Mathematics

Research article

A note on the generalized Gaussian Estrada index and Gaussian subgraph centrality of graphs

Yang Yang[1,2,3]**, Yanyan Song**[4]**, Haifeng Fan**[1,*]**and Haiyan Qiao**[5,*]

1 College of Artificial Intelligence, Tianjin University of Science and Technology, Tianjin 300457, China

2 Key Laboratory of Dual Dielectric Power Technology, Hebei Hanguang Industry Co. Ltd., Handan 056017, China

3 College of Aerospace and Civil Engineering, Harbin Engineering University, Harbin 150001, China

4 School of Mathematics and Statistics, Qinghai Normal University, Xining 810008, China

5 School of Information and Electrical Engineering, Hebei University of Engineering, Handan 056038, China

* **Correspondence:** Email: hffan@tust.edu.cn; qiaohaiyan@hebeu.edu.cn.

Abstract: Let H be a simple, undirected, connected graph represented by its adjacency matrix A. For a vertex $u \in V(H)$, the generalized Gaussian subgraph centrality of u in H is $GSC(u, \beta) = \exp\left(-\beta A^2\right)_{uu}$, where $\beta > 0$ is the real number and represents the temperature. Furthermore, the generalized Gaussian Estrada index of H is $GEE(H, \beta) = \sum_{i=1}^{n} \exp\left(-\beta \mu_i^2\right) = \sum_{u=1}^{n} GSC(u, \beta)$, where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of A and $\beta > 0$. This study presents new computational formulas for the $GSC(u, \beta)$ of graphs by employing an equitable partition and the star sets technique. We also investigated the influence of the parameter β on the robustness of the formula through experiments. Additionally, we established some bounds for $GEE(H, \beta)$.

Keywords: generalized Gaussian Estrada index; generalized Gaussian subgraph centrality; statistical mechanics; adjacency matrix; equitable partition

Mathematics Subject Classification: 05C92, 81P05, 05C09, 81Q05

1. Introduction

For a simple, undirected, connected graph $H = (V(H), E(H))$, let A represent the adjacency matrix of H, and let d_u denote the degree of vertex u in H. Assuming that the eigenvalues of A are $\mu_1 > \mu_2 \geq \cdots \geq \mu_n$.

The centrality of the node study is a significant research direction in network science and graph theory. The centrality of a node describes how important a node is in a network [1, 2]. The concept of node centrality comes from Leavitt's analysis of the influence between the behavior of small groups and their mode of communication in 1951 [3]. Soon after, many scholars defined and studied the centrality index of nodes from different perspectives, such as degree centrality [4], closeness centrality [5], energy centrality [6], and so on [7]. The research on node centrality has excellent significance for the solution of practical problems such as the robustness of the actual network [8], the propagation efficiency in the control network [9], and the understanding of the structural characteristics of the network [10].

The matrix functions have become an essential mathematical tool for studying network science [11]. The node centrality index is based on the matrix function with an adjacency matrix, including subgraph centrality [12, 13], total communicability centrality [14], Katz centrality [15], and so on [16]. The above definition of centrality gives weight to the adjacency matrix's extreme eigenvalues (the largest and the smallest). Such a weighting scheme is characterized by hiding the primary structural information in other eigenvalues [17]. For example, consider a connected graph H. If the spectral gap $\mu_1 - \mu_2$ is significantly large, then the matrix exponential $\exp(A)$ is primarily influenced by μ_1 and its corresponding eigenvector. Consequently, the information the remaining part of the spectrum provides is largely overlooked [18]. An exception to this is the Gaussian function $\exp(-A^2)$, which places greater emphasis on the zero eigenvalues (if they exist) and those eigenvalues that are close to it [19]. This matrix function explores the central part of the spectrum, revealing crucial structural information about the graphs and networks studied [17]. The zero eigenvalue and eigenvalues near zero of A play a critical role in determining molecules' magnetic and stability properties when A represents the tight-binding Hamiltonian in HMO (Hückel molecular orbital) theory [20, 21]. Many chemical reactivities are closely linked to the HOMO-LUMO gap, which corresponds to the smallest positive and the largest negative eigenvalues of A in frontier molecular orbital theory [22–25]. For example, the transfer of electrons from the HOMO of one molecule to the LUMO of another molecule is crucial in various organic chemical reactions [26]. Estrada et al. defined Gaussian subgraph centrality by exploring the influence of near-zero eigenvalues (i.e., "middle eigenvalues") on graph structure by the Gaussian function [17, 18].

For a vertex $u \in V(G)$, the generalized Gaussian subgraph centrality of u [18] is defined as

$$GSC(u, \beta) = \exp\left(-\beta A^2\right)_{uu},$$

where $\beta > 0$. Furthermore, the generalized Gaussian Estrada index of a graph [18] is defined as

$$GEE(H, \beta) = \sum_{u=1}^{n} \exp\left(-\beta A^2\right)_{uu} = \sum_{i=1}^{n} \exp\left(-\beta \mu_i^2\right),$$

where $\beta > 0$. Notice that the $GSC(u, 1)$ and $GEE(H, 1)$ are called the Gaussian subgraph centrality and the Gaussian Estrada index, respectively. According to the rules of quantum mechanics, in a network of particles, the generalized Gaussian Estrada index can be interpreted as the partition function of the system, utilizing a Hamiltonian derived from the A^2 folded spectrum method [27]. The $GEE(H, \beta)$ relates to the time-dependent Schrödinger equation involving the squared Hamiltonian, which uncovers information in the eigenvalues close to zero [28, 29]. In recent years, with the deepening research in network science [30–32]. Scholars have discovered that Gaussian functions

have important applications in capturing the structural signals of graphs [33], graph classification [34], and graph representation learning [35] in random and dynamic networks.

Equitable partition (EP) was initially introduced in [36,37] and is defined as follows. Consider H to be a graph with n vertices, and τ to be a partition of $V(H)$ with $V_1 \cup V_2 \cup \cdots \cup V_t$. If constants b_{ij} exist so that every vertex in the cell V_i has b_{ij} neighbors in the cell V_j for all $i, j \in \{1, 2, \ldots, t\}$, then τ is an EP. The matrix $\left(b_{ij}\right)_{t \times t}$ is the divisor matrix of τ. Every graph G possesses EP, as the orbits of any group of automorphisms of G create an EP [38]. EP has many applications in fields such as control theory, chemical analysis, and data clustering [39–41]. The spectrum of $(b_{ij})_{t \times t}$ is contained in that of H [37]. The matrix C serves as the characteristic matrix for τ, with its columns representing the characteristic vectors of the subsets $V_1, \ldots, V_t$.

