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EXTREMAL INVERSE EIGENVALUE PROBLEM FOR MATRICES DESCRIBED BY A CONNECTED UNICYCLIC GRAPH

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Abstract. In this paper, we deal with the construction of symmetric matrix whose corresponding graph is connected and unicyclic using some pre-assigned spectral data. Spectral data for the problem consist of the smallest and the largest eigenvalues of each leading principal submatrices. Inverse eigenvalue problem (IEP) with this set of spectral data is generally known as the extremal IEP. We use a standard scheme of labeling the vertices of the graph, which helps in getting a simple relation between the characteristic polynomials of each leading principal submatrix. Sufficient condition for the existence of the solution is obtained. The proof is constructive, hence provides an algorithmic procedure for finding the required matrix. Furthermore, we provide the condition under which the same problem is solvable when two particular entries of the required matrix satisfy a linear relation.

Keywords: inverse eigenvalue problem; unicyclic graph; leading principal submatrices

MSC 2020: 05C50, 15A24, 65F18

1. Introduction

Inverse eigenvalue problem has been of great importance in various fields of science and engineering such as control theory, mass spring vibration, pole assignment problem, circuit theory and graph theory. The reader is referred to different books and papers, such as [6], [14], [11], [23] for thorough discussion on it. The objective of an inverse eigenvalue problem is to construct a matrix of a certain structure using the pre-assigned spectral data. One can refer to [4] to see a detailed classification of the various inverse eigenvalue problems. IEP for different matrix structure like Jacobi, arrow, doubly arrow, Leslie, doubly Leslie matrices etc. have been studied by several authors [15], [16], [17], [18].

One of the interesting ways of describing the structure of a matrix is to consider its associated graph, where the nonzero nondiagonal entries correspond to the edges of

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the graph. Graph spectra has various applications in different fields: physics, chemistry, computer science, geography [6], [5]. The problem of constructing the matrices whose smallest and largest eigenvalues of each leading principal submatrices are given is generally known as the *extremal inverse eigenvalue problem*. Extremal eigenvalue problem has lots of applications in different research areas. In chemistry, problems on largest eigenvalues are very much useful in molecular context [13]. Several authors have studied the inverse eigenvalue problems for matrices whose graph is a certain type of tree. Extremal IEP for matrix whose corresponding graph is broom has been studied by [20]. The problem with the same eigendata has been studied for matrices described by dense centipede [21]. Several other authors also studied the extremal IEP for matrices described by generalized stars [10], banana trees [2], double-starlike trees or double comets [1] and generalised star of depth 2 (see [22]). Recently, the problem is solved completely for distinct eigendata for which corresponding matrix is any general tree [19]. Motivated by the above works, we study the extremal IEP for matrix whose corresponding graph is connected unicyclic. Unicyclic graphs have many applications in various problems of organic chemistry, computer science, network analysis, graph theory etc. [3], [12], [8]. In telecommunication network, unicyclic graphs are frequently used. The cycle guarantees a particular degree of survivability against link failure that happens on the cycle's outer edges (see [7]).

This paper is organized as follows: Section 2 provides some basic definitions of graphs and some preliminary results. In Section 3, we define an extremal IEP for connected unicyclic graph and analyse the necessary and sufficient conditions for its solution. In Section 4, we consider a variation of the problem and analyse its solution. Numerical examples illustrating the applicability of the solutions are given for both the problems.

2. Preliminaries

Throughout this paper, by the term graph, we mean an undirected graph without any multi-edge or loop. A graph $G = (V(G), E(G))$ consists of a finite nonempty set $V(G)$, called the set of vertices, and a set $E(G)$, called the set of edges. The set $E(G)$ consists of unordered pairs of vertices in $V(G)$. The number of elements in the vertex set is called the order of the graph G. Any two vertices $v_1, v_2 \in V(G)$ are called adjacent vertices if $e = \{v_1, v_2\} \in E(G)$. A *walk* in G, joining vertices u and v, is a sequence of adjacent vertices $u = v_0, v_1, \dots, v_{k-1}, v_k = v$. If all the vertices and edges in a walk are distinct, then it is called a path. If the first and the last vertex of the sequence are equal and the remaining vertices are distinct then it is called a cycle. The graph G is called *connected* if for each pair of distinct vertices u and v there is a path joining u and v. Usually, $V(G)$ is assumed as $\{1, 2, \dots, n\}$.

A *tree* is a connected graph without any cycles and a *connected unicyclic graph* is a connected graph having exactly one cycle. A graph H is said to be a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, and each edge of H has the same end vertices in H as in G and a subgraph H is said to be an *induced subgraph* of G if each edge of G having its ends in $V(H)$ is also an edge of H.

Given an $n \times n$ symmetric matrix $A = (a_{ij})_{n\times n}$, the graph of A is denoted by $G(A)$, it has vertex set $V = \{1, 2, \ldots, n\}$ and edge set $E = \{\{i, j\}\colon\ i \neq j, a_{ij} \neq 0\}$. For a graph $G = (V, E)$ of degree n, $S(G)$ denotes the set of all $n \times n$ symmetric matrices A such that $G(A) = G$. Figure 1 shows examples of two connected unicyclic graphs. For a matrix A, A_j denotes the $j \times j$ leading principal submatrix of A and $P_j(\lambda)$ denotes the characteristic polynomial of A_j.

