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REMARKS ON SOME GRAPHS WITH LARGE NUMBER OF EDGES

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Abstract

Using interlacing inequalities and matrix factorization techniques, we provide alternate methods for computing the spectra, hence the energy, of some graphs with large number of edges discussed in the paper *Bulletin de l'Academie Serbe des Sciences at des Arts (Cl. Math. Natur.)* 118 (1999) 35–50. Moreover, two conjectures on the hyper-energeticity of these graphs are resolved positively.

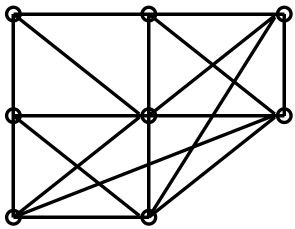

Figure 1:

1 Introduction

Let G be a simple graph on n vertices. In the paper [3], Gutman defined the *energy* $\mathcal{E}(G)$ of G to be the sum of the absolute values of the eigenvalues of G, i.e. the eigenvalues of its adjacency matrix $A(G)$, and he conjectured that $\mathcal{E}(G) \leq 2(n-1) = \mathcal{E}(K_n)$ for any graph G on n vertices, where K_n denotes the complete graph on n vertices. This conjecture can easily be verified for $n \leq 7$ (See [1]), but there are graphs on 8 vertices with energy exceeding $2(8-1) = 14 = \mathcal{E}(K_8)$. For example, the energy of the graph in Figure 1 is 14.0017. These graphs are called *hyper-energetic* graphs, i.e., graph on n vertices with energy greater than $2n-2$. There was an interest in literature [5, 7, 8] to construct and to understand the structure of hyper-energetic graphs for $n \geq 9$. It is natural to consider graphs with large number of edges because they tend to have higher energy in general. Indeed, there is a lower bound [2] by the number m of edges of a graph:

$$\mathcal{E}(G) \geq 2\sqrt{m}.$$

In the paper [4], Gutman and Pavlovic studied the following four families of graphs with large number of edges. For $n \geq 3$,

1. $K_{a_n}(k)$ denotes a graph obtained from K_n by deleting k edges sharing a common endpoint where $0 \leq k \leq n-1$.

2. $K_{b_n}(k)$ denotes a graph obtained from K_n by deleting k independent edges where $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

3. $K_{c_n}(k)$ denotes a graph obtained from K_n by deleting the edges of a clique of size k where $0 \leq k \leq n$.

4. $K_{d_n}(k)$ denotes a graph obtained from K_n by deleting a cycle of length k where $3 \leq k \leq n$.

Their characteristic polynomials were computed by evaluating determinant. Hence the spectra and so the energy were obtained. Then parameters giving rise to hyper-energetic graphs are determined.

In this paper, we provide alternate methods of computing the characteristic polynomials of these four families of graphs. Moreover, two conjectures in [4] are resolved positively. The rest of the paper is organized as follows. In section 2, we use interlacing inequalities for principal submatrix to help determining the spectrum of $K_{a_n}(k)$. Section 3 considers the spectra of $K_{b_n}(k)$, $K_{c_n}(k)$, and $K_{d_n}(k)$ when k takes on extreme values. Section 4 provides a unified approach for determining spectra of $K_{b_n}(k)$, $K_{c_n}(k)$, and $K_{d_n}(k)$ by matrix factorization.

2 The graph $K_{a_n}(k)$

Let $n \geq 3$ and $0 \leq k \leq n-1$. The adjacency matrix of $K_{a_n}(k)$ is of the form

$$A = \begin{bmatrix} 0 & x_r^T \\ x_r & B \end{bmatrix}$$

where x_r is an $(n-1)$-vector with the first $r = n-k-1$ entries equal to 1 and the rest equal to 0, and B is the adjacency matrix of K_{n-1}.