The concept of the star set and the star complement was introduced by [38,45]. For an eigenvalue μ of the graph H with multiplicity k, a star set for μ in H is a subset of vertices $\mathbb{X} \subseteq V(H)$ such that $|\mathbb{X}| = k$ and the induced subgraph $G - \mathbb{X}$ do not possess μ as an eigenvalue. In this scenario, $G - \mathbb{X}$ is referred to as the star complement for μ in H. As well known, a star set exists for any eigenvalue of any graph [46,47]. Further investigations into star set and star complement are studied in [48,49].

Since EP and star set exist for any eigenvalue of any graph, this study employs the methods of EP and star set to derive new equations for the $GSC(u, \beta)$ of graphs. These equations can assist in calculating the $GSC(u, \beta)$ of a large graph by utilizing the structures of a smaller graph. Moreover, some bounds for the $GSC(u, \beta)$ of H are established based on the graph parameters of H. The rest of this paper is structured as follows. In Section 2, we give some lemmas used later. Section 3 details the generalized Gaussian subgraph centrality calculation formula in the context of the equitable partitions of graphs and star complements technique method. The influence of the parameter β on the robustness of the formula is explored through experiments. Section 4 introduces some bounds for the generalized Gaussian Estrada index using the graph parameters for graph H. Section 5 conclusions are given.

2. Preliminaries

In this paper, let I denote the identity matrix and A represent the adjacency matrix of the graph H. For a graph H with order n that has an EP with $V(H) = V_1 \cup V_2 \cup \cdots \cup V_t$, the corresponding characteristic matrix C is an $n \times t$ matrix whose columns consist of the characteristic vectors of $V_1, \ldots, V_t$.

Next, we present the relationship between the characteristic, adjacency, and divisor matrices.

Lemma 2.1. *[36] Let τ be an EP of graph H with characteristic matrix C and divisor matrix B. Then*

$$AC = CB.$$

Here is the standard for determining whether a vertex subset qualifies as a star set.

Lemma 2.2. *[46, 47] Let $\mathbb{X} \subseteq V(H)$ and the adjacency matrix of the subgraph induced by $\mathbb{X}$ be $A_{\mathbb{X}}$, and $A = \begin{pmatrix} A_{\mathbb{X}} & T^{\top} \\ T & P \end{pmatrix}$. Then $\mathbb{X}$ is a star set for an eigenvalue μ of H if and only if μ is not an eigenvalue of P and*

$$\mu I - A_{\mathbb{X}} = T^{\top}(\mu I - P)^{-1} T.$$

Lemma 2.3. *[54] Let G be a graph with n vertices and m edges. Then*

$$\sum_{i=1}^{n} d_i^2 \leq m \left(\frac{2m}{n-1} + n - 2 \right).$$

3. Calculation of generalized Gaussian subgraph centrality for graph

We formulate the generalized Gaussian subgraph centrality using the EP for graph H and compute its values with a smaller order matrix as follows.

Theorem 3.1. *Suppose that H has an EP with $V(G) = V_1 \cup V_2 \cup \cdots \cup V_t$ and $V_1 = \{u\}$, then*

$$GSC(u, \beta) = (\exp(-\beta \boldsymbol{B}^2))_{V_1 V_1},$$

where B is the divisor matrix of EP.

Proof. Consider $\boldsymbol{C}$ and $\boldsymbol{B}$ as the characteristic and divisor matrices of EP, respectively. According to Lemma 2.1, then

$$\exp(-\beta \boldsymbol{A}^2)\boldsymbol{C} = \sum_{k=0}^{\infty} \frac{1}{k!} (-\beta)^k \boldsymbol{A}^{2k} \boldsymbol{C} = \boldsymbol{C} \sum_{k=0}^{\infty} \frac{1}{k!} (-\beta)^k \boldsymbol{B}^{2k} = \boldsymbol{C} \exp(-\beta \boldsymbol{B}^2).$$

Since $V_1 = \{u\}$, we get

$$(\exp -\beta \boldsymbol{A}^2)_{uu} = (\exp(-\beta \boldsymbol{A}^2)\boldsymbol{C})_{uV_1} = (\boldsymbol{C} \exp(-\beta \boldsymbol{B}^2))_{uV_1} = (\exp(-\beta \boldsymbol{B}^2))_{V_1 V_1}.$$

Hence

$$GSC(u, \beta) = (\exp(-\beta \boldsymbol{A}^2))_{uu} = (\exp(-\beta \boldsymbol{B}^2))_{V_1 V_1}.$$

$\square$

Let H_1 and H_2 be two graphs; the join of H_1 and H_2 is the graph $H_1 \otimes H_2$ such that $V(H_1 \otimes H_2) = V(H_1) \cup V(H_2)$ and $E(H_1 \otimes H_2) = E(H_1) \cup E(H_2) \cup \{xy : x \in V(H_1) \text{ and } y \in V(H_2)\}$. Furthermore, if H_2 is a complete graph K_1, then $H_1 \otimes K_1$ is also called a cone over H_1 [38].

Theorem 3.2. *Let H_1 be an r-regular graph on n vertices and $H = H_1 \otimes K_1$. If $u \in V(K_1)$, then*

$$GSC(u, \beta) = \frac{-r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4} \beta \right)$$
$$+ \frac{r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4} \beta \right).$$

Proof. Since H has an EP with $V(H) = \{u\} \cup V(H_1)$, it follows that the divisor matrix of EP is $\boldsymbol{B} = \begin{pmatrix} 0 & n \\ 1 & r \end{pmatrix}$. By matrix diagonalization, we have

$$\boldsymbol{B} = \boldsymbol{S} \begin{pmatrix} \frac{r + \sqrt{r^2 + 4n}}{2} & 0 \\ 0 & \frac{r - \sqrt{r^2 + 4n}}{2} \end{pmatrix} \boldsymbol{S}^{-1},$$

where the eigenvalues of divisor matrix $\boldsymbol{B}$ are $\mu_1(\boldsymbol{B}) = \frac{r + \sqrt{r^2 + 4n}}{2}$ and $\mu_2(\boldsymbol{B}) = \frac{r - \sqrt{r^2 + 4n}}{2}$, respectively.

