

λ -Core Distance Partitions

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Abstract

The λ -core vertices of a graph correspond to the non-zero entries of some eigenvector of λ for a universal adjacency matrix \mathbf{U} of the graph. We define a partition of the vertex set V based on the λ -core vertex set and its neighbourhoods at a distance r , and give a number of results relating the structure of the graph to this partition. For such partitions, we also define an entropic measure for the information content of a graph, related to every distinct eigenvalue λ of \mathbf{U} , and discuss its properties and potential applications.

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

1. Introduction

1.1. Nomenclature

An undirected graph $G = (V, E)$ has a finite vertex set $V = \{v_1, \dots, v_n\}$ and an edge set E of 2-element subsets of V . We use n exclusively to denote the number of vertices. The graphs we consider are connected and without loops or multi-edges. We predominantly use the definitions of Cvetković et al. (2009), with notation adapted accordingly.

The adjacency matrix of a graph G is the $n \times n$ matrix $\mathbf{A} = (a_{ij})$ such that $a_{ij} = 1$ if the vertices v_i and v_j are adjacent and $a_{ij} = 0$ otherwise. The degree matrix is the $n \times n$ matrix $\mathbf{D} = \text{diag}(\rho(v_1), \dots, \rho(v_n))$, where $\rho(v)$ is the number of edges incident to v . Let \mathbf{I} and \mathbf{J} denote the $n \times n$ identity and all-ones matrices, respectively. Haemers and Omid (2011) defined the universal adjacency matrix $\mathbf{U} = \gamma_A \mathbf{A} + \gamma_D \mathbf{D} + \gamma_I \mathbf{I} + \gamma_J \mathbf{J}$, for some scalars $\gamma_A \neq 0, \gamma_D, \gamma_I$ and γ_J . Depending on the choice of parameters, \mathbf{U} encodes a number of well-known and important matrices in graph theory, most notably the adjacency and Laplacian matrices.

The eigenvalue spectrum of a symmetric $n \times n$ matrix \mathbf{M} is a multi-set denoted by $\text{spec}(\mathbf{M})$, where for $\lambda^{(m_{\mathbf{M}}(\lambda))} \in \text{spec}(\mathbf{M})$, λ is the eigenvalue and $m_{\mathbf{M}}(\lambda)$ is the multiplicity of λ in the spectrum. For brevity, we shall (with some abuse of notation) simply write $\lambda \in \text{spec}(\mathbf{M})$.

A vertex v_i of a graph G is a λ -core vertex for \mathbf{U} if there exists an eigenvector \mathbf{x} of \mathbf{U} such that $\mathbf{U}\mathbf{x} = \lambda\mathbf{x}$ and the i^{th} entry of \mathbf{x} is non-zero. Otherwise, v_i is said to be a λ -core-forbidden vertex. The sets of λ -core and λ -core-forbidden vertices for \mathbf{U} are denoted by CV_λ and CFV_λ respectively. Diagrammatically, we draw  to represent λ -core vertices,  for vertices which have a λ -core neighbour but are not λ -core themselves, and  otherwise.

The terms *core* and *core-forbidden* vertices were first introduced by Sciriha (1997) for the kernel of \mathbf{A} . Similar concepts exist: for example, in linear algebra the core-forbidden vertices that increase the multiplicity of λ are termed as *Parter* vertices (after the work of S. Parter during the 1960s), while those that leave the multiplicity unchanged are called *neutral* vertices. The core vertices are termed as *downer* vertices, since they decrease the multiplicity of λ . In the context of the Laplacian, the core-forbidden vertices are typically known as the *Fiedler* vertices, after the pioneering work by M. Fiedler throughout the 1970s and 1980s.

More recently, new terminology has been introduced for different contexts. Of significant importance are the 0-core and 0-core-forbidden vertices, which have been studied greatly for singular trees. The nullity $\eta(G)$ of a graph is the dimension of the kernel of \mathbf{A} . In Fernandes and da Cruz (2018), the 0-core-forbidden vertices of a tree are termed as *F*-vertices. Those vertices that, in particular, increase the nullity of T or the multiplicity of 0 for the Laplacian of T , are termed as *P*-vertices.

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1.2. Overview

For a graph G with independent λ -core vertices, the set of their neighbours $N(CV_\lambda)$ is disjoint from CV_λ . Hence one can define a partition of V with blocks CV_λ , $N(CV_\lambda)$, and $CFV_{R,\lambda}$ (which is the set of remaining vertices not in CV_λ and $N(CV_\lambda)$). Such a partitioning was studied closely for the eigenvalue $\lambda = 0$ of \mathbf{A} by Sciriha et al. (2020) for graphs with independent CV_0 , and by Jaume and Molina (2018) for the case of singular trees (which always have an independent CV_0). In Section 2, we introduce the λ -Core Distance Partition (λ -CDP), which is a natural generalisation for the case when CV_λ is not an independent set and hence $N(CV_\lambda)$ is not disjoint from CV_λ . Moreover, we study the relation between the λ -CDP and the symmetries of the graph, and how the core distance partitions of two distinct eigenvalues relate to each other.

In Section 3 we define an index for the information content of a graph related to its λ -CDP, and study its lower and upper bounds for a fixed number of vertices n and varying number of λ -core vertices, $|CV_\lambda|$. Lastly in Section 4 we consider a number of applications related to this index and the structure of graphs with a singular adjacency matrix, most notably molecular graphs.