Let the eigenvalues of A be $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Since the spectrum of B is $\{n-2, -1^{(n-2)}\}$, by interlacing inequalities for principal submatrix, we have

$$\lambda_1 \geq n-2 \geq \lambda_2 \geq -1 \geq \lambda_3 \geq -1 \geq \cdots \geq -1 \geq \lambda_{n-1} \geq -1 \geq \lambda_n. \tag{1}$$

Hence $\lambda_3 = \cdots = \lambda_{n-1} = -1$. Note that the spectral moments of A can be computed in two different ways. In particular,

$$\begin{aligned} \lambda_1 + \lambda_2 + (n-3)(-1) + \lambda_n &= trA = 0, \\ \lambda_1^2 + \lambda_2^2 + (n-3)(-1)^2 + \lambda_n^2 &= trA^2 = 2r + (n-2)^2 + (n-2), \\ \lambda_1^3 + \lambda_2^3 + (n-3)(-1)^3 + \lambda_n^3 &= trA^3 = 3(r^2-r) + (n-2)^3 + (n-2)(-1). \end{aligned}$$

After simplification, we have

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_n &= n-3, \\ \lambda_1^2 + \lambda_2^2 + \lambda_n^2 &= 2r + n^2 - 4n + 5, \\ \lambda_1^3 + \lambda_2^3 + \lambda_n^3 &= 3(r^2-r) + n^3 - 6n^2 + 12n - 9. \end{aligned}$$

It follows from Newton's identities that

$$\begin{aligned} \lambda_1 + \lambda_2 + \lambda_n &= n-3, \\ \lambda_1\lambda_2 + \lambda_2\lambda_n + \lambda_n\lambda_1 &= 2-n-r, \\ \lambda_1\lambda_2\lambda_n &= r^2 + 2r - nr. \end{aligned}$$

Consequently, λ_1, λ_2 and λ_n are the roots of the cubic polynomial $x^3 - (n-3)x^2 + (2-n-r)x - (r^2+2r-nr)$, and we obtain

Lemma 2.1 For $n \geq 3$ and $0 \leq k \leq n-1$, the characteristic polynomial of $K_{a_n}(k)$ is

$$(x+1)^{n-3}[x^3 + (3-n)x^2 + (3+k-2n)x + (k-1)(n-k-1)].$$

Corollary 2.2 If $n \geq 3$ and $k = n-1$ then $K_{a_n}(n-1)$ is the disjoint union of two complete graphs K_{n-1} and K_1, and its characteristic polynomial is $(x+1)^{n-3}[x^3 + (3-n)x^2 + (2-n)x]$. Hence the spectrum is $\{n-2, 0, (-1)^{(n-2)}\}$ and the energy is $2n-4 < 2n-2$. Therefore $K_{a_n}(n-1)$ is not hyper-energetic.

Corollary 2.3 If $n \geq 3$ and $k = 1$ then $K_{a_n}(1)$ is the complete graph K_n with an edge deleted, and its characteristic polynomial is $(x+1)^{n-3}[x^3+(3-n)x^2+(4-2n)x]$. Hence the spectrum is $\{0, (-1)^{(n-3)}, \frac{n-3\pm\sqrt{n^2+2n-7}}{2}\}$ and the energy is $n-3+\sqrt{n^2+2n-7} < 2n-2$. Therefore $K_{a_n}(1)$ is not hyper-energetic.

Corollary 2.4 If $n \geq 3$ and $k = 0$ then $K_{a_n}(0)$ is the complete graph K_n, and its characteristic polynomial is $(x+1)^{n-3}[x^3+(3-n)x^2+(3-2n)x+(1-n)]$. Hence the spectrum is $\{(-1)^{(n-1)}, n-1\}$ and the energy is $2n-2$. Therefore $K_{a_n}(0)$ is not hyper-energetic.

Theorem 2.5 For $n \geq 4$ and $2 \leq k \leq n-2$, $K_{a_n}(k)$ is hyper-energetic if and only if $n > k+3+\frac{4}{k-1}$.

