



QUALITATIVE, STATISTICAL, AND EXTREME PROPERTIES OF SPECTRAL INDICES OF SIGNABLE PSEUDO-INVERTIBLE GRAPHS*

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Abstract. In this paper, we investigate the Moore-Penrose inversion of a simple connected graph. We analyze qualitative, statistical, and extreme properties of spectral indices of signable pseudo-invertible graphs. We introduce and analyze a wide class of signable pseudo-invertible simple connected graphs. It is a generalization of the classical concept of positively integrally invertible graphs due to Godsil. We present several constructions of signable pseudo-invertible graphs. We also discuss statistical properties of various spectral indices of the class of signable pseudo-invertible graphs.

Key words. Pseudo-invertible graph; Signability of Moore-Penrose inverse matrix; Signable pseudo-invertible graph; Spectral index of a graph.

AMS subject classifications. 05C50, 05B20, 05C22, 15A09, 15A18, 15B36.

1. Introduction. In this paper, we investigate a class of signable pseudo-invertible graphs. A graph is called signable pseudo-invertible if the Moore-Penrose inverse matrix of its adjacency matrix can be signed to a matrix containing elements of the same sign. Recall that inversion of an adjacency matrix does not need to define a graph again because it may contain both positive and negative elements (see Harari and Minc [23]). To overcome this difficulty, Godsil [21] introduced the concept of positively integrally invertible graphs by defining a graph to be invertible if the inverse of its non-singular adjacency matrix is integral and diagonally similar (cf. Zaslavski [43]) to a non-negative integral matrix representing the adjacency matrix of the inverse graph in which positive labels determine edge multiplicities. In the series of papers [32, 33], Pavlíková and Ševčovič extended this notion to a broader class of graphs by introducing the concept of negative invertibility of a graph. Both positively and negatively invertible graphs have the appealing property that inverting an inverse graph gives back the original graph. Related results, including a unifying approach to inverting graphs, were proposed in a recent survey paper by McLeman and McNicholas [28] focusing on the inverses of bipartite graphs and the diagonal similarity to non-negative matrices. For other results on graph inverses based on Godsil's ideas, we refer to Akbari and Kirkland [2], Kirkland and Tifenbach [25], and Bapat and Ghorbani [4] (see also [5]). Ye *et al.* [42] investigated graph inverses in the context of median eigenvalues. In [41], Tifenbach investigated a class of graphs whose adjacency matrices are non-singular with integral inverses and strongly self-dual graphs. Pavlíková [31] developed constructive methods to generate invertible graphs by the method of edge overlapping. Our main purpose is to extend and investigate the concept of positive and negative invertibility of a graph due to Godsil [21], Pavlíková, and Ševčovič [32] to the case when its adjacency matrix is not invertible but its Moore-Penrose inverse matrix is still signable to a matrix containing elements of the same sign. Such a signed Moore-Penrose inverse matrix can represent a weighted graph with non-negative weights.

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In applications including chemistry, biology, or statistics, various spectral indices of graphs representing the structure of organic molecules or transition diagrams for finite Markov chains play an important role (cf. Cvetković [14, 16], Brouwer, and Haemers [8] and references therein). All of them are related to various graph energies and spectral indices, which are characterized by means of eigenvalues of the adjacency matrix of a graph. Recall that the sum of absolute values of eigenvalues is called the matching energy index Λ^{pow} (cf. Chen and Jinfeng [11]), the maximum of absolute values of the least positive and largest negative eigenvalue is known as the HOMO-LUMO index Λ^{ind} (see Mohar [30], Jaklić *et al.* [24], Fowler *et al.* [20]), their difference is the HOMO-LUMO separation gap Λ^{gap} (cf. Gutman and Rouvray [22]). Regarding Aihara [1], a larger HOMO-LUMO gap implies higher kinetic stability and lower chemical reactivity of a molecule. According to Bacalis and Zdetsis [3] the spectral separation gap Λ^{gap} generally decreases with the number of vertices of the structural graph. The spectral indices Λ^{gap} and Λ^{ind} are closely related to the Moore-Penrose (group) inverse matrix A^\dagger of the adjacency matrix A of a given graph G^A . Following Pavlíková and Ševčovič [32, 33], we have

$$\Lambda^{gap}(A) = \lambda_{max}(A^\dagger)^{-1} - \lambda_{min}(A^\dagger)^{-1}, \quad \Lambda^{ind}(A) = \max(\lambda_{max}(A^\dagger)^{-1}, -\lambda_{min}(A^\dagger)^{-1}),$$

where $\lambda_{max}(A^\dagger)$, $\lambda_{min}(A^\dagger)$ are the maximal and minimal eigenvalues of A^\dagger . As a consequence, properties of maximal and minimal eigenvalues of the pseudo-inverse graph can be used to analyze the spectral indices Λ^{gap} and Λ^{ind} of the graphs.

Recently, McDonald, Raju, and Sivakumar [29] studied the Moore-Penrose (group) inverses of adjacency matrices associated with certain graph classes. They derived formulae for the Moore-Penrose inverses of matrices that are associated with a class of digraphs obtained from stars. This new class contains both bipartite and non-bipartite graphs. A representation of the Moore-Penrose inverse matrix corresponding to the Dutch windmill graph has been derived by McDonald *et al.* [29]. In [34], Pavlíková and Širáň constructed a pseudo-inverse of a weighted tree in terms of maximal matchings and alternating paths.

The maximum and minimal eigenvalues of the pseudo-inverse graph can be used to determine the spectral indices Λ^{gap} and Λ^{ind} (see also Pavlíková and Ševčovič [31, 32, 33]).

The objective of this paper is two-fold. In Section 2, we introduce and investigate the wide class of signable pseudo-invertible simple connected graphs. Section 3 is devoted to computational and statistical results on this class of graphs. More precisely, in Section 2 we introduce the notion of positive/negative/positive and negative pseudo-invertible graphs, which is based on the signability of the Moore-Penrose inverse matrix A^\dagger of the adjacency matrix A corresponding to a graph G^A . The signed Moore-Penrose inverse matrix A^\dagger defines a weighted graph $(G^A)^\dagger$. We investigate special classes of cycle and path graphs. We completely characterize which cycle and path graphs admit signable pseudo-inversion. We show that the complete graph K_m is signable pseudo-invertible only for order $m = 2$. Furthermore, we show that the complete multipartitioned graphs K_{m_1, \dots, m_k} are signable pseudo-invertible only for $k = 2$. Furthermore, we introduce and analyze a novel concept of $G^{\mathcal{A}}$ -complete multipartitioned graph which is constructed from the original labeled graph $G^{\mathcal{A}}$ by replacing a vertex i with the set of m_i vertices and connecting them with the set of m_j vertices iff $\mathcal{A}_{ij} = 1$. It can be viewed as a natural generalization of a complete multipartitioned graph. In Section 3, we discuss statistical properties of the class of signable pseudo-invertible graphs. We focus on maximal and minimal eigenvalues, as well as spectral indices Λ^{gap} , Λ^{ind} , and Λ^{pow} . In general, we present results for the order $m \leq 10$ although some properties of extreme eigenvalues and indices hold for a general order m . Our descriptive statistical results are based on the complete list of simple connected graphs provided by McKay [27] (see also [7]) for orders $m \leq 10$ in combination of a survey of signable pseudo-invertible graphs due to Pavlíková and Ševčovič [35].

2. Signable pseudo-invertible graphs. Let $G = (V, E)$ be an undirected connected graph with the set of m vertices V and the set of edges E . The graph G may contain loops, and its edges can be weighted.

By A_G we denote its symmetric adjacency matrix that contains non-negative elements. On the contrary, if A is a non-negative symmetric matrix, then G^A denotes the graph with the adjacency matrix A .

The spectrum $\sigma(G^A)$ of a graph G^A consists of eigenvalues $\lambda_{min} \equiv \lambda_m \leq \dots \leq \lambda_1 \equiv \lambda_{max}$ of its symmetric adjacency matrix A_G , that is $\sigma(G^A) = \sigma(A_G)$, (cf. Cvetković *et al.* [13, 16]). Notice that the diagonal of an adjacency matrix A representing a simple graph is zero, and so its trace is zero. As a consequence, we have $\lambda_{min}(A) < 0 < \lambda_{max}(A)$ where $\lambda_{min}(A), \lambda_{max}(A)$ are minimal and maximal eigenvalues of A , respectively.

If K is an $n \times m$ real matrix, then its Moore-Penrose inverse matrix is an $m \times n$ matrix K^\dagger that is uniquely determined by the following identities (see Ben-Israel and Greville [6]):

$$(2.1) \quad (KK^\dagger)^T = KK^\dagger, \quad (K^\dagger K)^T = K^\dagger K, \quad KK^\dagger K = K, \quad K^\dagger K K^\dagger = K^\dagger.$$

In the case when A is an $m \times m$ real symmetric matrix, Moore-Penrose can be constructed explicitly in the following way: Let \mathcal{P} be an orthogonal matrix such that $\mathcal{P}A\mathcal{P}^T = \Lambda = \text{diag}(\lambda_1, \dots, \lambda_m)$, where $\lambda_i, i = 1, \dots, m$, are real eigenvalues of the symmetric square matrix A .

Given a number $\lambda \in \mathbb{R}$, its Moore-Penrose inverse is as follows: $\lambda^\dagger = 0$ when $\lambda = 0$ and $\lambda^\dagger = 1/\lambda$, otherwise.

Then, the Moore-Penrose inverse matrix A^\dagger that satisfies the axioms (2.1) is given uniquely by $A^\dagger = \mathcal{P}^T \Lambda^\dagger \mathcal{P}$ where $\Lambda^\dagger = \text{diag}(\lambda_1^\dagger, \dots, \lambda_m^\dagger)$.

The Moore-Penrose inverse A^\dagger of a real symmetric square matrix A is also known as the group inverse of A . Note that the concept of a Moore-Penrose matrix inversion is more general than a matrix inversion. If a square symmetric matrix A is invertible, then it is also Moore-Penrose invertible and $A^\dagger = A^{-1}$.

DEFINITION 2.1. *Let A be a real symmetric matrix. Its Moore-Penrose inverse matrix A^\dagger is called positively (negatively) signable if there exists a diagonal ± 1 signature matrix D such that the matrix $DA^\dagger D$ contains non-negative (nonpositive) elements only.*

DEFINITION 2.2. *An undirected weighted graph G^A is called positively (negatively) pseudo-invertible if the Moore-Penrose inverse matrix A^\dagger is a positively (negatively) signable matrix. If D is the corresponding signature matrix, the undirected pseudo-inverse graph $(G^A)^\dagger$ is defined by the weighted non-negative symmetric adjacency matrix $DA^\dagger D$, if A^\dagger is positively signable ($-DA^\dagger D$, if A^\dagger is negatively signable). A graph G^A is called signably pseudo-invertible if it is positively or negatively pseudo-invertible.*

In general, the symmetric Moore-Penrose inverse matrix A^\dagger may contain non-integral elements (including its diagonal elements). The pseudo-inverse graph $(G^A)^\dagger$ is a uniquely defined undirected nonsimple graph containing weighted loops even if the graph G^A is a simple graph.

