

Article

Joining Forces for Reconstruction Inverse Problems

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Abstract: A spectral inverse problem concerns the reconstruction of parameters of a parent graph from prescribed spectral data of subgraphs. Also referred to as the P–NP *Isomorphism Problem, Reconstruction* or *Exact Graph Matching*, the aim is to seek sets of parameters to determine a graph uniquely. Other related inverse problems, including the *Polynomial Reconstruction Problem (PRP)*, involve the recovery of graph invariants. The PRP seeks to extract the spectrum of a graph from the deck of cards each showing the spectrum of a vertex-deleted subgraph. We show how various algebraic methods join forces to reconstruct a graph or its invariants from a minimal set of restricted eigenvalue–eigenvector information of the parent graph or its subgraphs. We show how functions of the entries of eigenvectors of the adjacency matrix \mathbf{A} of a graph can be retrieved from the spectrum of eigenvalues of \mathbf{A} . We establish that there are two subclasses of disconnected graphs with each card of the deck showing a common eigenvalue. These could occur as possible counter examples to the positive solution of the PRP.

Keywords: eigenvalue–eigenvector-inverse problems; Ulam’s reconstruction conjecture; polynomial reconstruction problem; adjacency matrix; characteristic polynomial

1. Introduction

An undirected graph G has a vertex set $\mathcal{V}(G) = \{1, 2, \dots, n\}$ of n vertices and an edge set E joining pairs of the vertices. The graphs we consider are simple, that is, they are without loops or multiple edges. By convention, its *adjacency matrix* \mathbf{A} is such that the (i, j) entry is 1 if $(i, j) \in E$, and 0 otherwise. For all i , let μ_i be the i th largest eigenvalue of \mathbf{A} , with multiplicity η_i . The entries on the diagonal of \mathbf{A} are 0.

The eigenvalues of G are the eigenvalues of \mathbf{A} ; λ_i is an eigenvalue of \mathbf{A} if $\mathbf{A}\mathbf{x} = \lambda_i\mathbf{x}$, for some $\mathbf{x} \neq 0$. The characteristic polynomial of \mathbf{A} is denoted by $\phi(G, \lambda)$ and

$$\phi(G, \lambda) = \text{Det}(\lambda\mathbf{I} - \mathbf{A}) = \sum_{j=0}^n a_j \lambda^j = \prod_{i=1}^n (\lambda - \lambda_i). \quad (1)$$

As \mathbf{A} is real and symmetric, the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of G are real and are said to form the spectrum, $Sp(G)$, of G . The eigenspace \mathcal{E}_i associated with an eigenvalue μ_i is $\{\mathbf{x}_i \in \mathbb{R}^n : \mathbf{A}\mathbf{x}_i = \mu_i\mathbf{x}_i\}$.

In 1941, S. M. Ulam and P. J. Kelly were working on what has become known as Ulam’s Reconstruction Conjecture (R.C.) [1–4]. In 1964, Harary proposed the RC as follows: *We are presented with a deck \mathcal{D} of $n \geq 3$ cards each showing a one-vertex-deleted unlabeled subgraph $G - v$ for each $v \in \mathcal{V}(G)$. The problem is to recover the parent graph G from \mathcal{D} .*

Although the classical graph reconstruction problem, RC, has been around for a long time, this topic is significant in the context of modern problems such as those encountered in graph mining.

An algebraic variation of the R.C., first posed by D. M. Cvetković in 1973 and later considered by I. Gutman and D. M. Cvetković in [5], is the Polynomial Reconstruction Problem (PRP): *Is it possible to recover the characteristic polynomial of a graph of order at least 3, from the **p-deck**, $\mathcal{PD}(H)$, of H , consisting of the characteristic polynomials of the one-vertex-deleted subgraphs (with multiplicities)?*



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The restriction on the order is necessary as the pair of graphs on two vertices form a counter example to both RC and PRP. Both have been solved for some classes of graphs but are still open in general.

Other studies on the PRP can be found in [6–11]. If a p-deck determines that the parent graph belongs to a particular class \mathcal{C} of graphs, then recognition is established. If furthermore, a p-deck provides sufficient information for the parent graph to be constructed, then reconstruction follows. If both stages are performed successfully, then the graphs in class \mathcal{C} are said to be *polynomial reconstructible* and the PRP is said to be solved positively for \mathcal{C} .

Another approach, mainly used regarding the PRP, is the *counter example technique* [7,12]. A graph H is assumed not to be polynomial reconstructible and that there exists a counter example G . Thus, G has the same p-deck as H but a different spectrum. This approach rules out certain classes \mathcal{C}' of graphs. The existence of polynomial reconstruction would then be established for \mathcal{C}' without demonstrating the actual reconstruction.

W.T.Tutte combined the combinatorial and algebraic aspects. He showed that $\phi(G, \lambda)$ is reconstructible from \mathcal{D} [13]. To date only the two graphs K_2 and $2K_1$, on two vertices are known to have the same deck and the same p-deck. If there were to be another pair of non-isomorphic graphs G_1 and G_2 , of higher order, with the same deck, then by Tutte's theorem on reconstruction [13], they would be cospectral.

