Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2026 (44)** : 1–13.
ISSN-0037-8712
doi:10.5269/bspm.78034

On Extended Adjacency Matrices Associated with Eccentricity-Based Topological Indices

Balkishbanu Khaji, Shahistha Hanif and K. Arathi Bhat

ABSTRACT: Several investigations of the extended adjacency matrices associated with various degree-based topological indices have been undertaken in recent years, leading to sharper theorems and conclusions. Motivated by this, we explore eccentricity-based topological indices and the extended adjacency matrices associated with them. Suppose F is a symmetric function associated with an eccentricity-based topological index, then a generalised extended adjacency matrix $A^e_F(G)$ has $(i,j)^{th}-$ entry as the value of F at the eccentricities of the corresponding vertices v_i, v_j if they are adjacent, else it is 0. The expressions and bounds for parameters like the trace, determinant, and eigenvalues associated with this matrix are derived in this article. The expression for the determinant indicates that it depends on the number of elementary spanning subgraphs present in the graph.

Keywords: Eccentricity, determinant, trace, extended adjacency matrix, quality education.

Contents

1. Introduction

All graphs considered in this article are finite, simple and connected. As usual, the degree and neighborhood of a vertex v_i are denoted by $d_G(v_i)$ and $N_G(v_i)$, respectively. The adjacency and non-adjacency between two vertices v_i, v_j are denoted by $v_i \sim_G v_j$ and $v_i \nsim_G v_j$, respectively. The suffix G in the notations $\sim_G$, $\nsim_G$, $d_G(v_i)$ and $N_G(v_i)$ are conveniently ignored if the graph under discussion is clearly understood. The distance $d(v_i, v_j)$ between the two vertices v_i and v_j of G is the length of the shortest path between them and the eccentricity of v_i is $e(v_i) = max\{d(v_i, v_j) : v_j \in V(G)\}$. The radius $R(G)$ and diameter $D(G)$ of G is measured from eccentricity, which are defined as $min\{e(v_i) : v_i \in V(G)\}$ and $max\{e(v_i) : v_i \in v(G)\}$, respectively. For any unfamiliar terms within graph theory, readers may refer to [1].

The prediction of physicochemical, pharmacological, and toxicological properties of compounds directly from their molecular structure has become an important tool in molecular chemistry and pharmaceutical drug design. The parameters called topological indices derived from a graph-theoretic model are used extensively in QSPR studies and analysis [2]. The Wiener index is the first topological index, introduced by H. Wiener in 1947 to determine the physical properties of paraffin [3]. Hundreds of topological indices are currently being researched and developed since then. Although most of the topological graph indices are degree and distance-based, researchers have recently begun replacing degrees with eccentricities in well-known degree-based topological indices in the verge of refining the existing topological indices. The general formula is given.

$$TI = TI(G) = \sum_{v_i \sim v_j} F(deg(v_i), deg(v_j))$$

where $F(x, y)$ is a symmetric function of vertex degrees [4]. On replacing the degree with eccentricity, one can get the corresponding eccentricity-based index. For example, the eccentric connectivity index

2020 *Mathematics Subject Classification:* 05C10, 05C30, 05C90.
Submitted July 24, 2025. Published March 22, 2026

(denoted by $\xi^c(G)$) is one of the eccentricity-based topological indices, where $F(x,y) = x + y$ [5]. Few eccentricity-based indices are successfully used for mathematical models of biological activities of diverse nature [6,7]. Analytically closed formulas for these descriptors are provided in [8,9,10], which may be used to investigate the underlying topologies of chemical compounds. The eccentricity-based topological indices like total eccentricity index, average eccentricity index, atom-bond connectivity index, etc. for benzenoid structure are studied extensively in [11]. Several eccentricity-based topological indices like the average eccentricity, eccentric version of Zagreb indices, etc. for first type of hex-derived network are contemplated and the basic topologies of these networks are investigated in [12].
The concept of the extended adjacency matrix of a graph was introduced by Yang et al. in 1994 [13], which is explored from the perspective of chemical molecular graphs to expand some beneficial molecular topological indices. The extended adjacency matrix $A_F(G)$ of a graph G is a matrix whose rows and columns are indexed by $V(G)$, and is defined as

$$A_F(G) = (a_F)_{ij} = \begin{cases} F(v_i, v_j), & if \quad v_i \sim v_j \\ 0, & otherwise \end{cases}$$

where $F(x,y)$ is the symmetric function associated with a degree-based topological index. The utilisation of extended adjacency matrices to investigate various combinatorial properties of graphs is one of the most recent research directions in spectral graph theory. For studying properties and relations between the extended adjacency index and other matrices associated with topological indices, see Refs. [14,15, 16,17,18,19].

Inspired by this, the extended adjacency matrix associated with the eccentricity-based topological indices are taken up and explored in this article. The generalized extended adjacency matrix associated with an eccentricity-based topological index is denoted by $A_F^e(G)$(or simply A_F^e), where $F(v_i, v_j)$ is a symmetric function of vertex eccentricities associated with an eccentricity-based topological index. After this notion of extended adjacency matrices, the usual adjacency matrix is often referred to as the classical adjacency matrix. Since $A_F^e(G)$ is a real symmetric matrix, its eigenvalues are real. Analogous to the classical adjacency matrix, the A_F^e-spectrum of a graph G, often denoted by $spec(A_F^e(G))$ comprises the eigenvalues of the matrix $A_F^e(G)$. Various kinds of graph spectra have been defined and used to study many properties of graphs like the number of spanning trees, the number of walks, etc. For example, from the spectrum of classical adjacency matrix $A(G)$ one can read off the number of closed walks of a given length.