Let

$$S = \begin{pmatrix} \frac{-r + \sqrt{r^2 + 4n}}{2} & -\frac{r + \sqrt{r^2 + 4n}}{2} \\ 1 & 1 \end{pmatrix},$$

and

$$S^{-1} = \begin{pmatrix} \frac{1}{\sqrt{r^2 + 4n}} & \frac{r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \\ -\frac{1}{\sqrt{r^2 + 4n}} & \frac{-r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \end{pmatrix}.$$

So, we can obtain

$$\boldsymbol{B}^2 = S \begin{pmatrix} \frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4} & 0 \\ 0 & \frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4} \end{pmatrix} S^{-1}.$$

Therefore,

$$\exp\left(-\beta \boldsymbol{B}^2\right)$$
$$= S \begin{pmatrix} \exp\left(-\frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4}\beta\right) & 0 \\ 0 & \exp\left(-\frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4}\beta\right) \end{pmatrix} S^{-1}$$
$$= S \begin{pmatrix} \frac{1}{\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4}\beta\right) & \frac{r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4}\beta\right) \\ -\frac{1}{\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4}\beta\right) & \frac{-r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4}\beta\right) \end{pmatrix}.$$

According to Theorem 3.1, we have

$$GSC(u, \beta) = \frac{-r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n + 2r\sqrt{r^2 + 4n}}{4}\beta\right)$$
$$+ \frac{r + \sqrt{r^2 + 4n}}{2\sqrt{r^2 + 4n}} \exp\left(-\frac{2r^2 + 4n - 2r\sqrt{r^2 + 4n}}{4}\beta\right).$$

$\square$

Next, we calculate the generalized Gaussian subgraph centrality for a windmill graph by Theorem 3.2.

Example 3.3. *The $F_s = K_1 \otimes (sK_2)$ is also called the windmill graph with order $2s + 1$. The spectra of F_s are $\left\{ \frac{1 \pm \sqrt{8s+1}}{2}, -1^{[m]}, 1^{[m-1]} \right\}$ [38]. From Theorem 3.2, if $u \in V(K_1)$, where its degree is $2s$, then*

$$GSC(u, \beta) = \frac{-1 + \sqrt{8s + 1}}{2\sqrt{8s + 1}} \exp\left(-\frac{\sqrt{8s + 1} + 4s + 1}{2}\beta\right)$$
$$+ \frac{1 + \sqrt{8s + 1}}{2\sqrt{8s + 1}} \exp\left(\frac{\sqrt{8s + 1} - 4s - 1}{2}\beta\right).$$

The eigenvalues of F_s are known; we have

$$GEE(F_s, \beta) = (2s - 1) \exp(-\beta) + \exp\left(-\frac{\sqrt{8s+1}+4s+1}{2}\beta\right) + \exp\left(\frac{\sqrt{8s+1}-4s-1}{2}\beta\right).$$

If $v \in V(sK_2)$, where their degree is 2. Obviously, the $GSC(v, \beta)$ values of these vertices are the same, then

$$GSC(v, \beta) = \frac{1}{2s}\left((2s - 1)\exp(-\beta) + \frac{1+\sqrt{8s+1}}{2\sqrt{8s+1}}\exp\left(-\frac{\sqrt{8s+1}+4s+1}{2}\beta\right)\right.$$
$$\left. + \frac{-1+\sqrt{8s+1}}{2\sqrt{1+8s}}\exp\left(\frac{\sqrt{8s+1}-4s-1}{2}\beta\right)\right).$$

We further give the generalized Gaussian subgraph centrality formula of a class multicone graph by Theorem 3.2.

Example 3.4. *The $R_{s,n} = K_1 \otimes (sC_n)$ is called the multicone graph with order $sn + 1$, where $n \geq 3$. If $s > 1$, the spectra of $R_{s,n}$ are $\{1 \pm \sqrt{sn+1}, 2\cos\frac{2k\pi}{n}^{[s]}, 2^{[s-1]}\}$, where $k = 1, 2, \cdots, n-1$. If $s = 1$, the spectra of $R_{s,n}$ are $\{1 \pm \sqrt{n+1}, 2\cos\frac{2k\pi}{n}\}$, where $k = 1, 2, \cdots, n-1$ [50]. From Theorem 3.2, if $u \in V(K_1)$, where its degree is sn, then*

$$GSC(u, \beta) = \frac{-1+\sqrt{sn+1}}{2\sqrt{sn+1}}\exp\left(-\left(2 + sn + 2\sqrt{sn+1}\right)\beta\right)$$
$$+ \frac{1+\sqrt{sn+1}}{2\sqrt{sn+1}}\exp\left(-\left(2 + sn - 2\sqrt{sn+1}\right)\beta\right).$$

The eigenvalues of $R_{s,n}$ are known; we have
Case 1. *If $s = 1$, then*

$$GEE(R_{1,n}, \beta) = \sum_{k=1}^{n-1}\exp\left(-4\cos^2\frac{2k\pi}{n}\beta\right) + \exp\left(-\left(2 + n + 2\sqrt{n+1}\right)\beta\right)$$
$$+ \exp\left(-\left(2 + n - 2\sqrt{n+1}\right)\beta\right).$$

If $v \in V(sC_n)$, where their degree is 3. Obviously, the $GSC(v, \beta)$ values of these vertices are the same, then

$$GSC(v, \beta) = \frac{1}{n}\left(GEE(R_{1,n}, \beta) - GSC(u, \beta)\right)$$
$$= \frac{1}{n}\left(\sum_{i=1}^{n-1}\exp\left(-4\cos^2\frac{2k\pi}{n}\beta\right) + \frac{1+\sqrt{n+1}}{2\sqrt{n+1}}\exp\left(-\left(2 + n + 2\sqrt{n+1}\right)\beta\right)\right.$$
$$\left. + \frac{\sqrt{n+1}-1}{2\sqrt{n+1}}\exp\left(-\left(2 + n - 2\sqrt{n+1}\right)\beta\right)\right).$$

Case 2. *If $s > 1$, then*

$$GEE(R_{s,n}, \beta) = s\sum_{k=1}^{n-1}\exp\left(-4\cos^2\frac{2k\pi}{n}\beta\right) + \exp\left(-\left(2 + sn + 2\sqrt{sn+1}\right)\beta\right)$$
$$+ \exp\left(-\left(2 + sn - 2\sqrt{sn+1}\right)\beta\right) + (s - 1)\exp(-4\beta).$$

