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# Computing the maximal signless Laplacian index among graphs of prescribed order and diameter

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#### Abstract

A bug  $\operatorname{Bug}_{p,r_1,r_2}$  is a graph obtained from a complete graph  $K_p$ by deleting an edge uv and attaching the paths  $P_{r_1}$  and  $P_{r_2}$  by one of their end vertices at u and v, respectively. Let Q(G) be the signless Laplacian matrix of a graph G and  $q_1(G)$  be the spectral radius of Q(G). It is known that the bug  $B_0 = \operatorname{Bug}_{n-d+2,\lfloor\frac{d}{2}\rfloor,\lceil\frac{d}{2}\rceil}$  maximizes  $q_1(G)$  among all graphs G of order n and diameter d. For a bug B of order n and diameter d, n-d is an eigenvalue of Q(B) with multiplicity n-d-1. In this paper, we prove that remainder d +1 eigenvalues of Q(B), among them  $q_1(B)$ , can be computed as the eigenvalues of a symmetric tridiagonal matrix of order d+1. Finally, we show that  $q_1(B_0)$  can be computed as the largest eigenvalue of a symmetric tridiagonal matrix of order  $\frac{d}{2} + 1$  whenever d is even.

Keyword : Signless Laplacian index, diameter, bug, H-join. 2000 AMS classification : 05C50, 05C35, 15A18.

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## 1. Introduction

Let G = (V(G), E(G)) be a simple undirected graph of order n with vertex set V(G) and edge set E(G). Let D(G) be the diagonal matrix of order n whose (i, i) – entry is the degree of the i - th vertex of G and let A(G)be the adjacency matrix of G. The matrices L(G) = D(G) - A(G) and Q(G) = D(G) + A(G) are the Laplacian matrix and signless Laplacian matrix of G, respectively. These matrices are both positive semidefinite matrices and they have the same characteristic polynomial if and only if Gis a bipartite graph. The eigenvalues of A(G), L(G) and Q(G) are called the eigenvalues, Laplacian eigenvalues and signless Laplacian eigenvalues of G, respectively. In particular, the spectral radius of Q(G) is called the signless Laplacian index of G and it is usually denoted by  $q_1(G)$ . From the Perron - Frobenius Theory for nonnegative matrices, it follows that if G is a connected graph then  $q_1(G)$  is a simple eigenvalue of Q(G).

Let  $K_n$  and  $P_n$  be a complete graph and a path on n vertices, respectively. A bug  $Bug_{p,r_1,r_2}$  is a graph obtained from  $K_p$  by deleting an edge uvand attaching the paths  $P_{r_1}$  and  $P_{r_2}$  by one of their end vertices at u and v, respectively. Observe that  $Bug_{p,r_1,r_2}$  is a graph of order  $p + r_1 + r_2 - 2$ and diameter  $r_1 + r_2$ .

**Example 1.** For instance  $Bug_{6,3,4}$  is the graph



of 11 vertices and diameter 7.

Let  $\mathcal{G}_n$  be the class of all connected graphs on n vertices and let  $\mathcal{G}_{n,d}$ be the subclass of graphs in  $\mathcal{G}_n$  with diameter d. Since  $\mathcal{G}_{n,1} = \{K_n\}$  and  $\mathcal{G}_{n,n-1} = \{P_n\}$ , throughout this paper, we assume  $2 \leq d \leq n-2$ . Let

$$\mathcal{B}_{n,d} = \{ Bug_{n-d+2,i,d-i} : 1 \le i \le d-1 \}.$$

Clearly  $\mathcal{B}_{n,d}$  is a subclass of  $\mathcal{G}_{n,d}$ .

Some results such that  $q_1(G)$  is maximal among graphs with fixed invariants are known. For instance, in [4] the graph having the largest  $q_1(G)$  among the graphs with fixed numbers of vertices and edges is found, in [6] the graphs with the largest  $q_1(G)$  and the largest adjacency index among all graphs with a fixed vertex connectivity or a fixed edge connectivity are characterized and in [7] the author characterizes the graphs having the largest  $q_1(G)$  among all the graphs on n vertices and a given matching number. of trees in  $\mathcal{T}_{n,d}$  are characterized.

