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On Unicyclic Graphs Spectra: New Results

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Abstract—Let $G = (V, E)$ be a unicyclic simple undirected graph. In this paper, we investigate the spectra of a particular class of unicyclic graphs $G(q, n_1)$ where q is the size of the unique cycle. Each vertex of the unique cycle is attached to n_1 vertices. We provide the “exact values” of the extremal eigenvalues of the adjacency matrix A and the Laplacian matrix L of G , in contrast to lower and upper bounds reported in the literature.

Index Terms—Unicyclic graph, Laplacian eigenvalues, Algebraic connectivity, Circulant matrices

I. INTRODUCTION

Given an undirected graph $G = (V, E)$, in which V represents the set of vertices and E the set of edges, if G is connected with the property $|V| = |E|$, then G is said to be a *unicyclic graph*. In other words, if G is connected and has the same number of vertices and edges then G is unicyclic (i.e. contains one and unique cycle).

Unicyclic graphs have applications in different research areas and domains. For example, unicyclic graphs are often used in telecommunications. They allow end-users connected in the same unicyclic component or graph to communicate using the two directions of the cycle. The cycle ensures a certain level of survivability to link failure that occurs on the edges of this cycle (commonly known as a “ring” in telecommunications). The traffic demands between nodes on the same cycle are then fully protected against failures while the other demands can be disrupted.

This paper focuses on a particular class of unicyclic graphs $G(q, n_1)$ where q is the size of the unique cycle and n_1 represents the number of nodes connected to each vertex on the cycle. The degree of each vertex of the cycle is $n_1 + 2$ (i.e., each vertex of the cycle has n_1 neighbors not on the cycle). We can easily deduce that the total number of vertices of this class of unicyclic graph is given by $q + (q \times n_1)$ (see Figure 1 for more details through a simple example).

Given a graph G with n vertices and m edges, we denote by A the adjacency matrix of G and by L the Laplacian matrix of G . The matrix L is the result of the difference between the degree matrix D (D is a diagonal matrix, and each value represents the degree of a vertex in G) and the adjacency matrix A , inducing $L = D - A$.

Let d_1, d_2, \dots, d_n be the degrees of the vertices $1, 2, \dots, n$ respectively in graph G . Without loss of generality, we

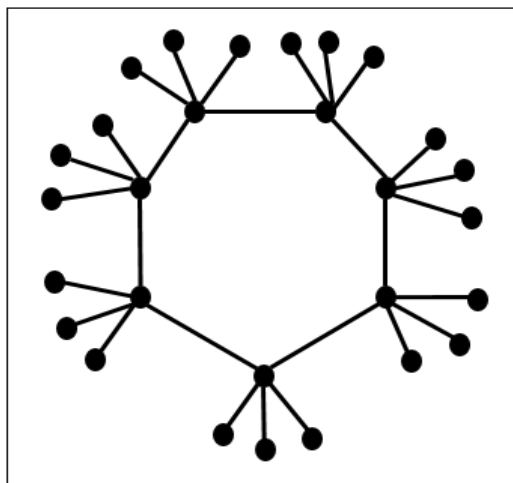


Fig. 1. Example of a unicyclic graph $G(7, 3)$

suppose that the degrees of the vertices are ranked in the following decreasing order ($d_1 \geq d_2 \geq \dots \geq d_n$). In addition, let $d_1 = \Delta$ be the maximum degree and $d_n = \delta$ the minimum degree of G .

Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of the adjacency matrix A of G (we suppose that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$) and $\mu_1, \mu_2, \dots, \mu_{n-1}, \mu_n = 0$ are the eigenvalues of the Laplacian matrix (we suppose also that $\mu_1 \geq \mu_2 \geq \dots \mu_{n-1} \geq \mu_n = 0$). Note that we are interested only by connected graphs, and according to [1], the smallest eigenvalue of the Laplacian matrix of a connected graph, is equal to zero. Graphs with different connected components are not in the scope of this paper.

Our key contributions consist of proposing exact values of the extremal eigenvalues of the Laplacian and the adjacency matrices of a particular class of unicyclic graphs $G(q, n_1)$, in contrast to lower and upper bounds provided by the current literature. Our results improve the quality of the spectral lower and upper bounds for any graphs.

Section II of this paper is dedicated to related work on lower and upper bounds of the eigenvalues of the adjacency and Laplacian matrices of a given graph. Section III provides the extremal and exact eigenvalues of A and L of unicyclic graphs $G = (q, n_1)$. Scalability analysis and performance

evaluations of our results are found in Section IV. Further work is presented in Section V.