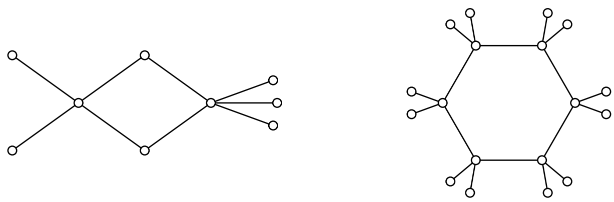


Figure 1. Connected unicyclic graphs.

3. IEP for unicyclic graph (IEPU)

We consider the following extremal inverse eigenvalue problem for a connected unicyclic graph:

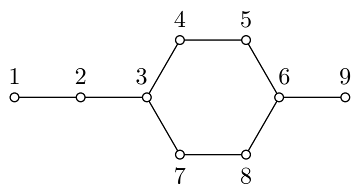
Problem 3.1 (IEPU). Given $2n - 1$ distinct real numbers γ_j, δ_j, $j = 1, \ldots, n$ with $\gamma_1 = \delta_1$ and a connected unicyclic graph U with n vertices, find a matrix $A \in S(U)$ such that γ_j and δ_j are respectively the smallest and the largest eigenvalues of the jth leading principal submatrix A_j of A.

The structure of a matrix associated with a graph depends upon the labelling of vertices of the graph. To solve the problem, we label the vertices of the unicyclic graph following a suitable scheme. Labelling plays a vital role in getting a simpler recurrence relation between the characteristic polynomials of the leading principal submatrices of the required matrix. We have the following lemma:

Lemma 3.1. *A necessary condition for solvability of the IEPU is that the vertices of U should be labelled so that for each $j \in \{1, 2, 3, \ldots, n\}$, the subgraph U_j of U induced by the vertices $\{1, 2, \ldots, j\}$ is connected.*

P r o o f. Suppose the vertices of U be labelled in such a way that the induced subgraph U_j is disconnected for some $j \in \{1, 2, \dots, n\}$ but U_{j-1} is connected. Then the vertex j in U_j is an isolated vertex. Let $A \in S(U)$. Then the eigenvalues of A_j are the same as the eigenvalues of A_{j-1} with an extra eigenvalue equal to a_{jj} that is the diagonal entry corresponding to the vertex j but by the definition of the problem, $\gamma_j \neq \gamma_{j-1}$ and $\delta_{j-1} \neq \delta_j$, which is not admissible as A_{j-1} and A_j can have atmost one eigenvalue that differs. Thus, the problem is not solvable if U_j is disconnected for any j. □

It is always possible to label the vertices of U in such a way that it follows the condition of Lemma 3.1. Let U be a unicyclic graph on n vertices. We label the vertices of the graph by following the process of successively connected labelling as adopted in [19]. We label any vertex as 1 and then label any other vertex adjacent to 1 as 2. We continue this process, at each step labelling a vertex which is adjacent to one of the already labeled vertices keeping the serial numbers of the labels in the natural order. We continue this process until all the vertices of U are labelled from 1 to n. With this scheme of labelling, at any step j, the graph with the vertices $\{1, 2, \dots, j\}$ remains connected and hence it is called *successively connected labelling.* Figure 2 shows an example of a unicyclic graph with successively connected labelling of vertices.



$$\begin{pmatrix} a_{11} & a_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{12} & a_{22} & a_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a_{23} & a_{33} & a_{34} & 0 & 0 & a_{37} & 0 & 0 \\ 0 & 0 & a_{34} & a_{44} & a_{45} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a_{45} & a_{55} & a_{56} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a_{56} & a_{66} & 0 & a_{68} & a_{69} \\ 0 & 0 & a_{37} & 0 & 0 & 0 & a_{77} & a_{78} & 0 \\ 0 & 0 & 0 & 0 & 0 & a_{68} & a_{78} & a_{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & a_{69} & 0 & 0 & a_{99} \end{pmatrix}$$

Figure 2. Unicyclic graph and its corresponding matrix.

Lemma 3.2. *In a successively connected scheme of labelling the vertices of a unicyclic graph U, there exists a unique vertex k that is adjacent to two of the vertices from $\{1, 2, \dots, k-1\}$.*

P r o o f. Since the graph U is unicyclic, it will have a unique induced subgraph C that is a cycle. After labelling the vertices as per the successively connected scheme, let k be the largest label among all the vertices of C. Since each vertex of a cycle has degree equal to 2, k has at least two adjacent vertices k_1, k_2 from $\{1, 2, \dots, k-1\}$. If possible, let k be adjacent to three vertices k_1, k_2, k_3 from $\{1, 2, \dots, k-1\}$ with

$k_1 < k_2 < k_3$. As per the successively connected labelling, there is a path joining k_1 to k_2 that does not contain k_3. Since k_1 and k_2 are adjacent to k, so there is a cycle through k_1, k_2 and k that does not contain k_3. Also, there is a cycle through k_2, k_3 and k. So, there are two distinct cycles in U, which is not possible as U is unicyclic. Hence, k is adjacent to two vertices k_1, k_2 from $\{1, 2, \ldots, k-1\}$. This proves the existence of vertex k.