For a bug B of order n and diameter d, n-d is an eigenvalue of Q(B) with multiplicity n-d-1. In this paper, we prove that remainder d+1 eigenvalues of Q(B) can be computed as the eigenvalues of a symmetric tridiagonal matrix of order d+1.

A conjecture proposed by Hansen and Lucas [5] states that, for a given  $n \geq 9$ , the bug  $B_{\lfloor \frac{n}{2} \rfloor + 1, \lfloor \frac{D}{2} \rfloor, \lceil \frac{D}{2} \rceil}$ , where  $D = \lceil \frac{n+1}{2} \rceil$ , is the unique connected graph of order n that maximizes the product  $q_1(G)diam(G)$  over all connected graphs G of order n. This conjecture was studied by H. Liu and M. Lu [3]. They proved that the bug  $B_0 = Bug_{n-d+2,\lfloor \frac{d}{2} \rfloor, \lceil \frac{d}{2} \rceil}$  maximizes  $q_1(G)$  among all graphs G of order n and diameter d and that, for a given n, the bug  $B_{\lfloor \frac{n}{2} \rfloor + 2, \lfloor \frac{D}{2} \rfloor, \lceil \frac{D}{2} \rceil}$ , where  $D = \lceil \frac{n+1}{2} \rceil$ , is the unique connected graph of order n that maximizes the product  $q_1(G)diam(G)$  over all connected graphs of order n.

Moreover, in this paper, we prove that  $q_1(B_0)$  can be computed as the largest eigenvalue of a symmetric tridiagonal matrix of order  $\frac{d}{2}+1$  whenever d is even.

We recall the notion of the join operation of graphs. Given two vertex disjoint graphs  $G_1$  and  $G_2$ , the join of  $G_1$  and  $G_2$  is the graph  $G = G_1 \lor G_2$  such that  $V(G) = V(G_1) \cup V(G_2)$  and  $E(G) = E(G_1) \cup E(G_2) \cup \{xy : x \in V(G_1), y \in V(G_2)\}$ .

The join operation of two vertex disjoint graphs can be generalize as follows [1, 2]. Let H be a graph of order k. Let  $V(H) = \{1, \ldots, k\}$  be the vertex set of H. Let  $\{G_1, G_2, \ldots, G_k\}$  be a set of pairwise vertex disjoint graphs. For  $1 \leq j \leq k$ , the vertex  $j \in V(H)$  is assigned to the graph  $G_j$ . Let G be the graph obtained from the graphs  $G_1, G_2, \ldots, G_k$  and the edges connecting each vertex of  $G_i$  with all the vertices of  $G_j$  if and only if  $ij \in E(H)$ . That is, G is the graph with vertex set  $V(G) = \bigcup_{i=1}^k V(G_i)$  and edge set  $E(G) = \left(\bigcup_{i=1}^k E(G_i)\right) \cup \left(\bigcup_{ij \in E(H)} \{uv : u \in V(G_i), v \in V(G_j)\}\right)$ . This graph is called the H - join of the graphs  $G_1, \ldots, G_k$  and it is denoted by  $G = \bigvee_H \{G_j : 1 \leq j \leq k\}$ .

We see that if  $n_i$  is the order of  $G_i$ , i = 1, 2, ..., k, then H - join of  $G_1, ..., G_k$  is a graph of order  $n_1 + n_2 + ... + n_k$ .

Important examples of this graph operation are the bugs  $Bug_{n-d+2,i,d-i}$ . In fact, the bug  $Bug_{n-d+2,i,d-i}$  is the  $P_{d+1} - join$  of the regular graphs  $G_1 = \ldots = G_i = K_1, G_{i+1} = K_{n-d}, G_{i+2} = \ldots = G_{d+1} = K_1$ .