If $v \in V(sC_n)$, where their degree is 3. Obviously, the $GSC(v, \beta)$ values of these vertices are the same, then

$$
\begin{aligned}
GSC(v, \beta) =& \frac{1}{sn} \left(GEE\left(R_{s,n}, \beta\right) - GSC(u, \beta) \right) \\
=& \frac{1}{sn} \left(s \sum_{k=1}^{n-1} \exp\left(-4 \cos^2 \frac{2k\pi}{n} \beta\right) \right. \\
& + (s-1) \exp(-4\beta) + \frac{1 + \sqrt{sn+1}}{2\sqrt{sn+1}} \exp\left(-\left(2 + sn + 2\sqrt{sn+1}\right)\beta\right) \\
& \left. + \frac{\sqrt{sn+1} - 1}{2\sqrt{sn+1}} \exp\left(-\left(2 + sn - 2\sqrt{sn+1}\right)\beta\right) \right).
\end{aligned}
$$

Remark 1. *More studies of eigenvalues of multicone graphs (e.g., $K_1 \otimes (sK_n)$, $K_1 \otimes (s\overline{C_n})$) are shown in [38]. Similar to the proof of examples 3.3 and 3.4, these graphs' generalized Gaussian subgraph centrality can be immediately obtained from the conclusion of Theorem 3.2. In addition, for some classes of graphs, such as the transitive graph (e.g., K_n, Petersen graph) and the large symmetries graph (e.g., Dandelion graph, Cayley tree), the quotient matrix of the graphs used by Theorem 3.1 will be much smaller than the order of the adjacency matrix, so the convergence rate may be faster when using Theorems 3.1 and 3.2 to calculate the generalized Gaussian subgraph centrality than the adjacency matrix.*

Furthermore, we discuss the influence of the parameter β on the robustness of the generalized Gaussian subgraph centrality by calculating the parameter β change in examples 3.3 and 3.4. First, we give the change of the value of the generalized Gaussian subgraph centrality with the windmill and wheel graphs, respectively, by the formulas in examples 3.3 and 3.4, as shown in Tables 1 and 2 (the results are to be retained to four decimal places).

Table 1. Values of $GSC(u, \beta)$ are obtained for windmill graph F_s.

Graph	d_u	$\beta = 0.5$	$\beta = 0.7$	$\beta = 1$	$\beta = 1.5$	$\beta = 2$
F_3	6	0.0856	0.0372	0.0110	0.0015	0.0001
	2	0.5156	0.4181	0.3780	0.1861	0.1128
F_4	8	0.0366	0.0116	0.0021	0.0001	-
	2	0.5341	0.4355	0.3221	0.1953	0.1184
F_5	10	0.0155	0.0035	0.0004	-	-
	2	0.5470	0.4472	0.3311	0.2008	0.1218
F_6	12	0.0065	0.0011	0.0001	-	-
	2	0.5564	0.4553	0.3372	0.2045	0.1241
F_7	14	0.0027	0.0003	-	-	-
	2	0.5634	0.4611	0.3416	0.2072	0.1257

Table 2. Values of $GSC(u,\beta)$ are obtained for wheel graph $R_{1,n}$.

Graph	d_u	$\beta = 0.5$	$\beta = 0.7$	$\beta = 1$	$\beta = 1.5$	$\beta = 2$
$R_{1,3}$	3	0.4517	0.3729	0.2759	0.1673	0.1015
	3	0.4517	0.3729	0.2759	0.1673	0.1015
$R_{1,4}$	4	0.3385	0.2485	0.1570	0.0731	0.0341
	3	0.5670	0.5390	0.5196	0.5076	0.5033
$R_{1,5}$	5	0.2470	0.1619	0.0861	0.0301	0.0105
	3	0.4596	0.3838	0.3094	0.2360	0.1893
$R_{1,6}$	6	0.1783	0.1035	0.0459	0.0119	0.0031
	3	0.4404	0.3490	0.2518	0.1501	0.0905
$R_{1,7}$	7	0.1274	0.0652	0.0239	0.0045	0.0008
	3	0.4552	0.3788	0.3075	0.2425	0.2055

Sandwich coordination compounds, also known as metallocenes, are a fascinating class of organometallic compounds characterized by a metal atom sandwiched between two cyclopentadienyl anions [51]. The molecular graph for metallocenes can be represented as $R_{2,5} = K_1 \otimes (2C_5)$, where K_1 stands for a transition metal (e.g., iron atoms, chromium atom), and C_5 represents the cyclopentadienyl ring [52]. Like ferrocene and chromocene, many molecular structures can be represented by the molecular graph $R_{2,n}$ of the molecular sandwich structure. Therefore, our discussion on the influence of parameter β of generalized Gaussian subgraph centrality may further explain the physical and chemical properties of the molecular map of the sandwich structure, as shown in Table 3.

Table 3. Values of $GSC(u,\beta)$ are obtained for multicone graph $R_{2,n}$.

Graph	d_u	$\beta = 0.5$	$\beta = 0.7$	$\beta = 1$	$\beta = 1.5$	$\beta = 2$
$R_{2,3}$	6	0.1783	0.1035	0.0459	0.0119	0.0034
	3	0.4404	0.3490	0.2518	0.1501	0.0905
$R_{2,4}$	8	0.0903	0.0405	0.0122	0.0017	0.0002
	3	0.5564	0.5253	0.5076	0.5010	0.5001
$R_{2,5}$	10	0.0445	0.0152	0.0030	0.0002	-
	3	0.4544	0.3770	0.3042	0.2337	0.1885
$R_{2,6}$	12	0.0214	0.0055	0.0007	-	-
	3	0.4392	0.3465	0.2499	0.1494	0.0903
$R_{2,7}$	14	0.0164	0.0019	0.0001	-	-
	3	0.4565	0.3788	0.3071	0.2424	0.2055

As seen from the results in Tables 1, 2, and 3. When $\beta = 1$ is used as the basis for calculating the generalized Gaussian subgraph centrality, F_7 requires more digits to compute. As the number of F_n nodes increases, higher precision is required to obtain the results for F_n. Therefore, when $\beta \leq 0.7$, the result is conducive to the numerical analysis of the graph (network) and structural analysis. From a chemical analysis perspective, taking the molecular structure of ferrocene as an example, nodes with a higher degree are prone to substitution reactions, which correspond to nodes with generalized Gaussian subgraph centrality values close to 0. Therefore, appropriately increasing β may be beneficial in identifying the positions of atoms that are prone to substitution. So, the parameter

β plays a significant role in understanding how variations in the molecular configuration can impact the reactivity and stability of metallocenes.