Proof. From the discussion before Lemma 2.1, the spectrum of $K_{a_n}(k)$ is

$$\{\lambda_1, \lambda_2, (-1)^{(n-3)}, \lambda_n\}$$

where $\lambda_1, \lambda_2, \lambda_n$ are the roots of the cubic polynomial

$$f(x) = x^3 + (3-n)x^2 + (3+k-2n)x + (k-1)(n-k-1).$$

Moreover the interlacing inequalities (1) give $\lambda_1 \geq n-2 \geq \lambda_2 \geq -1$, and so $\lambda_1 > 0$ and $\lambda_n < 0$. Since $n \geq 4$ and $2 \leq k \leq n-2$, the product $\lambda_1\lambda_2\lambda_n = -(k-1)(n-k-1) < 0$, it follows that $\lambda_2 > 0$. Consequently, $\mathcal{E}(K_{a_n}(k)) = n-3+|\lambda_1|+|\lambda_2|+|\lambda_n| = n-3+\lambda_1+\lambda_2-\lambda_n$. Now $K_{a_n}(k)$ is hyper-energetic if and only if $\mathcal{E}(K_{a_n}(k)) = n-3+\lambda_1+\lambda_2-\lambda_n > 2n-2$, i.e., $\lambda_1+\lambda_2-\lambda_n > n+1$. Note that $\lambda_1+\lambda_2+\lambda_n = n-3$, it follows that $K_{a_n}(k)$ is hyper-energetic if and only if $\lambda_n < -2$ which, by the Intermediate Value Theorem, is equivalent to $f(-2) > 0$, i.e., $n > k+3+\frac{4}{k-1}$ since λ_n is the only negative root of $f(x)$. ■

Corollary 2.6 For $n \geq 3$ and $0 \leq k \leq n-1$, $K_{a_n}(k)$ is hyper-energetic if and only if

$$\begin{aligned} k = 2 &\text{ and } n \geq 10 \text{ or} \\ k = 3 &\text{ and } n \geq 9 \text{ or} \\ k = 4 &\text{ and } n \geq 9 \text{ or} \\ k = 5 &\text{ and } n \geq 10 \text{ or} \\ k \geq 6 &\text{ and } n \geq k+4. \end{aligned}$$

Proof. (Necessity) Suppose that $K_{a_n}(k)$ is hyper-energetic. Then, by Corollaries 2.2, 2.3, and 2.4, we have $n \geq 4$ and $2 \leq k \leq n-2$. Hence the conclusion follows from the condition $n > k + 3 + \frac{4}{k-1}$ of Theorem 2.5.

(Sufficiency) It is straight forward to check that the conclusion on n and k satisfies the conditions $n \geq 4$, $2 \leq k \leq n-2$, and $n > k+3+\frac{4}{k-1}$. Hence $K_{a_n}(k)$ is hyper-energetic by Theorem 2.5. ■

Remark 2.7 Corollary 2.6 resolves Conjecture 1 in [4] positively. Lemma 2.1 can also be obtained by other methods like the one in [9]. However our approach yields more information about the eigenvalues, and so the proof of Theorem 2.5 becomes relatively simple.

3 Complement of a regular graph

In this section, we consider the three families of graphs $K_{b_n}(k), K_{c_n}(k)$, and $K_{d_n}(k)$ with extreme values of k. Our goal is to determine when they are hyper-energetic. The next lemma is a well established fact in spectral graph theory. We include a proof using matrix factorization.

Lemma 3.1 Let G be a regular graph with eigenvalues $k \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then the complement graph $\overline{G}$ is also regular with eigenvalues $n-k-1 \geq -1-\lambda_n \geq \cdots \geq -1-\lambda_2$.

Proof. Denote the orthonormal eigenvectors $e/\sqrt{n}, x_2, \ldots, x_n$ of the eigenvalues $k \geq \lambda_2 \geq \cdots \geq \lambda_n$ respectively, where e is the vector with all entries equal to 1. Then

$$U^T A(G) U = Diag(k, \lambda_2, \cdots, \lambda_n)$$

is a diagonal matrix, where U is the orthogonal matrix with columns $e/\sqrt{n}, x_2, \ldots, x_n$. If J denotes the matrix with all entries equal to 1 and I donotes the identity matrix of the appropriate size then

$$\begin{aligned} U^T A(\overline{G}) U &= U^T [J - I - A(G)] U \\ &= U^T J U - I - U^T A(G) U \\ &= Diag(n, 0, \cdots, 0) - I - Diag(k, \lambda_2, \cdots, \lambda_n) \\ &= Diag(n-k-1, -1-\lambda_2, \cdots, -1-\lambda_n). \ ■ \end{aligned}$$