Theorem 1.1 *[20] Let k be a non-negative integer. Then $(A(G)^k)_{xy}$ is the number of walks of length k from x to y. In particular, $(A(G)^2)_{xx}$ is the degree of the vertex x, and $trace(A(G))^2$ equals twice the number of edges of G; similarly, $trace(A(G))^3$ is six times the number of triangles in G.*

In a similar vein regarding the classical adjacency matrices, the sum of absolute values of the eigenvalues of $A_F^e(G)$ is known as A_F^e-energy of the graph G. In an attempt to explore properties and parameters associated with $A_F^e(G)$, some of the preliminary results from matrix theory are used, which are stated below.

Lemma 1.1 *[21] The Cauchy – Schwarz inequality: If $(a_1, a_2, \dots, a_p)$ and $(b_1, b_2, \dots, b_p)$ are real p – vectors then,*

$$\left(\sum_{i=1}^{p} a_i b_i\right)^2 \leq \sum_{i=1}^{p} a_i^2 \sum_{i=1}^{p} b_i^2$$

Lemma 1.2 *[22] Cauchy interlacing theorem: Suppose $A \in R^{n\times n}$ is symmetric. Let $B \in R^{m\times m}$ with $m < n$ be a principal submatrix of A (submatrix whose rows and columns are indexed by the same index set $i_1, ..., i_m$, for some m). Suppose A has eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$, and B has eigenvalues $\beta_1 \leq \cdots \leq \beta_m$. Then, $\lambda_k \leq \beta_k \leq \lambda_{k+n-m}$ for $k = 1, \dots m$, and if $m = n-1$, then $\lambda_1 \leq \beta_1 \leq \lambda_2 \leq \beta_2 \leq \cdots \leq \beta_{n-1} \leq \lambda_n$.*

Lemma 1.3 *[22] Let $A = (a_{ij})$ be a square matrix of order n. Then the determinant of A is given by*

$$det(A) = \sum_{\sigma \in S_n} sign(\sigma) a_{1\sigma(1)} a_{2\sigma(2)} \dots . a_{n\sigma(n)}$$

The summation is over all permutations $\sigma \in S_n$, where S_n is the set of all permutations of $1, 2, \ldots, n$.

Lemma 1.4 *[23] Let $C \in M_{m,n}$ and $q = min\{n, m\}, \alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_q$ be the ordered singular values of C, and define the Hermitian matrix $H = \begin{pmatrix} 0 & C \\ C^* & 0 \end{pmatrix}$. The ordered eigenvalues of H are $-\alpha_1 \leq \cdots \leq -\alpha_q \leq 0 = 0 \cdots = 0 \leq \alpha_q \leq \ldots \alpha_1$.*

Lemma 1.5 *[23] Let $A \subset M_n$ be a Hermitian matrix and let eigenvalues of A be ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ then $\lambda_n y^* y \leq y^* A y \leq \lambda_1 y^* y \; \forall \; y \in C^n$.*

A partition D of a square matrix A is said to be equitable if all the blocks of the partitioned matrix have constant row sums and each of the diagonal blocks is of square order. A quotient matrix B of a square matrix A corresponding to an equitable partition is a matrix whose entries are the constant row sums of the corresponding blocks of A. The quotient matrices are useful in finding some eigenvalues of block matrices, which are comparatively larger in size. In the theory of graph spectra, equitable partitions play an important role, mostly because of the following results.

Theorem 1.2 *[24] Let A be a real symmetric matrix with a quotient matrix B. Then the characteristic polynomial of B divides the characteristic polynomial of A.*

Theorem 1.3 *[20] Let D be an equitable partition of the connected graph G. Then $A(G)$ and the quotient matrix B of D has the same spectral radius λ_1.*

2. Main Results

The following propositions give the basic properties of $A_F^e(G)$, which are analogous to the ones available for classical adjacency matrices. We omit the proofs whenever they are straightforward. Throughout the article, by extended adjacency matrix $A_F^e(G)$, we mean the one associated with the eccentricity-based topological index. Further, suppose $F(x, y)$ is a function associated with an eccentricity-based topological index, then we simply write $F(i, j)$ for $F(e(v_i), e(v_j))$. Also, we use the convention of denoting the $(i, j)^{th}-$ entry of A_F^e corresponding to the vertices v_i and v_j by a_{ij}.

Proposition 2.1 *Let G be a connected graph with the extended adjacency matrix $A_F^e(G)$. For $i \neq j$, the principal submatrix of $A_F^e(G)$ formed by i^{th} row and j^{th} column of order 2×2 is the zero matrix if $v_i \nsim v_j$ and otherwise it equals $\begin{pmatrix} 0 & F(i,j) \\ F(i,j) & 0 \end{pmatrix}$.*

Using the above proposition, one can easily derive the following bounds for the sum of all principal minors of order 2×2 of $A_F^e(G)$.

Proposition 2.2 *Let G be a connected graph with the extended adjacency matrix $A_F^e(G)$. Let S_2 be the sum of all principal minors of order 2×2 of the matrix $A_F^e(G)$. Then*

$$mF(R, R)^2 \leq |S_2| \leq mF(D, D)^2$$

where m, R, D are the size, radius and diameter of G, respectively.

Next, we look in to the principal submatrix of order 3.