II. RELATED WORK

A. Bounds on λ_1 and λ_n

Computation of extremal eigenvalues of graph spectra is a classical problem, investigated using different numerical methods (see references [2] and [3], for example) to characterize the exact values for small graphs. Since characterizing the eigenvalues becomes harder for large graphs, prior art resorted to lower and upper bounds to estimate the spectra of these graphs. We review some of these upper and lower bounds results from the literature.

If A is a symmetric matrix with values in \mathcal{R} and x is a vector with norm 1, then a function $f(x) = x^t Ax$ reaches its maximum (resp. minimum) value at the eigenvector associated to the largest (respectively, smallest) eigenvalue.

Proposition II.1. [1] *If G is a graph with n vertices and m edges and we note $\bar{d} = \frac{\sum_{i=1}^n d_i}{n}$, then we can write:*

$$\begin{aligned} \Delta &\geq \lambda_1 \geq \bar{d} \\ \sum_{i=1}^n \lambda_i &= 0 \\ \sum_{i=1}^n \lambda_i^2 &= 2m \\ \lambda_1 &\geq 2\cos\left(\frac{\pi}{n+1}\right) \end{aligned}$$

In order to propose tighter lower and upper bounds, previous work proposed different bounds improving the distance to the exact value. For instance, reference [4], proposed a new tight bound on λ_1 as established in the following proposition, for a given graph:

Proposition II.2. *Let λ_1 be the largest eigenvalue (index) of the adjacency matrix of a graph G . Then*

$$\lambda_1 \geq \sqrt{\Delta}$$

In case of unicyclic graph, reference [5] proposed an upper bound on λ_1 , given as follows:

Proposition II.3. *If G is a unicyclic graph then:*

$$\lambda_1 \leq 2\sqrt{\Delta - 1}$$

References [1] and [6] proposed also upper bounds on λ_1 using different parameters of graph G . Their results are given in Propositions II.4 and II.5 respectively.

Proposition II.4. *Let G be a connected graph with n vertices and m edges, this new bound is valid :*

$$\lambda_1 \leq \sqrt{2m - (n-1)\delta + (\delta-1)m_{max}}$$

with $m_{max} = \max_{i=1,n} m_i$ and $m_i = \frac{1}{d_i} \sum_{j \sim i} d_j$

Proposition II.5. *Let G be a graph with n vertices and m edges. Then we have :*

- $1 \leq \lambda_1 \leq n-1$
- $-\lambda_1 \leq \lambda_n \leq -1$

In the same manner, authors of [7] proposed new bounds on λ_n to reduce the separation of the obtained bounds and the exact value. This result is indicated in Proposition II.6.

Proposition II.6. *Let G be a connected graph with n vertices and m edges. Then*

$$\lambda_n \geq -\sqrt{2m - (n-1)\delta + (\delta-1)\Delta}.$$

Another reference dealing with spectral radius of some unicyclic graphs is proposed in [8]. Authors of this reference investigate new upper bounds on μ_1 and λ_1 as proposed in the following proposition:

Proposition II.7. *Let G be a simple undirected unicyclic graph, then:*

$$\begin{aligned} \mu_1 &< \Delta + 2\sqrt{\Delta-1} \cos\left(\frac{\pi}{2k(G)+1}\right) \\ \lambda_1 &< 2\sqrt{\Delta-1} \cos\left(\frac{\pi}{2k(G)+1}\right) \end{aligned}$$

where $k(G)$ is the maximum distance between all couples of vertices in the forest obtained by $G \setminus E(C)$, where C is the unique cycle of G .

B. Bounds on μ_1 and μ_{n-1}

In this section, we briefly review some interesting results on tight lower and upper bounds of the algebraic connectivity of any graph G , and we specify some particular results when G is unicyclic.

Authors of reference [9] proposed a lower bound on the algebraic connectivity (i.e. the smallest eigenvalue of the matrix L). This bound depends on the edge connectivity which is the minimum number of edges whose deletion from a graph G disconnects G .

Proposition II.8. *Let G be a connected graph with n vertices and m edges. We denote by $e(G)$ the edge connectivity. Then :*

$$\mu_{n-1} \geq 2e(G) \left(1 - \cos\left(\frac{\pi}{n}\right)\right)$$

A well-known result on the exact value of the algebraic connectivity is given in Proposition II.9. A detailed proof can be found in [9].