Note that the pseudo-inverse graph $(G^A)^\dagger$ is defined by the non-negative weighted adjacency matrix $DA^\dagger D$ ($-DA^\dagger D$). The matrix $(DA^\dagger D)^\dagger$ is signable by the same signature matrix and $D(DA^\dagger D)^\dagger D = DD(A^\dagger)^\dagger DD = A$. One can proceed similarly if G^A is a negatively pseudo-invertible graph. As a consequence, we obtain

$$(G^\dagger)^\dagger = G.$$

It means that inverting an inverse graph gives the original graph. Furthermore, it is easy to verify by a simple contradiction argument that the weighted pseudo-inverse graph is connected, provided that the original graph is connected.

Examples of simple connected graphs on five vertices and their weighted pseudo-invertible graphs with loops are shown in Fig. 1.

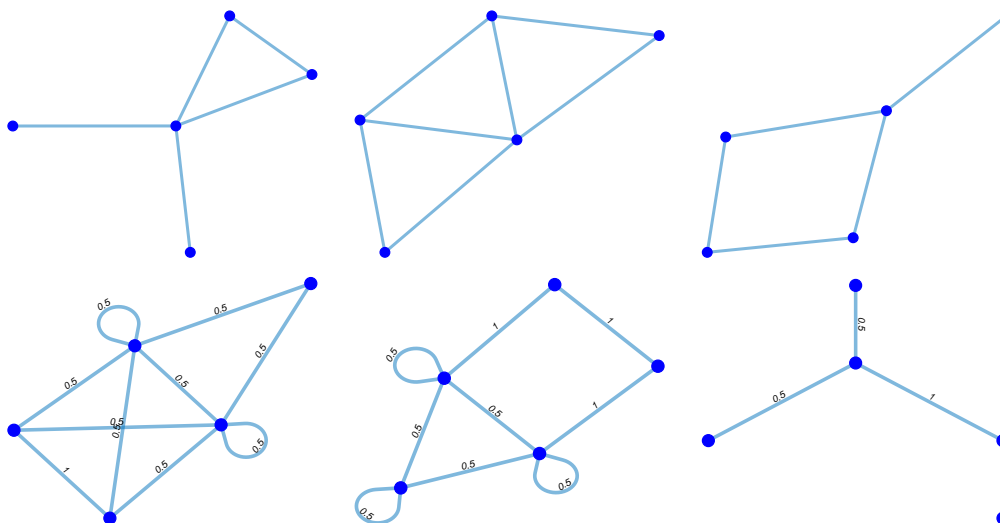


FIGURE 1. Top row: examples of a positively (left), negatively (middle), positively and negatively (right) pseudo-invertible graphs on $m = 5$ vertices. Bottom row: corresponding weighted pseudo-inverse graphs.

The explicit form of the Moore-Penrose (group) inverse of tridiagonal circulant matrices has been derived, e.g., by Encinas, Carmona *et al.* [10, 19] and references therein. To our knowledge, the signability of the Moore-Penrose inverse matrix of a circulant or tridiagonal matrix has not been investigated so far. In the next proposition, we analyze positive/negative pseudo-invertibility of cycle C_m and path P_m graphs on m vertices.

PROPOSITION 2.3. *Let C_m be a cycle graph of order m , $m \geq 3$. The graph C_m is neither positively nor negatively pseudoinvertible for $m \neq 4$. The bipartite graph C_4 is positively and negatively pseudo-invertible. Path graphs P_m are integrally positively and negatively invertible bipartite graphs for any even order m . The path graph P_3 is positively and negatively pseudo-invertible. The path graph P_m is neither positively nor negatively pseudo-invertible for any odd degree $m \neq 3$.*

Proof. There are several papers dealing with the form of the Moore-Penrose inverse matrix to the adjacency matrix of a circular graph C_m (see Sivakumar and Nandi [39], and references therein). Here, we present the approach taking into account the circulant form of the adjacency matrix. Notice that the adjacency matrix A has the form of a circular Toeplitz matrix, $A_{ij} = a_{i-j}$, $i, j = 1, \dots, m$, where a_p , $p \in \mathbb{Z}$, is an m -periodic sequence such that $a_{m-p} = a_{-p} = a_p$, $a_1 = a_{-1} = a_{m-1} = 1$, and $a_p = 0$ for $p \neq \pm 1, m-1, -m+1$. The Moore-Penrose inverse matrix A^\dagger can be searched again in the form of a circular Toeplitz matrix, $A^\dagger_{ij} = a^\dagger_{i-j}$, $i, j = 1, \dots, m$. Taking into account the form of the sequence a_p , $p \in \mathbb{Z}$, it is straightforward to verify that A^\dagger satisfies the Moore-Penrose axioms provided that $\sum_{p=1}^m (a_{s-p-1} + a_{s-p+1})a_p^\dagger = a_s$, for each $s = 1, \dots, m$. Calculating the solution of this equation and taking into account the fact $a_p^\dagger = a_{-p}^\dagger = a_{m-p}^\dagger$, we obtain:

- if $m \equiv 0 \pmod{4}$, then $a_p^\dagger = \frac{1}{m} \left(\frac{m}{2} - |p|\right) (-1)^{\frac{|p|-1}{2}}$ for p odd, $a_p^\dagger = 0$ for p even;
- if $m \not\equiv 0 \pmod{4}$, then $a_p^\dagger = \frac{1}{2}(-1)^{\frac{|p|-1}{2}}$ for p odd. For p even, we have:
 $a_p^\dagger = \frac{1}{2}(-1)^{\frac{|p|}{2}}$, if $m \equiv 1 \pmod{4}$; $a_p^\dagger = 0$, if $m \equiv 2 \pmod{4}$; $a_p^\dagger = \frac{1}{2}(-1)^{\frac{|p|}{2}+1}$, if $m \equiv 3 \pmod{4}$.

Note that $a_1^\dagger = 1/2$, and $a_3^\dagger = -1/2$ for any order $m \neq 4$. Assume that the cycle graph C_m is positively pseudo-invertible. Then, there exists a signature matrix $D = \text{diag}(d_1, \dots, d_m)$ signing A^\dagger to a non-negative matrix. Without loss of generality, we may assume $d_1 = 1$. Then, $d_{i+1}A_{i+1,i}^\dagger d_i = d_{i+1}a_1^\dagger d_i \geq 0$. Since $a_1^\dagger > 0$, then $d_2 > 0$, and subsequently $d_p = 1$, for $p = 2, \dots, m$, that is, $D = I$. As the matrix A^\dagger contains both positive and negative elements for $m \neq 4$, we conclude that A^\dagger is not positively signable for $m \neq 4$. Similarly, assuming A^\dagger is negatively signable matrix, i.e., $DA^\dagger D \leq 0$, by the signature matrix D leads to the conclusion $D = \text{diag}(1, -1, 1, \dots, (-1)^{m+1})$. For $m \geq 5$, we have $d_1A_{14}^\dagger d_4 = d_1a_3^\dagger d_4 = (-1/2)(-1) > 0$, a contradiction. For the triangle C_3 of order $m = 3$, we have $d_3A_{31}^\dagger d_1 = A_{31}^\dagger = a_2^\dagger = 1/2$, a contradiction. For $m = 4$, the matrix A^\dagger is proportional to the adjacency matrix A of the cycle graph C_4 . It is positively signable by the diagonal matrix $D = \text{diag}(1, 1, 1, 1)$ and negatively signable by the signature matrix $D = \text{diag}(1, -1, 1, -1)$. Hence, C_4 is the only signable cycle graph. It is positively and negatively signable.

The path graph P_m has the tridiagonal adjacency matrix A where $A_{ij} = 1$ for $|i - j| = 1$, and $A_{ij} = 0$, otherwise. It follows from the general results on the inverses of tridiagonal Toeplitz matrices due to Da Fonseca and Petronilho [17, Corollary 4.2, Section 3] that the Toeplitz matrix A is invertible for any even order m , and $\det(A) = (-1)^{\frac{m}{2}}$. Furthermore, for $i \leq j$, and m even we have

$$(A^{-1})_{ij} = (A^{-1})_{ji} = \begin{cases} 0, & \text{if } i \text{ is even, or } j \text{ is odd,} \\ 1, & \text{if } i + j \equiv 1 \pmod{4}, i \text{ is odd, and } j \text{ is even,} \\ -1, & \text{if } i + j \equiv 3 \pmod{4}, i \text{ is odd, and } j \text{ is even.} \end{cases}$$

For $i \leq j$, and m odd we have

$$(A^\dagger)_{ij} = (A^\dagger)_{ji} = (-1)^{\frac{j-i-1}{2}} \begin{cases} 0, & \text{if } i + j \text{ is even,} \\ \frac{i}{m+1}, & \text{if } i \text{ is even, } j \text{ is odd,} \\ \frac{m-j+1}{m+1}, & \text{if } i \text{ is odd, } j \text{ is even.} \end{cases}$$

If the order m is even, then the matrix A^{-1} is positively signable by the diagonal signature matrix $D = \text{diag}(d_1, \dots, d_m)$ where $d_i = 1$ for $i \equiv 1$, or $i \equiv 2 \pmod{4}$, and $d_i = -1$ for $i \equiv 3$, or $i \equiv 4 \pmod{4}$. It is also negatively signable $DA^{-1}D \leq 0$ by the signature matrix D where $d_i = 1$ for $i \equiv 1$, or $i \equiv 4 \pmod{4}$ and $d_i = -1$ for $i \equiv 2$, or $i \equiv 3 \pmod{4}$. That is, the path graph P_m is positively and negatively integrally invertible bipartite graph for any even order m .

For the order $m = 3$, we have $A^\dagger = \frac{1}{2}A$. Therefore, the path P_3 is positively and negatively pseudo-invertible bipartite graph. On the other hand, if $m \geq 5$ is odd, then A^\dagger is neither positively nor negatively signable. In fact, suppose that A^\dagger is positively signable by the signature matrix D . As $(A^\dagger)_{i,i+1} > 0$, $(A^\dagger)_{i,i+3} < 0$, we have $d_1d_2 > 0$, $d_2d_3 > 0$, $d_3d_4 > 0$, but $d_1d_4 < 0$, a contradiction. A similar argument shows that A^\dagger cannot be a negatively signable matrix. \square

For the order $k = 2$, the complete graph K_2 is just the simple path graph P_2 which is a positive and negative integrally invertible graph. It is the only example of a simple connected graph that is self-invertible $K_2^{-1} \cong K_2$ (cf. Harary and Minc [23]). On the other hand, the complete graph K_k , $k \geq 3$ is neither positive nor negatively pseudo-invertible.