Now, suppose there exists another vertex i such that i is adjacent to two vertices of $\{1, 2, \ldots, i-1\}$. If $i < k$, U has a cycle containing vertex i but not k and it has another cycle containing k, which is not possible as U is unicyclic. Similarly, $i > k$ is also not possible. Hence, $i = k$, i.e., there exists a unique vertex k that is adjacent to exactly two vertices from $\{1, 2, \ldots, k-1\}$. □

We refer to the vertex k of a unicyclic graph U obtained as in Lemma 3.2 as the *peak vertex*. For the rest of this paper, U denotes a connected unicyclic graph on n vertices with successively connected labelling. We adopt some notations for the entries of a matrix $A \in S(U)$. It follows from Lemma 3.2 that each vertex j with $j > 1$ and $j \neq k$ is adjacent to exactly one vertex $v(j)$ from $\{1, 2, \ldots, j-1\}$. However, each vertex j may be adjacent to many other vertices from $\{j+1, j+2, \ldots, n\}$. Also, let r and s be the two vertices from $\{1, 2, \ldots, k-1\}$ that are adjacent to the peak vertex k. We adopt the convention that $r < s$. Figure 2 gives an example of a unicyclic graph with successively connected labelling, where $k = 8$, $r = 6$ and $s = 7$.

We shall require the following standard lemmas for further analysis of the extremal IEPs:

Lemma 3.3 ([19]). *Let $P(\lambda)$ be a monic polynomial of degree n with all real zeros and $\lambda_{\min}$ and $\lambda_{\max}$ be the minimal and maximal zeros of P. Then*

(1) *if $\mu < \lambda_{\min}$, then $(-1)^n P(\mu) > 0$,*
(2) *if $\mu > \lambda_{\max}$, then $P(\mu) > 0$.*

Lemma 3.4 (Cauchy's Interlacing Theorem, [9]). *Let $\lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$ be the eigenvalues of any $n \times n$ real smmetric matrix A and $\mu_1 \leqslant \mu_2 \leqslant \ldots \leqslant \mu_{n-1}$ be the eigenvalues of any of its submatrices of order $(n-1) \times (n-1)$. Then*

$$\lambda_1 \leqslant \mu_1 \leqslant \lambda_2 \leqslant \mu_2 \leqslant \ldots \leqslant \lambda_{n-1} \leqslant \mu_{n-1} \leqslant \lambda_n.$$

From the above theorem, it follows that the eigenvalues of an $n \times n$ real symmetric matrix and those of any of its $(n-1) \times (n-1)$ principal submatrices interlace each other.

Lemma 3.5. *A necessary condition for the solvability of Problem* 3.1 *is*

$$\gamma_n < \gamma_{n-1} < \ldots < \gamma_2 < \gamma_1 = \delta_1 < \delta_2 < \ldots < \delta_{n-1} < \delta_n.$$

P r o o f. For each $j \in \{1, 2, \ldots, n\}$, γ_{j-1}, γ_j are the smallest eigenvalues of A_{j-1}, A_j, respectively, and δ_{j-1},δ_j are the largest eigenvalues of A_{j-1} and A_j, respectively. By applying *Cauchy's interlacing theorem* (Lemma 3.4), we can say that the eigenvalues of A_{j-1} and A_j interlace with each other and since all the eigenvalues are distinct, we have the following relation:

$$\gamma_n < \gamma_{n-1} < \ldots < \gamma_2 < \gamma_1 = \delta_1 < \delta_2 < \ldots < \delta_{n-1} < \delta_n.$$

□

Lemma 3.6. *Let $A \in S(U)$ be such that the vertices of U are labelled following the scheme of successive labelling and A_j be the $j \times j$ leading principal submatrix of A. The sequence $P_j(\lambda) = \det(\lambda I_j - A_j)$ of characteristic polynomials of A_j satisfies the following recurrence relation:*

$$\begin{aligned}
&P_1(\lambda) = \lambda - a_{11},\\
&P_j(\lambda) = (\lambda - a_{jj})P_{j-1}(\lambda) - a_{v(j)j}^2 Q_j(\lambda) \quad \text{for } j \neq k,\\
&P_k(\lambda) = (\lambda - a_{kk})P_{k-1}(\lambda) - a_{rk}^2 R_r(\lambda) - a_{sk}^2 R_s(\lambda) - (-1)^{r+s} 2a_{rk}a_{sk}R_{[r:s]}(\lambda),
\end{aligned}$$

where $Q_j(\lambda)$ is the characteristic polynomial of the principal submatrix of A_j obtained by deleting the rows and columns indexed by j and $v(j)$ with the convention $Q_2(\lambda) = 1$, $R_r(\lambda)$ and $R_s(\lambda)$ are the characteristic polynomials of the principal submatrix of A_{k-1} obtained by deleting rows and columns indexed by r and s, respectively, and $R_{[r:s]}(\lambda)$ is the characteristic polynomial of the submatrix of A_{k-1} obtained by deleting the rth row and the sth column.