Proposition II.9. *If G is a graph with n vertices, then :*

$$\mu_{n-1} = 2n \min_{x \neq 0} \frac{\sum_{uv \in E} a_{uv} (x_u - x_v)^2}{\sum_{u \in V} \sum_{v \in V} (x_u - x_v)^2}$$

The two following propositions that can be found respectively in [10] and [11], provide lower and upper bounds on

μ_1 and μ_{n-1} , and give relations between the two eigenvalues. More details and information on proofs of the previous propositions, can be found in [10], [12], [13], [14] and [15].

Proposition II.10.

$$\mu_{n-1} \leq \frac{n}{n-1} \delta \leq \frac{n}{n-1} \Delta \leq \mu_1 \leq 2\Delta.$$

If G is a unicyclic graph, then

$$\Delta + 1 \leq \mu_1 \leq \Delta + 2\sqrt{\Delta - 1}$$

Proposition II.11. *Let G be a graph with a diameter $D \geq 4$. Then*

$$\mu_{n-1} \leq 1 - \frac{2\sqrt{\Delta - 1}}{\Delta} \left(1 - \frac{2}{D}\right) + \frac{2}{D}$$

III. EXTREMAL EIGENVALUES OF $G(q, n_1)$

In this Section, we consider unicyclic graphs $G(q, n_1)$ as already shown in Figure 1, and propose extremal exact eigenvalues of A and L of G .

Lemma III.1. *Let G be a unicyclic graph of the class $G(q, n_1 = \Delta - 2)$, then*

$$\lambda_1 = 1 + \sqrt{\Delta - 1} \quad (1)$$

Proof. Let x be an eigenvector associated to λ_1 . Each component of x is associated to each vertex of the graph G . The vertices of the unique cycle are indexed by c_1, \dots, c_q . For each vertex c_i on the cycle ($i = 1, \dots, q$), there are $\Delta - 2$ leaves connected to c_i . Each leaf j connected to c_i is denoted by f_i^j where $1 \leq j \leq \Delta - 2$.

Assuming that x is an eigenvector, we obtain the two following equations ($\forall j = 1, \dots, (\Delta - 2)$ and $i = 1, \dots, q$):

$$\lambda_1 x_{f_i^j} = x_{c_i} \quad (2)$$

$$\lambda_1 x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}} + \sum_{j=1}^{\Delta-2} x_{f_i^j} \quad (3)$$

By combining these two equations, we obtain :

$$\left(\lambda_1 - \frac{\Delta - 2}{\lambda_1}\right) x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}} \quad (4)$$

By summing the two sides of (4) on each vertex on the cycle, we obtain:

$$\left(\lambda_1 - \frac{\Delta - 2}{\lambda_1} - 2\right) \times \sum_i x_{c_i} = 0 \quad (5)$$

Following the Perron-Frobenius theorem (Theorem III.2 given below), we know that $\sum_i x_{c_i} \neq 0$.

Theorem III.2. [16] *Let A be a $n \times n$ real and non-negative matrix of a connected graph G . Then the index of G is simple (its multiplicity is equal to one). Each component of the eigenvector x associated to this eigenvalue is different from zero and has the same sign.*

From the equality (5) we have:

$$\lambda_1 - \frac{\Delta - 2}{\lambda_1} = 2$$

We multiply the two sides of (5) by λ_1 , and we obtain :

$$\lambda_1^2 - (\Delta - 2) = 2\lambda_1.$$

The discriminant of the equation III is then given by $Disc = 1 + \Delta - 2 = \Delta - 1 > 0$ ($\Delta \geq 3$), and we deduce the two following solutions :

$$\lambda_1^{(1)} = 1 - \sqrt{\Delta - 1}$$

$$\lambda_1^{(2)} = 1 + \sqrt{\Delta - 1}.$$

It is well known that the index of the adjacency matrix A verifies $\lambda_1 \geq 1$, and that $\Delta \geq 3$ (see Figure 1), then $\lambda_1^{(1)}$ is not a feasible solution. We can conclude that:

$$\lambda_1 = 1 + \sqrt{\Delta - 1}$$

□

In the same manner, we propose the exact and smallest eigenvalue of the adjacency matrix of the graph $G(q, n_1)$.