PROPOSITION 2.4. *The complete graph K_k of order $k \geq 3$ has an invertible adjacency matrix \mathcal{A} , but it is neither positively nor negatively Moore-Penrose invertible.*

Proof. The adjacency matrix \mathcal{A} of the complete graph $G^{\mathcal{A}} = K_k$ and its inverse matrix \mathcal{A}^{-1} have the form:

$$\mathcal{A} = \mathbf{1}\mathbf{1}^T - I = (\alpha_{ij})_{i,j=1,\dots,k}, \quad \mathcal{A}^{-1} = \frac{1}{k-1}\mathbf{1}\mathbf{1}^T - I,$$

where $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^k$, and $\alpha_{ii} = 0, \alpha_{ij} = 1$ for $i \neq j$. Let $\mathcal{D} = \text{diag}(d_1, \dots, d_k)$ be a signature matrix. Then, inspecting the diagonal terms of $\mathcal{D}\mathcal{A}^{-1}\mathcal{D}$ we conclude $(\mathcal{D}\mathcal{A}^{-1}\mathcal{D})_{ii} = (1/(k-1) - 1)(d_{ii})^2 < 0$. Therefore, $G^{\mathcal{A}}$ cannot be positively pseudo-invertible. On the other hand, the matrix \mathcal{A}^{-1} contains positive off-diagonal and negative diagonal entries. Therefore, any signature matrix \mathcal{D} that signs \mathcal{A}^{-1} to a non-positive matrix should have two elements $d_{i'}$ and $d_{j'}$ of the same sign, $i' \neq j'$. Then, $(\mathcal{D}\mathcal{A}^{-1}\mathcal{D})_{i'j'} = d_{i'}(\mathcal{A}^{-1})_{i'j'}d_{j'} > 0$, a contradiction. Therefore, $G^{\mathcal{A}} = K_k$ is neither positively nor negatively pseudo-invertible graph, as claimed. \square

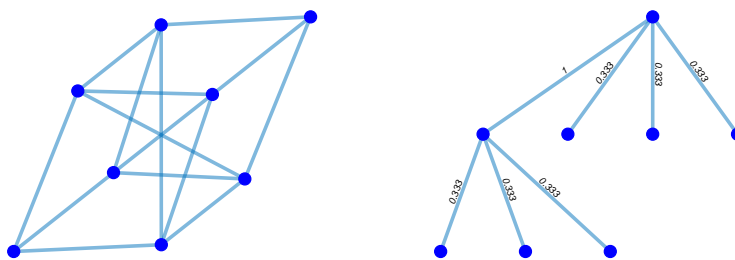


FIGURE 2. *The uncomplete positively and negatively pseudoinvertible bipartite graph $K_{m,m}^-$ with $m = 4$ (left) and its pseudo-inverse weighted graph $(K_{m,m}^-)^\dagger$ (right).*

In the next proposition, we show that the complete bipartite graph K_{m_1,m_2} of the order $m = m_1 + m_2$ is positively and negatively pseudo-invertible. Notice that $K_{m-1,1} = S_m$ is just the star graph and $K_{2,2} = C_4$ is the cycle graph.

PROPOSITION 2.5. *The complete multipartitioned graph K_{m_1,m_2} of the order $m = m_1 + m_2$ is positively and negatively pseudo-invertible. The pseudo-inverse graph $(K_{m_1,m_2})^\dagger$ is the weighted bipartite graph K_{m_1,m_2} with all weights equal to $1/(m_1m_2)$.*

Proof. Let \mathcal{E}_{m_1,m_2} be an $m_1 \times m_2$ matrix consisting of ones. It is easy to verify that $(\mathcal{E}_{m_1,m_2})^\dagger = (1/(m_1m_2))\mathcal{E}_{m_2,m_1}$. Therefore, the adjacency matrix A of the graph K_{m_1,m_2} and its Moore-Penrose inverse matrix A^\dagger have the form

$$A = \begin{pmatrix} 0 & \mathcal{E}_{m_1,m_2} \\ (\mathcal{E}_{m_1,m_2})^T & 0 \end{pmatrix}, \quad A^\dagger = \frac{1}{m_1m_2} \begin{pmatrix} 0 & \mathcal{E}_{m_1,m_2} \\ (\mathcal{E}_{m_1,m_2})^T & 0 \end{pmatrix} = \frac{1}{m_1m_2}A.$$

The matrix A^\dagger is positively (negatively) signable by the signature matrix $D = \text{diag}(I, I)$ ($D = \text{diag}(I, -I)$). The proof of the proposition follows. \square

Let us denote by $K_{m,m}^-$ the noncomplete bipartite graph constructed from the complete bipartite graph $K_{m,m}$ by deleting exactly one edge. In [36], Pavlíková, Ševčovič, and Širáň showed that its spectrum consists of $2m-4$ zeros and four real eigenvalues $\lambda^{\pm,\pm} = \pm(1 - m \pm \sqrt{m^2 + 2m - 3})/2$. In the following proposition, we will prove the positive and negative pseudo-invertibility of $K_{m,m}^-$, and we completely characterize the pseudo-inverse weighted graph $(K_{m,m}^-)^\dagger$.

PROPOSITION 2.6. *The bipartite noncomplete graph $K_{m,m}^{-e}$ is positively and negatively pseudo-invertible. The pseudo-inverse graph $(K_{m,m}^{-e})^\dagger$ is the weighted graph consisting of two star graphs S_m having edge weights equal to $1/(m-1)$ and connected through the central vertices by an edge with unit weight.*

Proof. Without loss of generality, we may assume that the adjacency matrix A of the graph $K_{m,m}^{-e}$ has the form

$$A = \begin{pmatrix} 0 & K \\ K^T & 0 \end{pmatrix}, \quad K = \mathbf{1}\mathbf{1}^T - e_1 e_1^T,$$

where $\mathbf{1} = (1, \dots, 1)^T$, $e_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^m$. It is straightforward to verify that the Moore-Penrose inverse A^\dagger has the form

$$(2.2) \quad A^\dagger = \begin{pmatrix} 0 & (K^\dagger)^T \\ K^\dagger & 0 \end{pmatrix}, \quad K^\dagger = \frac{1}{m-1} (e_1 \mathbf{1}^T + \mathbf{1} e_1^T - (m+1)e_1 e_1^T).$$

Clearly, if $D_+ = \text{diag}(-1, 1, \dots, 1)$, and $D_- = \text{diag}(1, -1, \dots, -1)$, then the matrix $D_+ K^\dagger D_-$ contains non-negative elements only. Therefore, $DA^\dagger D \geq 0$ where $D = \text{diag}(D_+, D_-)$. Thus, the graph $G^A = K_{m,m}^{-e}$ is positively pseudo-invertible. If we take the signature matrix $D = \text{diag}(D_+, -D_-)$, then $DA^\dagger D \leq 0$. As a consequence, the graph $K_{m,m}^{-e}$ is also negatively pseudo-invertible.

Finally, $(K^\dagger)_{11} = -1$, and $(K^\dagger)_{1j} = (K^\dagger)_{i1} = 1/(m-1)$ for $i, j \neq 1$. Therefore, the pseudo-inverse graph $(K_{m,m}^{-e})^\dagger$ is the weighted graph consisting of two star graphs S_m having edge weights equal to $1/(m-1)$ and connected through the central vertices by an edge with unit weight (see Fig. 2). \square

The spectrum of a complete multipartitioned graph K_{m_1, \dots, m_k} has been investigated by Delorme [18] (see also S. Pavlíková, D. Ševčovič, J. Širáň [36]). In what follows, we propose a novel concept of $G^{\mathcal{A}}$ -complete multipartitioned graph denoted by $G_{m_1, \dots, m_k}^{\mathcal{A}}$. It is a natural generalization of a complete multipartitioned graph K_{m_1, \dots, m_k} . If $G^{\mathcal{A}} = K_k$ is the complete graph, then $G_{m_1, \dots, m_k}^{\mathcal{A}}$ is just the complete multipartitioned graph K_{m_1, \dots, m_k} .

DEFINITION 2.7. *Let $G^{\mathcal{A}}$ be a simple connected vertex labeled graph of the order k with an adjacency matrix \mathcal{A} , and vertex labels $\{1, \dots, k\}$. Assume $m_1, \dots, m_k \geq 1$. We denote by $G_{m_1, \dots, m_k}^{\mathcal{A}}$ the $G^{\mathcal{A}}$ -complete multipartitioned vertex labeled graph of the order $m = m_1 + \dots + m_k$, constructed as follows: Each vertex i of $G^{\mathcal{A}}$ is replaced by the set V_i of m_i vertices. Each vertex of V_i is connected to every vertex of V_j provided there is an edge connecting the vertex i and j in the original graph $G^{\mathcal{A}}$, that is, $\mathcal{A}_{ij} = 1$.*

An example is shown in Figure 3.

PROPOSITION 2.8. *Let $G^{\mathcal{A}}$ be a simple connected vertex labeled graph of the order k with an adjacency matrix \mathcal{A} , and vertex labels $\{1, \dots, k\}$. Assume $m_1, \dots, m_k \geq 1$. Let $G_{m_1, \dots, m_k}^{\mathcal{A}}$ be the $G^{\mathcal{A}}$ -complete multipartitioned graph of order $m = m_1 + \dots + m_k$. Then*

- (i) *its spectrum $\sigma(G_{m_1, \dots, m_k}^{\mathcal{A}})$ consists of the zero eigenvalue with multiplicity $m - k$ and all eigenvalues of the $k \times k$ matrix $\mathcal{M}^{1/2} \mathcal{A} \mathcal{M}^{1/2}$ where $\mathcal{M} = \text{diag}(m_1, \dots, m_k)$.*
- (ii) *The Moore-Penrose inverse matrix $(\mathcal{M}^{1/2} \mathcal{A} \mathcal{M}^{1/2})^\dagger$ is positively (negatively) signable iff the graph $G_{m_1, \dots, m_k}^{\mathcal{A}}$ is positively (negatively) pseudo-invertible.*
- (iii) *Suppose that the adjacency matrix \mathcal{A} is invertible. Then, the graph $G^{\mathcal{A}}$ is positively (negatively) invertible iff the graph $G_{m_1, \dots, m_k}^{\mathcal{A}}$ is positively (negatively) pseudo-invertible.*

Proof. The adjacency matrix A of $G_{m_1, \dots, m_k}^{\mathcal{A}}$ has the block form $A = (\alpha_{ij} \mathcal{E}_{m_i, m_j})_{i, j=1, \dots, k}$ where the elements α_{ij} form the adjacency matrix $\mathcal{A} = (\alpha_{ij})_{i, j=1, \dots, k}$ of the underlying graph $G^{\mathcal{A}}$, and \mathcal{E}_{m_i, m_j} is the $m_i \times m_j$ matrix consisting of ones.

To prove (i), the vector $x = (x^{(1)}, \dots, x^{(k)}) \in \mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_k} \equiv \mathbb{R}^m$, where $x^{(i)} \in \mathbb{R}^{m_i}$, is an eigenvector of the adjacency matrix A , that is, $Ax = \lambda x$, iff $\sum_{j=1}^k \alpha_{ij} \xi_j = \lambda x_p^{(j)}$ for each $p = 1, \dots, m_i$, and $i = 1, \dots, k$, where $\xi_j = \sum_{p=1}^{m_j} x_p^{(j)} = m_j x_1^{(j)}$, that is, $x_1^{(i)} = x_2^{(i)} = \dots = x_{m_j}^{(i)}$. As $x \neq 0$, we have $\xi \neq 0$. Therefore, the non-trivial vector $\xi \in \mathbb{R}^k$ is a solution to the linear system of equations $\sum_{j=1}^k \alpha_{ij} m_j \xi_j = \lambda \xi_i$ for $i = 1, \dots, k$. That is, $\lambda \in \sigma(\mathcal{A}\mathcal{M}) = \sigma(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})$, as claimed in part (i).