2. λ -Core Distance Partitions

Consider a connected graph G , and $\lambda \in \text{spec}(\mathbf{U})$. The function $d(u, v): V \times V \rightarrow \mathbb{N} \cup \{0\}$ gives the length of the shortest path between any two vertices u and v . We define the minimum distance from any vertex $v \in V$ to some λ -core vertex $u \in CV_\lambda$ by the function $d_\lambda(v): V \rightarrow \mathbb{N} \cup \{0\}$,

$$d_\lambda(v) = \min \{d(v, u) : u \in CV_\lambda\}. \quad (2.1)$$

The non-negative integer $D_\lambda = \max \{d_\lambda(v) : v \in V\}$ is the maximum distance assigned by d_λ to a vertex, which is bounded above by the diameter of the graph. We define the set of vertices at a minimum distance $0 \leq i \leq D_\lambda$ from λ -core vertex as the set $V_{\lambda,i} = \{v \in V : d_\lambda(v) = i\}$. It follows then that $CV_\lambda = V_{\lambda,0}$.

Proposition 2.1 (λ -Core Distance Partition). *Let $\lambda \in \text{spec}(\mathbf{U})$. The collection $\mathcal{V}_\lambda = \{V_{\lambda,0}, \dots, V_{\lambda,D_\lambda}\}$ is a partition of V .*

Proof. Since G is connected, there exists a path between any pair of vertices. In particular, every vertex $v \in V$ has a shortest path to some λ -core vertex. Hence d_λ exists for every vertex $v \in V$ and therefore v belongs to some $V_{\lambda,i} \in \mathcal{V}_\lambda$, for $0 \leq i \leq D_\lambda$. Clearly then, V is the union of $V_{\lambda,0}, \dots, V_{\lambda,D_\lambda}$.

Moreover, since d_λ is clearly not one-to-many, we have that the intersection of $V_{\lambda,i}$ and $V_{\lambda,j}$ is empty, for $i \neq j$. The result follows. \square

Remark 2.2. Note that d_λ gives an equivalence relation, where two vertices u and v are said to be related if $d_\lambda(u) = d_\lambda(v)$. Hence the λ -CDP \mathcal{V}_λ is in fact a collection of equivalence classes.

2.1. λ -Core Distance Partitions and Orbit Structure

The automorphism group $\text{Aut}(G)$ of a graph is the group from G onto itself. If v_i is adjacent to v_j then for any automorphism $\sigma \in \text{Aut}(G)$, $\sigma(v_i)$ is adjacent to $\sigma(v_j)$. The *orbit* of $\text{Aut}(G)$ on $v \in V$ is the set $\pi(v) = \{\sigma(v) : \sigma \in \text{Aut}(G)\}$. We denote the set of orbits by Π . A graph G is vertex-transitive if it has a single orbit. The orbits of $\text{Aut}(G)$ induce a partition $\Pi = \{\pi_1, \pi_2, \dots, \pi_s\}$ of V , known as the *orbital partition* of G .

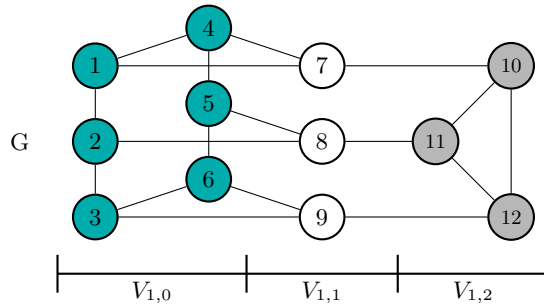


Figure 1: 1-CDP of the graph G , for $\mathbf{U} = \mathbf{A}$.

Consider the cubic graph G in Figure 1 as a motivating example. The spectrum of its adjacency matrix (up to 3 decimal places) is: $\{3^{(1)}, 2.115^{(1)}, 2^{(1)}, 1.303^{(1)}, 1^{(1)}, -0.254^{(1)}, -1^{(3)}, -1.861^{(1)}, -2^{(1)}, -2.303^{(1)}\}$. For $\lambda = 1$, the 1-CDP for $\mathbf{U} = \mathbf{A}$ is:

$$\mathcal{V}_1 = \{V_{1,0} = \{1, 2, 3, 4, 5, 6\}, V_{1,1} = \{7, 8, 9\}, V_{1,2} = \{10, 11, 12\}\}$$

Moreover, the orbits of $\text{Aut}(G)$ acting on V are,

$$\Pi = \{\pi_1 = \{1, 3, 4, 6\}, \pi_2 = \{2, 5\}, \pi_3 = \{7, 9\}, \pi_4 = \{8\}, \pi_5 = \{10, 12\}, \pi_6 = \{11\}\}$$

Notice that each block in the 1-CDP is a disjoint union of orbits in Π . In this section we will show that this holds for every λ -CDP of any universal adjacency matrix \mathbf{U} of G .

Given a permutation $\sigma \in \text{Aut}(G)$, there exists a corresponding permutation matrix \mathbf{P}_σ such that $\mathbf{P}_\sigma \mathbf{A} = \mathbf{A} \mathbf{P}_\sigma$. Since \mathbf{D} and \mathbf{I} have constant entries with respect to each orbit, and since \mathbf{J} is a constant matrix, then \mathbf{P}_σ also commutes with \mathbf{D} , \mathbf{I} , and \mathbf{J} . Since matrix multiplication is distributive, then \mathbf{U} and \mathbf{P}_σ commute: $\mathbf{U} \mathbf{P}_\sigma = \mathbf{P}_\sigma \mathbf{U}$. The following result is due to Akbari et al. (2013).