$K_{b_n}(0)$ is the complete graph and so it is not hyper-energetic. If n is even, then $K_{b_n}(\lfloor \frac{n}{2} \rfloor)$ is the complement graph of the 1-regular graph on n vertices. Hence, by Lemma 3.1, it has eigevalues $\{n-2, 0^{(\lfloor \frac{n}{2} \rfloor)}, (-2)^{(\lfloor \frac{n}{2} \rfloor - 1)}\}$ and so the energy is $2n-4 < 2n-2$. Therefore $K_{b_n}(\lfloor \frac{n}{2} \rfloor)$ is not hyper-energetic.

$K_{c_n}(0)$ is the complete graph and $K_{c_n}(n)$ is the empty graph. Therefore both are not hyper-energetic.

$K_{d_n}(n)$ is the complement graph of a Hamiltonian cycle in K_n, hence it is a $(n-3)-$regular graph on n vertices. It is known that regular graphs with degree less than 4 are not hyper-energetic [11]. However it may not be the case for regular graphs with higher degree, see Corollary 3.3. By Lemma 3.1, $K_{d_n}(n)$ has eigenvalues $\{n-3, -(1+2\cos\frac{2\pi}{n}), \ldots, -(1+2\cos\frac{2(n-1)\pi}{n})\}$ and so the energy is $n-3+\sum_{j=1}^{n-1}|1+2\cos\frac{2j\pi}{n}|$. The next lemma is taken from [10].

Lemma 3.2 For $n \geq 3$, $\sum_{j=1}^{n-1}|1+2\cos\frac{2j\pi}{n}| > n+1$ if and only if $n \geq 10$.

Proof. Note that

$$\lim_{n\to\infty}\frac{2\pi}{n}\sum_{j=0}^{n-1}|1+2\cos\frac{2j\pi}{n}| = \int_0^{2\pi}|1+2\cos x|\,dx = \frac{2\pi+12\sqrt{3}}{3}.$$

Hence $\lim_{n\to\infty}\frac{1}{n+1}\sum_{j=0}^{n-1}|1+2\cos\frac{2j\pi}{n}| = \frac{\pi+6\sqrt{3}}{3\pi} = 1.4359 > 1$, and so there exists an integer n_0 such that

$$\sum_{j=1}^{n-1}|1+2\cos\frac{2j\pi}{n}| > n+1$$

for $n \geq n_0$. Numerical calculation shows that $n_0 = 10$. ■

Corollary 3.3 For $n \geq 3$, $K_{d_n}(n)$ is hyper-energetic if and only if $n \geq 10$.

Proof. $K_{d_n}(n)$ is hyper-energetic if and only if $\mathcal{E}(K_{d_n}(n) = n-3+\sum_{j=1}^{n-1}|1+2\cos\frac{2j\pi}{n}| > 2n-2$ if and only if $\sum_{j=1}^{n-1}|1+2\cos\frac{2j\pi}{n}| > n+1$ if and only if $n \geq 10$, by Lemma 3.2. ■

4 Joint of complements of two regular graphs

Let G be a regular graph on $s \geq 1$ vertices with eigenvalues $k_s \geq \lambda_2 \geq \cdots \geq \lambda_s$ and orthonormal eigenvectors $e/\sqrt{s}, x_2, \ldots, x_s$. Denote U the orthogonal matrix with columns $e/\sqrt{s}, x_2, \ldots, x_s$. Then, from the proof of Lemma 3.1,

$$U^T A(\overline{G})U = Diag(n-k_s-1, -(\lambda_2+1), \ldots, -(\lambda_s+1)).$$

Similarly, let H be a regular graph on $t \geq 1$ vertices with eigenvalues $k_t \geq \mu_2 \geq \cdots \geq \mu_t$ and orthonormal eigenvectors $e/\sqrt{t}, y_2, \ldots, y_t$. Then

$$V^T A(\overline{H})V = Diag(n-k_t-1, -(\mu_2+1), \ldots, -(\mu_t+1))$$

where V denotes the orthogonal matrix with columns $e/\sqrt{t}, y_2, \ldots, y_t$.