Proposition 2.3 *Let G be a connected graph with the extended adjacency matrix $A_F^e(G)$. The principal submatrix formed by any three distinct rows and columns i, j, k of order 3×3 is non-singular only when the corresponding vertices v_i, v_j, v_k constitute a triangle. In that case, the submatrix is given by $\begin{pmatrix} 0 & F(i,j) & F(i,k) \\ F(i,j) & 0 & F(j,k) \\ F(i,k) & F(j,k) & 0 \end{pmatrix}$.*

Analogous to the case of 2×2 principal submatrices, one can obtain the bounds for the sum of all principal minors of A_F^e of order 3×3.

Proposition 2.4 *Let G be a connected graph with the extended adjacency matrix $A_F^e(G)$. Let S_3 be the sum of all principal minors of order 3×3 of the matrix A_F^e. Then*

$$2tF(R,R)^3 \le S_3 \le 2tF(D,D)^3$$

where R, D, t are the radius, diameter and the number of triangles in G, respectively.

Proposition 2.5 *Let G be a connected graph with diameter D and the extended adjacency matrix $A_F^e(G)$. Suppose $A_F^e(G)$ has k distinct eigenvalues, then $k > D$.*

Proof: The proof follows from the fact that the matrices $A_F^e(G), (A_F^e(G))^2, (A_F^e(G))^3, \ldots, (A_F^e(G))^D$ are linearly independent and the degree of minimal polynomial of $A_F^e(G)$ is k and it must exceed D. □

Theorem 2.1 *Let G be a connected graph and $trace(A_F^e)$ denotes the trace of the extended adjacency matrix $A_F^e(G)$. Then*

1. $trace(A_F^e) = 0$.
2. $trace\left((A_F^e)^2\right) = 2\sum\limits_{(v_i,v_j)\in E} F(i,j)^2$.
3. $trace\left((A_F^e)^3\right) = 6\sum\limits_{(v_i,v_j,v_k)\in S} F(i,j)F(j,k)F(k,i)$.

where E and S are the set of all edges and the set of all triangles in G, respectively. And $F(x,y)$ be any function associated with an eccentricity-based topological index.

Proof: (i) : The first result is obvious from the definition.
(ii) : We know that $a_{ij}^2 = \sum\limits_{v_k\sim v_i,v_j} a_{ik}a_{kj}$. Consider

$$\begin{aligned} trace((A_F^e)^2) &= \sum_{i=1}^n a_{ii}^2 = \sum_{i=1}^n \sum_{v_j\sim v_i} a_{ij}a_{ji} \\ &= \sum_{i=1}^n \sum_{v_j\sim v_i} F(i,j)^2 \\ &= 2\sum_{(v_i,v_j)\in E} F(i,j)^2 \end{aligned}$$

(iii) : Similarly,

$$\begin{aligned} trace((A_F^e)^3) &= \sum_{i=1}^n a_{ii}^3 = \sum_{i=1}^n \sum_{v_j\sim v_i} a_{ij}(a_{ji})^2 \\ &= \sum_{i=1}^n \sum_{v_j\sim v_i} a_{ij} \sum_{v_k\sim v_j} a_{jk}a_{ki} \\ &= \sum_{i=1}^n \sum_{v_j\sim v_i} \sum_{v_k\sim v_j} a_{ij}a_{jk}a_{ki} \end{aligned}$$

Here, the summation runs over the set S of all the triangles in G. One can note that each triangle formed by the vertices v_i, v_j, v_k is counted twice in the corresponding terms $a_{ii}^3, a_{jj}^3, a_{kk}^3$, which implies a triangle formed by the vertices v_i, v_j, v_k is counted six times in total. Thus

$$trace((A_F^e)^3) = 6\sum_{(v_i,v_j,v_k)\in S} a_{ij}a_{jk}a_{ki} = 6\sum_{(v_i,v_j,v_k)\in S} F(i,j)F(j,k)F(k,i).$$

□

The expressions in the trace of $(A_F^e)^2$ and $(A_F^e)^3$ take the simplest form when the graph is eccentricity regular, that is $e(v_i) = r$ for all v_i in G and r is an integer. In this case, we get $trace\left((A_F^e)^2\right) = 2mF(r,r)^2$ and $trace\left((A_F^e)^3\right) = 6tF(r,r)^3$, where m, t are the number of edges and triangles in G, respectively.

Theorem 2.2 *A graph is bipartite if and only if the A_F^e- spectrum of G is symmetric about the origin.*

Proof: Let G be a bipartite graph with the bipartition $V(G) = V_1 \cup V_2$ with $|V_1| = n_1$ and $|V_2| = n_2$. Then the vertices of G can be labeled in such a way that the matrix $A_F^e(G)$ can be written as

$$A_F^e(G) = \begin{pmatrix} 0_{n_1\times n_2} & B_{n_1\times n_2} \\ B^T_{n_2\times n_1} & 0_{n_1\times n_2} \end{pmatrix}.$$

where B is a non-negative matrix of order $n_1 \times n_2$. Then by Lemma 1.4, the A_F^e-spectrum is symmetric about the origin.
Conversely, suppose the A_F^e-spectrum is symmetric about the origin, then for all the odd integers k, the $trace(A_F^e(G)^k) = 0$. The matrix $A_F^e(G)$ has a nonzero entry if and only if the corresponding entry in the classical adjacency matrix $A(G)$ is nonzero. That is, $trace(A_F^e(G)^k) > 0$ if and only if $trace(A(G)^k) > 0$. Suppose G has an odd cycle of length p, by Theorem 1.1, $trace(A(G)^p) > 0$, which in turn means that $trace(A_F^e(G)^k) > 0$, a contradiction. Thus G has no cycles of odd length and hence is bipartite. □