Proposition 2.3 (Akbari et al. (2013)). *Let G be vertex-transitive and $\lambda \in \text{spec}(\mathbf{A})$. Then every vertex of G is a λ -core vertex.*

The following proposition is a generalisation of Proposition 2.3, of which it is a special case for when G is vertex-transitive and hence has a single orbit.

Proposition 2.4. *Let $\lambda \in \text{spec}(\mathbf{U})$ and let u, v belong to the same orbit $\pi \in \Pi$. If u is a λ -core vertex, then v is also a λ -core vertex.*

Proof. Since u and v belong to the same orbit, it follows by the definition of an orbit that there exists a permutation $\sigma \in \text{Aut}(G)$, such that $\sigma(u) = v$. Let \mathbf{P}_σ be the corresponding permutation matrix. Since u is λ -core, there exists an eigenvector \mathbf{x} for λ such that the u^{th} entry of \mathbf{x} is non-zero. Now, $\mathbf{U} \mathbf{P}_\sigma \mathbf{x} = \mathbf{P}_\sigma \mathbf{U} \mathbf{x} = \lambda \mathbf{P}_\sigma \mathbf{x}$, since $\mathbf{U} \mathbf{P}_\sigma = \mathbf{P}_\sigma \mathbf{U}$ and $\mathbf{U} \mathbf{x} = \lambda \mathbf{x}$. Hence $\mathbf{P}_\sigma \mathbf{x}$ is an eigenvector of \mathbf{U} as well. Since \mathbf{P}_σ permutes the u^{th} entry of \mathbf{x} with the v^{th} entry, it follows that the v^{th} entry of $\mathbf{P}_\sigma \mathbf{x}$ is non-zero. Therefore v is a λ -core vertex. \square

Remark 2.5. It follows that all the vertices in the same orbit are either λ -core or λ -core forbidden. Hence, CV_λ is the disjoint union of some collection of orbits $\{\pi_{i_1}, \dots, \pi_{i_s}\} \subseteq \Pi$.

Theorem 2.6. *Let $\lambda \in \text{spec}(\mathbf{U})$ and $0 \leq i \leq D_\lambda$. Then $V_{\lambda,i}$ is the disjoint union of a collection of orbits $\{\pi_1, \dots, \pi_{s_i}\} \subseteq \Pi$.*

Proof. That $V_{\lambda,0} = CV_\lambda$ is the disjoint union of orbits is discussed in Remark 2.5. Suppose that up to some $0 \leq i < D_\lambda$, $\forall 0 \leq k \leq i$, $V_{\lambda,k}$ is the disjoint union of some collection of orbits $\Pi_k = \{\pi_1^{(k)}, \dots, \pi_{s_k}^{(k)}\} \subseteq \Pi$. We show that the claim holds for $i+1$.

Suppose that $V_{\lambda,i+1}$ is not the disjoint union of some collection of orbits. Then there exists two vertices u and v in an orbit π , such that v is in $V_{\lambda,i+1}$ and u is in $V_{\lambda,j}$, for some $i+2 \leq j \leq D_\lambda$. Note that π is distinct from those in the collection $\cup_{k=0}^i \Pi_k$.

By definition of the λ -CDP, v in $V_{\lambda,i+1}$ must have a neighbour in $V_{\lambda,i}$. Moreover, there must exist a permutation $\sigma \in \text{Aut}(G)$ which maps v to u while preserving adjacency. In particular, $V_{\lambda,k}$ for $0 \leq k \leq i$ are preserved since they are the disjoint union of orbits, and hence u must have a neighbour in $V_{\lambda,i}$. Since $i+1 < j$, then u has a path to some λ -core vertex of length less than j , and hence cannot be in $V_{\lambda,j}$, a contradiction. Therefore $V_{\lambda,i+1}$ is the disjoint union of some collection of orbits, completing the proof. \square

2.2. Relating the Core Distance Partitions of Two Distinct Eigenvalues

We continue our study of the relation between the spectrum of \mathbf{U} and the structure of G , in light of the λ -CDP. We say that for two distinct eigenvalues λ and μ , the μ -CDP can be *constructed* from the λ -CDP if every block in the μ -CDP is a disjoint union of blocks in the λ -CDP. In particular, we are interested in the following problem.

Problem 2.7. Let $\lambda \in \text{spec}(\mathbf{U})$ and let the λ -CDP be given. When does there exist an eigenvalue $\mu \neq \lambda$ of \mathbf{U} , such that the μ -CDP can be constructed from the λ -CDP?

As it turns out, if the λ -CDP is an equitable partition, then under certain circumstances reconstruction is possible. First however we require some preliminary definitions and results. The *characteristic matrix* \mathbf{C} of a partition $\{V_1, \dots, V_k\}$ is an $n \times k$ matrix, where the i^{th} column \mathbf{c}_i is associated with the block V_i , such that for every vertex in V_i the corresponding entry in \mathbf{c}_i is 1, and 0 otherwise. An *equitable partition* with k blocks is a partition of V such that there exists a $k \times k$ matrix \mathbf{B} , known as the *divisor matrix*, satisfying $\mathbf{U}\mathbf{C} = \mathbf{C}\mathbf{B}$.