P r o o f. The expressions for $P_j(\lambda)$ can be obtained by expanding the determinant $\det(\lambda I_j - A_j)$ for each $j = 1, 2, 3, \ldots, n$. □

For any $A \in S(U)$ with the successively connected labelling of vertices, as γ_j and δ_j are the smallest and largest eigenvalues of A_j, we obtain the following system of linear equations:

$$P_j(\gamma_j) = 0 \quad \text{and} \quad P_j(\delta_j) = 0. \tag{3.1}$$

Using equation 3.1 and Lemma 3.6, we get $a_{11} = \gamma_1$ and for $2 \leqslant j \neq k$ we have

$$\begin{aligned}
a_{jj}P_{j-1}(\gamma_j) + a_{v(j)j}^2 Q_j(\gamma_j) &= \gamma_j P_{j-1}(\gamma_j),\\
a_{jj}P_{j-1}(\delta_j) + a_{v(j)j}^2 Q_j(\delta_j) &= \delta_j P_{j-1}(\delta_j).
\end{aligned} \tag{3.2}$$

For $j = k$, $P_k(\gamma_k) = 0$ and $P_k(\delta_k) = 0$ gives

(3.3)

$$a_{kk}P_{k-1}(\gamma_k) + a_{rk}^2 R_r(\gamma_k) + a_{sk}^2 R_s(\gamma_k) + (-1)^{r+s} 2a_{rk}a_{sk}R_{[r:s]}(\gamma_k) = \gamma_k P_{k-1}(\gamma_k),$$
$$a_{kk}P_{k-1}(\delta_k) + a_{rk}^2 R_r(\delta_k) + a_{sk}^2 R_s(\delta_k) + (-1)^{r+s} 2a_{rk}a_{sk}R_{[r:s]}(\delta_k) = \delta_k P_{k-1}(\delta_k).$$

Equating the expression of a_{kk} from both the equations (3.3), we get the following quadratic equation in two variables a_{rk} and a_{sk}:

$$U_k a_{rk}^2 + 2V_k a_{rk}a_{sk} + W_k a_{sk}^2 + X_k = 0, \tag{3.4}$$

where U_k, V_k, W_k, X_k are given by

$$\begin{aligned} U_k &= R_r(\delta_k)P_{k-1}(\gamma_k) - R_r(\gamma_k)P_{k-1}(\delta_k),\\ V_k &= (-1)^{r+s}(R_s(\delta_k)P_{k-1}(\gamma_k) - R_s(\gamma_k)P_{k-1}(\delta_k)),\\ W_k &= R_s(\delta_k)P_{k-1}(\gamma_k) - R_s(\gamma_k)P_{k-1}(\delta_k),\\ X_k &= (\gamma_k - \delta_k)P_{k-1}(\gamma_k)P_{k-1}(\delta_k). \end{aligned}$$

Based on the above discussion, we conclude the following theorem.

Theorem 3.1. *For $2n-1$ distinct real numbers satisfying*

$$\gamma_n < \gamma_{n-1} < \ldots < \gamma_2 < \gamma_1 = \delta_1 < \delta_2 < \ldots < \delta_{n-1} < \delta_n$$

the IEPU has a solution.

Proof. For $j = 1$, equation (3.1) gives $a_{11} = \gamma_1$. For $j \geqslant 2$ and $j \neq k$, determinant of the co-efficient matrix of the linear system of equations (3.2) is given by

$$D_j = P_{j-1}(\gamma_j)Q_j(\delta_j) - P_{j-1}(\delta_j)Q_j(\gamma_j). \tag{3.5}$$

Since γ_{j-1} and δ_{j-1} are respectively the smallest and largest zeros of polynomial $P_{j-1}(\lambda)$ of degree $j-1$ and $\gamma_j < \gamma_{j-1}$, $\delta_{j-1} < \delta_j$, by applying Lemma 3.3, we get

$$(-1)^{j-1}P_{j-1}(\gamma_j) > 0 \quad \text{and} \quad P_{j-1}(\delta_j) > 0. \tag{3.6}$$

Let γ_j and δ_j be respectively the smallest and largest zeros of the polynomial Q_j of degree $j-2$. By Lemma 3.5, $\gamma_j < \gamma_{j-1} \leqslant \gamma_j$ and $\delta_j \leqslant \delta_{j-1} < \delta_j$ and by Lemma 3.3,

$$(-1)^{j-2}Q_j(\gamma_j) > 0 \quad \text{and} \quad Q_j(\delta_j) > 0. \tag{3.7}$$

Hence, from (3.5) we have

$$(-1)^{j-1}D_j = (-1)^{j-1}P_{j-1}(\gamma_j)Q_j(\delta_j) + P_{j-1}(\delta_j)(-1)^{j-2}Q_{j-1}(\gamma_j) > 0. \tag{3.8}$$

In particular, $D_j \neq 0$, hence the system of equations (3.2) has a unique solution. a_{jj}, $a^2_{v(j)j}$ are given by

$$a_{jj} = \frac{\gamma_j Q_j(\delta_j)P_{j-1}(\gamma_j) - \delta_j Q_j(\gamma_j)P_{j-1}(\delta_j)}{D_j}, \tag{3.9}$$

$$a^2_{v(j)j} = \frac{(\delta_j - \gamma_j)P_{j-1}(\gamma_j)P_{j-1}(\delta_j)}{D_j}. \tag{3.10}$$

It follows from (3.6) and (3.8) that the expression of $a^2_{v(j)j}$ is positive as

$$a^2_{v(j)j} = \frac{(-1)^{j-1}(\delta_j - \gamma_j)P_{j-1}(\gamma_j)P_{j-1}(\delta_j)}{(-1)^{j-1}D_j} > 0.$$

For $j = k$, we get (3.4), the solutions of which are the elements of the following set

$$\{(X, Y)\colon\ U_k X^2 + 2V_k XY + W_k Y^2 + X_k = 0,\ X, Y \in \mathbb{R} \setminus \{0\}\}. \tag{3.11}$$