We search the Moore-Penrose inverse matrix A^\dagger in block matrix form $A^\dagger = (\beta_{ij} \mathcal{E}_{m_i, m_j})_{i,j=1, \dots, k}$ where the elements β_{ij} form the symmetric matrix $\mathcal{B} = (\beta_{ij})_{i,j=1, \dots, k}$. Since $\mathcal{E}_{m_i, m_p} \mathcal{E}_{m_p, m_j} = m_p \mathcal{E}_{m_i, m_j}$, we have

$$AA^\dagger = ((\mathcal{A}\mathcal{M}\mathcal{B})_{ij} \mathcal{E}_{m_i, m_j})_{i,j=1, \dots, k}, \quad A^\dagger A = ((\mathcal{B}\mathcal{M}\mathcal{A})_{ij} \mathcal{E}_{m_i, m_j})_{i,j=1, \dots, k},$$

where $\mathcal{M} = \text{diag}(m_1, \dots, m_k)$. Taking $\mathcal{B} = \mathcal{M}^{-1/2}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger \mathcal{M}^{-1/2}$, we obtain

$$AA^\dagger = (AA^\dagger)^T = \left((\mathcal{M}^{-1/2}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger \mathcal{M}^{-1/2})_{ij} \mathcal{E}_{m_i, m_j} \right)_{i,j=1, \dots, k}.$$

Now, it is easy to verify $AA^\dagger A = A$, $A^\dagger AA^\dagger = A^\dagger$, and so A^\dagger is indeed the Moore-Penrose inverse of the adjacency matrix A .

In order to prove statement (ii), let us assume that the graph $G_{m_1, \dots, m_k}^{\mathcal{A}}$ is a positively (negatively) pseudo-invertible graph. Then, there exists a $m \times m$ diagonal signature matrix:

$$(2.3) \quad D = \text{diag}(d_1^{(1)}, \dots, d_{m_1}^{(1)}, \dots, \dots, d_1^{(k)}, \dots, d_{m_k}^{(k)})$$

such that $DA^\dagger D \geq 0$ (≤ 0). Let $\mathcal{D} = \text{diag}(d_1^{(1)}, \dots, d_1^{(k)})$ be the $k \times k$ signature diagonal matrix. Since $A^\dagger = (\beta_{ij} \mathcal{E}_{m_i, m_j})_{i,j=1, \dots, k}$, then $\mathcal{D}\mathcal{B}\mathcal{D} \geq 0$ (≤ 0) where $\mathcal{B} = (\beta_{ij})_{i,j=1, \dots, k} = \mathcal{M}^{-1/2}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger \mathcal{M}^{-1/2}$. As $\mathcal{D}\mathcal{M}^{-1/2} = \mathcal{M}^{-1/2}\mathcal{D}$, and $\mathcal{M}^{-1/2} > 0$, the matrix $\mathcal{D}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger \mathcal{D}$ has the same sign of elements as the matrix \mathcal{B} we conclude that Moore-Penrose inverse matrix $(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger$ is positively (negatively) signable. On the contrary, if the Moore-Penrose inverse matrix $(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger$ is positively (negatively) signable, then the matrix \mathcal{A}^\dagger is signable to a non-negative (nonpositive) matrix by a signature matrix $\mathcal{D} = \text{diag}(d^1, \dots, d^k)$. Then, the matrix A^\dagger is signable to a positive (negative) matrix by the signature matrix of the form (2.3) with $d_j^{(i)} = d^i$ for $j = 1, \dots, m_i$, $i = 1, \dots, k$, and the proof follows.

To prove (iii), we suppose that the matrix \mathcal{A} is invertible. Since the diagonal matrices \mathcal{D} and $\mathcal{M}^{1/2}$ commute, we have $\mathcal{D}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger \mathcal{D} = \mathcal{D}(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^{-1} \mathcal{D} = \mathcal{M}^{-1/2} \mathcal{D} \mathcal{A}^{-1} \mathcal{D} \mathcal{M}^{-1/2}$. It means that the matrix $(\mathcal{M}^{1/2}\mathcal{A}\mathcal{M}^{1/2})^\dagger$ is positively (negatively) signable if and only if the graph $G^{\mathcal{A}}$ is positively (negatively) pseudo-invertible. The rest of the proof of (iii) now follows from part (ii). \square

PROPOSITION 2.9. *The complete multipartitioned graph K_{m_1, \dots, m_k} of the order $m = m_1 + \dots + m_k$, where $k \geq 3$ is neither positively nor negatively pseudo-invertible. If $k < m$, then the adjacency matrix A is singular.*

Proof. With regard to Proposition 2.4, the complete graph K_k , $k \geq 3$, is neither positively nor negatively pseudo-invertible. Its adjacency matrix \mathcal{A} is invertible. The rest of the proof now follows from Proposition 2.8, part (iii).

DEFINITION 2.10. *Let G^A be a simple connected graph of order m with an adjacency matrix A . We say that the graph G^A is homothetically self-pseudo-invertible iff G^A is a signable pseudo-invertible graph, and $(G^A)^\dagger \sim G^A$. i.e., there exists $\kappa \in \mathbb{R}$ and a permutation matrix P of order m such that $DA^\dagger D = \kappa PAP^T$ where D is the signature matrix such that $DA^\dagger D$ (or $-DA^\dagger D$) is the adjacency matrix of G^\dagger .*

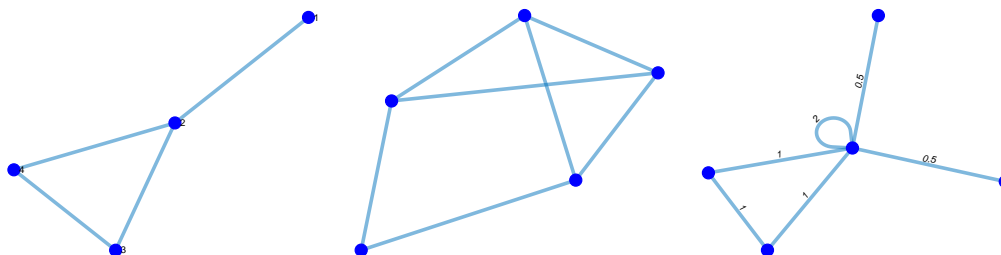


FIGURE 3. A positively integrally invertible vertex labeled graph G^{sd} with $k = 4$ vertices (left); the G^{sd} complete graph $G_{1,2,1,1}^{\text{sd}}$ complete graph (middle); the weighted signable pseudo-inverse graph $(G_{1,2,1,1}^{\text{sd}})^{\dagger}$ (right).

REMARK 2.11. Path graphs P_2, P_3, P_4 and the cycle graph C_4 are homothetically self-pseudo-invertible graphs. Furthermore, complete bipartite graphs $K_{m_1, m_2}, m = m_1 + m_2, m \geq 2$, form an infinite family of homothetically self-pseudo-invertible graphs. In Proposition 3.2, we show that a graph G^A constructed from a given graph G^B by adding a pendant vertex to each vertex of G^B is always a signable integrally invertible graph whose inverse graph $(G^A)^{-1}$ is homothetically similar to G^A .

3. Statistical and extreme properties of eigenvalues and spectral indices of signable pseudo-invertible and signable integrally invertible graphs. Let G^A be a simple connected graph with an adjacency matrix A . Then A has positive and negative eigenvalues, because $\text{trace}(A) = 0$. In what follows, we shall denote $\lambda_{\pm}(G^A) \equiv \lambda_{\pm}(A)$, the least positive and largest negative eigenvalues of the adjacency matrix A . Let us denote by $\Lambda^{\text{gap}}(A) = \lambda_+(A) - \lambda_-(A)$ and $\Lambda^{\text{ind}}(A) = \max(|\lambda_+(A)|, |\lambda_-(A)|)$ the spectral gap and the spectral index of A . Furthermore, we define the spectral power $\Lambda^{\text{pow}}(A) = \sum_{k=1}^m |\lambda_k|$. Clearly, all three spectral indices $\Lambda^{\text{gap}}, \Lambda^{\text{ind}}$, and Λ^{pow} depend on the positive $\sigma_+(A) = \{\lambda \in \sigma(A), \lambda > 0\}$ and negative $\sigma_-(A) = \{\lambda \in \sigma(A), \lambda < 0\}$ parts of the spectrum of the matrix A . In fact, $\lambda_+(A) = \min \sigma_+(A), \lambda_-(A) = \max \sigma_-(A)$, and $\Lambda^{\text{pow}} = \sum_{\lambda \in \sigma_+(A)} \lambda - \sum_{\lambda \in \sigma_-(A)} \lambda = 2 \sum_{\lambda \in \sigma_+(A)} \lambda$. In the context of spectral graph theory, the eigenvalues of the adjacency matrix A representing a structural chemical graph of an organic molecule play an important role. The spectral gap $\Lambda^{\text{gap}}(A)$ is also known as the HOMO-LUMO energy separation gap of the energy of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). Generally speaking, the molecule is more stable when the spectral gap is larger (cf. Aihara [1]).

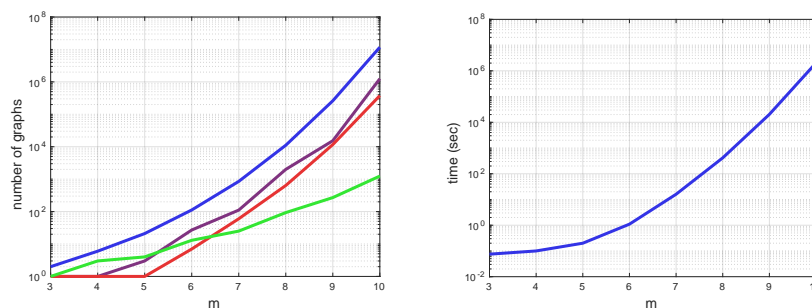


FIGURE 4. Left: the number of all simple connected graphs of order $m \leq 10$ (blue). The numbers of positively but not negatively pseudo-invertible graphs (magenta), the number of negatively but not positively pseudo-invertible graphs (red), the number of positively and negatively (bipartite) pseudo-invertible graphs (green). Right: computational time complexity of the results summarized in Table 2.