Since  $Bug_{n-d+2,i,d-i}$  and  $Bug_{n-d+2,d-i,i}$ , are isomorphic graphs, we may take  $1 \leq i \leq \lfloor \frac{d}{2} \rfloor$ .

**Example 2.** Below are the non-isomorphic bugs of order 11 and diameter 7.

 $Bug_{6,1,6}$  is the  $P_8-join$  of  $G_1 = K_1, G_2 = K_4$  and  $G_i = K_1$  for  $i = 3, \ldots, 8$ :



 $Bug_{6,2,5}$  is the  $P_8 - join$  of  $G_1 = G_2 = K_1$ ,  $G_3 = K_4$  and  $G_i = K_1$  for  $i = 4, \ldots, 8$ :



 $Bug_{6,3,4}$  is the  $P_8-join$  of  $G_1 = G_2 = G_3 = K_1$ ,  $G_4 = K_4$  and  $G_i = K_1$  for  $i = 5, \ldots, 8$ :



### 2. The signless Laplacian eigenvalues of bugs

In [1], Theorem 5, the spectrum of the adjacency matrix of the H- join of regular graphs is obtained. The version of this result for the signless Laplacian matrix is given below and its proof is similar.

**Theorem 1.** Let *H* be a graph with *k* vertices. Let  $G = \bigvee_H \{G_j : 1 \le j \le k\}$ . For j = 1, ..., k, let  $G_j$  be a  $r_j$ -regular graph of order  $n_j$ . Then

 $(2.1) \sigma \left( Q \left( G \right) \right) = \cup_{G_j \neq K_1} \left\{ s_j + \lambda : \lambda \in \sigma \left( Q \left( G_j \right) \right) \setminus \left\{ 2r_j \right\} \right\} \cup \sigma \left( M(G) \right)$ 

where M(G) is a matrix of order  $k \times k$  given by

$$M(G) = \begin{bmatrix} s_1 + 2r_1 & \delta_{12}\sqrt{n_1n_2} & \dots & \delta_{1k}\sqrt{n_1n_k} \\ \delta_{12}\sqrt{n_1n_2} & s_2 + 2r_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \delta_{(k-1)k}\sqrt{n_{k-1}n_k} \\ \delta_{1k}\sqrt{n_1n_k} & \dots & \delta_{(k-1)k}\sqrt{n_{k-1}n_k} & s_k + 2r_k \end{bmatrix}$$

(2.2)

with

$$\delta_{ij} = \begin{cases} 1 \text{ if } ij \in E(H) \\ 0 \text{ otherwise} \end{cases}$$

and, for j = 1, 2, ..., k, (2.3)  $s_j = \sum_{jl \in E(H)} n_l$ .

For brevity, let  $B(i) = Bug_{n-d+2,i,d-i}$ . Remember that we may take  $1 \le i \le \lfloor \frac{d}{2} \rfloor$ .

We already observed  $B(i) = Bug_{n-d+2,i,d-i}$  is the  $P_{d+1} - join$  of the regular graphs  $G_1 = \ldots = G_i = K_1, G_{i+1} = K_{n-d}, G_{i+2} = \ldots = G_{d+1} = K_1$ . Hence Theorem 1 can be applied to determine its signless Laplacian eigenvalues. For all the bugs B(i), the graph H in Theorem 1 is the path  $P_{d+1}$ . Hence the matrix M(B(i)) in (2.2) becomes a symmetric tridiagonal

matrix of order  $(d+1) \times (d+1)$ :

For convenience, we define the matrices

#### **Definition 1.** Let

$$R(n-d) = \begin{bmatrix} n-d+1 & \sqrt{n-d} & 0\\ \sqrt{n-d} & 2(n-d) & \sqrt{n-d}\\ 0 & \sqrt{n-d} & n-d+1 \end{bmatrix},$$
$$T_1 = [1]$$

and, for  $s \ge 2$ , let

(2.5) 
$$T_{s} = \begin{bmatrix} 1 & 1 & & \\ 1 & 2 & 1 & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 2 & 1 \\ & & & 1 & 2 \end{bmatrix}.$$

of order  $s \times s$ .