Clearly, (3.4) represents a conic, hence set (3.11) is always nonempty. For any particular value of $a_{sk} = b_s$ (say), equation (3.4) reduces to

$$U_k a^2_{rk} + 2V_k a_{rk} b_s + W_k b_s^2 + X_k = 0. \tag{3.12}$$

Above (3.12) gives the real solution if the discriminant is nonnegative, i.e.,

$$V_k^2 b_s^2 - U_k(W_k b_s^2 + X_k) \geqslant 0 \Rightarrow (V_k^2 - U_k W_k)b_s^2 \geqslant U_k X_k. \tag{3.13}$$

Since all γ_j's are distict and by Lemma 3.3, $(-1)^{k-1}R_r(\gamma_k), (-1)^{k-1}R_s(\gamma_k) > 0$, which imply $(-1)^{k-1}U_k, (-1)^{k-2}X_k > 0$, $U_k X_k < 0$. Depending on the value of $V_k^2 - U_k W_k$, the following two cases arise:

- ▷ If $V_k^2 - U_k W_k < 0$, for any $b_s \in (-\sqrt{U_k X_k/(V_k^2 - U_k W_k)}, \sqrt{U_k X_k/(V_k^2 - U_k W_k)})$, condition (3.13) is satisfied.
- ▷ For $V_k^2 - U_k W_k \geqslant 0$, any value of b_s satisfies condition (3.13).

Then a_{sk} is obtained by

$$a_{rs} = \frac{-V_k b_s \pm \sqrt{V_k^2 b_s^2 - U_k(W_k b_s^2 + X_k)}}{U_k},$$

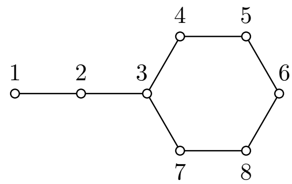
a_{kk} is obtained by putting the values of a_{rk}, a_{sk} in equation (3.3). By Lemma 3.5 and Theorem 3.1 the following theorem can be concluded:

Theorem 3.2. *For $2n - 1$ distinct real numbers γ_j, δ_j, $j = 1, \ldots, n$ with $\gamma_1 = \delta_1$, the IEPU has a solution if and only if*

$$\gamma_n < \gamma_{n-1} < \ldots < \gamma_2 < \gamma_1 = \delta_1 < \delta_2 < \ldots < \delta_{n-1} < \delta_n.$$

We illustrate the procedure with the help of an example:

E x a m p l e 3.1. Given 15 real numbers −8, −7, −6, −5, −4, −3, −2, −1, 1, 2, 3, 4, 5, 6, 7, label them as $\gamma_j, \delta_j, j \in \{1, 2, \dots, 8\}$ following the inequality condition of Lemma 3.5, find a symmetric matrix A such that γ_j, δ_j are respectively the smallest and largest eigenvalues of the $j \times j$ leading principal submatrix of A, where A is the adjacency matrix of the following unicyclic graph.



P r o o f of Theorem 3.2. Here $k = 8$, $r = 6$, $s = 7$. Using Theorem 3.1, we obtain the following matrix:

$$A = \begin{pmatrix} -1.0000 & 1.4142 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.4142 & 0 & 2.0000 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2.0000 & -1.0000 & 2.6833 & 0 & 0 & 5.0812 & 0 \\ 0 & 0 & 2.6833 & 0 & 3.2776 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3.2776 & -1.0000 & 3.8832 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3.8832 & 0 & 0 & 2 \\ 0 & 0 & 5.0812 & 0 & 0 & 0 & 0 & 4.1178 \\ 0 & 0 & 0 & 0 & 0 & 2 & 4.1178 & -1.0000 \end{pmatrix}.$$

From the above matrix A, we recompute the eigenvalues of each leading principal submatrix A_j, we denote it by $\sigma(A_j)$:

$$\begin{aligned}
\sigma(A_1) &= \{-\mathbf{1}\},\\
\sigma(A_2) &= \{-\mathbf{2}, \mathbf{1}\},\\
\sigma(A_3) &= \{-\mathbf{3}, -1, \mathbf{2}\},\\
\sigma(A_4) &= \{-\mathbf{4}, -1.7042, 0.7042, \mathbf{3}\},\\
\sigma(A_5) &= \{-\mathbf{5}, -2.5476, -1, 1.5476, \mathbf{4}\},\\
\sigma(A_6) &= \{-\mathbf{6}, -3.3952, -1.5677, 0.5677, 2.3952, \mathbf{5}\},\\
\sigma(A_7) &= \{-\mathbf{7}, -5.1196, -1.9144, 0, 0.9144, 4.1196, \mathbf{6}\},\\
\sigma(A_8) &= \{-\mathbf{8}, -5.1616, -3.1779, -1.7827, 0.7827, 2.1779, 4.1616, \mathbf{7}\}.
\end{aligned}$$

□

4. A variation of IEPU

Now, we consdier the extremal IEPU when some particular entries of the matrix have a linear relation. The problem is defined as below:

Problem 4.1. Given $2n-1$ distinct real numbers γ_j, δ_j, $j=1,\ldots,n$, with $\gamma_1=\delta_1$, a connected unicyclic graph U with n vertices and a real number x, the vertices of the graph U are successively connected. Find a matrix $A\in S(U)$ such that γ_j and δ_j are respectively the smallest and the largest eigenvalues of the jth leading principal submatrix A_j of A and $a_{sk}=xa_{rk}$, where r and k are the vertices as defined in Section 3.

