*

5. Conclusion

In this paper we obtained bound for Hamming energy of a graph in terms of number of vertices and egdes. We also obtained the largest eigenvalue of the Hamming matrix of regular graph. Also gave explicit formula for the eigenvalues of Hamming matrix and for Hamming energy of a complete bipartite graph. The obtained results are better than the existing results.

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DEPARTMENT OF MATHEMATICS, KARNATAK UNIVERSITY, DHARWAD - 580003, INDIA
Email address: hsramane@yahoo.com
Email address: shivap942@gmail.com
Email address: sheenachowri@gmail.com