Remark 2.8. Let \mathbf{x} be an eigenvector for μ of \mathbf{B} such that its i^{th} entry x_i is non-zero. If $\mathbf{C}\mathbf{x}$ is also an eigenvector for some $\lambda \in \text{spec}(\mathbf{U})$, then all the vertices in V_i must be λ -core vertices, since the corresponding entry in $\mathbf{C}\mathbf{x}$ is x_i by definition of \mathbf{C} .

It is well-known that for the case when $\mathbf{U} = \mathbf{A}$, the characteristic polynomial of \mathbf{B} divides the characteristic polynomial of \mathbf{A} (Theorem 3.9.5, Cvetković et al. (2009)). More generally, the result holds for any universal adjacency matrix \mathbf{U} , which we state as follows without proof.

Theorem 2.9. *Let \mathcal{C} be an equitable partition of V with divisor and characteristic matrices \mathbf{B} and \mathbf{C} , respectively. The characteristic polynomial of \mathbf{B} divides the characteristic polynomial of \mathbf{U} .*

Remark 2.10. Consider some λ -CDP \mathcal{V}_λ to be equitable. By combining Remark 2.8 and Theorem 2.9 we observe that for every eigenvalue of \mathbf{U} that is also an eigenvalue of \mathbf{B} , the core vertex set has a subset which is the disjoint union of some blocks in \mathcal{V}_λ .

Theorem 2.11. *Let $\lambda \in \text{spec}(\mathbf{U})$ and \mathcal{V}_λ be an equitable partition with divisor and characteristic matrices \mathbf{B} and \mathbf{C} , respectively. Let $\mu \in \text{spec}(\mathbf{B})$. Then there exists a subset of CV_μ which is the disjoint union of a finite collection of blocks in \mathcal{V}_λ . Moreover, if $m_{\mathbf{U}}(\mu) = m_{\mathbf{B}}(\mu)$ then equality holds between the two sets and \mathcal{V}_μ can be constructed from \mathcal{V}_λ .*

Proof. Let B be a basis for the eigenspace of μ for \mathbf{B} . Define the indexing set X_B of row-indices corresponding to some non-zero row of any vector \mathbf{b} in B : $X_B = \{i \in \{1, \dots, D_\lambda + 1\} : \exists \mathbf{b} \in B, \mathbf{b} \cdot \mathbf{e}_i \neq 0\}$. By definition of an equitable partition, each index i in X_B corresponds to the block $V_{\lambda, i-1}$ of \mathcal{V}_λ . As discussed in Remark 2.10 we have that $\bigcup_{i \in X_B} V_{\lambda, i-1} \subseteq CV_\mu$ and the first part of the result follows.

Let the basis B be $\{\mathbf{b}_1, \dots, \mathbf{b}_r\}$ and consider the set $B' = \{\mathbf{C}\mathbf{b}_1, \dots, \mathbf{C}\mathbf{b}_r\}$. Since B is an independent set, then B' must also be an independent set. By Remark 2.8 and Theorem 2.9, B' is a basis for some sub-space of the eigenspace of μ for \mathbf{U} . In the case that $m_{\mathbf{U}}(\mu) = m_{\mathbf{B}}(\mu)$, it follows that B' is a basis for the eigenspace of μ for \mathbf{U} . Since every vertex in CV_μ must correspond to a non-zero entry for some eigenvector in B' , it follows that $\bigcup_{i \in X_B} V_{\lambda, i-1} = CV_\mu$. Let $X_B = X_B^0$. For $d \in \mathbb{N}$, recursively define,

$$X_B^d = \{i \in \{1, \dots, D_\lambda + 1\} : \exists j \in X_B^{d-1}, i = j \pm 1\} \setminus \bigcup_{k=0}^{d-1} X_B^k$$

which is the set of indices, not already appearing in some X_B^j for $0 \leq j < d$, of blocks whose vertices are at a distance 1 from the vertices in the blocks with indices in X_B^{d-1} . Hence the union of the blocks $V_{\lambda, i-1}$ with indices in X_B^d gives the vertices at a distance d from CV_μ . Moreover, $\exists D_\mu \in \mathbb{N}$ such that $X_B^{D_\mu} \neq \emptyset$ and for every $d > D_\mu$, $X_B^d = \emptyset$. Hence \mathcal{V}_μ can be constructed from the indexing sets $X_B^0, \dots, X_B^{D_\mu}$. \square

2.2.1. Worked Example

Consider once again the cubic graph G in Figure 1. The 1-CDP is also an equitable partition, having the following divisor and characteristic matrices \mathbf{B} and \mathbf{C} , respectively,

$$\mathbf{B} = \begin{pmatrix} 2 & 1 & 0 \\ 2 & 0 & 1 \\ 0 & 1 & 2 \end{pmatrix} \quad \mathbf{C} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \end{pmatrix}^T.$$

The spectrum of \mathbf{B} is $\{3^{(1)}, 2^{(1)}, -1^{(1)}\}$. Consider $\mu = 2$, which is in both $\text{spec}(\mathbf{A})$ and $\text{spec}(\mathbf{B})$, with the same multiplicity (equal to 1). The basis of the eigenspace for 2 of \mathbf{B} is $\{(-1, 0, 2)^T\}$, which is non-zero with respect to each block of \mathcal{V}_1 . On the other hand, the eigenspace for 2 of \mathbf{A} is spanned by a single vector, $(-1, -1, -1, -1, -1, -1, 0, 0, 0, 2, 2, 2)^T$. In this case, CV_2 is the disjoint union of the blocks $V_{1,0}$ and $V_{1,2}$ from \mathcal{V}_1 . Moreover, \mathcal{V}_2 can be constructed from \mathcal{V}_1 : $\mathcal{V}_2 = \{V_{2,0} = V_{1,0} \dot{\cup} V_{1,2}, V_{2,1} = V_{1,1}\}$.