TABLE 1

The number of all simple connected graphs G^A on $m \leq 10$ vertices, graphs G^A with invertible adjacency matrix ($\det(A) \neq 0$), and graphs G^A with integrally invertible adjacency matrix ($\det(A) = \pm 1$). Source: own computations [35] based on McKay's list of all simple connected graphs [27].

m	2	3	4	5	6	7	8	9	10
All graphs	1	2	6	21	112	853	11,117	261,080	11,716,571
$\det(A) \neq 0$	1	1	3	8	52	342	5724	141,063	7,860,195
$\det(A) = \pm 1$	1	–	2	–	29	–	2381	–	1,940,904

If we denote by c_m the number of simple nonisomorphic connected graphs on m vertices, then the number c_m can be approximated by the quadratic exponential function: $c_m \approx \omega_0 10^{\omega_1(m-9) + \omega_2(m-9)^2}$, where $\omega_0 = 261080$, $\omega_1 = 1.4$, $\omega_2 = 0.09$ (cf. [36]). This formula is exact for the order $m = 9$ and gives accurate approximation results for other $m \leq 10$ (see Fig. 4, left (blue line)). Moreover, $\log(c_m) = O(m^2)$ as $m \rightarrow \infty$. The class of multipartitioned complete graphs is completely characterized by its partitions $\{m_1, \dots, m_k\}$. The number \hat{c}_m of multipartitioned complete graphs is therefore given by the number of partitions of order $m = m_1 + \dots + m_k$, for $k = 1, \dots, m$. According to Hardy-Ramanujan's 1918 result, we have $\hat{c}_m \approx \frac{1}{4m\sqrt{3}} \exp(\pi\sqrt{2m/3})$, i.e., $\log(\hat{c}_m) = O(\sqrt{m})$ as $m \rightarrow \infty$. This means that the number of all multipartitioned complete graphs of a given order m is considerably smaller than the number of all simple connected graphs of that order.

Recall the following well-known facts regarding the minimal and maximal eigenvalues of a graph. The maximal value of $\lambda_{max} = \lambda_1$ on all simple connected graphs on m vertices is equal to $m - 1$ and is reached by the complete graph K_m . The minimal value of λ_{max} is equal to $2 \cos(\pi/(m+1))$ and is achieved for the path graph P_m . The lower bound for the minimal eigenvalue $\lambda_{min} = \lambda_m \geq -\sqrt{\lceil m/2 \rceil \lceil m/2 \rceil}$ was independently proved by Constantine [12] and Powers [37]. The lower bound is attained for the complete bipartite graph K_{m_1, m_2} where $m_1 = \lceil m/2 \rceil$, $m_2 = \lfloor m/2 \rfloor$. The maximal value of λ_{min} on all simple connected graphs on the m vertices is equal to -1 . It is attained for the complete graph K_m . Unfortunately, neither the complete graph K_k nor the complete multipartitioned graph K_{m_1, \dots, m_k} are signable pseudo-invertible graphs for $k \geq 3$. This is why we have to investigate the properties of extreme spectral indices within the class of signable pseudo-invertible graphs that do not include complete graphs K_k , or complete multipartitioned graphs K_{m_1, \dots, m_k} with $k \geq 3$.

In Table 1, we present the number of all simple connected graphs G^A on $m \leq 10$ vertices, graphs G^A with an invertible adjacency matrix ($\det(A) \neq 0$), and graphs G^A with an integrally invertible adjacency matrix ($\det(A) = \pm 1$) based on our calculations [35], and McKay's list of all simple connected graphs [27]. In Table 2, we present the number of positively but not negatively pseudo-invertible graphs (+signable), the number of negatively but not positively pseudo-invertible graphs (–signable), and the number of simultaneously positively and negatively invertible and pseudo-invertible graphs (\pm signable). Complete characterization of these classes of graphs and their spectrum can be found in [35]. In Fig. 4, we depict the dependence of the number of all simple connected graphs of the order $m \leq 10$ (blue), the number of (+signable) graphs (magenta), the number (–signable) of graphs (red), and the number of (\pm signable) bipartite graphs (green). We also show the computational time complexity of the results summarized in Table 2.

Finally, in Table 3 we present the number of positively but not negatively integrally invertible graphs (+signable) and then the number of negatively but not positively integrally invertible graphs (–signable). We also present the number of positively and negatively integrally invertible graphs (\pm signable).

TABLE 2

The number of positively but not negatively pseudo-invertible graphs (+signable). The number of negatively but not positively pseudo-invertible graphs (-signable). The number of simultaneously positively and negatively invertible and pseudo-invertible graphs (\pm signable). Source: own computations [35].

m	2	3	4	5	6	7	8	9	10
+signable	0	0	1	3	27	111	2001	15,310	1,247,128
-signable	0	0	0	1	7	60	638	11,643	376,137
\pm signable	1	1	3	4	13	25	93	270	1243
all signable	1	1	4	8	47	196	2732	27,223	1,624,508

TABLE 3

The number of signable positively but not negatively integrally invertible graphs (+signable). The number of negatively but not positively integrally invertible graphs (-signable). The number of positively and negatively integrally invertible graphs (\pm signable). Source: own computations [35] based on McKay's list of all simple connected graphs [27].

m	2	3	4	5	6	7	8	9	10
+signable	0	-	1	-	20	-	1626	-	1,073,991
-signable	0	-	0	-	4	-	260	-	105,363
\pm signable	1	-	1	-	4	-	25	-	349
all signable	1	0	2	0	28	0	1911	0	1,179,703

3.1. All simple connected signable pseudo-invertible graphs. In Table 4, we present descriptive statistics of maximal(minimal) eigenvalues $\lambda_{max}(\lambda_{min})$, spectral gap Λ^{gap} , spectral index Λ^{ind} , and spectral power Λ^{pow} for all signable pseudo-invertible simple connected graphs on $m \leq 10$ vertices. The symbols E, σ, \mathcal{S} and \mathcal{K} represent the mean value, standard deviation, skewness, and kurtosis of the corresponding sets of eigenvalues λ_{max} , and λ_{min} , respectively. Skewness $\mathcal{S}(\lambda_{max})$ is close to zero, and kurtosis $\mathcal{K}(\lambda_{max})$ tends to 3. This means that the distribution of maximal eigenvalues of all signable pseudo-invertible simple connected graphs on m vertices becomes normally distributed as m increases. On the other hand, $\mathcal{S}(\lambda_{min}) < 0$ and $\mathcal{K}(\lambda_{min}) > 3$. It reveals that the distribution of minimal eigenvalues is slightly skewed to the left, and it has a leptokurtic distribution with fat tails. The signatures (+)/(-)/(\pm) after the extreme value indicate (positive)/(negative)/(positive and negative) pseudo-invertibility of the graph attaining this extreme value.

Recall that the lower bound for λ_{min} is achieved for the complete bipartite graph K_{m_1, m_2} where $m_1 = \lceil m/2 \rceil, m_2 = \lfloor m/2 \rfloor$. The graph K_{m_1, m_2} is positively and negatively pseudo-invertible. In Fig. 5, we show signable pseudo-invertible graphs on $3 \leq m \leq 10$ vertices with the maximal value of λ_{max} . For values of λ_{max} , we refer to Table 4.

In the next proposition, we derive upper and lower bounds of the spectral indices $\Lambda^{gap}, \Lambda^{ind}$, and Λ^{pow} in the class of all signable pseudo-invertible graphs.

PROPOSITION 3.1. Assume G^A is a signable pseudo-invertible graph of order m . Then,

- (i) $\Lambda^{gap}(G^A) \leq 2\sqrt{\lceil m/2 \rceil \lfloor m/2 \rfloor}$, and $\Lambda^{ind}(G^A) \leq \sqrt{\lceil m/2 \rceil \lfloor m/2 \rfloor}$. The equalities are attained by the complete bipartite graph K_{m_1, m_2} where $m_1 = \lceil m/2 \rceil, m_2 = \lfloor m/2 \rfloor$.
- (ii) $\Lambda^{pow}(G^A) \geq 2\sqrt{m-1}$. The equality is attained by the complete bipartite star graph $K_{m-1, 1} \equiv S_m$.

Proof. The proof of part i) is based on the properties of the second largest eigenvalue $\lambda_2(A)$ of the graph G^A . With regard to Powers [37, 38], and Cvetković and Simić [15], we have the following estimate for the second largest eigenvalue: $-1 \leq \lambda_2(A) \leq \lfloor m/2 \rfloor - 1$. According to Smith [40], a simple connected graph G^A has exactly one positive eigenvalue $\lambda_1(A) = \lambda_{max} > 0$, i.e., $\lambda_2(A) \leq 0$, if and only if it is a complete multipartitioned graph K_{m_1, \dots, m_k} where $1 \leq m_1 \leq \dots \leq m_k$ denote the sizes of the partitions,

TABLE 4

Descriptive statistics of the maximal(minimal) eigenvalues λ_{max} (λ_{min}), spectral gap Λ^{gap} , spectral index Λ^{ind} , and spectral power Λ^{pow} for all signable pseudo-invertible simple connected graphs on $m \leq 10$ vertices.

m	3	4	5	6	7	8	9	10
$E(\lambda_{max})$	1.4142	1.8800	2.4066	2.8107	3.3106	3.7471	4.2491	4.7634
$\sigma(\lambda_{max})$	-	0.2510	0.3993	0.5074	0.5640	0.6160	0.6553	0.6309
$S(\lambda_{max})$	-	0.1191	-0.0036	-0.0101	-0.1702	-0.0756	-0.0282	-0.1001
$\mathcal{K}(\lambda_{max})$	-	1.3963	1.6392	2.0501	2.2927	2.7045	2.9230	2.9675
$\max(\lambda_{max})$	1.4142 (\pm)	2.1701 (+)	2.9354 (-)	3.7321 (+)	4.4253 (+)	5.9164 (-)	7.0315 (-)	8.1231 (-)
$\min(\lambda_{max})$	1.4142 (\pm)	1.6180 (\pm)	1.8478 (\pm)	1.8019 (\pm)	1.9319 (\pm)	1.8794 (\pm)	1.9616 (\pm)	1.9190 (\pm)
$E(\lambda_{min})$	-1.4142	-1.7078	-1.9739	-2.1375	-2.3811	-2.4676	-2.6930	-2.7947
$\sigma(\lambda_{min})$	-	0.2201	0.2708	0.3243	0.3311	0.3198	0.3259	0.2838
$S(\lambda_{min})$	-	-0.4543	-0.4438	-0.6230	-0.5321	-0.6962	-0.5011	-0.4281
$\mathcal{K}(\lambda_{min})$	-	1.8907	2.2189	2.9493	2.9185	3.8455	3.3743	3.4984
$\max(\lambda_{min})$	-1.4142 (\pm)	-1.4812 (+)	-1.6180 (-)	-1.6180 (-)	-1.7823 (-)	-1.6180 (-)	-1.8384 (+)	-1.6180 (-)
$\min(\lambda_{min})$	-1.4142 (\pm)	-2.0000 (\pm)	-2.4495 (\pm)	-3.0000 (\pm)	-3.4641 (\pm)	-4.0000 (\pm)	-4.4721 (\pm)	-5.0000 (\pm)
$\max(\Lambda^{gap})$	2.8284 (\pm)	4.0000 (\pm)	4.8990 (\pm)	6.0000 (\pm)	6.9282 (\pm)	8.0000 (\pm)	8.9442 (\pm)	10.000 (\pm)
$\max(\Lambda^{ind})$	1.4142 (\pm)	2.0000 (\pm)	2.4495 (\pm)	3.0000 (\pm)	3.4641 (\pm)	4.0000 (\pm)	4.4721 (\pm)	5.0000 (\pm)
$\max(\Lambda^{pow})$	2.8284 (\pm)	4.9624 (+)	7.1068 (-)	8.8284 (+)	11.2176 (-)	14.000 (+)	16.7446 (-)	19.4136 (-)
$\min(\Lambda^{gap})$	2.8284 (\pm)	1.2360 (\pm)	1.0806 (-)	0.7423 (+)	0.6429 (-)	0.3877 (+)	0.3310 (-)	0.1647 (+)
$\min(\Lambda^{ind})$	1.4142 (\pm)	0.6180 (\pm)	0.6180 (-)	0.4142 (\pm)	0.3573 (-)	0.2624 (+)	0.1937 (-)	0.1092 (+)
$\min(\Lambda^{pow})$	2.8284 (\pm)	3.4642 (\pm)	4.0000 (\pm)	4.4722 (\pm)	4.8990 (\pm)	5.2916 (\pm)	5.6568 (\pm)	6.0000 (\pm)