For $j\neq k$, the entries $a_{jj}, a_{v(j)j}$ can be obtained using (3.9) and (3.10). We consider the entries a_{rk} and a_{sk} as

$$a_{sk}=xa_{rk} \tag{4.1}$$

for some $x\in\mathbb{R}$. Hence, the system of equations (3.3) becomes

$$\begin{aligned} a_{kk}P_{k-1}(\gamma_k)+a_{rk}^2\{R_r(\gamma_k)+x^2R_s(\gamma_k)+(-1)^{r+s}2xR_{[r:s]}(\gamma_k)\}&=\gamma_kP_{k-1}(\gamma_k),\\ a_{kk}P_{k-1}(\delta_k)+a_{rk}^2\{R_r(\delta_k)+x^2R_s(\delta_k)+(-1)^{r+s}2xR_{[r:s]}(\delta_k)\}&=\delta_kP_{k-1}(\delta_k). \end{aligned} \tag{4.2}$$

Determinant of the coefficient matrix of the system of linear equations (3.3) corresponding to $j=k$ is given by

$$\begin{aligned} D_k(x)=x^2\{P_{k-1}(\gamma_k)R_s(\delta_k)-P_{k-1}(\delta_k)R_s(\gamma_k)\}+(-1)^{r+s}2x\{P_{k-1}(\gamma_k)R_{[r:s]}(\delta_k)\\ -P_{k-1}(\delta_k)R_{[r:s]}(\gamma_k)\}+\{P_{k-1}(\gamma_k)R_r(\delta_k)-P_{k-1}(\delta_k)R_r(\gamma_k)\}. \end{aligned} \tag{4.3}$$

Here $D_k(x)$ is a quadratic polynomial in x and so D_k is zero for atmost two values of x, say x_1, x_2. Thus, choosing $x\in\mathbb{R}\setminus\{x_1,x_2\}$, we get $D_k(x)\neq 0$ and the solution of the system of equations (4.2) is given by

$$a_{kk}=\frac{\gamma_kA_xP_{k-1}(\gamma_k)-\delta_kB_xP_{k-1}(\delta_k)}{D_k}, \tag{4.4}$$

$$a_{rk}^2=\frac{(\delta_k-\gamma_k)P_{k-1}(\gamma_k)P_{k-1}(\delta_k)}{D_k}, \tag{4.5}$$

$$a_{sk}=xa_{rk}, \tag{4.6}$$

where A_x and B_x are given by

$$\begin{aligned} A_x&=R_r(\delta_k)+x^2R_s(\delta_k)+(-1)^{r+s}2xR_{[r:s]}(\delta_k),\\ B_x&=R_r(\gamma_k)+x^2R_s(\gamma_k)+(-1)^{r+s}2xR_{[r:s]}(\gamma_k). \end{aligned}$$

□

R e m a r k 4.1. It is to be noted that the expression for a_{rk}^2 in (4.5) is not necessarily positive for all values of x. However, under some restrictions on the value of x, a_{rk}^2 can be made positive. We consider the following expression:

$$
\begin{aligned}
(-1)^{k-1}D_k(x) &= x^2\{(-1)^{k-1}P_{k-1}(\gamma_k)R_s(\delta_k) + P_{k-1}(\delta_k)(-1)^{k-2}R_s(\gamma_k)\} \\
&\quad + (-1)^{r+s}2x\{(-1)^{k-1}P_{k-1}(\gamma_k)R_{[r:s]}(\delta_k) + P_{k-1}(\delta_k)(-1)^{k-2}R_{[r:s]}(\gamma_k)\} \\
&\quad + \{(-1)^{k-1}P_{k-1}(\gamma_k)R_r(\delta_k) + P_{k-1}(\delta_k)(-1)^{k-2}R_r(\gamma_k)\}.
\end{aligned}
$$

Under the condition $(-1)^{r+s}2x > 0$, by virtue of Lemma 3.3, each term of the above expression is positive. Consider the following expression of a_{rk}^2:

$$
a_{rk}^2 = \frac{(\delta_k - \gamma_k)(-1)^{k-1}P_{k-1}(\gamma_k)P_{k-1}(\delta_k)}{(-1)^{k-1}D_k(x)}.
$$

Clearly, it is positive under the condition $(-1)^{r+s}2x > 0$. Hence, a_{rk} is real when x is taken as a positive real number if $r+s$ is even and as a negative real number if $r+s$ is odd.

The following theorem gives a sufficient condition for the solvability of problem 4.1.

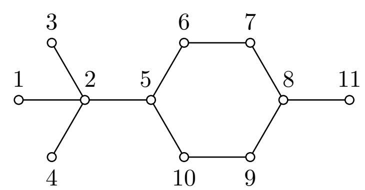
Theorem 4.1. *For* $2n-1$ *distinct real numbers satisfying*

$$
\gamma_n < \gamma_{n-1} < \ldots < \gamma_2 < \gamma_1 = \delta_1 < \delta_2 < \ldots < \delta_{n-1} < \delta_n,
$$

the Inverse Eigenvalue Problem 4.1 *has a solution if* $D_k(x) \neq 0$ *and* $(-1)^{r+s}x > 0$.