3. Information Content of Graphs and Topological Indices

3.1. Information Content and Structure of λ -Core Distance Partitions

The study of the information content of graphs is an important and active field, which is at the intersection of graph and information theory. The notion of information content of graphs was first introduced by Rashevsky (1955); Trucco (1956), and was generalised and formalised by Mowshowitz (1968) as follows: Given a graph G with a vertex set V and a partition of V into equivalence classes, a finite probability scheme can be assigned to this partitioning, by assigning the probability $\frac{|V_i|}{n}$ to each equivalence class V_i . An entropic measure associated with this finite probability scheme could then be defined as $I = -\sum_{i=0}^k \frac{|V_i|}{n} \log\left(\frac{|V_i|}{n}\right)$, which is based on Shannon's Entropy. Such measures form part of a broader class of indices, known as *topological indices*. Note that the logarithms we consider are typically of base 2, e or 10, all of which are monotonically increasing.

Since the orbital partition Π is in fact a collection of equivalence classes, Mowshowitz studied the entropy measure I_a associated with Π : $I_a = -\sum_{i=0}^s \frac{|\pi_i|}{n} \log\left(\frac{|\pi_i|}{n}\right)$. Similarly, for $\lambda \in \text{spec}(\mathbf{U})$, the λ -CDP \mathcal{V}_λ is a collection of equivalence classes, as discussed in Remark 2.2, and hence a finite probability scheme may be associated with it. In this manner, we can define a topological index for every distinct eigenvalue of \mathbf{U} , related to the structure of the neighbourhoods $V_{\lambda,i}$ of CV_λ at a distance i , and their size.

Theorem 3.1. *Let $\lambda \in \text{spec}(\mathbf{U})$ and \mathcal{V}_λ be the associated λ -CDP. Then for each equivalence class $V_{\lambda,i}$ in \mathcal{V}_λ , we can associate the probability $\frac{|V_{\lambda,i}|}{n}$, defining a finite probability scheme with entropy*

$$I_\lambda = -\sum_{i=0}^{D_\lambda} \frac{|V_{\lambda,i}|}{n} \log\left(\frac{|V_{\lambda,i}|}{n}\right).$$

3.2. Relating I_λ and I_μ for Two Distinct Eigenvalues

Consider a value x_i associated with each block $V_{\lambda,i}$ in some λ -CDP. Then, $W_\lambda(x_0, \dots, x_{D_\lambda}) = \frac{1}{n} \sum_{i=0}^{D_\lambda} |V_{\lambda,i}| x_i$ is the arithmetic mean of these values, weighted by the size of each block. For brevity, we write $W_\lambda(\{x_i\})$, where $0 \leq i \leq D_\lambda$. Let \mathcal{P} be a partition of V such that each block $V_{\lambda,i}$ in \mathcal{V}_λ is the disjoint union of $k_i \in \mathbb{N}$ blocks in \mathcal{P} .

It can be shown that $-\sum_{i=1}^{|\mathcal{P}|} \frac{|P_i|}{n} \log\left(\frac{|P_i|}{n}\right)$ is bounded above by $I_\lambda + W_\lambda(\{\log(k_i)\})$. We first require the following well-known inequality in information theory.

Theorem 3.2 (Theorem 2.7.1, Cover and Thomas (2005)). *For non-negative numbers x_1, \dots, x_n and y_1, \dots, y_n ,*

$$\sum_{k=1}^n x_k \log\left(\frac{x_k}{y_k}\right) \geq \left(\sum_{k=1}^n x_k\right) \log\left(\frac{\sum_{k=1}^n x_k}{\sum_{k=1}^n y_k}\right)$$

with equality if and only if $\frac{x_k}{y_k} = \text{constant}$.

Proposition 3.3. *Let $\lambda \in \text{spec}(\mathbf{U})$ and \mathcal{V}_λ be the associated λ -CDP. Let \mathcal{P} be a partition of V such that each block $V_{\lambda,i}$ of \mathcal{V}_λ is the disjoint union of $k_i \in \mathbb{N}$ blocks of \mathcal{P} . Then,*

$$-\sum_{i=1}^{|\mathcal{P}|} \frac{|P_i|}{n} \log\left(\frac{|P_i|}{n}\right) \leq I_\lambda + W_\lambda(\{\log(k_i)\}) \quad (3.1)$$

Proof. Let $V_{\lambda,i}$ be the disjoint union of $k_i \in \mathbb{N}$ blocks $\{P_1^{(i)}, \dots, P_{k_i}^{(i)}\}$ in \mathcal{P} . Then,

$$\begin{aligned} & \frac{1}{n} \sum_{k=1}^{k_i} |P_k^{(i)}| \log\left(\frac{|P_k^{(i)}|}{n}\right) && \text{since } V_{\lambda,i} \text{ is the union of } \{P_1^{(i)}, \dots, P_{k_i}^{(i)}\}, \\ & \geq \frac{1}{n} \left(\sum_{k=1}^{k_i} |P_k^{(i)}|\right) \log\left(\frac{\sum_{k=1}^{k_i} |P_k^{(i)}|}{n k_i}\right) && \text{by Theorem 3.2 for } x_k = |P_k^{(i)}|, y_k = n, \\ & = \frac{|V_{\lambda,i}|}{n} \left[\log\left(\frac{|V_{\lambda,i}|}{n}\right) - \log(k_i)\right] && \text{by properties of logs and } |V_{\lambda,i}| = \sum_{k=1}^{k_i} |P_k^{(i)}|. \end{aligned}$$

Applying this inequality to each term in I_λ , the bound follows immediately. \square

Such an inequality is closely associated with Problem 2.7. For two distinct eigenvalues $\lambda, \mu \in \text{spec}(\mathbf{U})$, such that the μ -CDP can be constructed from the λ -CDP, the following result follows immediately.