Below is the generalized Gaussian subgraph centrality formula for the graph, which utilizes a star set of graphs.

Theorem 3.5. *Let $\mathbb{X} \subseteq V(H)$ and the adjacency matrix of the subgraph induced by $\mathbb{X}$ be $A_{\mathbb{X}}$. Consider $\mathbb{X}$ as a star set corresponding to an eigenvalue μ of graph H, and $A = \begin{pmatrix} A_{\mathbb{X}} & T^{\top} \\ T & P \end{pmatrix}$. Suppose that $Q = P - \mu I$, $C = Q^{-1}TT^{\top} + Q$. Then,*
(1) *For any vertex $u \in \mathbb{X}$, we have*

$$GSC(u,\beta) = \sum_{u_1,u_2 \in N_u(\widetilde{\mathbb{X}})} \left(C^{-1} \left(\exp\left(-(C+\mu I)^2 \beta\right) - \exp\left(-\mu^2\beta\right) I \right) Q^{-1} \right)_{u_1 u_2}$$
$$+ \exp\left(-\mu^2\beta\right),$$

where $N_u(\widetilde{\mathbb{X}})$ denotes the set of all adjacent vertices of u in $\widetilde{\mathbb{X}} = V(H)\backslash\mathbb{X}$.
(2) *For any $v \in \widetilde{\mathbb{X}} = V(H)\backslash\mathbb{X}$, we can obtain*

$$GSC(v,\beta) = \left(\exp\left(-\mu^2\beta\right) Q^{-1}TT^{\top}C^{-1} + \left(I - Q^{-1}TT^{\top}C^{-1}\right) \exp\left(-(C+\mu I)^2\beta\right) \right)_{vv}.$$

Proof. According to Lemma 2.2 and $C = Q^{-1}TT^{\top} + Q = Q^{-1}\left(TT^{\top} + Q^2\right)$, we can obtain

$$A - \mu I = \begin{pmatrix} A_{\mathbb{X}} - \mu I & T^{\top} \\ T & Q \end{pmatrix} = \begin{pmatrix} I & 0 \\ -Q^{-1}T & I \end{pmatrix} \begin{pmatrix} 0 & T^{\top} \\ 0 & C \end{pmatrix} \begin{pmatrix} I & 0 \\ Q^{-1}T & I \end{pmatrix}.$$

Since $TT^{\top} + Q^2$ is positive definite and C is nonsingular, it follows that

$$A = S \begin{pmatrix} \mu I & 0 \\ 0 & C + \mu I \end{pmatrix} S^{-1},$$

where

$$S = \begin{pmatrix} I & 0 \\ -Q^{-1}T & I \end{pmatrix} \begin{pmatrix} I & T^{\top}C^{-1} \\ 0 & I \end{pmatrix} = \begin{pmatrix} I & T^{\top}C^{-1} \\ -Q^{-1}T & I - Q^{-1}TT^{\top}C^{-1} \end{pmatrix},$$

$$S^{-1} = \begin{pmatrix} I & -T^{\top}C^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ Q^{-1}T & I \end{pmatrix} = \begin{pmatrix} I - T^{\top}C^{-1}Q^{-1}T & -T^{\top}C^{-1} \\ Q^{-1}T & I \end{pmatrix}.$$

Then

$$\exp\left(-\beta A^2\right)$$
$$= S \begin{pmatrix} \exp\left(-\mu^2\beta\right)I & 0 \\ 0 & \exp\left(-(C+\mu I)^2\beta\right) \end{pmatrix} S^{-1}$$
$$= \begin{pmatrix} I & T^{\top}C^{-1} \\ -Q^{-1}T & I - Q^{-1}TT^{\top}C^{-1} \end{pmatrix} \begin{pmatrix} \exp\left(-\mu^2\beta\right)I & 0 \\ 0 & \exp\left(-(C+\mu I)^2\beta\right) \end{pmatrix} S^{-1}$$
$$= \begin{pmatrix} \exp\left(-\mu^2\beta\right)I & T^{\top}C^{-1}\exp\left(-(C+\mu I)^2\beta\right) \\ -\exp\left(-\mu^2\beta\right)Q^{-1}T & \exp\left(-(C+\mu I)^2\beta\right) - Q^{-1}TT^{\top}C^{-1}\exp\left(-(C+\mu I)^2\beta\right) \end{pmatrix} S^{-1}.$$

Therefore, we can obtain the generalized Gaussian subgraph centrality of H as follows:

(1) For any vertex $u \in \mathbb{X}$, we can obtain

$$GSC(u,\beta) = \sum_{u_1,u_2 \in N_u(\widetilde{\mathbb{X}})} \left(C^{-1} \left(\exp\left(-(C + \mu I)^2 \beta \right) - \exp\left(-\mu^2 \beta \right) I \right) Q^{-1} \right)_{u_1 u_2}$$
$$+ \exp\left(-\mu^2 \beta \right),$$

where $N_u(\widetilde{\mathbb{X}})$ denotes the set of all adjacent vertices of u in $\widetilde{\mathbb{X}} = V(H) \backslash \mathbb{X}$.

(2) For any vertex $v \in \widetilde{\mathbb{X}}$, we can obtain

$$GSC(v,\beta) = \left(\exp\left(-\mu^2 \beta \right) Q^{-1} TT^{\top} C^{-1} + \left(I - Q^{-1} TT^{\top} C^{-1} \right) \exp\left(-(C + \mu I)^2 \beta \right) \right)_{vv}.$$

$\square$

Remark 2. *The emergence of the star complement technique is a method to study the problem of graph space and graph isomorphism. However, it is still challenging to find the maximal graphs corresponding to nice star complements; literature [53] still gives some small μ-rank (the value of $t = n - s$ is as small as possible, where s is the multiplicity of the eigenvalues of μ) graphs with good structural characteristics. The order of the matrices of these small μ-rank graphs is much smaller than that of the adjacency matrices. Therefore, Theorem 3.5 can significantly improve the convergence rate of calculating the centrality of generalized Gaussian subgraphs in theory. However, we cannot find a good way to obtain nice star complements of graphs, which is also our future research direction.*

4. Bounds of generalized Gaussian Estrada index

In this section, we get some bounds of the generalized Gaussian Estrada index based on the count of vertices and edges in graph H. We determine the bounds of $GEE(H,\beta)$ by some graph parameters as follows.