In this article, there are two main aims. Combinatorial and algebraic properties of a parent graph and of its deck join forces to produce minimal collections of parameters that suffice to reconstruct the parent graph or its invariants. First, a graph invariant C_v^i equal to the sum of squares of the v entries of certain eigenvectors associated with an eigenvalue μ_i is reconstructed. Second, the PRP for disconnected graphs is investigated. In particular, disconnected graphs $\{H\}$ with a common eigenvalue deck lend themselves to interesting algebraic techniques for the recovery of the graph or certain graph invariants, enabling combinatorial characterizations.

In Section 2, we derive an expression for the characteristic polynomial of a vertex-deleted subgraph from the eigenspaces of the parent graph leading to new proofs of two well known theorems, namely Clarke's derivative of the characteristic polynomial and Cauchy's Inequalities for non-negative matrices (also referred to as the Interlacing Theorem). The techniques in the proofs are useful in the sequel. We then define the graph invariant, C_v^i , depending on v and the eigenspace \mathcal{E}_i . For simple eigenvalues, C_v^i yields the associated unit eigenvector entries up to sign. In Section 3, we focus on counter examples to the positive resolution of the PRP for the class of disconnected graphs $\{H\}$ with a common eigenvalue deck, which is shown to be partitioned into two subclasses depending on whether H has the eigenvalue. We give a characterization of the graphs in the two classes.

2. The Characteristic Polynomial of a Vertex-Deleted Subgraph

In this section, we derive an expression for the characteristic polynomial of a vertex-deleted subgraph from the eigenspaces of the parent graph. The information this expression provides leads to new proofs of two well known theorems, namely, Clarke's derivative of the characteristic polynomial and Cauchy's Inequalities for non-negative matrices (also referred to as the Interlacing Theorem). These two theorems are among the most powerful in spectral graph theory. The notation and techniques used in the proofs of these two theorems has facilitated the new theory developed in the rest of the paper. We proceed to determine C_v^i , from the eigenvalues of the graph. These graph parameters provide eigenvector entries, up to sign, for one dimensional eigenspaces. Moreover, the non-zero values of C_v^i reveal the vertices v of the graph of *type* known as μ_i -core vertex.

Theorem 1. *Let an n -vertex graph G have the n eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, written in non-increasing order. Let $\{\mathbf{y}^i\}$, $1 \leq i \leq n$, be an ordered orthonormal set of eigenvectors. If y_v^r is the v th entry of the eigenvector \mathbf{y}^r , then the characteristic polynomial $\phi(G - v, \lambda)$ of $G - v$ is given by*

$$\phi(G - v, \lambda) = \sum_{r=1}^n \frac{(y_v^r)^2}{(\lambda - \lambda_r)} \phi(G, \lambda). \quad (2)$$

Proof. The characteristic polynomial $\phi(G - v, \lambda)$ of $G - v$ is the v th diagonal entry of the adjugate of $\lambda \mathbf{I} - \mathbf{A}$, where \mathbf{A} is the adjacency matrix of G .

Let $Diag[\alpha_i]$ denote the diagonal matrix with entries $\{\alpha_i\}$ on the main diagonal and 0 on the off-diagonal entries. The orthogonal matrix $\mathbf{P} := (\mathbf{y}^1 | \mathbf{y}^2 | \dots | \mathbf{y}^n)$ diagonalizes G such that $\mathbf{P}^t(\mathbf{A})\mathbf{P} = Diag[\lambda_i]$ and thus $\mathbf{P}^t(\lambda \mathbf{I} - \mathbf{A})^{-1}\mathbf{P} = Diag[\frac{1}{\lambda - \lambda_i}]$. It follows that

$$(\lambda \mathbf{I} - \mathbf{A})_{vv}^{-1} = (y_v^1 | y_v^2 | \dots | y_v^n) Diag[\frac{1}{\lambda - \lambda_i}] (y_v^1 | y_v^2 | \dots | y_v^n)^t = \sum_{r=1}^n \frac{(y_v^r)^2}{(\lambda - \lambda_r)}.$$

$$\text{Thus } \phi(G - v, \lambda) = adj(\lambda \mathbf{I} - \mathbf{A})_{vv} = (\lambda \mathbf{I} - \mathbf{A})_{vv}^{-1} \phi(G, \lambda) = \sum_{r=1}^n \frac{(y_v^r)^2}{(\lambda - \lambda_r)} \phi(G, \lambda). \quad \square$$

As \mathbf{A} is real symmetric, its eigenvalues are real. As shown in the proof of Theorem 1, the columns of an orthogonal diagonalizing matrix \mathbf{P} are mutually orthonormal eigenvectors $\{\mathbf{y}^i\}$, $1 \leq i \leq n$. Let the multiplicity of the distinct eigenvalues $\mu_1, \mu_2, \dots, \mu_s$ of $\mathbf{A}(G)$ be $\eta_1, \eta_2, \dots, \eta_s$. From $\mathbf{P}^T \mathbf{A} \mathbf{P} = \Sigma$ where Σ is a diagonal matrix with the eigenvalues of \mathbf{A} on its diagonal, one can deduce the spectral decomposition $\mathbf{A}(G) = \mu_1 \mathbf{P}_1 + \mu_2 \mathbf{P}_2 + \dots + \mu_s \mathbf{P}_s$ of \mathbf{A} , where \mathbf{P}_i is the orthogonal projection of \mathbb{R}^n onto \mathcal{E}_i for $1 \leq i \leq n$.