Proposition 3.4. *Let $\lambda, \mu \in \text{spec}(\mathbf{U})$ be two distinct eigenvalues. If the μ -CDP can be constructed from the λ -CDP, then there exist $|D_\mu| + 1$ positive integers k_i such that $I_\lambda \leq I_\mu + W_\mu(\{\log(k_i)\})$.*

In particular, as an immediate consequence of Theorem 2.11, we have the following corollary.

Corollary 3.5. *Let $\lambda \in \text{spec}(\mathbf{U})$ and \mathcal{V}_λ be an equitable partition with divisor and characteristic matrices \mathbf{B} and \mathbf{C} , respectively. Let $\mu \in \text{spec}(\mathbf{B})$ such that $m_{\mathbf{U}}(\mu) = m_{\mathbf{B}}(\mu)$. Then $I_\lambda \leq I_\mu + W_\mu(\{\log(k_i)\})$.*

Consider the 1-CDP and 2-CDP for the adjacency matrix \mathbf{A} of the graph G in Figure 1. As in the worked example of Section 2.2.1, the 2-CDP can be constructed from the 1-CDP. In particular, the 2-CDP has two blocks $V_{2,0}$ and $V_{2,1}$, which are the disjoint union of $k_0 = 2$ and $k_1 = 1$ blocks from the 1-CDP, respectively. Up to 4 decimal places, we have that $W_2(\ln(2), \ln(1)) \simeq 0.5199$ and $I_2 \simeq 0.5623$. Moreover, $I_1 \simeq 1.0397$ and hence $I_1 \leq I_2 + W_2(\ln(2), \ln(1)) \simeq 1.0822$.

3.3. Note on the Minimum–Maximum Attainable Bounds of I_λ

Of interest are the minimum and maximum bounds attainable by I_λ for a fixed number of vertices n , and varying number of λ -core vertices. These bounds are given in the following theorem, and visualised in Figure 2.

Proposition 3.6. *Let $\lambda \in \text{spec}(\mathbf{U})$ and let $|CV_\lambda| = k, 1 \leq k \leq n$. Then,*

$$\left. \begin{array}{l} 0 \\ -\frac{n-k}{n} \log\left(\frac{n-k}{n}\right) \end{array} \right\} \begin{array}{l} k = n \\ k < n \end{array} \leq I_\lambda + \frac{k}{n} \log\left(\frac{k}{n}\right) \leq -\frac{n-k}{n} \log\left(\frac{1}{n}\right)$$

Proof. Let $|CV_\lambda| = k$, where $1 \leq k < n$. Then $1 \leq D_\lambda \leq n - k$. Consider,

$$I_\lambda + \frac{k}{n} \log\left(\frac{k}{n}\right) = -\sum_{i=1}^{D_\lambda} \sum_{j=1}^{|V_{\lambda,i}|} \frac{1}{n} \log\left(\frac{|V_{\lambda,i}|}{n}\right) \leq -\sum_{i=1}^{D_\lambda} \sum_{j=1}^{|V_{\lambda,i}|} \frac{1}{n} \log\left(\frac{1}{n}\right)$$

since $-\log(x)$ is monotonically decreasing and $1 \leq |V_{\lambda,i}|$. Since $n - k = \sum_{i=1}^{D_\lambda} |V_{\lambda,i}|$, the upper-bound $I_\lambda + \frac{k}{n} \log\left(\frac{k}{n}\right) \leq -\frac{n-k}{n} \log\left(\frac{1}{n}\right)$ follows. For $1 \leq k < n$, by a similar argument we have $-\frac{n-k}{n} \log\left(\frac{n-k}{n}\right) \leq I_\lambda + \frac{k}{n} \log\left(\frac{k}{n}\right)$. For the case that $k = n$, then $I_\lambda = \frac{n}{n} \log\left(\frac{n}{n}\right) = 0$, completing the proof. \square

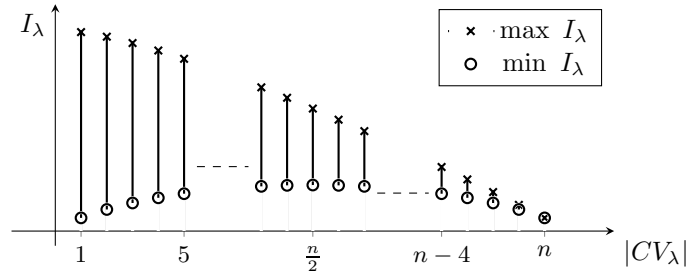


Figure 2: Discrete plot of the range of I_λ for fixed n and varying $|CV_\lambda|$, between the Minimum–Maximum bounds in Proposition 3.6. For n even (as shown here), the maximum lower-bound occurs at $n/2$.