Theorem 2.3 *Let G be a self centered and regular graph with $deg(v_i) = d$ and $e(v_i) = r$ for all the vertices v_i in G. Then $2rd \in A_F^e(G)-$ spectrum.*

Proof: Suppose G is a graph of order n and $v = \begin{pmatrix} 1 & 1 & 1 & \dots & 1\end{pmatrix}^T$ be a vector in R^n. On considering $A_F^e(G)v = \mu v$, we get $\mu = 2rd$. □

The next theorem gives an expression for the determinant of A_F^e, which in turn determines if the matrix is of positive nullity. Before moving into the expression, we define the following convention of associating a permutation to an elementary spanning subgraph. For a graph of order n, with labels $v_1, v_2, \dots, v_n$, we associate a special type of permutation of $\begin{pmatrix} 1 & 2 & \dots & n\end{pmatrix}$. Suppose H is an elementary spanning subgraph, then

1. for each component K_2 present in H formed by the vertices v_i,v_j, we associate the permutation $\begin{pmatrix} i & j \\ j & i\end{pmatrix} = \begin{pmatrix} i & j\end{pmatrix}$.

2. for each cycle $C_k : v_1 \sim v_2 \sim v_3 \sim \dots \sim v_k \sim v_1$ present in H, we associate two permutations $\begin{pmatrix} 1 & 2 & 3 & \dots & k \\ 2 & 3 & 4 & \dots & 1\end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & \dots & k\end{pmatrix}$ and $\begin{pmatrix} 1 & 2 & 3 & \dots & k \\ k & 1 & 2 & \dots & k-1\end{pmatrix} = \begin{pmatrix} 1 & k & k-1 & \dots & 2\end{pmatrix}$.

For example, if H is an elementary subgraph given in Figure 1, then we can associate $2^c(H) = 2^2$ permutations of $\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9\end{pmatrix}$ to H, say $\sigma_1(H), \sigma_2(H), \sigma_3(H)$ and $\sigma_4(H)$ which are listed below

1. $\sigma_1(H) = \begin{pmatrix} 1 & 2 & 3\end{pmatrix}\begin{pmatrix} 4 & 5 & 6 & 7\end{pmatrix}\begin{pmatrix} 8 & 9\end{pmatrix}$

2. $\sigma_2(H) = \begin{pmatrix} 1 & 3 & 2\end{pmatrix}\begin{pmatrix} 4 & 7 & 6 & 5\end{pmatrix}\begin{pmatrix} 8 & 9\end{pmatrix}$

3. $\sigma_3(H) = \begin{pmatrix} 1 & 2 & 3\end{pmatrix}\begin{pmatrix} 4 & 7 & 6 & 5\end{pmatrix}\begin{pmatrix} 8 & 9\end{pmatrix}$

4. $\sigma_4(H) = \begin{pmatrix} 1 & 3 & 2\end{pmatrix}\begin{pmatrix} 4 & 5 & 6 & 7\end{pmatrix}\begin{pmatrix} 8 & 9\end{pmatrix}$

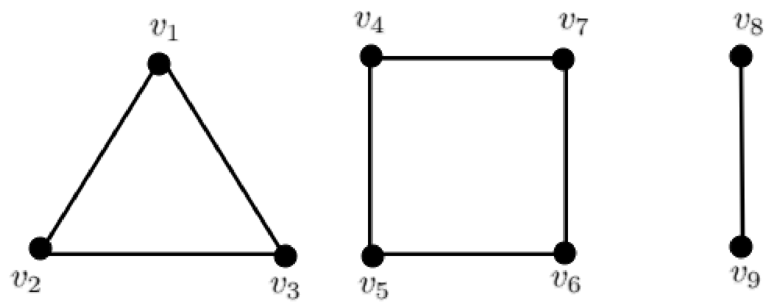

Figure 1: An elementary spanning subgraph H

Theorem 2.4 *Let G be a graph of order n and $det(A_F^e)$ denotes the determinant of the matrix A_F^e of the graph G. Then*

$$det(A_F^e) = \sum_H (-1)^{n-c_1(H)-c(H)} \sum_{\substack{\sigma_j(H)\\ j=1}}^{2^{c(H)}} \prod_{i=1}^{n} F(i, \sigma_j(i))$$

where the first summation is over all the elementary spanning subgraphs H in G, and the second summation is over all the permutations $\sigma_j(H)$, associated with the elementary spanning subgraph H in G. And $c(H), c_1(H)$ are the number of components in H which are cycles and K_2's, respectively.

Proof: Since A_F^e is of order n, from Lemma 2.4,

$$det(A_F^e) = \sum_\sigma sign(\sigma) a_{1\sigma(1)} a_{2\sigma(2)} \ldots\ldots a_{n\sigma(n)}$$

where the summation is over all permutations of $1, 2, \ldots, n$. If $\sigma(i) = i$ for any $1 \le i \le n$, then the term $a_{1\sigma(1)} a_{2\sigma(2)} \ldots\ldots a_{n\sigma(n)}$ is zero as it contains the diagonal entry a_{ii}. Consider a nonzero term $a_{1\sigma(1)} a_{2\sigma(2)} \ldots\ldots a_{n\sigma(n)}$ in the summation of $det(A_F^e)$. Since a permutation σ admits a cyclic decomposition, such a term will correspond to either of the following or the combinations of the following:

1. a 2-cycle $\begin{pmatrix} i & j \end{pmatrix}$, which designates an edge joining the vertices v_i and v_j in G.