Lemma III.3. *Let G be a unicyclic graph of the class $G(q, n_1)$. Then*

- For even values of q :

$$\lambda_n = -1 - \sqrt{\Delta - 1} \quad (6)$$

- For odd values of q :

$$\lambda_n = -\cos\left(\frac{\pi}{q}\right) - \sqrt{\cos^2\left(\frac{\pi}{q}\right) + \Delta - 2} \quad (7)$$

Proof. To prove this result, we can use the same approach as in the proof of Lemma 1. We find ($\forall j = 1, \dots, (\Delta - 2)$ and $i = 1, \dots, q$):

$$\lambda_n x_{f_i^j} = x_{c_i} \quad (8)$$

$$\lambda_n x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}} + \sum_{j=1}^{\Delta-2} x_{f_i^j} \quad (9)$$

We obtain:

$$\left(\lambda_n - \frac{\Delta - 2}{\lambda_n}\right) x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}}$$

We recall that $\lambda_n \leq -1$, then $\lambda_n \neq 0$.

Then, we obtain a system of q equations associated to a circulant matrix [17], which is given by:

$$C = \begin{pmatrix} \gamma & -1 & -1 & 0 & \dots & 0 \\ -1 & \gamma & -1 & 0 & \dots & 0 \\ 0 & -1 & \gamma & -1 & \dots & 0 \\ \dots & 0 & -1 & \gamma & -1 & 0 \\ 0 & \dots & 0 & -1 & \gamma & -1 \\ -1 & 0 & \dots & 0 & -1 & \gamma \end{pmatrix}$$

with $\gamma = \lambda_n - \frac{\Delta-2}{\lambda_n}$, and this leads to an eigenvalue $\gamma - 2 \cos\left(\frac{2k\pi}{q}\right) \forall k = 1, \dots, q$.

It is easy to see that 0 should be an eigenvalue of C , which is equivalent to justify the existence of k , such that $\gamma - 2 \cos\left(\frac{2k\pi}{q}\right) = 0$ (see [1], [12], [17]).

Finally, we solve the following equation:

$$\lambda_n - \frac{\Delta-2}{\lambda_n} = 2 \cos\left(\frac{2k\pi}{q}\right)$$

which is a second degree equation equivalent to :

$$\lambda_n^2 - 2 \cos\left(\frac{2k\pi}{q}\right) \lambda_n - (\Delta-2) = 0$$

The discriminant of equation (III) is given by:

$$Disc = \cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2 > 0, \quad \forall k = 0, \dots, q$$

the solution of this equation is given by the two following roots, $\forall k = 0, \dots, q-1$

$$\lambda_n^{(1)} = \cos\left(\frac{2k\pi}{q}\right) - \sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}$$

$$\lambda_n^{(2)} = \cos\left(\frac{2k\pi}{q}\right) + \sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}$$

As $\Delta \geq 3$ then $\sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2} \geq 1$ and we can deduce that

$$\sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2} + \cos\left(\frac{2k\pi}{q}\right) \geq 0$$

This is in contradiction with $\lambda_n < 0$ (see [1]). Thus, the solution is given by:

$$\lambda_n^{(1)} = \cos\left(\frac{2k\pi}{q}\right) - \sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}$$

Let $f(k) = \cos\left(\frac{2k\pi}{q}\right) - \sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}$.

The derivative form of f is given by :

$$f'(k) = \sin\left(\frac{2k\pi}{q}\right) \left[\frac{\cos\left(\frac{2k\pi}{q}\right)}{\sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}} - 1 \right]$$

the expression between the square brackets is negative, because

$$\cos\left(\frac{2k\pi}{q}\right) < \sqrt{\cos^2\left(\frac{2k\pi}{q}\right) + \Delta - 2}$$

this derivative is equal to zero for the values of $k = 0$, and $\frac{q}{2}$. According to [1], one can see that λ_n is bounded. The function $f(k)$ is then :

- decreasing : for $k \in [0, \frac{q}{2}]$.
- increasing : for $k \in [\frac{q}{2}, q]$

and reaches its minimum value for $k = \lfloor \frac{q}{2} \rfloor$. This gives us :

- q even : $\lambda_n^{(1)} = -1 - \sqrt{\Delta-1}$
- q odd : $\lambda_n^{(1)} = -\cos\left(\frac{\pi}{q}\right) - \sqrt{\cos^2\left(\frac{\pi}{q}\right) + \Delta - 2}$

With these values of λ_n , we can verify that 0 is an eigenvalue of C . Then, we have an eigenvector x_C of C .

It is not difficult to reconstruct the rest of the vector using the relations (8) and (9). \square

In the following, and according to the unicyclic graph $G(q, n_1)$, we investigate exact and extremal values of the eigenvalues of the Laplacian matrix L .