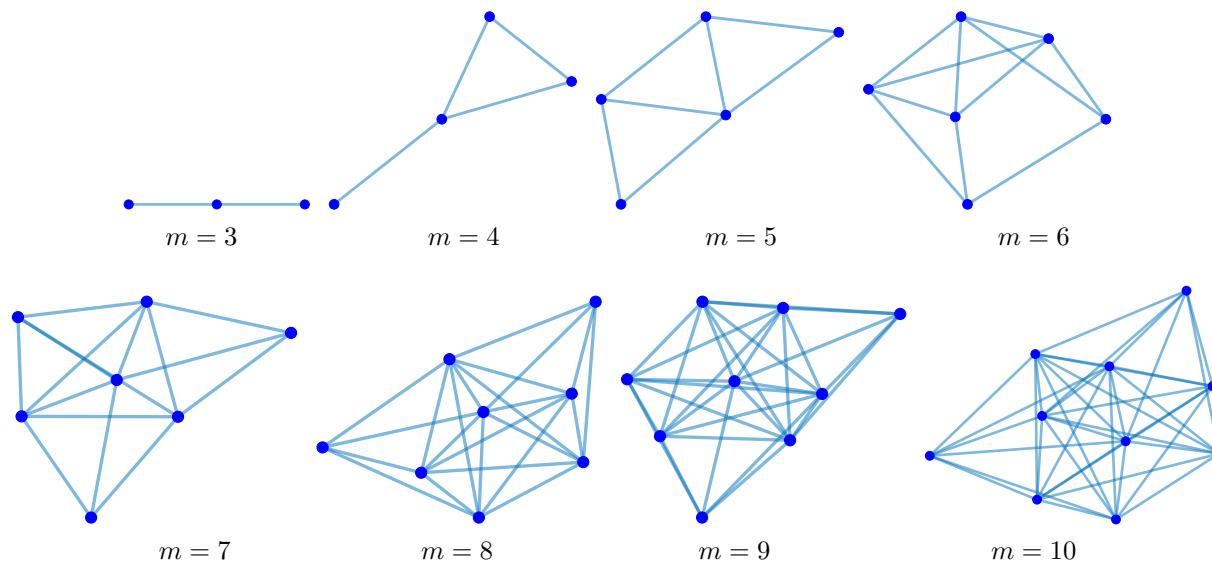


FIGURE 5. Signable pseudo-invertible graphs on $3 \leq m \leq 10$ vertices with a maximal value of λ_{max} (see Table 4).

$m_1 + \dots + m_k = m$, and $k \geq 2$ is the number of partitions (see also Cvetković *et al.* [16, Theorem 6.7]). Therefore, for a graph G^A different from any complete multipartitioned graph K_{m_1, \dots, m_k} we have $\lambda_2(A) > 0$, and consequently, $-\sqrt{\lfloor m/2 \rfloor \lceil m/2 \rceil} \leq \lambda_{min}(A) \leq \lambda_-(A) < 0 < \lambda_+(A) \leq \lambda_2(A) \leq \lfloor m/2 \rfloor - 1$. Hence, the spectral gap $\Lambda^{gap}(G^A) = \lambda_+(A) - \lambda_-(A) \leq \sqrt{\lfloor m/2 \rfloor \lceil m/2 \rceil} + \lfloor m/2 \rfloor - 1 \leq 2\sqrt{\lfloor m/2 \rfloor \lceil m/2 \rceil}$ because $\lfloor m/2 \rfloor - 1 \leq \sqrt{\lfloor m/2 \rfloor \lceil m/2 \rceil}$ for any m . Similarly, $\Lambda^{ind}(A) \leq \sqrt{\lfloor m/2 \rfloor \lceil m/2 \rceil}$.

To prove (ii), we recall that $\Lambda^{pow}(G^A) \geq 2\sqrt{m-1}$ for a general simple connected graph G^A (cf. Caporossi *et al.* [9, Theorem 2]). The minimal value of $\Lambda^{pow}(G^A) = 2\sqrt{m-1}$ is attained by the star graph $S_m \equiv K_{m-1,1}$ which is a signable positively and negatively pseudo-invertible bipartite graph, and the proof follows. \square

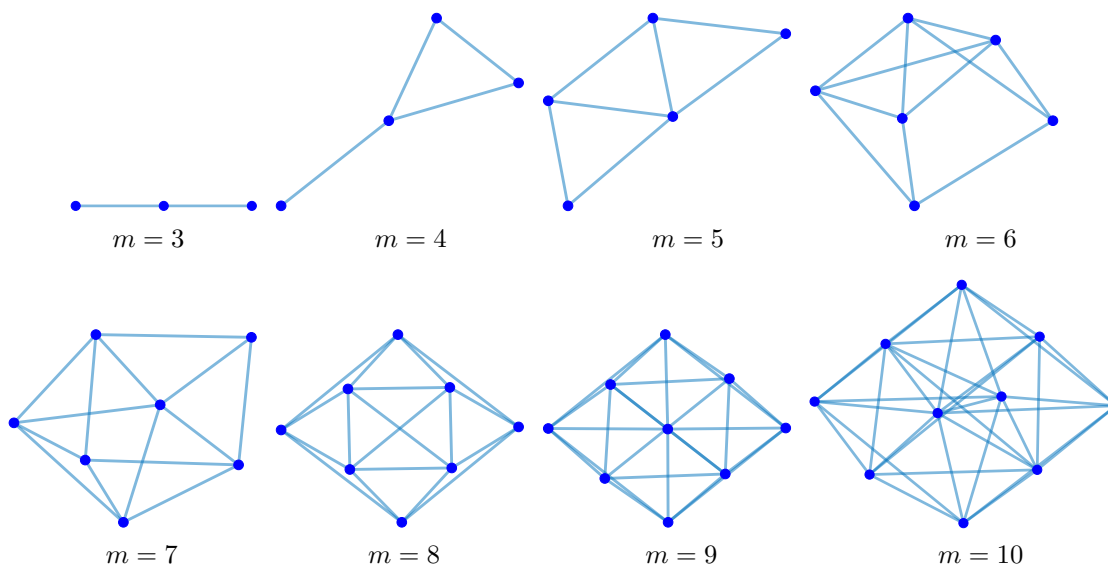


FIGURE 6. Signable pseudo-invertible graphs on $3 \leq m \leq 10$ vertices with a maximal value of Λ^{pow} (see Table 4).

In Fig. 6, we present signable pseudo-invertible graphs on the $4 \leq m \leq 10$ vertices with maximal values of Λ^{pow} . Graphs that achieve minimal values of Λ^{gap} are shown in Fig. 7. For m , even the minimal values of Λ^{gap} and Λ^{ind} are attained by signable integrally invertible graphs.

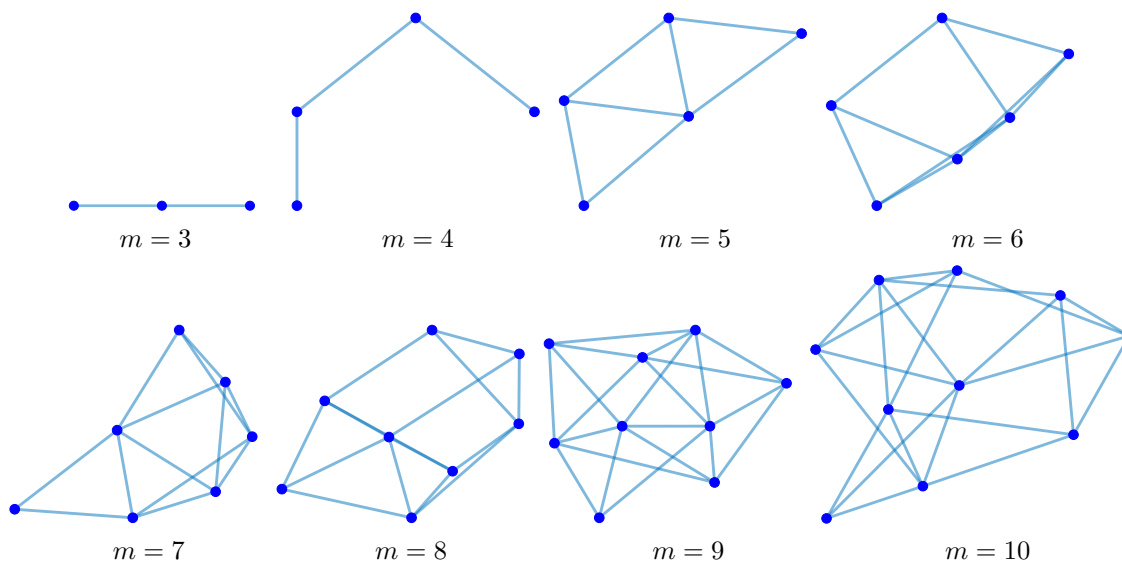


FIGURE 7. Signable pseudo-invertible graphs on $3 \leq m \leq 10$ vertices with a minimal value of Λ^{gap} (see Table 4).

3.2. All simple connected signable integrally invertible graphs. In this section, we present signable integrally invertible graphs attaining extreme values of spectral indices. First, we present a simple construction of an infinite family of signable integrally invertible graphs. For arbitrary simple connected

graph G^B (not necessarily even pseudo-invertible), we can construct a signable integrally invertible graph just by adding a pendant vertex to each vertex of G^B . An adjacency matrix A is integrally invertible ($|\det(A)| = 1$), iff m is even. If G_B is a graph, the graph G_A formed from G_B by adding a pendant vertex to each vertex of G_B is known in the literature as the corona graph of G_B .

PROPOSITION 3.2. *Assume G^A is a graph of even order m constructed from a simple connected G^B of order $m/2$ by adding a pendant vertex to each vertex of G^B . Then*

- (i) G^A is a signable negatively integrally invertible graph.
- (ii) If G^B is a bipartite graph, then G^A is a signable positively integrally invertible bipartite graph.
- (iii) $\Lambda^{pow}(G^A) = \sum_{\mu \in \sigma(B)} \sqrt{\mu^2 + 4} \geq \max\{\Lambda^{pow}(G^B), m\}$.
- (iv) The graph G^A is homothetically pseudo-invertible.