2. a cycle of length $k > 2$, say $\begin{pmatrix} i_1 & i_2 & \ldots & i_k \end{pmatrix}$, designating a cycle $v_{i_1} \sim v_{i_2} \sim \cdots \sim v_{i_k} \sim v_{i_1}$ in G

Thus, any nonzero term in the summation corresponds to an elementary spanning subgraph of G. The sign of the permutation σ, which is associated with the elementary spanning subgraph H is $sign(\sigma) = (-1)^{n-c_1(H)-c(H)}$, where $c_1(H), c(H)$ are the number of components which are K_2's and cycles in H, respectively. Since each cycle can be associated with a cyclic permutation in two ways (as explained earlier), each elementary spanning subgraph H gives rise to $2^c(H)$ permutations, say $\sigma_1(H), \sigma_2(H), \ldots, \sigma_{2^c}(H)$ and hence there are $2^c(H)$ terms in the second summation. Thus

$$det(A_F^e) = \sum_H (-1)^{n-c_1(H)-c(H)} \sum_{\substack{\sigma_j(H)\\ j=1}}^{2^{c(H)}} a_{1\sigma_j(1)} a_{2\sigma_j(2)} \ldots\ldots a_{n\sigma_j(n)}.$$

On substituting $a_{i\sigma_j(i)} = F(i, \sigma_j(i))$, we get the expression. □

From the above proof, one can note that the second summation is over all the permutations $\sigma(H)$, corresponding to the elementary spanning subgraph H in G and hence contains $2^c(H)$ terms in it (explained with an illustration for one of the specific index called eccentric connectivity index).

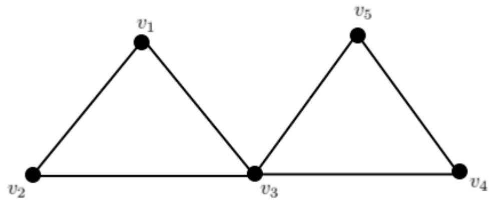

Figure 2: The graph G_1

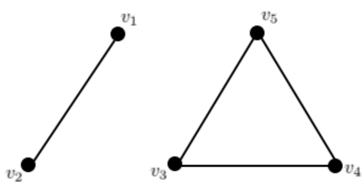

Figure 3: H_1, the elementary subgraph of G_1

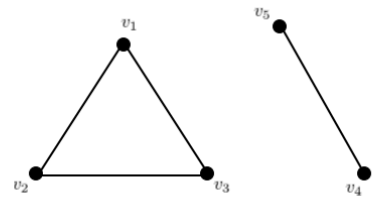

Figure 4: H_2, the elementary subgraph of G_1

Example 2.1 *Consider the graph G_1 as shown in Figure 2. Then the graph G_1 has two elementary spanning subgraphs H_1(Figure 3) and H_2(Figure 4). Each of H_i for $i = 1, 2$ induces 2 permutations on $\begin{pmatrix}1 & 2 & 3 & 4 & 5\end{pmatrix}$. Thus, there are 4 permutations $\sigma_1(H_1), \sigma_2(H_1), \sigma_1(H_2)$ and $\sigma_2(H_2)$ given by,*

1. $\sigma_1(H_1) = \begin{pmatrix}1 & 2 & 3\end{pmatrix}\begin{pmatrix}4 & 5\end{pmatrix}$
2. $\sigma_2(H_1) = \begin{pmatrix}1 & 3 & 2\end{pmatrix}\begin{pmatrix}4 & 5\end{pmatrix}$
3. $\sigma_1(H_2) = \begin{pmatrix}1 & 2\end{pmatrix}\begin{pmatrix}3 & 4 & 5\end{pmatrix}$
4. $\sigma_1(H_2) = \begin{pmatrix}1 & 2\end{pmatrix}\begin{pmatrix}3 & 5 & 4\end{pmatrix}$

On substituting $F(x, y) = x + y$ for eccentric connectivity index, we get $det(A^e_F) = -2304$.

One can note that if a graph G has no elementary spanning subgraph, then $det(A_{\varepsilon^c}) = 0$, but the converse may not be true. The graph in Figure 5 is a counterexample.

Example 2.2 *The graph G_2 is shown in Figure 5. has three elementary spanning subgraphs (H_1 : $2K_2, H_2 : 2K_2, H_3 : C_4$),*

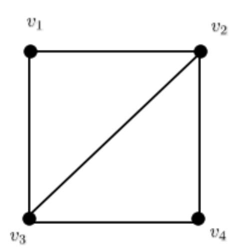

Figure 5: A graph G_2

but the determinant of the extended adjacency matrix corresponding to the eccentric connectivity index is zero. That is $det(A^e_F(G_2)) = det \begin{pmatrix} 0 & 3 & 3 & 0 \\ 3 & 0 & 2 & 3 \\ 3 & 2 & 0 & 3 \\ 0 & 3 & 3 & 0 \end{pmatrix} = 0$, *where* $F(x, y) = x + y$.

Theorem 1.3 leads to the following observations and results.

Remark 2.1 *If* G *is a bipartite graph on an odd number of vertices, then* $det(A^e_F) = 0$.

The expression in Theorem 1.3 is simplified as follows for eccentric regular graphs.