Theorem 4.1. *Let H be a graph with n vertices and m edges, then*

$$\sqrt{n - 4\beta m + n(n-1)e^{-\frac{4\beta m}{n}}} \le GEE(H,\beta) \le n - 2\beta m - 1 - \omega + e^{\omega},$$

where $\omega = \sqrt{2m\beta^2 + m\beta^2 \left(\frac{2m}{n-1} + n - 2 \right)}$ and the equality mentioned above is valid if and only if $H \cong \overline{K_n}$.

Proof. According to the generalized Gaussian Estrada index definition, we have

$$GEE^2(H,\beta) = \sum_{i=1}^{n} e^{-2\beta\mu_i^2} + 2 \sum_{1 \le i < j \le n} e^{-\beta\mu_i^2} e^{-\beta\mu_j^2}.$$

From the arithmetic-geometric inequality $\frac{\sum_{i=1}^{n} x_i}{n} \ge \sqrt[n]{\prod_{i=1}^{n} x_i}$ for positive number x, in which equality holds if and only if $x_1 = x_2 = \cdots = x_n$. For $\sum_{i=1}^{n} \mu_i^2 = 2m$, we can obtain

$$2 \sum_{1 \le i < j \le n} e^{-\beta\mu_i^2} e^{-\beta\mu_j^2} \ge n(n-1) \left(\prod_{1 \le i < j \le n} e^{-\beta\mu_i^2} e^{-\beta\mu_j^2} \right)^{\frac{2}{n(n-1)}} = n(n-1) \left(\prod_{1 \le i \le n} e^{-\beta\mu_i^2} \right)^{\frac{2}{n}}$$

$$= n(n-1) \left(e^{-\beta \sum_{i=1}^{n} \mu_i^2} \right)^{\frac{2}{n}} = n(n-1)e^{-\frac{4\beta m}{n}}.$$

From the expansion of Taylor series $e^{-x} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!}$ and $e^{-x} \geq 1-x$ for positive number x, it follows that

$$\sum_{k=2}^{\infty} \frac{(-x)^k}{k!} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!} - (1-x) = e^{-x} - (1-x) \geq 0.$$

So we can obtain

$$\sum_{i=1}^{n} e^{-2\beta\mu_i^2} = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\left(-2\beta\mu_i^2\right)^k}{k!} = n - 4\beta m + \sum_{i=1}^{n} \sum_{k=2}^{\infty} \frac{\left(-2\beta\mu_i^2\right)^k}{k!} \geq n - 4\beta m.$$

By substituting the mentioned formula and solving for $GEE(H,\beta)$, we obtained

$$GEE^2(H,\beta) \geq n - 4\beta m + n(n-1)e^{-\frac{4\beta m}{n}},$$

then

$$GEE(H,\beta) \geq \sqrt{n - 4\beta m + n(n-1)e^{-\frac{4\beta m}{n}}},$$

where $\beta > 0$.

We also give an upper bound by Lemma 2.3.

$$\begin{aligned}
GEE(H,\beta) &= n - 2\beta m + \sum_{i=1}^{n} \sum_{k=2}^{\infty} \frac{\left(-\beta\mu_i^2\right)^k}{k!} \\
&\leq n - 2\beta m + \sum_{k=2}^{\infty} \frac{1}{k!} \sum_{i=1}^{n} \left|\beta\mu_i^2\right|^k \\
&\leq n - 2\beta m + \sum_{k=2}^{\infty} \frac{1}{k!} \left(\sum_{i=1}^{n} \beta^2 \mu_i^2\right)^{k/2} \\
&\leq n - 2\beta m + \sum_{k=2}^{\infty} \frac{1}{k!} \left(2mt^2 + mt^2\left(\frac{2m}{n-1} + n - 2\right)\right)^{k/2} \\
&= n - 2\beta m - 1 - \omega + \sum_{k=0}^{\infty} \frac{\omega^k}{k!} \\
&= n - 2\beta m - 1 - \omega + e^{\omega},
\end{aligned}$$

where $\omega = \sqrt{2m\beta^2 + m\beta^2\left(\frac{2m}{n-1} + n - 2\right)}$.

Based on the previous derivation, it is evident that equality holds if and only if graph H has all eigenvalues equal to zero. This condition is only satisfied by the empty graph $\overline{K_n}$.

$\square$

Next, we give another simple lower bound for $GEE(H,\beta)$.

Theorem 4.2. *Let H be a graph with n vertices and m edges, then*

$$GEE(H, \beta) \geq n - 2\beta m,$$

the equality holds if and only if $H \cong \overline{K_n}$.

Proof. Similar to the analysis of Theorem 4.1, we have

$$GEE(H, \beta) = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\left(-\beta \mu_i^2\right)^k}{k!} = n - 2\beta m + \sum_{i=1}^{n} \sum_{k=2}^{\infty} \frac{\left(-\beta \mu_i^2\right)^k}{k!}$$

From the expansion of Taylor series $e^{-x} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!}$ and $e^{-x} \geq 1 - x$ for positive number x, it follows that

$$\sum_{k=2}^{\infty} \frac{(-x)^k}{k!} = \sum_{k=0}^{\infty} \frac{(-x)^k}{k!} - (1 - x) = e^{-x} - (1 - x) \geq 0.$$

Consequently, for any $\epsilon \in [0, 1]$, we have

$$GEE(H, \beta) \geq n - 2\beta m + \epsilon \sum_{i=1}^{n} \sum_{k=2}^{\infty} \frac{\left(-\beta \mu_i^2\right)^k}{k!}$$

$$= n - 2\beta m - \epsilon n + 2\beta m \epsilon + \epsilon \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\left(-\beta \mu_i^2\right)^k}{k!}$$

$$= (1 - \epsilon)n + 2(\epsilon - 1)\beta m + \epsilon \, GEE(H, \beta).$$

For $\epsilon < 1$, it follows that

$$GEE(H, \beta) \geq \frac{(1 - \epsilon)n + 2(\epsilon - 1)\beta m}{1 - \epsilon} = n - 2\beta m.$$

Based on the previous derivation, it is evident that equality holds if and only if graph H has all eigenvalues equal to zero. This condition is only satisfied by the empty graph $\overline{K_n}$. $\qquad \square$

5. Conclusions

The Estrada index and subgraph centrality for exploring network structure and properties focus more on the influence of extreme eigenvalues on network structure and properties. Unlike the well-known Estrada index and subgraph centrality, $GSC(u, \beta)$ and $GEE(H, \beta)$, under the Gaussian function definition, assign more weight to zero eigenvalues (if they exist) and near-zero eigenvalues to the network structure. At the same time, $GSC(u, \beta)$ and $GEE(H, \beta)$ are highly related to frontier orbital theory in quantum chemistry, so studying $GSC(u, \beta)$ and $GEE(H, \beta)$ is valuable. In this paper, since every graph has EP and a star set, against this background, we give some new formulas to calculate $GSC(u, \beta)$. We can obtain $GSC(u, \beta)$ formulas using a smaller matrix than the adjacency matrix. The influence of the parameter β on the robustness of the formula is explored through experiments. In addition, we also give some bounds for $GEE(H, \beta)$. Based on the above research and recent research results, our future work will study $GSC(u, \beta)$ and $GEE(H, \beta)$ of random and dynamic graphs.