Remark 3.7. There are a number of observations that one can make on the range of values that I_λ may take as the number of λ -core vertices changes and n remains fixed. Firstly, the lower-bound is attained when the number of blocks in \mathcal{V}_λ is exactly two, while the upper-bound is attained when the number of blocks is $n - |CV_\lambda| + 1$. Hence for fixed n and $|CV_\lambda|$, the entropy I_λ increases as D_λ increases. Secondly, the maximum lower-bound is attained when \mathcal{V}_λ has two blocks of more or less equal size. Entropy values below this threshold indicate graphs with either very few or almost all vertices being λ -core. Moreover, D_λ must be very small and hence few vertices must be distant from a λ -core vertex.

4. Applications

For every eigenvalue λ of a universal adjacency matrix \mathbf{U} associated with a graph G , a notion of information content related to that eigenvalue may be defined, based on the structure of the λ -CDP. We say that a graph G is *singular* if its adjacency matrix is singular. Partitions of the vertex set based on neighbourhoods of λ -core vertices have been studied greatly in Sciriha et al. (2020); Jaume and Molina (2018) for singular graphs with independent CV_λ . Such partitions, as well as topological indices, have many applications in the study of networks and molecular graphs.

4.1. Singular Graphs

In the study of singular graphs, *minimal configurations* (MCs) are of importance, as they are considered to be the building blocks for such graphs, through graph operations such as coalescence.

Definition 4.1 (Sciriha (1998)). A minimal configuration is a singular graph which is either K_1 or if $n \geq 3$ then it has a core-graph F induced by CV_0 and a periphery $\mathcal{P} \setminus CV_0$ satisfying the following conditions:

- (i) $\eta(G) = 1$,
- (ii) $\mathcal{P} = \emptyset$ or the graph induced by \mathcal{P} consists of isolated vertices,
- (iii) $|\mathcal{P}| + 1 = \eta(F)$.

In particular, MCs are connected (Theorem 2, Sciriha (1998)). Of interest are bipartite MCs, which are closely associated with *slim graphs*. Slim graphs were defined for the case of independent 0-core vertices in Definition 8 of Sciriha et al. (2020). The following definition generalises the notion of slim graphs to include those graphs for which CV_0 is not an independent set.

Definition 4.2. A connected singular graph G with 0-core distance partition \mathcal{V}_0 for $\mathbf{U} = \mathbf{A}$, is a *slim graph* if CFV_0 is precisely $V_{0,1}$.

In the case that CV_0 is independent, then CFV_0 is exactly $N(CV_0)$ for a slim graph. The following proposition characterises such graphs as being those graphs for which the entropic measure I_0 is at a minimum, for a given number of vertices n and λ -core vertices $|CV_0|$.

Proposition 4.3. Let G be a connected singular graph. Then, G is a slim graph if and only if I_0 is equal to the lower-bound for the given n and $|CV_0|$.

Proof. If G is a slim graph, then by definition, for $\mathbf{U} = \mathbf{A}$, we have that $\mathcal{V}_0 = \{V_{0,0} = CV_0, V_{0,1}\}$, where $|V_{0,1}| = n - |CV_0|$. Therefore by Proposition 3.6, I_0 is equal to the lower-bound for the given n and $|CV_0|$. Conversely, let I_0 be equal to the lower-bound, given n and $|CV_0|$. Suppose that the 0-CDP for $\mathbf{U} = \mathbf{A}$ has at least three blocks. Then I_0 has the term $-\frac{|CV_0|}{n} \log\left(\frac{|CV_0|}{n}\right)$, and all the other terms are of the form $-\frac{n-k}{n} \log\left(\frac{n-k}{n}\right)$, where $|CV_0| < k < n$. Since $-\log(x)$ is strictly monotonically decreasing, then $-\log\left(\frac{n-|CV_0|}{n}\right) < -\log\left(\frac{n-k}{n}\right)$ and hence I_0 is greater than the lower-bound, a contradiction. The result follows. \square

It was shown by Sciriha et al. (2020) that bipartite MCs, which have an independent 0-core vertex set, are in fact slim graphs with partite sets $V_1 = CV_0$ and $V_2 = N(CV_0)$, such that $|CV_0| = |N(CV_0)| + 1$. The following is an immediate consequence of Proposition 4.3.

Proposition 4.4. If G is a bipartite minimal configuration then I_0 is equal to the lower-bound for the given n and $|CV_0|$.

4.2. Chemical Considerations

Let G be the n -atomic molecular graph of a conjugated hydrocarbon system. In *Hückel Molecular Orbital Theory*, the *Hamiltonian* for such a system is given by $\mathbf{H}(\alpha, \beta) = \alpha\mathbf{I} + \beta\mathbf{A}$, where \mathbf{A} is the adjacency matrix of G and α, β are two parameters. Notice that \mathbf{H} may be represented by a universal adjacency matrix, by setting $\gamma_A = \beta$, $\gamma_I = \alpha$, and $\gamma_D = 0 = \gamma_J$. Clearly, $\mathbf{H}(\alpha, \beta)$ and \mathbf{A} commute and hence have the same eigenvectors. If λ_i is an eigenvalue in the ordered spectrum of \mathbf{A} , then $E_i = \alpha + \beta\lambda_i$ is the corresponding eigenvalue of $\mathbf{H}(\alpha, \beta)$.