Corollary 2.1 *Let* G *be an eccentric regular graph with regularity* r. *Then*

$$det(A^e_F) = \sum_H (-1)^{n-c_1(H)-c(H)} 2^{c(H)} (F(r, r))^n$$

where the summation is over all the elementary spanning subgraphs H *in* G *and* $c(H), c_1(H)$ *are the number of components in* H *which are cycles and* K_2*'s, respectively.*

Theorem 2.5 *Let* T *be a tree of order* n. *Then*

$$det(A^e_F) = \begin{cases} (-1)^{\frac{n}{2}} \prod\limits_{(v_i,v_j)\in E(H)} (F(i, j))^2 & if\ n\ is\ even \\ 0 & else \end{cases}$$

where H *is the unique elementary spanning subgraph of* T, *if present.*

Proof: We know that a tree has at most one elementary spanning subgraph. Further, if T has an odd number of vertices, then it has no elementary spanning subgraph, due to which $det(A^e_F) = 0$. Let T be a tree on an even number of vertices. Then T has at most one elementary spanning subgraph in which every component is K_2 and hence $c_1(H) = \frac{n}{2}$ and $c(H) = 0$. Suppose T has an elementary spanning subgraph H, then there is one and only one term in both the summations of the expression given in Theorem 1.3. That is, $det(A^e_F) = (-1)^{\frac{n}{2}} \prod\limits_{(v_i,v_j)\in E(H)} (F(i, j))^2$, where the product is over all the edges in H.
If T is a graph on an even number of vertices with no elementary spanning trees, then again $det(A^e_F) = 0$. □

3. Bounds for Spectral Radius of A^e_F

Let $\mu_1(G)$ denote the largest eigenvalue of the matrix A^e_F. Some bounds for $\mu_1(G)$ are derived in this section.

Theorem 3.1 *Let* G *be a connected graph of order* n *having diameter* D. *Let* $\mu_1(G)$ *and* $\mu_n(G)$ *be the largest and smallest eigenvalues of* $A^e_F(G)$, *respectively. Then,*

1. $\mu_n(G) \leq -F(D, D)$
2. $F(D, D) \leq \mu_1(G)$

Furthermore, if $D \geq 3$, *then* $\mu_n \leq -6$.

Proof: Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be the eigenvalues of the matrix A^e_F. Since D is the diameter, there exists at least one pair of vertices v_i, v_j such that $d(v_i, v_j) = D$. The principal submatrix of A^e_F corresponding to these vertices is given by $B = \begin{pmatrix} 0 & F(D, D) \\ F(D, D) & 0 \end{pmatrix}$. Suppose $\beta_1 \geq \beta_2$ are the two eigenvalues of B, then $\beta_1 = F(D, D)$ and $\beta_2 = -F(D, D)$. Since $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$, by interlacing theorem, $\mu_n \leq \beta_2 \leq \mu_2$ and $\mu_{n-1} \leq \beta_1 \leq \mu_1$. On substituting β_1, β_2, we get the inequality. □

Theorem 3.2 *Let $\mu_1 \geq \mu_2 \geq ..... \geq \mu_n$ be the eigenvalues of $A_F^e(G)$. Then*

$$\mu_1 \leq \sqrt{\frac{(n-1)S}{n}}$$

where $S = \sum_{i=1}^{n} \mu_i^2$.

Proof: From Theorem 2.1, $trace(A_F^e) = 0$ and $\mu_1 = -\sum_{i=2}^{n} \mu_i$. On applying the Cauchy-Schwarz inequality,

$$\begin{aligned} \mu_1^2 = \left| -\sum_{i=2}^{n} \mu_i \right|^2 &\leq (n-1) \sum_{i=2}^{n} |\mu_i|^2 \\ \mu_1^2 = \left(-\sum_{i=2}^{n} \mu_i \right)^2 &\leq (n-1) \sum_{i=2}^{n} \mu_i^2 \\ &= (n-1) \left(\sum_{i=1}^{n} \mu_i^2 - \mu_1^2 \right) \\ &= (n-1) \left(S - \mu_1^2 \right) \end{aligned}$$

□

Theorem 3.3 *Let G be a graph of order n and $\mu_1 \geq \mu_2 \geq ..... \geq \mu_n$ be the eigenvalues of $A_F^e(G)$. Let $TI_F(G)$ be the topological index based on which the extended adjacency matrix $A_F^e(G)$ is defined. Then*

$$\mu_n \leq \frac{2TI_F(G)}{n} \leq \mu_1$$

Proof: Let $y = \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \end{pmatrix}^T$. Then

$$y^T A_F^e y = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \quad = 2 \sum_{v_i \sim v_j} F(i,j) = 2TI_F(G)$$

From Lemma 1.5, $\mu_1 y^T y \leq y^T A y \leq \mu_p y^T y$ for all vectors $y \in R^n$. Thus

$$\begin{aligned} &\mu_n y^T y \leq 2TI_F(G) \leq \mu_1 y y^T \\ &\Rightarrow \mu_n n \leq 2TI_F(G) \leq \mu_1 n \\ &\Rightarrow \mu_n \leq \frac{2TI_F(G)}{n} \leq \mu_1 \end{aligned}$$

□

Theorem 3.4 *Let G be a graph of order n and size m with the diameter $D(G)$. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_p$ be the eigenvalues of A_F^e. Then*

$$\mu_p \leq F(D,D)\sqrt{2m-n+1}$$

with equality if and only if G is a complete graph on n vertices.