We illustrate this result with the help of the following example:

E x a m p l e 4.1. Given 21 real numbers -10.1, -10, -9, -8.3, -8, -6, -5, -4.5, -3, -2.9, -1, 2, 2.3, 2.9, 3, 3.9, 4, 5, 6, 7.9, 8, label them as γ_j, δ_j, $j \in \{1, 2, \ldots, 11\}$ following the inequality condition of Lemma 3.5, find a symmetric matrix A such that γ_j, δ_j are, respectively, the smallest and largest eigenvalues of the $j \times j$ leading principal submatrix of A, where A is the adjacency matrix of the following unicyclic graph and $a_{5\,10} = a_{9\,10}$.



S o l u t i o n o f E x a m p l e 4.1. Here $k = 10$, $r = 5$, $s = 9$. We obtain the solution considering $x = 1$:

$$\begin{pmatrix}
-1.0000 & 2.3875 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2.3875 & 0.1000 & 0.9309 & 2.3194 & 1.0914 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.9309 & 0.4667 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2.3194 & 0 & -2.5766 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1.0914 & 0 & 0 & -4.0813 & 3.5566 & 0 & 0 & 0 & 3.8670 & 0 \\
0 & 0 & 0 & 0 & 3.5566 & 2.1467 & 1.2789 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1.2789 & -7.7578 & 2.0308 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2.0308 & 4.6441 & 3.7564 & 0 & 2.7327 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 3.7564 & -7.5475 & 3.8670 & 0 \\
0 & 0 & 0 & 0 & 3.8670 & 0 & 0 & 0 & 3.8670 & 4.9020 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.7327 & 0 & 0 & -4.8068
\end{pmatrix}.$$

From the above matrix A, we recompute the eigenvalues of each leading principal submatrix A_j, we denote it by $\sigma(A_j)$:

$$\begin{aligned}
\sigma(A_1) &= \{-\mathbf{1}\},\\
\sigma(A_2) &= \{-\mathbf{2.9}, \mathbf{2}\},\\
\sigma(A_3) &= \{-\mathbf{3}, 0.2667, \mathbf{2.3}\},\\
\sigma(A_4) &= \{-\mathbf{4.5}, -1.7309, 0.3210, \mathbf{2.9}\},\\
\sigma(A_5) &= \{-\mathbf{5}, -3.7127, -1.7053, 0.3267, \mathbf{3}\},\\
\sigma(A_6) &= \{-\mathbf{6}, -4.2865, -1.7201, 0.3233, 2.8388, \mathbf{3.9}\},\\
\sigma(A_7) &= \{-\mathbf{8}, -5.8895, -4.2726, -1.7196, 0.3234, 2.8560, \mathbf{4}\},\\
\sigma(A_8) &= \{-\mathbf{8.3}, -5.9066, -4.2742, -1.7197, 0.3234, 2.8532, 3.9657, \mathbf{5}\},\\
\sigma(A_9) &= \{-\mathbf{9}, -7.8746, -5.8996, -4.2737, -1.7197, 0.3234, 2.8543, 3.9842, \mathbf{6}\},\\
\sigma(A_{10}) &= \{-\mathbf{10}, -8.0410, -6.5874, -4.3626, -1.7225, 0.3229, 2.8427, 3.3857,\\
&\qquad 5.5585, \mathbf{7.9}\},\\
\sigma(A_{11}) &= \{-\mathbf{10.1}, -8.0476, -6.6593, -5.2454, -4.3573, -1.7225, 0.3229,\\
&\qquad 2.8427, 3.3927, 6.0632, \mathbf{8}\}.
\end{aligned}$$

We illustrate the effectiveness of our results by measuring the error for a certain type of unicyclic graphs with orders ranging from 10 to 100. For any unicyclic graph of order n, we define $\gamma = (\gamma_1, \gamma_2, \dots, \gamma_n)$, $\delta = (\delta_1, \delta_2 \dots, \delta_n)$ as the vectors of the prescribed eigendata and $\widehat{\gamma} = (\widehat{\gamma}_1, \widehat{\gamma}_2, \dots, \widehat{\gamma}_n), \hat{\delta} = (\hat{\delta}_1, \hat{\delta}_2, \dots, \hat{\delta}_n)$ as the vectors of the extremal eigendata obtained from solution matrix, where $\widehat{\gamma}_j, \hat{\delta}_j$ are respectively the smallest and the largest eigenvalues of the jth leading principal submatrix of the solution matrix. We compute the error by $e = \|\gamma - \widehat{\gamma}\| + \|\delta - \hat{\delta}\|$, the eigendata considered in each problem are randomly generated. Table 1 shows the order of the unicyclic graphs and the corresponding errors.

Order of graph (n)	10	30	50
Error (e)	7.1471e − 15	2.7041e − 14	4.6893e − 14
	80	100	
	1.1760e − 13	1.4622e − 13	

Table 1. Order of the graphs and the corresponding errors.

The solutions found in this study are analytically sound, but for larger matrices, computational time and error will be substantial. In the future, any numerically effective approach can be studied to address this problem.