Moreover, we introduce the following matrices: I is the identity matrix, 0 is the zero matrix, J is the exchange matrix (the matrix with ones in the secondary diagonal and zeros elsewhere) and F is the matrix whose entries are zeros except for the entry in the last row and first column which is equal to 1. The orders of these matrices will be clear from the context in which they are used.

**Theorem 2.** The eigenvalues of  $B(i) = Bug_{n-d+2,i,d-i}$  are n-d with multiplicity n-d-1 and the eigenvalues of the  $(d+1) \times (d+1)$  symmetric tridiagonal matrix

(2.6) 
$$M(B(i)) = \begin{bmatrix} X_i & F \\ F^T & JT_{d-i-1}J \end{bmatrix}$$

where

(2.7) 
$$X_{1} = \begin{bmatrix} n-d & \sqrt{n-d} & 0\\ \sqrt{n-d} & 2(n-d) & \sqrt{n-d}\\ 0 & \sqrt{n-d} & n-d+1 \end{bmatrix}$$

whenever i = 1,

(2.8) 
$$X_{i} = \begin{bmatrix} T_{i-1} & F \\ F^{T} & R(n-d) \end{bmatrix}$$

whenever  $2 \le i \le \left\lfloor \frac{d}{2} \right\rfloor$  and F is the matrix defined above.

**Proof.** We know that  $B(i) = Bug_{n-d+2,i,d-i}$  is the  $P_{d+1} - join$  of the regular graphs  $G_1 = \ldots = G_i = K_1, G_{i+1} = K_{n-d}, G_{i+2} = \ldots = G_{d+1} = K_1$ . Thus  $G_j = K_1$  for all j except for j = i + 1. For j = i + 1, we have  $G_{i+1} = K_{n-d}$  which is a (n - d - 1) - regular graph. From (2.3),  $s_{i+1} = n_i + n_{i+2} = 1 + 1 = 2$ . Then, from (2.1), we have

$$\sigma(Q(B(i))) = \{2 + \lambda : \lambda \in Q(K_{n-d}) \setminus \{2(n-d-1)\}\} \cup \sigma(M(B(i)))$$

(2.9)
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At this point, we recall that the signless Laplacian eigenvalues of  $K_{n-d}$  are 2(n-d-1) and n-d-2 with multiplicity n-d-1. Using this fact in (2.9), we obtain  $\sigma(Q(B(i))) = \{(n-d)^{[n-d-1]}\} \cup \sigma(M(B(i)))$  where  $(n-d)^{[n-d-1]}$  means that n-d is an eigenvalue of multiplicity n-d-1.

We now search for the entries of M(B(i)) in (2.4). We begin with M(B(1)). The bug B(1) is the  $P_{d+1} - join$  of  $G_1 = K_1$ ,  $G_2 = K_{n-d}$  and  $G_3 = G_4 = \ldots = G_{d+1} = K_1$ . For this bug

$$n_{1} = 1 r_{1} = 0$$

$$n_{2} = n - d r_{2} = n - d - 1$$

$$n_{3} = 1 r_{3} = 0$$

$$\vdots \vdots$$

$$n_{d} = 1 r_{d} = 0$$

$$n_{d+1} = 1 r_{d+1} = 0$$

Then  $s_1 = n_2 = n - d$ ,  $s_2 = n_1 + n_3 = 2$ ,  $s_3 = n_2 + n_4 = n - d + 1$ ,  $s_4 = n_3 + n_5 = 2, \ldots, s_d = n_{d-1} + n_{d+1} = 2$ ,  $s_{d+1} = n_d = 1$ . Replacing these values in (2.4), we obtain

$$\mathbf{M}(\mathbf{B}(1)) = \begin{bmatrix} X_1 & F \\ F^T & JT_{d-2}J \end{bmatrix} \text{ with } \mathbf{X}_1 = \begin{bmatrix} n-d & \sqrt{n-d} & 0 \\ \sqrt{n-d} & 2(n-d) & \sqrt{n-d} \\ 0 & \sqrt{n-d} & n-d+1 \end{bmatrix}$$

and  $T_{d-2}$  as in (2.5). The theorem has been proved for B(1). Let  $2 \leq i \leq \lfloor \frac{d}{2} \rfloor$ . The bug B(2) is the  $P_{d+1} - join$  of the regular graphs  $G_1 = G_2 = K_1, G_3 = K_{n-d}, G_4 = \ldots = G_{d+1} = K_1$ . For B(2), we have