Within the Hückel framework, E_i corresponds to the i^{th} energy level. Each eigenvector corresponds to one of the n -molecular orbitals, where the eigenvector entries give a linear combination of the n -atomic orbitals. The normalised values of these entries represent the probability of electron occupation at each atomic orbital, for the i^{th} molecular orbital. For an in-depth treatment of the Hückel framework, see Gutman and Polansky (1986).

Since $\mathbf{H}(\alpha, \beta)$ takes the form of a universal adjacency matrix, then the E_i -CDP is defined for every $E_i \in \text{spec}(\mathbf{H})$. Hence for the i^{th} energy level, we can associate a topological index I_{E_i} . Such an index I_{E_i} has appealing interpretations, related to the probabilistic distribution of electrons amongst the atomic orbitals. For example, for large values of I_{E_i} , the number of atomic orbitals with non-zero probability of electron occupation is very small, with a relatively large probability of occupation for each. Moreover the corresponding vertices in the molecular graph are very ‘localised’, as there exists a substantial number of E_i -core-forbidden vertices which are ‘distant’ from these E_i -core vertices. Further interpretations are discussed in Remark 3.7, in a more general context.

For simplicity, we shall consider $\mathbf{H} = \mathbf{A}$. Singular graphs have an important role in the Hückel framework, as the zero energy level $E = 0$, and its multiplicity, correspond to the non-bonding orbitals of the molecule. The 0-core vertices correspond to the atomic orbitals of which the molecular orbitals for $E = 0$ are a linear combination. Consider the 0-CDP for $\mathbf{U} = \mathbf{A}$. By Proposition 4.3, I_0 attains a minimum if and only if G is a slim graph. In particular bipartite MCs, which are a sub-class of MCs and the building blocks of singular graphs, always have I_0 at a minimum.

Example 4.5. More generally, suppose we have two slim graphs $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$, where v_1 and v_2 are not cut vertices and are both 0-core vertices. Let H_1 have n_1 vertices and $k_1 = |CV_0(H_1)|$. Similarly for $G_2 + v_2$. Ali et al. (2016) showed that the coalescence of H_1 and H_2 on v_1 and v_2 yields the graph $H_1 \circ H_2 = G_1 + G_2 + v$, where v is also a 0-core vertex, and the nullity is $\eta(H_1) + \eta(H_2) - 1$. Clearly the 0-core vertices in H_1 which are not v_1 are preserved, and similarly for H_2 . Hence $|CV_0(H_1 \circ H_2)| = k_1 + k_2 - 1$. It is also worth noting that $H_1 \circ H_2$ is also a slim graph and therefore $I_0(H_1 \circ H_2)$ is at a minimum. Without loss of generality, let $\frac{k_1}{n_1} < \frac{k_2-1}{n_2-1}$. Then $\frac{k_1}{n_1} < \frac{k_1+k_2-1}{n_1+n_2-1} < \frac{k_2}{n_2}$. It follows that $I_0(H_1 \circ H_2)$ is some value between $I_0(H_1)$ and $I_0(H_2)$, reflecting the ‘averaged’ distribution of 0-core vertices from H_1 and H_2 in $H_1 \circ H_2$, both in probabilistic terms for electron occupation, and in terms of the distribution of 0-core vertices within the molecular graph.

Future directions include the study of changes in I_0 as larger molecular graphs are constructed, through *eg.* edge additions or graph coalescence operations.

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References

- Akbari, S., Ghorbani, E., Mahmoodi, A., 2013. Nowhere-zero eigenvectors of graphs. *Linear and Multilinear Algebra* 61, 273–279.
- Ali, D.A., Gauci, J.B., Sciriha, I., 2016. Coalescing fiedler and core vertices. *Czechoslovak Mathematical Journal* 66, 971–985.
- Cover, T.M., Thomas, J.A., 2005. *Elements of Information Theory*. John Wiley & Sons, Ltd. doi:10.1002/047174882X.
- Cvetković, D., Rowlinson, P., Simić, S., 2009. *An Introduction to the Theory of Graph Spectra*. London Mathematical Society Student Texts, Cambridge University Press. doi:10.1017/CB09780511801518.
- Fernandes, R., da Cruz, H.F., 2018. The number of p-vertices in a matrix with maximum nullity. *Linear Algebra and its Applications* 547, 168–182.
- Gutman, I., Polansky, O.E., 1986. *Mathematical Concepts in Organic Chemistry*. Springer-Verlag.
- Haemers, W., Omid, G., 2011. Universal adjacency matrices with two eigenvalues. *Linear Algebra and its Applications* 435, 2520–2529.
- Jaume, D.A., Molina, G., 2018. Null decomposition of trees. *Discrete Mathematics* 341, 836–850.
- Mowshowitz, A., 1968. Entropy and the complexity of the graphs: I. an index of the relative complexity of a graph. *The Bulletin of Mathematical Biophysics* 30, 175–204.
- Rashevsky, N., 1955. Life, information theory, and topology. *The Bulletin of Mathematical Biophysics* 17, 229–235.
- Sciriha, I., 1997. On the coefficient of λ in the characteristic polynomial of singular graphs. *Utilitas Mathematica* 52, 97–111.
- Sciriha, I., 1998. On the construction of graphs of nullity one. *Discrete Mathematics* 181, 193–211.
- Sciriha, I., Mifsud, X., Borg, J.L., 2020. Nullspace vertex partition in graphs. *Journal of Combinatorial Optimization*.
- Trucco, E., 1956. A note on the information content of graphs. *The Bulletin of Mathematical Biophysics* 18, 129–135.