5. Conclusion

Unicyclic graph has lots of applications in different fields of science and engineering. Unicyclic graphs are commonly used in the field of chemical graph theory to model different chemical structures. In network analysis, unicyclic graphs are used to model the topology of communication networks. We have solved the extremal inverse eigenvalue problem for matrices whose graph is connected unicyclic. Labelling plays a significant role in solving the extremal IEPs. We studied the problem under a fixed labelling format. Unicyclic graph under other form of labelling can also be studied in the future.

References

[1] *M. Babaei Zarch, S. A. Shahzadeh Fazeli*: Inverse eigenvalue problem for a kind of acyclic matrices. Iran. J. Sci. Technol. Trans. A Sci. *43* (2019), 2531–2539. MR doi

[2] *M. Babaei Zarch, S. A. Shahzadeh Fazeli, S. M. Karbassi*: Inverse eigenvalue problem for matrices whose graph is a banana tree. J. Algorithms Comput. *50* (2018), 89–101.

[3] *W. Y. Chen, X. Li, C. Wang, X. Zhang*: Linear time algorithms to the minimum all-ones problem for unicyclic and bicyclic graphs. Workshop on Graphs and Combinatorial Optimization. Electronic Notes Discrete Mathematics 17. Elsevier, Amsterdam, 2004, pp. 93–98. zbl MR doi

[4] *M. T. Chu*: Inverse eigenvalue problems. SIAM Rev. *40* (1998), 1–39. zbl MR doi

[5] *D. Cvetković*: Applications of graph spectra: An introduction to the literature. Applications of Graph Spectra. Zbornik Radova 13. Matematički Institut SANU, Beograd, 2009, pp. 7–31. zbl MR

[6] *G. M. L. Gladwell*: Inverse problems in vibration. Appl. Mech. Rev. *39* (1986), 1013–1018. zbl doi

[7] *M. Hadji, M. Chau*: On unicyclic graphs spectra: New results. IEEE Intl Conference on Computational Science and Engineering (CSE) and IEEE Intl Conference on Embedded and Ubiquitous Computing (EUC) and 15th Intl Symposium on Distributed Computing and Applications for Business Engineering (DCABES). IEEE, Paris, 2016, pp. 586–593. doi

[8] *R. S. Haoer, K. A. Atan, M. R. Said, A. M. Khalaf, R. Hasni*: Zagreb-eccentricity indices of unicyclic graph with application to cycloalkanes. J. Comput. Theor. Nanosci. *13* (2016), 8870–8873. doi
[9] *R. A. Horn, C. R. Johnson*: Matrix Analysis. Cambridge University Press, Cambridge, 2013. zbl MR doi
[10] *C. R. Johnson, A. Leal Duarte, C. M. Saiago*: Inverse eigenvalue problems and lists of multiplicities of eigenvalues for matrices whose graph is a tree: The case of generalized stars and double generalized stars. Linear Algebra Appl. *373* (2003), 311–330. zbl MR doi
[11] *N. Li*: A matrix inverse eigenvalue problem and its application. Linear Algebra Appl. *266* (1997), 143–152. zbl MR doi
[12] *X. Li, C. Magnant, Z. Qin*: Properly Colored Connectivity of Graphs. SpringerBriefs in Mathematics. Springer, Cham, 2018. zbl MR doi
[13] *X. Li, J. Wang*: On the ABC spectra radius of unicyclic graphs. Linear Algebra Appl. *596* (2020), 71–81. zbl MR doi
[14] *P. Nylen, F. Uhlig*: Inverse eigenvalue problems associated with spring-mass systems. Linear Algebra Appl. *254* (1997), 409–425. zbl MR doi
[15] *J. Peng, X.-Y. Hu, L. Zhang*: Two inverse eigenvalue problems for a special kind of matrices. Linear Algebra Appl. *416* (2006), 336–347. zbl MR doi
[16] *H. Pickmann, J. Egaña, R. L. Soto*: Extremal inverse eigenvalue problem for bordered diagonal matrices. Linear Algebra Appl. *427* (2007), 256–271. zbl MR doi
[17] *H. Pickmann, J. C. Egaña, R. L. Soto*: Two inverse eigenproblems for symmetric doubly arrow matrices. Electron. J. Linear Algebra *18* (2009), 700–718. zbl MR doi
[18] *H. Pickmann-Soto, S. Arela-Pérez, H. Nina, E. Valero*: Inverse maximal eigenvalues problems for Leslie and doubly Leslie matrices. Linear Algebra Appl. *592* (2020), 93–112. zbl MR doi
[19] *D. Sharma, B. K. Sarma*: Extremal inverse eigenvalue problem for irreducible acyclic matrices. Appl. Math. Sci. Eng. *30* (2022), 192–209. MR doi
[20] *D. Sharma, M. Sen*: Inverse eigenvalue problems for two special acyclic matrices. Mathematics *4* (2016), Article ID 12, 11 pages. zbl doi
[21] *D. Sharma, M. Sen*: Inverse eigenvalue problems for acyclic matrices whose graph is a dense centipede. Spec. Matrices *6* (2018), 77–92. zbl MR doi
[22] *D. Sharma, M. Sen*: The minimax inverse eigenvalue problem for matrices whose graph is a generalized star of depth 2. Linear Algebra Appl. *621* (2021), 334–344. zbl MR doi
[23] *Y. Wei, H. Dai*: An inverse eigenvalue problem for the finite element model of a vibrating rod. J. Comput. Appl. Math. *300* (2016), 172–182. zbl MR doi

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