 $\begin{array}{ll} n_1 = 1 & r_1 = 0 \\ n_2 = 1 & r_2 = 0 \\ n_3 = n - d & r_3 = n - d - 1 \\ n_4 = 1 & r_4 = 0 \\ \vdots & \vdots \\ n_d = 1 & r_d = 0 \\ n_{d+1} = 1 & r_{d+1} = 0 \end{array}$ 

Then  $s_1 = n_2 = 1$ ,  $s_2 = n_1 + n_3 = n - d + 1$ ,  $s_3 = n_2 + n_4 = 2$ ,  $s_4 = n_3 + n_5 = n - d + 1$ ,  $s_5 = n_4 + n_6 = 2$ , ...,  $s_d = n_{d-1} + n_{d+1} = 2$ ,  $s_{d+1} = n_d = 1$ . Replacing these values in (2.4), we get

$$\mathbf{M}(\mathbf{B}(2)) = \left[\begin{array}{cc} X_2 & F\\ F^T & JT_{d-3}J \end{array}\right]$$

where

$$\mathbf{X}_{2} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & n-d+1 & \sqrt{n-d} & 0 \\ 0 & \sqrt{n-d} & 2(n-d) & \sqrt{n-d} \\ 0 & 0 & \sqrt{n-d} & n-d+1 \end{bmatrix}$$

and  $T_{d-3}$  as in (2.5). The bug B(3) is the  $P_{d+1} - join$  of  $G_1 = G_2 = G_3 = K_1$ ,  $G_4 = K_{n-d}$ ,  $G_5 = \ldots = G_{d+1} = K_1$ . Similarly

$$\mathbf{M}(\mathbf{B}(3)) = \left[ \begin{array}{cc} X_3 & F \\ F^T & JT_{d-4}J \end{array} \right]$$

where

$$\mathbf{X}_{3} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & n-d+1 & \sqrt{n-d} & 0 \\ 0 & 0 & \sqrt{n-d} & 2(n-d) & \sqrt{n-d} \\ 0 & 0 & 0 & \sqrt{n-d} & n-d+1 \end{bmatrix}$$

and  $T_{d-4}$  as in (2.5). We continue in this fashion obtaining that the result also holds for  $i = 4, \ldots, \lfloor \frac{d}{2} \rfloor$ .  $\Box$ 

# 3. Computing the largest signless Laplacian index of graphs of prescribed order and diameter

We already mentioned that H. Liu and M. Lu, Theorem 3.2 in [3] characterized the largest signless Laplacian index among the graphs in  $\mathcal{G}_{n,d}$ . **Theorem 3.** Among all the graphs G on n vertices and diameter  $d, 2 \leq d \leq n-2$ , the largest  $q_1(G)$  is attained by the bug  $B(\lfloor \frac{d}{2} \rfloor) = Bug_{n-d+2,\lfloor \frac{d}{2} \rfloor, \lfloor \frac{d}{2} \rfloor}$ .