Proof: Let $X = \begin{pmatrix} X_1 & X_2 & \dots & X_n \end{pmatrix}^T$ be the eigenvector of length one corresponding to the largest eigenvalue μ_1 of A_F^e, then

$$A_F^e(G)X = \mu_1 X$$

By $(A_F^e(G))_i$ and X_i we mean the i^{th} row of $A_F^e(G)$ and X, respectively. Let $X(i)$ be the new vector obtained from X by replacing X_j with zero whenever the corresponding vertex $v_j \nsim v_i$, for all $1 \leq j \leq n$ and $i \neq j$.

$$(A_F^e(G))_i X(i) = \mu_1 X(i)$$

On applying the Cauchy-Schwarz inequality, we get

$$|(\mu_1 X(i)|^2 = |(A_F^e(G))_i X(i)|^2 \leq |(A_F^e(G))_i|^2 |X(i)|^2$$

Also, $(A_F^e(G))_i$, the i^{th} row of $A_F^e(G)$ has the non-zero entry $F(i,j)$ if and only if the corresponding vertex $v_j \sim v_i$. Thus

$$\begin{aligned} |(A_F^e(G))_i|^2 &= \sum_{v_j \sim v_i} (F(i,j))^2 \\ &\leq \sum_{v_i \sim v_j} F(D,D)^2 \\ &\leq d(v_i) F(D,D)^2 \end{aligned} \tag{3.1}$$

where $d(v_i)$ is the degree of the vertex v_i and $D(G)$ is the diameter of G. We have

$$\begin{aligned} |X(i)|^2 &= X_i^2 + \sum_{v_i \sim v_j} X_j^2 \\ &= 1 - \sum_{v_i \nsim v_j} X_j^2 \end{aligned} \tag{3.2}$$

From Equations 3.1 and 3.2,

$$\begin{aligned} \mu_1^2 X(i)^2 &\leq d(v_i) F(D,D)^2 \left(1 - \sum_{v_i \nsim v_j} X_j^2\right) \\ &= d(v_i) F(D,D)^2 - d(v_i) F(D,D)^2 \sum_{v_i \nsim v_j} X_j^2 \end{aligned}$$

Now, taking summation over i for $1 \leq i \leq n$, we get

$$\begin{aligned} \mu_1^2 \sum_{i=1}^{n} X(i)^2 &\leq \sum_{i=1}^{n} d(v_i) F(D,D)^2 - \sum_{i=1}^{n} d(v_i) F(D,D)^2 \sum_{v_i \nsim v_j} X_j^2 \\ &\leq 2m F(D,D)^2 - F(D,D)^2 \sum_{i=1}^{n} d(v_i) \sum_{v_i \nsim v_j} X_j^2 \end{aligned} \tag{3.3}$$

Now

$$\begin{aligned} \sum_{i=1}^{n} d(v_i) \sum_{v_i \nsim v_j} X_j^2 &= \sum_{i=1}^{n} d(v_i) X_i^2 + \sum_{i=1}^{n} d(v_i) \sum_{\substack{v_i \nsim v_j \\ i \neq j}} X_j^2 \\ &\geq \sum_{i=1}^{n} d(v_i) X_i^2 + \sum_{i=1}^{n} \sum_{\substack{v_i \nsim v_j \\ i \neq j}} X_j^2 \\ &= \sum_{i=1}^{n} d(v_i) X_i^2 + \sum_{i=1}^{n} (n-1-d(v_i)) X_j^2 \\ &= n-1 \end{aligned} \tag{3.4}$$

Thus $F(D,D)^2 \sum_{i=1}^{n} d(v_i) \sum_{v_i \nsim v_j} X_j^2 \geq F(D,D)^2(n-1)$.
On substituting Equation 3.4 in Equation 3.3, we get

$$\mu_1^2 \sum_{i=1}^{n} X(i)^2 = \mu_1^2 \leq 2mF(D,D)^2 - F(D,D)^2(n-1)$$
$$\leq F(D,D)^2(2m-n+1)$$

Thus $\mu_p \leq F(D,D)\sqrt{2m-n+1}$.

In order for equality to hold in the Theorem, all the inequalities in the above arguments must be equalities, especially the ones in Equations 3.1 and 3.4. That is, $|(A_F^e(G))_i|^2 = d(v_i)F(D,D)^2$ and $\sum_{i=1}^{n} d(i) \sum_{v_i \nsim v_j} X_j^2 = n-1$. This is possible only when both of the following conditions hold:

1. $e(v_i) = D$ for all $1 \leq i \leq n$
2. $d(v_i) = (n-1)$ for all $1 \leq i \leq n$

That is, when the graph is complete.
Conversely, the extended adjacency matrix of a complete graph K_n is given by

$$A_F^e(K_n) = \begin{pmatrix} 0 & F(D,D) & F(D,D) & \dots & F(D,D) \\ F(D,D) & 0 & F(D,D) & \dots & F(D,D) \\ \dots & & & & \\ F(D,D) & F(D,D) & F(D,D) & \dots & 0 \end{pmatrix}$$

whose spectral radius can be found easily as $\mu_1 = (n-1)F(D,D)$. □

The next corollary is an immediate consequence.

Corollary 3.1 *Let G be a planar graph on $n \geq 5$ vertices with $A_F^e(G)$. Suppose μ_1 is the largest eigenvalue of $A_F^e(G)$, then*

$$\mu_1 \leq F(2,2)\sqrt{5n-11}.$$

Proof: Since $n \geq 5$, the diameter of G is at least 2. Further, it follows from the fact that $m \leq 3n-6$. □

4. Conclusions

Linear algebraic tools like the determinant, rank, eigenvalues, etc., play a crucial role in concluding the various topological properties of graphs. The current article deals with a special type of generalized extended adjacency matrices associated with graphs, which makes a substantial contribution to the field of spectral graph theory. The properties and parameters associated with this matrix are explored in this article. The expression for the determinant derived states that it depends on the number of elementary spanning subgraphs in it. This enables us to characterize the graphs with zero determinant, in turn, the ones with positive nullity. Various bounds for the largest eigenvalue in terms of parameters like the diameter, the number of edges and the topological index itself are derived.