Lemma III.4. *Let G be a unicyclic graph of the class $G(q, n_1)$. The exact value of the algebraic connectivity is given by*

$$\mu_{n-1} = \frac{1}{2} \times \left(\Delta - 1 + 4 \sin^2\left(\frac{\pi}{q}\right) - \sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{\pi}{q}\right)} \right) \quad (10)$$

Proof. Starting from the definition of an eigenvalue of a Laplacian matrix, we have ($\forall j = 1, \dots, \Delta - 2$ and $\forall i = 1, \dots, q$):

- 1) $i \notin C_q : (1 - \mu_{n-1})x_{f_i^j} = x_{c_i}$
 - 2) $i \in C_q : (\Delta - \mu_{n-1})x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}} + \sum_{j=1}^{\Delta-2} x_{f_i^j}$
- by substituting $x_{f_i^j}$ in the second case, we obtain:

$$\left(\Delta - \mu_{n-1} - \frac{\Delta-2}{1-\mu_{n-1}} \right) x_{c_i} = x_{c_{i+1}} + x_{c_{i-1}}$$

which is a system of q equations, and q variables. To solve it, we set $\gamma = \Delta - \mu_{n-1} - \frac{\Delta-2}{1-\mu_{n-1}}$, and we can remark that the associated matrix to this system is also circulant :

$$C = \begin{pmatrix} \gamma & -1 & -1 & 0 & \dots & 0 \\ -1 & \gamma & -1 & 0 & \dots & 0 \\ 0 & -1 & \gamma & -1 & \dots & 0 \\ \dots & 0 & -1 & \gamma & -1 & 0 \\ 0 & \dots & 0 & -1 & \gamma & -1 \\ -1 & 0 & \dots & 0 & -1 & \gamma \end{pmatrix}$$

and this leads to an eigenvalue $\gamma - 2 \cos\left(\frac{2k\pi}{q}\right) \forall k = 1, \dots, q$ such that $\exists k, \gamma - 2 \cos\left(\frac{2k\pi}{q}\right) = 0$.

From the proposition II.11, we see that $\mu_{n-1} \neq 1$.

Thus, we solve the following:

$$\Delta - \mu_{n-1} - \frac{\Delta-2}{1-\mu_{n-1}} = 2 \cos\left(\frac{2k\pi}{q}\right)$$

It is a second degree equation which can be reformulated as follows:

$$\Delta - \left(\frac{\mu_{n-1} - \mu_{n-1}^2 + \Delta - 2}{1 - \mu_{n-1}} \right) = 2 \cos\left(\frac{2k\pi}{q}\right)$$

$$\begin{aligned} \Rightarrow \Delta - \Delta\mu_{n-1} + \mu_{n-1}^2 - \mu_{n-1} - \Delta + 2 &= \\ &= 2 \cos\left(\frac{2k\pi}{q}\right) - 2 \cos\left(\frac{2k\pi}{q}\right) \mu_{n-1} \end{aligned}$$

with $\mu_{n-1} \neq 1$ and then

$$\mu_{n-1}^2 - (\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)) \mu_{n-1} + 2(1 - \cos\left(\frac{2k\pi}{q}\right)) = 0$$

The discriminant (*Disc*) of this last equation is given by

$$Disc = (\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right))^2 - 8 + 8 \cos\left(\frac{2k\pi}{q}\right)$$

$$Disc = [\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)$$

Thus, we obtain two solutions (11) and (12):

$$\mu_{n-1}^{(1)} = \frac{1}{2} \left(\Delta + 1 - 2(1 - 2 \sin^2\left(\frac{k\pi}{q}\right)) - \sqrt{[\Delta + 1 - 2(1 - 2 \sin^2\left(\frac{k\pi}{q}\right))]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)} \right) \quad (11)$$

$$\mu_{n-1}^{(2)} = \frac{1}{2} \left(\Delta + 1 - 2(1 - 2 \sin^2\left(\frac{k\pi}{q}\right)) + \sqrt{[\Delta + 1 - 2(1 - 2 \sin^2\left(\frac{k\pi}{q}\right))]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)} \right) \quad (12)$$

after some simplification, we can deduce:

$$\mu_{n-1}^{(1)} = \frac{1}{2} \left(\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right) - \sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)} \right) \quad (13)$$

$$\mu_{n-1}^{(2)} = \frac{1}{2} \left(\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right) + \sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)} \right) \quad (14)$$