Author contributions

Yang Yang: Writing-review & editing, Writing-original draft, Visualization, Validation, Supervision, Software, Project administration, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. Yanyan Song: Writing-review & editing. Haifeng Fan: Writing-review & editing, Writing-original draft, Methodology, Investigation, Funding acquisition. Haiyan Qiao: Writing-review & editing, Funding acquisition. Yang Yang and Yanyan Song contribute equally to the article.

Use of Generative-AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Acknowledgments

Conflict of interest

The authors declare no conflict of interest.

References

1. E. Estrada, *The structure of complex networks: theory and applications*, American Chemical Society, 2012. https://doi.org/10.1093/acprof:oso/9780199591756.001.0001

2. R. Cohen, S. Havlin, *Complex networks: Structure, robustness and function*, Cambridge University Press, 2010. https://doi.org/10.1017/cbo9780511780356

3. H. J. Leavitt, Some effects of certain communication patterns on group performance, *J. Abnorm. Soc. Psychol.,* **46** (1951), 38–50. https://doi.org/10.1037/h0057189

4. Y. Yustiawan, W. Maharani, A. A. Gozali, Degree centrality for social network with opsahl method, *Procedia Comput. Sci.,* **59** (2015), 419–426. https://doi.org/10.1016/j.procs.2015.07.559

5. U. Brandes, S. P. Borgatti, L. C. Freeman, Maintaining the duality of closeness and betweenness centrality, *Soc. Networks,* **44** (2016), 153–159. https://doi.org/10.1016/j.socnet.2015.08.003

6. S. Zhao, S. Sun, Identification of node centrality based on Laplacian energy of networks, *Physica A,* **609** (2023), 128353. https://doi.org/10.1016/j.physa.2022.128353

7. Z. Li, T. Ren, X. Ma, S. Liu, Y. Zhang, T. Zhou, Identifying influential spreaders by gravity model, *Sci. Rep.,* **9** (2019), 8387. https://doi.org/10.1038/s41598-019-44930-9

8. S. Iyer, T. Killingback, B. Sundaram, Z. Wang, Attack robustness and centrality of complex networks, *PloS one,* **8** (2013), e59613. https://doi.org/10.1371/journal.pone.0059613

9. V. Latora, M. Marchiori, A measure of centrality based on network efficiency, *New J. Phys.,* **9** (2007), 188. https://doi.org/10.1088/1367-2630/9/6/188

10. C. Salavati, A. Abdollahpouri, Z. Manbari, Ranking nodes in complex networks based on local structure and improving closeness centrality, *Neurocomputing,* **336** (2019), 36–45. https://doi.org/10.1016/j.neucom.2018.04.086

11. E. Estrada, D. J. Higham, Network properties revealed through matrix functions, *SIAM Rev.,* **52** (2010), 696–714. https://doi.org/10.1137/090761070

12. E. Estrada, J. A. Rodriguez-Velazquez, Subgraph centrality in complex networks, *Phys. Rev. E,* **71** (2005), 056103. https://doi.org/10.1103/PhysRevE.71.056103

13. S. Amirrahmat, K. A. Alshibli, Subgraph centrality: A complex network metric to characterize the contact network between sheared sand particles, *Comput. Geotech.,* **169** (2024), 106211. https://doi.org/10.1016/j.compgeo.2024.106211

14. E. Estrada, Communicability cosine distance: similarity and symmetry in graphs/networks, *Comput. Appl. Math.,* **43** (2024), 49. https://doi.org/10.1007/s40314-023-02571-9

15. K. Bakhat, K. Kifayat, M. S. Islam, M. M. Islam, Katz centrality based approach to perform human action recognition by using OMKZ, *Signal Image Video P.,* **17** (2023), 1677–1685. https://doi.org/10.1007/s11760-022-02378-x

16. F. Arrigo, F. Durastante, Mittag-Leffler functions and their applications in network science, *SIAM J. Matrix Anal. Appl.,* **42** (2021), 1581–1601. https://doi.org/10.1137/21M1407276

17. A. Alhomaidhi, F. Al-Thukair, E. Estrada, Double gaussianization of graph spectra, *Appl. Math. Model.,* **93** (2021), 134–147. https://doi.org/10.1016/j.apm.2020.12.018

18. E. Estrada, A. A. Alhomaidhi, F. Al-Thukair, Exploring the "Middle Earth" of network spectra via a Gaussian matrix function, *Chaos,* **27** (2017), 023109. https://doi.org/10.1063/1.4976015

19. Y. Shang, Lower bounds for Gaussian Estrada index of graphs, *Symmetry,* **10** (2018), 325. https://doi.org/10.3390/sym10080325

20. E. Estrada, The electron density function of the Hückel (tight-binding) model, *Proc. R. Soc. A,* **474** (2018), 20170721.https://doi.org/10.1098/rspa.2017.0721

21. E. Estrada, The many facets of the estrada indices of graphs and networks, *SeMA J.,* **79** (2022), 57–125.https://doi.org/10.1007/s40324-021-00275-w

22. B. Mazouin, A. A. Schöpfer, O. A. von Lilienfeld, Selected machine learning of HOMO-LUMO gaps with improved data-efficiency, *Mater. Adv.,* **3** (2022), 8306–8316. https://doi.org/10.1039/D2MA00742H

23. X. Li, Y. Li, Y. Shi, I. Gutman, Note on the HOMO-LUMO index of graphs, *MATCH Commun. Math. Comput. Chem.,* **70** (2013), 85–96.https://doi.org/10.1155/2013/397382

24. P. W. Fowler, T. Pisanski, HOMO-LUMO maps for chemical graphs, *MATCH Commun. Math. Comput. Chem.,* **64** (2010), 373–390.https://doi.org/10.1007/s10985-009-9124-6