Proof. The adjacency matrix A of the graph G^A and its inverse matrix A^{-1} have the following block matrix form:

$$(3.4) \quad A = \begin{pmatrix} 0 & I \\ I & B \end{pmatrix}, \quad A^{-1} = \begin{pmatrix} -B & I \\ I & 0 \end{pmatrix},$$

where B is the adjacency matrix of the graph G^B . The matrix A^{-1} is integral. Therefore, A is integrally invertible, $|\det(A)| = 1$. Furthermore, it is negatively signable by the signature matrix $D = \text{diag}(I, -I)$, and statement (i) follows.

To prove (ii), suppose that G^B is a bipartite graph. Then, there exists a $k \times k$ signature matrix D_- such that $D_-BD_- \leq 0$. In fact, if we set $(D_-)_{ii} = 1$ for a vertex i belonging to the first bipartition of G^B , and $(D_-)_{jj} = -1$ for a vertex j belonging to the second bipartition, then $D_-BD_- \leq 0$. Since $D_-D_- = I$, we have $DA^{-1}D \geq 0$ where $D = \text{diag}(D_-, D_-)$ is a diagonal $m \times m$ signature matrix. Hence, G^A is also a positively integrally invertible bipartite graph. Statement ii) now follows. To prove iii), notice that $\lambda \in \sigma(A)$ iff $\lambda = (\mu \pm \sqrt{\mu^2 + 4})/2$ for some $\mu \in \sigma(B)$. Therefore, $\lambda \in \sigma_+(A)$ iff $\lambda = (\mu + \sqrt{\mu^2 + 4})/2$ for some $\mu \in \sigma(B)$. As $\sum_{\lambda \in \sigma(A)} \lambda = 0$, and $\sum_{\mu \in \sigma(B)} \mu = 0$ we have

$$\Lambda^{pow}(A) = \sum_{\lambda \in \sigma(A)} |\lambda| = \sum_{\lambda \in \sigma_+(A)} \lambda - \sum_{\lambda \in \sigma_-(A)} \lambda = 2 \sum_{\lambda \in \sigma_+(A)} \lambda = \sum_{\mu \in \sigma(B)} \sqrt{\mu^2 + 4} \geq \max\{\Lambda^{pow}(G^B), m\},$$

because $\sqrt{\mu^2 + 4} \geq \max\{|\mu|, 2\}$. The proof of iii) now follows. Finally, if D is a signature matrix of the inverse graph $(G^A)^{-1}$ then $DA^{-1}D = \kappa PAP^T$ where $P = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}$ is a permutation matrix and $\kappa = 1$ or $\kappa = -1$. The proof of (iv) now follows. \square

In Table 5, we present descriptive statistics of the extreme eigenvalues λ_{max} , λ_{min} , spectral gap Λ^{gap} , spectral index Λ^{ind} , and spectral power Λ^{pow} for all signable integrally invertible simple connected graphs on $m \leq 10$ vertices. Interestingly enough, the maximal and minimal eigenvalues λ_{max} and λ_{min} , maximal gap Λ^{gap} and the power Λ^{pow} over all signable integrally invertible graphs on $m = 6$ vertices are attained by the same graph (see Fig. 8).

REMARK 3.3. *In the class of all pseudo-invertible graphs, the maximal and minimal values of spectral indices λ_{max} , λ_{min} , Λ^{gap} , Λ^{ind} , Λ^{pow} can be attained by graphs with varying signability (see Table 4). For example, there are four ($m = 5, 8, 9, 10$) negatively but only three ($m = 4, 6, 7$) positively pseudo-invertible graphs with a maximal value of λ_{max} for the order $4 \leq m \leq 10$. Similarly, maximal values of Λ^{pow} are attained by negative pseudo-invertible graphs for order $m = 5, 7, 9, 10$. On the other hand, it follows from the*

TABLE 5

Descriptive statistics of the maximal(minimal) eigenvalues λ_{max} (λ_{min}), spectral gap Λ^{gap} , spectral index Λ^{ind} , and spectral power Λ^{pow} for all signable integrally invertible simple connected graphs on $m \leq 10$ vertices.

m	4	6	8	10
$E(\lambda_{max})$	1.8941	2.7716	3.6912	4.7082
$\sigma(\lambda_{max})$	0.3904	0.5081	0.5868	0.6155
$S(\lambda_{max})$	0	0.0654	-0.0866	-0.1249
$\mathcal{K}(\lambda_{max})$	1	2.2008	2.6776	2.8808
$\max(\lambda_{max})$	2.1701 (+)	3.7321 (+)	5.3628 (+)	7.1205 (+)
$\min(\lambda_{max})$	1.6180 (\pm)	1.8019 (\pm)	1.8794 (\pm)	1.9190 (\pm)
$E(\lambda_{min})$	-1.5496	-1.9924	-2.4068	-2.7995
$\sigma(\lambda_{min})$	0.0967	0.2384	0.2555	0.2680
$S(\lambda_{min})$	0	-0.1743	-0.1380	-0.1912
$\mathcal{K}(\lambda_{min})$	1	1.8261	2.8754	2.9341
$\max(\lambda_{min})$	-1.4812 (+)	-1.6180 (+)	-1.6180 (+)	-1.6180 (+)
$\min(\lambda_{min})$	-1.6180 (\pm)	-2.4142 (+)	-3.3028 (+)	-4.2361 (+)
$\max(\Lambda^{gap})$	1.3111 (+)	1.2679 (+)	1.2947 (+)	1.4773 (+)
$\max(\Lambda^{ind})$	1.0000 (+)	1.0000 (+)	1.2501 (+)	1.4685 (+)
$\max(\Lambda^{pow})$	4.9624 (+)	8.8284 (+)	13.4838 (+)	18.8636 (+)
$\min(\Lambda^{gap})$	1.2360 (\pm)	0.7423 (+)	0.3877 (+)	0.1647 (+)
$\min(\Lambda^{ind})$	0.6180 (\pm)	0.4142 (\pm)	0.2624 (+)	0.1092 (+)
$\min(\Lambda^{pow})$	4.4720 (\pm)	6.8990 (\pm)	9.2916 (\pm)	11.6568 (\pm)

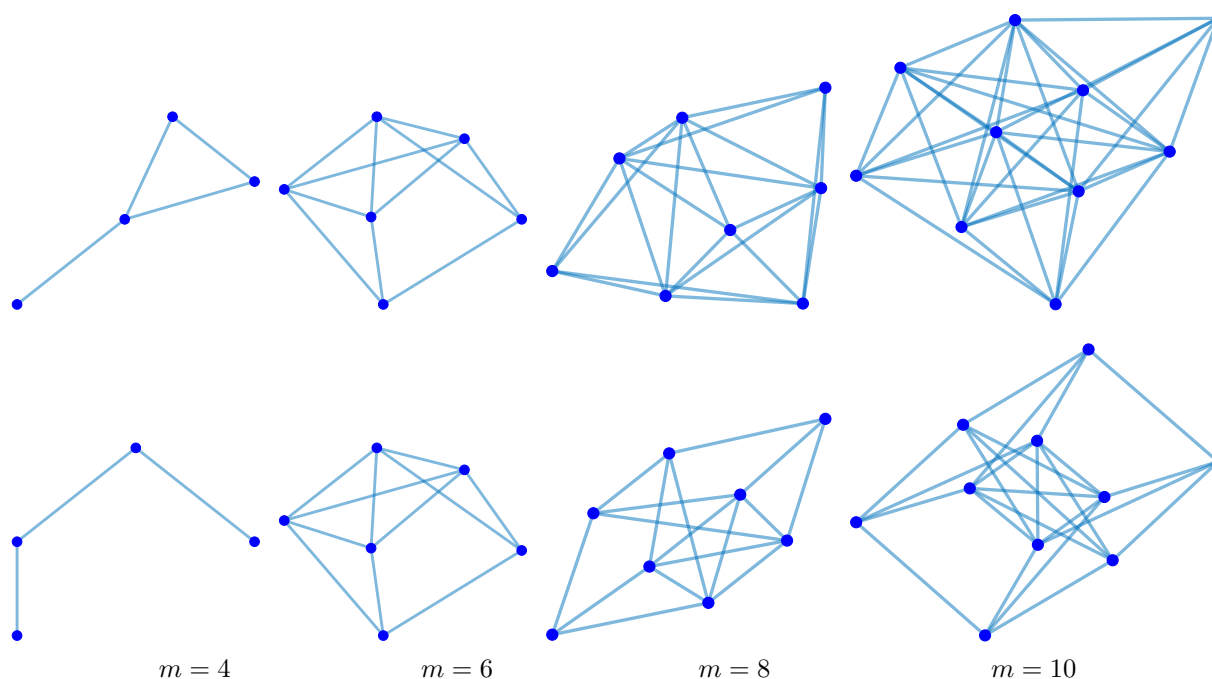


FIGURE 8. Signable integrally invertible graphs on the $m = 4, 6, 8, 10$ vertices with a maximal value of λ_{max} (top row) and a minimal value of λ_{min} (bottom row) (see Table 5).

results summarized in Table 5 that the extreme values of these spectral indices are achieved only by integrally invertible positive (+) or positively/negatively (\pm) integrally invertible graphs.

Finally, we present signable integrally invertible graphs of the order $m = 4, 6, 8, 10$ achieving extreme spectral indices. In Fig. 8, we plot signable integrally invertible graphs with a maximal value of λ_{max} and

minimal value of λ_{min} . In Fig. 9, we show signable integrally invertible graphs with maximal and minimal values of Λ^{pow} . The minimal value of $\Lambda^{pow} = m - 4 + 2\sqrt{m/2 + 3}$ in the class of all signable integrally invertible graphs is attained by a graph constructed from the star graph $S_{m/2}$ by adding one pendant vertex to each vertex of $S_{m/2}$ (see Fig. 9 and Proposition 3.2). In Fig. 10, we depict signable integrally invertible graphs with the maximal value of Λ^{gap} .