Theorem 3 tell us that the largest signless Laplacian index among the graph in  $\mathcal{G}_{n,d}$  is  $q_1(B(\lfloor \frac{d}{2} \rfloor))$ . From Theorem 2,  $q_1(B(\lfloor \frac{d}{2} \rfloor))$  can be computed as the largest eigenvalues of the symmetric tridiagonal matrix  $M(B(\lfloor \frac{d}{2} \rfloor))$  of order d + 1. More precisely

**Theorem 4.** Let  $G \in \mathcal{G}_{n,d}$ .

(a) If d = 3 then the largest  $q_1(G)$  can be computed as the largest eigenvalue of the symmetric tridiagonal matrix M(B(1)) of order 4 with diagonal entries

$$n-3, 2(n-3), n-2, 1$$

and codiagonal entries

$$\sqrt{n-3}, \sqrt{n-3}, 1$$

(b) If  $d \ge 4$  then the largest  $q_1(G)$  can be computed as the largest eigenvalue of the symmetric tridiagonal matrix  $M(B(\lfloor \frac{d}{2} \rfloor))$  of order d+1 with diagonal entries

$$1, \underbrace{\lfloor \frac{d}{2} \rfloor^{-2}}_{1, 1, 2, \dots, 2}, n - d + 1, 2(n - d), n - d + 1, \underbrace{\lceil \frac{d}{2} \rceil^{-2}}_{2, \dots, 2, 1}, 1$$

codiagonal entries

$$\underbrace{\lfloor \frac{d}{2} \rfloor^{-1}}_{1, \dots, 1}, \sqrt{n-d}, \sqrt{n-d}, \underbrace{\sqrt{n-d}}_{1, \dots, 1}.$$

We now prove that  $q_1(B(\lfloor \frac{d}{2} \rfloor))$  can be computed as the largest eigenvalue of a symmetric tridiagonal matrix of order  $\frac{d}{2} + 1$  whenever d is an even integer.

**Theorem 5.** If  $d \ge 4$  is an even integer then among the graphs G on n vertices and diameter d, the largest  $q_1(G)$  can be computed as the largest eigenvalue of a symmetric tridiagonal matrix of order  $\frac{d}{2} + 1$  with diagonal entries

$$1, 2, \ldots, 2, n - d + 1, 2(n - d)$$

and codiagonal entries

$$1,\ldots,1,\sqrt{2(n-d)}.$$

**Proof.** Let d be an even integer and  $\alpha = n - d$ . From Theorem 4,  $q_1(M(B(\frac{d}{2})))$  can be computed as the largest eigenvalue of

$$M(B(\frac{d}{2})) = \begin{bmatrix} U & \mathbf{b} & 0\\ \mathbf{b}^T & 2\alpha & \mathbf{b}^T J\\ 0 & J\mathbf{b} & JUJ \end{bmatrix}$$

of order d + 1 where

$$U = \begin{bmatrix} 1 & 1 & & & \\ 1 & 2 & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & 1 & 2 & 1 \\ & & & 1 & \alpha + 1 \end{bmatrix}$$

of order  $\frac{d}{2}$ ,  $\mathbf{b}^T = \begin{bmatrix} 0 & \cdots & 0 & \sqrt{\alpha} \end{bmatrix}$ , J is the reverse matrix and 0 is the zero matrix, all of them of the appropriate sizes. Consider the orthogonal matrix

$$Q = \frac{1}{\sqrt{2}} \begin{bmatrix} I & \mathbf{0} & J \\ \mathbf{0}^T & \sqrt{2} & \mathbf{0}^T \\ -J & \mathbf{0} & I \end{bmatrix}.$$

An easy calculation shows that

$$QM(B(\frac{d}{2}))Q^{T} = \begin{bmatrix} U & \sqrt{2}\mathbf{b} & 0\\ \sqrt{2}\mathbf{b}^{T} & 2\alpha & \mathbf{0}^{T}\\ 0 & \mathbf{0} & JUJ \end{bmatrix}.$$

Then the eigenvalues of  $M(B(\frac{d}{2}))$  are the eigenvalues of

 $\begin{bmatrix} U & \sqrt{2}\mathbf{b} \\ \sqrt{2}\mathbf{b}^T & 2\alpha \end{bmatrix}$  and the eigenvalues of U. Since the eigenvalues of U strictly interlace the eigenvalues of  $\begin{bmatrix} U & \sqrt{2}\mathbf{b} \\ \sqrt{2}\mathbf{b}^T & 2\alpha \end{bmatrix}$ , the proof is complete.

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