As $\Delta \geq 3$, then $\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right) \geq 2$, then we can write

knowing that $\mu_{n-1} < 1$, we can reject $\mu_{n-1}^{(2)}$ which is greater than 1, and we keep only the solution given by (15)

$$\mu_{n-1}^{(2)} \geq 1 + \frac{\sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)}}{2} > 1$$

$$\mu_{n-1} = \mu_{n-1}^{(1)} = \frac{1}{2} \left(\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right) - \sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{k\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{k\pi}{q}\right)} \right) \quad (15)$$

We investigate the value k (k ranging from $k = 0, \dots, q$) that minimizes the function $\mu_{n-1}(k)$. We remark that if $k = 0$, or $k = q$, we find $\mu_{n-1} = 0$, which is absurd. Thus, we are interested in integer values of $k \in [1, q - 1]$.

$$\left[1 - \frac{4 \sin^2\left(\frac{k\pi}{q}\right) + \Delta - 3}{\sqrt{(\Delta - 1)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) + 8(\Delta - 3) \sin^2\left(\frac{k\pi}{q}\right)}} \right] \quad (16)$$

The derivative function of $\mu_{n-1}(k)$ is given by:

$$\mu'_{n-1} = \frac{8\pi}{q} \sin\left(\frac{k\pi}{q}\right) \cos\left(\frac{k\pi}{q}\right) \times$$

$$\sqrt{(\Delta - 1)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) + 8(\Delta - 3) \sin^2\left(\frac{k\pi}{q}\right)} > 4 \sin^2\left(\frac{k\pi}{q}\right) + \Delta - 3 \quad (\Delta \geq 3) \quad (17)$$

thus if we write (with $\Delta \geq 3$):

$$(\Delta - 1)^2 > (\Delta - 3)^2$$

$$\begin{aligned} \Rightarrow (\Delta - 1)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) > \\ (\Delta - 3)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) \end{aligned}$$

$$\begin{aligned} \Rightarrow (\Delta - 1)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) + 8(\Delta - 3) \sin^2\left(\frac{k\pi}{q}\right) > \\ (\Delta - 3)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) + 8(\Delta - 3) \sin^2\left(\frac{k\pi}{q}\right) \end{aligned}$$

we observe that the square of the two sides of the inequality is given by

$$\begin{aligned} \sqrt{(\Delta - 1)^2 + 16 \sin^4\left(\frac{k\pi}{q}\right) + 8(\Delta - 3) \sin^2\left(\frac{k\pi}{q}\right)} > \\ 4 \sin^2\left(\frac{k\pi}{q}\right) + \Delta - 3 \end{aligned}$$

The derivative function is equal to zero only if $\sin\left(\frac{k\pi}{q}\right) = 0$ or $\cos\left(\frac{k\pi}{q}\right) = 0$, so it is equal to 0 for the following values of k : $k = 0, q, \frac{q}{2}, \frac{3q}{2}$ and as $k \in [1, q - 1]$, so it is equal to 0 only for $k = \frac{q}{2}$, with $\mu_{n-1}(k = \frac{q}{2}) = \frac{\Delta + 3 - \sqrt{\Delta^2 + 6\Delta - 7}}{2} < 1$.

The function μ is bounded and has the following behaviour:

- increasing : pour $k \in [1, \frac{q}{2}]$.
- decreasing : pour $k \in [\frac{q}{2}, q - 1]$

We conclude that $\mu_{n-1}(k = q - 1) = \mu_{n-1}(k = 1)$ and $k = 1$ (or $k = q - 1$), and obtain:

$$\begin{aligned} \mu_{n-1} &= \frac{1}{2} \times \\ &\left(\Delta - 1 + 4 \sin^2\left(\frac{\pi}{q}\right) - \sqrt{[\Delta - 1 + 4 \sin^2\left(\frac{\pi}{q}\right)]^2 - 16 \sin^2\left(\frac{\pi}{q}\right)} \right) \end{aligned}$$

$$\mu_1^{(1)} = \frac{\Delta + 1}{2} - \left(\frac{2 \cos\left(\frac{2k\pi}{q}\right) + \sqrt{[\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)]^2 - 8[1 - \cos\left(\frac{2k\pi}{q}\right)]}}{2} \right) < \Delta + 1 \quad (21)$$

thus, we reject it and consider the solution given by:

In the following, we provide the exact and largest eigenvalue of L of the unicyclic graph $G(q, n_1)$.