Let Γ be the joint graph of the complement graphs $\overline{G}$ and $\overline{H}$. Then the adjacency matrix of Γ is

$$A(\Gamma) = \begin{bmatrix} A(\overline{G}) & J \\ J^T & A(\overline{H}) \end{bmatrix}$$

where J is an $s \times t$ matrix with all entries equal to 1.

Lemma 4.1 For $s, t \geq 1$, the characteristic polynomial of Γ is

$$[x^2 - (s+t-k_s-k_t-2)x + (s-k_s-1)(t-k_t-1) - st]\prod_{i=2}^{s}(x+\lambda_i+1)\prod_{i=2}^{t}(x+\mu_i+1).$$

Proof. Denote P the orthogonal matrix $\begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix}$. Then

$$\begin{aligned}
& P^T A(\Gamma) P \\
= & \begin{bmatrix} U^T A(\overline{G}) U & U^T J V \\ V^T J^T U & V^T A(\overline{H}) V \end{bmatrix} \\
= & \left[\begin{array}{cccc|cccc}
s-k_s-1 & & & & \sqrt{st} & & & \\
 & -(\lambda_2+1) & & & & 0 & & \\
 & & \ddots & & & & \ddots & \\
 & & & -(\lambda_s+1) & & & & 0 \\
\hline
\sqrt{st} & & & & t-k_t-1 & & & \\
 & 0 & & & & -(\mu_2+1) & & \\
 & & \ddots & & & & \ddots & \\
 & & & 0 & & & & -(\mu_t+1)
\end{array}\right]
\end{aligned}$$

Hence the spectrum of $A(\Gamma)$ is $\{-(\lambda_2+1), \ldots, -(\lambda_s+1), -(\mu_2+1), \ldots, -(\mu_t+1)\}$ together with the eigenvalues of the 2×2 matrix $\begin{bmatrix} s-k_s-1 & \sqrt{st} \\ \sqrt{st} & t-k_t-1 \end{bmatrix}$. It follows that the characteristic polynomial of $A(\Gamma)$ is

$$[x^2 - (s+t-k_s-k_t-2)x + (s-k_s-1)(t-k_t-1) - st]\prod_{i=2}^{s}(x+\lambda_i+1)\prod_{i=2}^{t}(x+\mu_i+1). \blacksquare$$

Corollary 4.2 For $n \geq 3$ and $1 \leq k < \lfloor \frac{n}{2} \rfloor$, if G is the disjoint union of k edges and H is empty graph on $n-2k$ vertices, then Γ is the $K_{b_n}(k)$ and its characteristic polynomial is $[x^2 - (n-3)x - 2(n-k-1)]x^k(x+1)^{n-2k-1}(x+2)^{k-1}$. Hence the spectrum is $\{0^{(k)}, (-1)^{(n-2k-1)}, (-2)^{(k-1)}, \frac{n-3\pm\sqrt{(n+1)^2-8k}}{2}\}$ and the energy is $n-3+\sqrt{(n+1)^2-8k} \leq 2n-2$. Therefore $K_{b_n}(k)$ is not hyper-energetic.

Corollary 4.3 For $n \geq 3$ and $1 \leq k \leq n-1$, if G is a complete graph on k vertices and H is empty graph on $n-k$ vertices, then Γ is the $K_{c_n}(k)$ and its characteristic polynomial is $[x^2 - (n-k-1)x - k(n-k)]x^{k-1}(x+1)^{n-k-1}$. Hence the spectrum is $\{0^{(k-1)}, (-1)^{(n-k-1)}, \frac{n-k-1\pm\sqrt{(n-k-1)^2+4k(n-k)}}{2}\}$ and the energy is $n-k-1+\sqrt{(n-k-1)^2+4k(n-k)} \leq 2n-2$. Therefore $K_{c_n}(k)$ is not hyper-energetic.