25. K. Fukui, T. Yonezawa, H. Shingu, A molecular orbital theory of reactivity in aromatic hydrocarbons, *J. Chem. Phys.,* **20** (1952), 722–725. https://doi.org/10.1063/1.1700523

26. W. Kutzelnigg, What I like about Hückel theory, *J. Comput. Chem.,* **28** (2007), 25–34. https://doi.org/10.1002/jcc.20470

27. L. W. Wang, A. Zunger, Solving Schrödinger's equation around a desired energy: application to silicon quantum dots, *J. Chem. Phys.,* **100** (1994), 2394. https://doi.org/10.1063/1.466486

28. E. R. Gagliano, C. A. Balseiro, Dynamic correlation functions in quantum many-body systems at zero temperature, *Phys. Rev. B,* **38** (1988), 11766–11773. https://doi.org/10.1103/PhysRevB.38.11766

29. J. E. Hirsch, J. R. Schrieffer, Dynamic correlation functions in quantum systems: a monte carlo algorithm, *Phys. Rev. B,* **28** (1983), 5353–5356. https://doi.org/10.1103/PhysRevB.28.5353

30. Y. Shang, Resilient tracking consensus over dynamic random graphs: A linear system approach, *European J. Appl. Math.,* **34** (2023), 408–423. https://doi.org/10.1017/S0956792522000225

31. Y. Shang, Non-linear consensus dynamics on temporal hypergraphs with random noisy higher-order interactions, *J. Complex. Netw.,* **11** (2023), cnad009. https://doi.org/10.1093/comnet/cnad009

32. Y. Shang, Sombor index and degree-related properties of simplicial networks, *Appl. Math. Comput.,* **419** (2022), 126881. https://doi.org/10.1016/j.amc.2021.126881

33. Y. C. Zhi, Y. C. Ng, X. W. Dong, Gaussian processes on graphs via spectral kernel learning, *IEEE T. Signal. Inf. Pr.,* **9** (2023), 304–314. https://doi.org/10.1109/TSIPN.2023.3265160

34. L. Cosmo, G. Minello, A. Bicciato, A. Bronstein, M. M. Rodola, E. Rossi, Graph kernel neural networks, *IEEE Neur. Net. Lear.,* 2024, 1–14.https://doi.org/10.1109/TNNLS.2024.3400850

35. V. T. Hoang, H. J. Jeon, E. S. You, Y. Yoon, S. Jung, O. J. Lee, Graph representation learning and its applications: A survey, *Sensors,* **23** (2023), 4168. https://doi.org/10.3390/s23084168

36. C. D. Godsil, Compact graphs and equitable partitions, *Linear Algebra Appl.,* **255** (1997), 259–266.https://doi.org/10.1016/S0024-3795(97)83595-1

37. F. Atik, On equitable partition of matrices and its applications, *Linear Multilinear Algebra,* **68** (2020), 2143–2156. https://doi.org/10.1080/03081087.2019.1572708

38. D. Cvetković, P. Rowlinson, S. Simić, *An introduction to the theory of graph spectra*, Cambridge University Press, 2010. https://doi.org/10.1017/cbo9780511801518

39. C. O. Aguilar, Strongly uncontrollable network topologies, *IEEE Trans. Control Netw. Syst.,* **7** (2019), 878–886. https://doi.org/10.1109/TCNS.2019.2951665

40. I. Michos, V. Raptis, Graph partitions in chemistry, *Entropy,* **25** (2023), 1504. https://doi.org/10.3390/e25111504

41. M. T. Schaub, N. Oclery, Y. N. Billeh, J. C. Delvenne, R. Lambiotte, M. Barahona, Graph partitions and cluster synchronization in networks of oscillators, *Chaos,* **26** (2016), 27-41. https://doi.org/10.1063/1.4961065

42. H. Krovi, T. A. Brun, Quantum walks on quotient graphs, *Phys. Rev. A,* **75** (2007), 062332. https://doi.org/10.1103/PhysRevA.75.062332

43. C. Godsil, G. Royle. *Algebraic Graph Theory*, Springer, 2001.

44. L. You, M. Yang, W. So, W. G. Xi, On the spectrum of an equitable quotient matrix and its application, *Linear Algebra Appl.,* **577** (2019), 21–40. https://doi.org/10.1016/j.laa.2019.04.013

45. D. Cvetković, P. Rowlinson, Star complements and exceptional graphs, *Linear Algebra Appl.,* **423** (2007), 146–154. https://doi.org/10.1016/j.laa.2007.01.008

46. D. Cvetković, M. Lepović, P. Rowlinson, S. Simić, The maximal exceptional graphs, *J. Combin. Theory Ser. B.,* **86** (2002), 347–363. https://doi.org/10.1006/jctb.2002.2132

47. P. Rowlinson, I. Sciriha, Some properties of the Hoffman-Singleton graph, *Appl. Anal. Discrete Math.,* **1** (2007), 438–445.https://www.jstor.org/stable/43666073

48. C. Bu, X. Zhang, J. Zhou, A note on the multiplicities of graph eigenvalues, *Linear Algebra Appl.,* **442** (2014), 69–74. https://doi.org/10.1016/j.laa.2013.08.003

49. D. Stevanović, M. Milošević, A spectral proof of the uniqueness of a strongly regular graph with parameters (81, 20, 1, 6), *Eur. J. Comb.,* **30** (2009), 957–968. https://doi.org/10.1016/j.ejc.2008.07.021

50. A. Z. Abdian, L. W. Beineke, K. Thulasiraman, R. T. Khorami, M. R. Oboudi, The spectral determination of the connected multicone graphs $K_\omega \nabla r C_s$, *AKCE Int. J. Graphs Comb.,* **18** (2021), 47–52. https://doi.org/10.1080/09728600.2021.1917974

51. E. J. Maslowsky, Inorganic metallocenes: the structures and aromaticity of sandwich compounds of the transition elements with inorganic rings, *Coordin Chem. Rev. ,* **255** (2011), 2746–2763. https://doi.org/10.1016/j.ccr.2011.04.011

52. C. A. P. Goodwin, What is a sandwich complex?, *Inorg. Chem.,* **63** (2024), 9363–9365. https://doi.org/10.1021/acs.inorgchem.4c00243

53. B. Tayfeh-Rezai, The star complement technique online lecture note, 2009. `http://math.ipm.ac.ir/tayfehr/papersandpreprints/starcompl.pdf`

54. K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujev. J. Math.,* **25** (2003), 19–41. http://elib.mi.sanu.ac.rs/files/journals/kjm/25/d003download.pdf