Lemma III.5. *Let G be a unicyclic graph of the class $G(q, n_1)$. Then*

1) *If q is even:*

$$\mu_1 = \frac{\Delta + 3 + \sqrt{(\Delta + 3)^2 - 16}}{2} \quad (18)$$

The expression between the square brackets is non-negative as we can see it in (17)

2) *If q is odd:*

$$\begin{aligned} \mu_1 &= \frac{(\Delta + 1) + 2 \cos\left(\frac{\pi}{q}\right)}{2} + \\ &\frac{\sqrt{[(\Delta + 1) + 2 \cos\left(\frac{\pi}{q}\right)]^2 - 8(1 + \cos\left(\frac{\pi}{q}\right))}}{2} \end{aligned} \quad (19)$$

Proof. According to the proof of Lemma (10), and by using the associated circulant matrix of the current case, we obtain the following equation :

$$\mu_1^2 - \left(\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right) \right) \mu_1 + 2 \left(1 - \cos\left(\frac{2k\pi}{q}\right) \right) = 0$$

and we recall that for a unicyclic graph, we have:

$$\Delta + 1 \leq \mu_1 \leq \Delta + 2\sqrt{\Delta - 1} \quad (20)$$

The discriminant of this equation is non-negative (see proof of the Lemma (10)) and this leads to two solutions :

$$\begin{aligned} 1) \mu_1^{(1)} &= \frac{\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right) - \sqrt{[\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)]^2 - 8[1 - \cos\left(\frac{2k\pi}{q}\right)]}}{2} \\ 2) \mu_1^{(2)} &= \frac{\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right) + \sqrt{[\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)]^2 - 8[1 - \cos\left(\frac{2k\pi}{q}\right)]}}{2} \end{aligned}$$

It is easy to verify that $\mu_1^{(1)}$ violates the requirement (20), and this is due to formulas (21):

$$\begin{aligned} \mu_1 &= \frac{\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)}{2} + \\ &\frac{\sqrt{[\Delta + 1 - 2 \cos\left(\frac{2k\pi}{q}\right)]^2 - 8[1 - \cos\left(\frac{2k\pi}{q}\right)]}}{2} \end{aligned} \quad (22)$$

μ_1 is a function of k , which is symmetric around $\lfloor \frac{q}{2} \rfloor$. In other words, we find the same value of μ_1 for instances of $k = 0$ and $k = q$, then for $k = 1$ and $k = q - 1$, etc. According to this remark, we illustrate the behaviour of μ_1 for some values of $k = 0, \dots, q$ (see Figure (2)). We note that: $\cos\left(\frac{2(q-1)\pi}{2q}\right) = \cos\left(\pi - \frac{\pi}{q}\right) = -\cos\left(\frac{\pi}{q}\right)$.

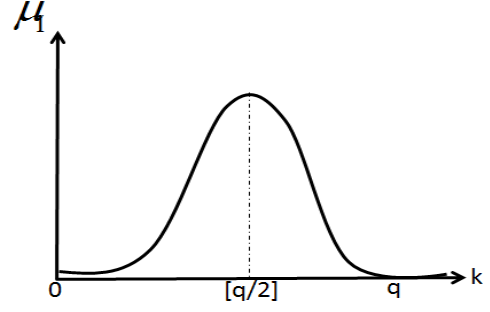


Fig. 2. μ_1 's behavior with k evolution

The derivative formula of μ_1 is given by (23) and simplified in (24):

$$\mu_1' = \frac{1}{2} \left[\frac{4\pi}{q} \sin\left(\frac{2k\pi}{q}\right) + \frac{2(\Delta + 1 - 2\cos(\frac{2k\pi}{q}))(\frac{4\pi}{q} \sin(\frac{2k\pi}{q})) - \frac{16\pi}{q} \sin(\frac{2k\pi}{q})}{2\sqrt{[\Delta + 1 - 2\cos(\frac{2k\pi}{q})]^2 - 8[1 - \cos(\frac{2k\pi}{q})]}} \right] \quad (23)$$

$$\mu_1' = \frac{2\pi}{q} \sin\left(\frac{2k\pi}{q}\right) \left[1 + \frac{(\Delta + 1 - 2\cos(\frac{2k\pi}{q})) - 2}{\sqrt{[\Delta + 1 - 2\cos(\frac{2k\pi}{q})]^2 - 8[1 - \cos(\frac{2k\pi}{q})]}} \right] \quad (24)$$

as $\Delta \geq 3$, the expression between the square brackets is non-negative. The derivative function is equal to zero for the values of $k = 0$ and $\frac{q}{2}$, and as we are interested by integer values of $k \in [1, q - 1]$, then we keep only $k = \lfloor \frac{q}{2} \rfloor$. The function reaches its maximum for $k = \lfloor \frac{q}{2} \rfloor$, and we find:

1) q even : $k = \frac{q}{2}$, and

$$\mu_1 = \frac{\Delta + 3 + \sqrt{(\Delta + 3)^2 - 16}}{2}$$

2) q odd : $k = \frac{q-1}{2}$, and

$$\mu_1 = \frac{(\Delta + 1) + 2\cos\left(\frac{\pi}{q}\right) + \sqrt{[(\Delta + 1) + 2\cos\left(\frac{\pi}{q}\right)]^2 - 8(1 + \cos\left(\frac{\pi}{q}\right))}}{2}$$

IV. NUMERICAL RESULTS AND VALIDATION

In this Section, we verify and validate numerically the provided results on different unicyclic graph instances of type $G(q, n_1)$, compared to a well-known numerical method that can be found in [18] for example.

We use an instance of unicyclic graphs of type $G(q, n_1)$ as shown in Table I and Table II. In this instance, we consider odd cycle sizes, when varying n_1 values from 1 to 10.

We used the LAPACK method [18] as a numerical analysis benchmark to get exact eigenvalues of the considered graphs. Thus, one can observe in Tables I and II that our proposed results are exactly the same as LAPACK. This reinforces and validates our provided proofs in the previous sections, and

□ leads to use our results for large unicyclic graph instances, when the numerical methods suffer from scaling-up and to provide exact eigenvalues solutions.

V. CONCLUSION

In this paper, we proposed exact values of the extremal eigenvalues of the adjacency matrix and the Laplacian matrix of a particular class of unicyclic graphs. The proposed results are often given by solving linear equation systems involving circulant matrices. The provided results are new and reinforce the lower and upper bounds of the spectra of any graphs with a topology close to the unicyclic graphs considered in our work.

In future work, we will investigate new results on the spectra of the adjacency and Laplacian matrices for larger classes of

TABLE I
COMPARISON OF EXTREMAL EIGENVALUES OF A : UNICYCLIC GRAPHS
 $G(q, n_1)$ WITH $q = 3$

n_1	(1)	num λ_1	(III.3)	num λ_n
1	2.414	2.414	-1.618	-1.618
2	2.732	2.732	-2	-2
3	3	3	-2.302	-2.302
4	3.236	3.236	-2.561	-2.561
5	3.449	3.449	-2.791	-2.791
6	3.645	3.645	-3	-3
7	3.828	3.828	-3.192	-3.192
8	4	3.999	-3.372	-3.372
9	4.162	4.162	-3.541	-3.541
10	4.316	4.316	-3.701	-3.701

TABLE II
COMPARISON OF EXTREMAL EIGENVALUES OF L : UNICYCLIC GRAPHS
 $G(q, n_1)$ WITH $q = 3$

n_1	(19)	num μ_1	(10)	num μ_{n-1}
1	4.302	4.302	0.697	0.697
2	5.449	5.449	0.550	0.550
3	6.541	6.541	0.458	0.458
4	7.605	7.605	0.394	0.394
5	8.653	8.653	0.346	0.346
6	9.690	9.690	0.309	0.309
7	10.720	10.720	0.279	0.279
8	11.744	11.744	0.255	0.255
9	12.764	12.764	0.235	0.235
10	13.782	13.782	0.217	0.217

unicyclic graphs noted by $G(q, n_1, n_2)$. Figure 3 illustrates an example of such a class of unicyclic graphs.

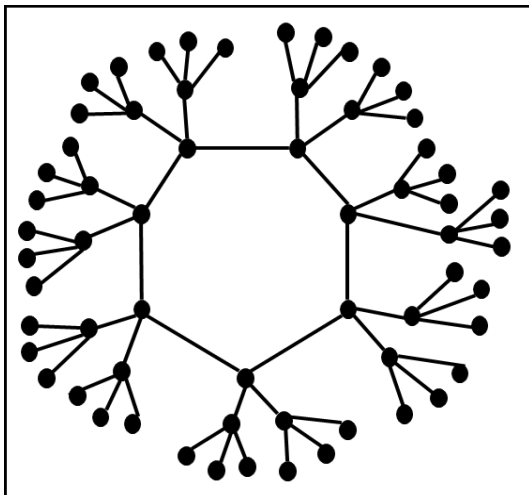


Fig. 3. Example of a unicyclic graph $G(7, 2, 3)$

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