References

1. West, D. B.: Introduction to Graph Theory(second edition). Prentice Hall (2000).
2. Nikolic, S., Trinajstic, N., *The Wiener index: Development and applications.* Croatica Chemica Acta. 68, 105–129, (1995).
3. Burch, K.J., *Chemical applications of graph theory.* In Mathematical Physics in Theoretical Chemistry. 261–294, (2019).
4. Islam, T.U., Mufti, Z.S., Ameen, A., Aslam, M.N. and Tabraiz, A., *On certain aspects of topological indices. Journal of Mathematics.* 2021, 9913529, (2021).

5. Sharma, V., Goswami, R. and Madan, A.K., *Eccentric Connectivity Index: A Novel Highly Discriminating Topological Descriptor for Structure-Property and Structure-Activity Studies.* The Journal for Chemical Information and Computer Scientists. 37, 273–282, (1997).

6. Dureja, H., Gupta, S., Madan, A.K., *Predicting anti-HIV-1 activity of 6-arylbenzonitriles: Computational approach using superaugmented eccentric connectivity topochemical indices.* Journal of Molecular Graphics and Modelling. 26, 1020–1029, (2008).

7. Gupta, S., Singh, M., Madan, A.K., *Eccentric distance sum: A novel graph invariant for predicting biological and physical properties.* Journal of Mathematical Analysis and Applications. 275, 386–401, (2002).

8. Padmapriya P., Veena Mathad, *Eccentricity-based topological indices of some graphs.* TWMS J. App. and Eng. Math. 10, 1084–1095, (2020).

9. Gul Ozkan Kizilirmak, *The eccentricity-based topological indices.* Acta Universitatis Sapientiae Informatica. 15, 294–305, (2023).

10. Balkishbanu Khaji, Shahistha Hanif, K Arathi Bhat, *Eccentricity-based topological indices of chain graphs.* IAENG International Journal of Applied Mathematics, 55, 1235–1241, (2025).

11. Kamel Jebreen, Hifza Iqbal, Muhammad Haroon Aftab, Iram Yaqoob, Mohammed Issa Sowaity, Amjad Barham, *Study of eccentricity-based topological indices for benzenoid structure.* South African Journal of Chemical Engineering. 45, 221–227, (2023).

12. Usman Babar, Asim Naseem, Hani Shaker, Mian Muhammad Zobair, Haidar Ali, *Eccentricity-Based Topological Descriptors of First Type of Hex-Derived Network.* Hindawi Journal of Chemistry. 2022, 3340057, (2023).

13. Yang, Y.Q., Xu, L. Hu, C.Y., *Extended adjacency matrix indices and their applications.* Journal of Chemical Information and Computer Sciences. 34, 1140–1145, (1994).

14. Modjtaba Ghorbani, Najaf Amraei, *A note on eigenvalue, spectral radius and energy of extended adjacency matrix, Extended adjacency matrix indices and their applications.* Discrete Applied Mathematics. 322, 102–116, (1994).

15. Modjtaba Ghorbani, Xueliang Li, Samaneh Zangi, Najaf Amraei, *On the eigenvalue and energy of extended adjacency matrix.* Applied Mathematics and Computation. 397, 125939, (2021).

16. Kinkar Ch. Das, Ivan Gutman, Boris Furtula, *On spectral radius and energy of extended adjacency matrix of graphs.* Applied Mathematics and Computation. 296, 116–123, (2017).

17. Ivan Gutman, Kinkar Ch. Das, Boris Furtula, *Extended energy and its dependence on molecular structure.* Canadian Journal of Chemistry. 95, 526–529, (2017).

18. Parikshit Das, Sourav Mondal, Biswajit Some, Anita Pal, *Extension of adjacency matrix in QSPR analysis.* Chemometrics and Intelligent Laboratory Systems. 243, 105024, (2023).

19. Balkishbanu Khaji, Shahistha Hanif, K Arathi Bhat, *Spectral properties of eccentricity sum matrix of graphs.* Communications in Combinatorics and Optimization (accepted).

20. Brouwer, A. E., Haemers, W. H., *Spectra of graphs.* Springer, New York (2011)

21. Alzer, H., *On the Cauchy-Schwarz inequality.* Journal of mathematical analysis and applications. 234, 6–14, (1999).

22. Bapat, R.B., *Graphs and matrices.* Springer, New York, (2010).

23. R. A. Horn, C. R. Johnson, *Matrix analysis. Cambridge University Press*, (2012).

24. Godsil, C., Royle, G.F., *Algebraic graph theory.* Springer Science and Business Media, (2001).

Balkishbanu khaji,
Manipal Institute of Technology,
Manipal Academy of Higher Education,
Manipal, India.
E-mail address: balkishbanu.dscmpl2023@learner.manipal.edu

and

Shahistha Hanif,
* *Corresponding author,*
Manipal Institute of Technology,
Manipal Academy of Higher Education,
Manipal, India.
E-mail address: shahistha.hanif@manipal.edu

and

K. Arathi Bhat,
Manipal Institute of Technology,
Manipal Academy of Higher Education,
Manipal, India.
E-mail address: arathi.bhat@manipal.edu