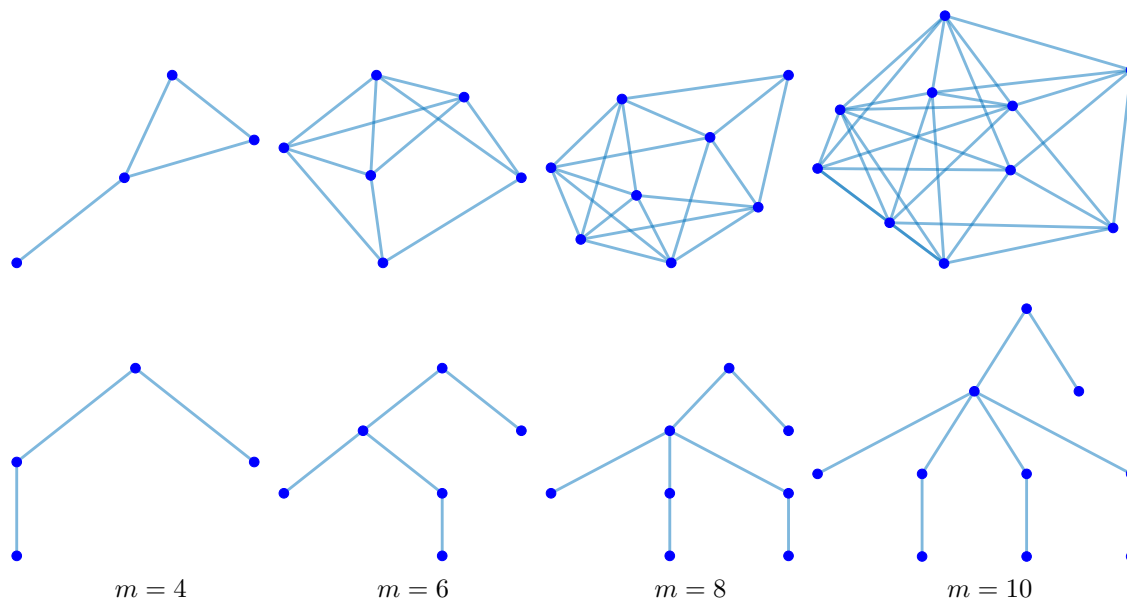


FIGURE 9. Signable integrally invertible graphs on $m = 4, 6, 8, 10$ vertices with a maximal (top row) and minimal (bottom row) value of Λ^{pow} (see Table 5).

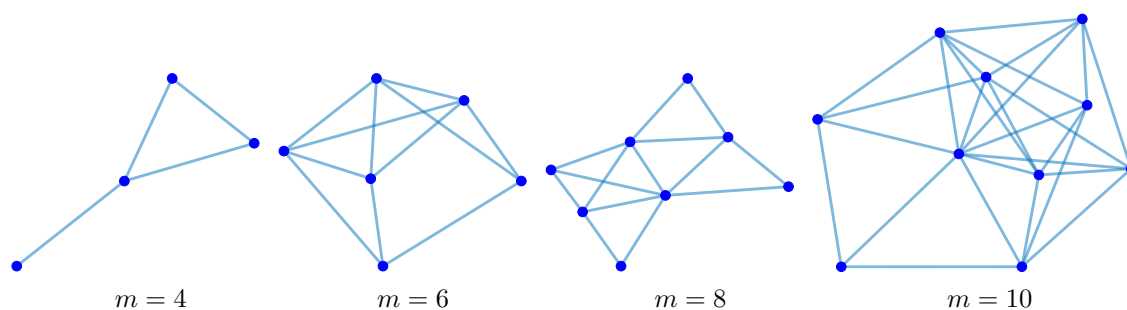


FIGURE 10. Signable integrally invertible graphs on $m = 4, 6, 8, 10$ vertices with a maximal value of Λ^{gap} (see Table 5).

4. Conclusions. In this paper, we investigated signable pseudo-invertible graphs. We analyzed various qualitative, statistical, and extreme properties of spectral indices of pseudo-invertible graphs. We derived various upper and lower bounds on maximal and minimal eigenvalues and spectral indices $\Lambda^{gap}, \Lambda^{ind}$, and Λ^{pow} . We showed that the complete multipartitioned graphs K_{m_1, \dots, m_k} are signable pseudo-invertible only for $k = 2$. A novel concept of G^{sc} -complete multipartitioned graph was introduced and analyzed. It is a natural generalization of a complete multipartitioned graph. We also presented computational and statistical

results for the class of signable pseudo-invertible and integrally invertible graphs of order $m \leq 10$. Some properties of extreme eigenvalues and indices were shown for arbitrary order m .

REFERENCES

- [1] Aihara, J.I. Reduced HOMO-LUMO gap as an index of kinetic stability for polycyclic aromatic hydrocarbons. *J. Phys. Chem. A*, 103:7487–7495, 1999.
- [2] Akbari S. and Kirkland, S.J. On unimodular graphs. *Linear Algebra Appl.*, 421:3–15, 2007.
- [3] Bacalis, N.C. and Zdetsis, A.D. Properties of hydrogen terminated silicon nanocrystals via a transferable tight-binding Hamiltonian, based on ab-initio results. *J. Math. Chem.*, 26:962–970, 2009.
- [4] Bapat, R.B. and Ghorbani, E. Inverses of triangular matrices and bipartite graphs. *Linear Algebra Appl.*, 447:68–73, 2014.
- [5] Bapat, R.B. *Graphs and Matrices*. Universitext. Springer, London; Hindustan Book Agency, New Delhi, 2010.
- [6] Ben-Israel, A. and Greville, T.N.E. *Generalized Inverses: Theory and Applications*. CMS Books Math., Springer, 2003.
- [7] Bender, E.A., Canfield, E.R., and McKay, B.D. The asymptotic number of labeled connected graphs with a given number of vertices and edges. *Random Struct. Algor.*, 1:127–169, 1990.
- [8] Brouwer, A. and Haemers, W. *Spectra of Graphs*. Universitext. Springer, New York, 2012.
- [9] Caporossi, G., Cvetković, D, Gutman, I, and Hansen, P. Variable neighborhood search for extreme graphs. 2. Finding graphs with extreme energy. *J. Chem. Inf. Comput. Sci.*, 39:984–996, 1999.
- [10] Carmona, A., Encinas, A.M., Jimeénez, M.J. and Mitjana, M. The group inverse of circulant matrices depending on four parameters. *Spec. Matrices*, 10:87–108, 2022.
- [11] Chen L. and Jinfeng, L. Extremal values of matching energies of one class of graphs. *Appl. Math. Comput.*, 273:976–992, 2016.
- [12] Constantine, G. Lower bounds on the spectra of symmetric matrices with non-negative entries. *Linear Algebra Appl.*, 65:171–178, 1985.
- [13] Cvetković, D., Gutman, I., and Simić, S. On self pseudo-inverse graphs. *Publikacije Elektrotehničkoga fakulteta. Serija Matematika i fizika*, 602/633:111–117, 1978.
- [14] Cvetković, D., Hansen, P., and Kovačević-Vučič, V. On some interconnections between combinatorial optimization and extreme graph theory. *Yugoslav J. Oper. Res.*, 14:147–154, 2004.
- [15] Cvetković, D. and Simić, S. The second largest eigenvalue of a graph (a survey). *Filomat*, 9:449–472, 1995.
- [16] Cvetković, D., Doob, M., and Sachs, H. *Spectra of Graphs – Theory and Application*, 3rd ed. Heidelberg-Leipzig, 1995.
- [17] Da Fonseca, C.M. and Petronilho, J. Explicit inverses of some tridiagonal matrices. *Linear Algebra Appl.* 325:7–21, 2001.
- [18] Delorme, C. Eigenvalues of complete multipartite graphs. *Discrete Math.* 312 (2012), 2532–2535.
- [19] Encinas, A.M. and Jimeénez, M.J. Explicit inverse of a tridiagonal (p, r) -Toeplitz matrix. *Linear Algebra Appl.*, 542:402–421, 2018.
- [20] Fowler, P.V. HOMO-LUMO maps for chemical graphs. *MATCH Commun. Math. Comput. Chem.*, 64:373–390, 2010.
- [21] Godsil, C.D. Inverses of trees. *Combinatorica*, 5:33–39, 1985.
- [22] Gutman, I. and Rouvray, D.H. An approximate topological formula for the HOMO-LUMO separation in alternant hydrocarbons. *Chem.-Phys. Lett.*, 62:384–388, 1979.
- [23] Harary, F. and Minc, H. Which non-negative matrices are self-inverse? *Math. Mag.*, 49:91–92, 1976.
- [24] Jaklić, G., Fowler, P.W., and Pisanski, T. HL-index of a graph. *Ars Math. Contempor.*, 5:99–105, 2012.
- [25] Kirkland, S.J. and Tifenbach, R.M. Directed intervals and the dual of a graph. *Linear Algebra Appl.*, 431:792–807, 2009.
- [26] Klein, D.J., Yang, Y., and Ye, D. HOMO-LUMO gaps for sub-graphenic and sub-buckytubic species. *Proc. Royal Soc. A*, 471, Paper No. 20150138, 2015.
- [27] McKay, B. Combinatorial data. Available online November 2022, <http://users.cecs.anu.edu.au/~bdm/data/graphs.html>
- [28] McLeman, C. and McNicholas, E. Graph invertibility. *Graphs Combin.*, 30:977–1002, 2014.
- [29] McDonald, J., Raju, N., and Sivakumar, K.C. Group inverses of matrices associated with certain graph classes. *Electron. J. Linear Algebra*, 38:204–220, 2022.
- [30] Mohar, B. Median eigenvalues and the HOMO-LUMO index of graphs. *J. Comb. Theory B*, 112:78–92, 2015.
- [31] Pavlíková, S. A note on inverses of labeled graphs. *Aust. J. Comb.*, 67(2):222–234, 2017.
- [32] Pavlíková, S. and Ševčovič, D. On a construction of integrally invertible graphs and their spectral properties. *Linear Algebra Appl.*, 532 (2017), 512–533.
- [33] Pavlíková, S. and Ševčovič, D. On the Moore-Penrose pseudo-inversion of block symmetric matrices and its application in the graph theory. *Linear Algebra Appl.*, 673:280–303, 2023.
- [34] Pavlíková, S. and Širáň, J. Inverting non-invertible weighted trees. *Australasian J. Combin.*, 75:246–255, 2019.
- [35] Pavlíková, S. and Ševčovič, D. Invertible and pseudo-invertible simple connected graphs, their spectra, positive and negative (pseudo)invertibility, July 2022. Available online at: www.iam.fmph.uniba.sk/institute/sevcovic/inversegraphs.

- [36] Pavlíková, S., Ševčovič, D., and Širáň, J. Extreme and statistical properties of eigenvalue indices of simple connected graphs. *Disc. Math.*, (2024), Paper No. 113635.
- [37] Powers, D. Graph partitioning by eigenvectors. *Linear Algebra Appl.*, 101:121–133, 1988.
- [38] Powers, D. Bounds on graph eigenvalues. *Linear Algebra Appl.*, 117:1–6, 1989.
- [39] Sivakumar, K.C. and Nandi, R. Group inverses of adjacency matrices of cycles, wheels and brooms. *Comp. Appl. Math.*, 41, Paper No. 196: 2022.
- [40] Smith, J.H. Some properties of the spectrum of a graph. In: R. Guy, H. Haxani, N. Saver, and J. Schonheim (editors). *Combinatorial Structures and Their Applications*. Gordon and Breach, New York–London–Paris 1970, 403–406.
- [41] Tifenbach, R. Strongly self-dual graphs. *Linear Algebra Appl.*, 435:3151–3167, 2011.
- [42] Ye, D., Yang, Y., Mandal, B. and Klein, D.J. Graph invertibility and median eigenvalues. *Linear Algebra Appl.*, 513:304–323, 2017.
- [43] Zaslavsky, T. Signed graphs. *Discrete Applied Math.*, 4:47–74, 1982.