Corollary 4.4 For $n \geq 4$ and $3 \leq k \leq n-1$, if G is the cycle graph on k vertices and H is the empty graph on $n-k$ vertices, then Γ is the $K_{d_n}(k)$ and its characteristic polynomial is $[x^2-(n-4)x-(3n-2k-3)](x+1)^{n-k-1}(x+1+2\cos\frac{2\pi}{k})(x+1+2\cos\frac{4\pi}{k})\cdots(x+1+2\cos\frac{2(k-1)\pi}{k})$. Hence the spectrum is $\{\frac{n-4\pm\sqrt{n+2)^2-8k}}{2}, (-1)^{(n-k-1)}, -1-2\cos\frac{2\pi}{k}, \ldots, -1-2\cos\frac{2(k-1)\pi}{k}\}$ and the energy is $n-k-1+\sqrt{(n+2)^2-8k}+\sum_{j=1}^{k-1}|1+2\cos\frac{2j\pi}{k}|$.

Corollary 4.5 For $n \geq 4$ and $3 \leq k \leq n-1$, $K_{d_n}(k)$ is hyper-energetic if and only if

$$\begin{aligned} &k = 4 \text{ and } n \geq 8 \text{ or} \\ &k = 5 \text{ and } n \geq 8 \text{ or} \\ &k = 6 \text{ and } n \geq 12 \text{ or} \\ &k = 7 \text{ and } n \geq 9 \text{ or} \\ &k \geq 8 \text{ and } n \geq k+1. \end{aligned}$$

Proof. For $k=3$, $K_{d_n}(3) = K_{c_n}(3)$ which is not hyper-energetic for any $n \geq 4$ by Corollary 4.3.

For $k=4$, $\mathcal{E}(K_{d_n}(4)) = n-2+\sqrt{n^2+4n-28}$. Hence $K_{d_n}(4)$ is hyper-energetic if and only if $n > 7$.

For $k=5$, $\mathcal{E}(K_{d_n}(5)) = n-6+\sqrt{n^2+4n-36}+\sum_{j=1}^{4}|1+2\cos\frac{2j\pi}{5}| = n-6+\sqrt{n^2+4n-36}+4.4721...$ Hence $K_{d_n}(5)$ is hyper-energetic if and only if $n > 7.3263$.

For $k=6$, $\mathcal{E}(K_{d_n}(6)) = n-2+\sqrt{n^2+4n-44}$. Hence $K_{d_n}(6)$ is hyper-energetic if and only if iff $n > 11$.

For $k=7$, $\mathcal{E}(K_{d_n}(7)) = n-8+\sqrt{n^2+4n-52}+\sum_{j=1}^{6}|1+2\cos\frac{2j\pi}{7}| = n-8+\sqrt{n^2+4n-52}+7.2078...$ Hence $K_{d_n}(7)$ is hyper-energetic if and only if $n > 8.3326$.

For $k=8$, $\mathcal{E}(K_{d_n}(8)) = n-6+4\sqrt{2}+\sqrt{n^2+4n-60}$. Hence $K_{d_n}(8)$ is hyper-energetic if and only if $n > \frac{27-8\sqrt{2}}{2\sqrt{2}-1} \approx 8.5791$.

For $k=9$, $\mathcal{E}(K_{d_n}(9)) = n-10+\sqrt{n^2+4n-68}+\sum_{j=1}^{8}|1+2\cos\frac{2j\pi}{9} = n-10+\sqrt{n^2+4n-68}+9.5175...$ Hence $K_{d_n}(9)$ is hyper-energetic if and only if $n > 9.9933$.

For $k \geq 10$, by Lemma 3.2, $\sum_{j=1}^{k-1}|1+2\cos\frac{2j\pi}{k}| > k+1$. Hence

$$\begin{aligned} \mathcal{E}(K_{d_n}(k)) &= n-k-1+\sqrt{(n+2)^2-8k}+\sum_{j=1}^{k-1}|1+2\cos\frac{2j\pi}{k}| \\ &> n-k-1+\sqrt{(n+2)^2-8k}+k+1 \\ &\geq 2n-2. \end{aligned}$$

The last inequality is due to the fact that $k \leq n-1$. ■

Remark 4.6 Corollary 4.5 resolves Conjecture 2 in [4] positively.

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