Using the notation in the proof of Theorem 1, let $C_v^i = \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2$ be associated with vertex v and the eigenspace of μ_i . In the case when the multiplicity of the eigenvalue μ_i is 1, it is equal to $(y_v^i)^2$, the square of entry v of the μ_i -eigenvector \mathbf{y}^i generating the one dimensional μ_i -eigenspace.

Note that (2) can be written as

$$\begin{aligned} \frac{\phi(G - v, \lambda)}{\phi(G, \lambda)} &= \frac{\sum_{\ell=1}^{\eta_1} (y_{v,\ell}^1)^2}{\lambda - \mu_1} + \dots + \frac{\sum_{\ell=1}^{\eta_s} (y_{v,\ell}^s)^2}{\lambda - \mu_s} \\ &= \frac{C_v^1}{\lambda - \mu_1} + \dots + \frac{C_v^s}{\lambda - \mu_s} \end{aligned} \tag{3}$$

We present our new proofs of Theorems 2 and 3 below, which will be used in the sequel. These follow directly from (2) and the concept of the type of vertex relative to \mathcal{E}_i .

2.1. Parameters Derived from the p-deck

Recall that the p -deck consists of the n characteristic polynomials of the subgraphs in \mathcal{D} .

Theorem 2. (F.H. Clarke) [14] *Let G be a graph and let $\phi(G, \lambda)$ be the characteristic polynomial of its 0-1-adjacency matrix. The derivative of the characteristic polynomial is given by*

$$\phi'(G, \lambda) = \sum_{i=1}^n \phi(G - v_i, \lambda) \tag{4}$$

Proof. Let the spectrum of an n -vertex graph G be $\mu_1, \mu_2, \dots, \mu_s$ with multiplicity $\eta_1, \eta_2, \dots, \eta_s$, respectively. Then, $\phi(G, \lambda) = (\lambda - \mu_1)^{\eta_1} (\lambda - \mu_2)^{\eta_2} \dots (\lambda - \mu_s)^{\eta_s}$. Denote the natural logarithmic function $\log_e(x)$ by $\ln(x)$. Differentiating $\ln(\phi(G, \lambda)) = \sum_{i=1}^s \eta_i \ln(\lambda - \mu_i)$ with respect to λ , we obtain

$$\frac{\phi'(G, \lambda)}{\phi(G, \lambda)} = \sum_{i=1}^s \eta_i \frac{1}{\lambda - \mu_i}. \tag{5}$$

Summing (3) up over v ,

$$\sum_{v=1}^n \frac{\phi(G - v, \lambda)}{\phi(G, \lambda)} = \sum_{i=1}^s \frac{\sum_{v=1}^n \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2}{(\lambda - \mu_i)}. \tag{6}$$

As a diagonalizing matrix \mathbf{P} is orthogonal, the length of each column vector is 1. Therefore, $\sum_{v=1}^n \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2 = \eta_i$. Comparing with (5), $\phi'(G, \lambda) = \sum_{v=1}^n \phi(G - v, \lambda)$. \square

By integration of $\phi'(G, \lambda)$, Theorem 2 of Clarke yields the following result immediately.

Corollary 2. From the polynomial deck of the subspectra, all the coefficients in $\phi(G, \lambda)$ are derived, except for the constant term a_0 . ■

One of the most useful theorems in spectral graph theory is the *Interlacing Theorem*, also known as *Cauchy's inequalities* for a Hermitian matrix \mathbf{M} . It gives the relative distribution of the eigenvalues of a graph and of those of a vertex-deleted subgraph. This is often key to establishing classes of polynomial reconstructible graphs.

The concept of the three possible types of vertices in a graph, associated with an eigenvalue μ of multiplicity η_μ , is needed in the proof of the Interlacing theorem and in the sections that follow.

The *type of a vertex* is determined by the v th entries of an orthonormal set of eigenvectors of G [15,16]. A non-zero entry at position v in some μ -eigenvector determines a μ -core vertex v and the dimension of the μ -eigenspace of $G - v$ is $\eta_\mu - 1$. A μ -core forbidden vertex corresponds to a non-zero entry in all the μ -eigenvectors. It is a *middle μ -core forbidden vertex* if the dimension of the μ -eigenspace of $G - v$ is η_μ and an *upper μ -core forbidden vertex* if the dimension of the μ -eigenspace of $G - v$ is $\eta_\mu + 1$. In linear algebraic literature, for $\mu = 0$, upper μ -core-forbidden vertices are sometimes referred to as *Parter* vertices. They form a subset of the core-forbidden vertices, also known as *Fiedler* vertices [17]. If each vertex of a graph G is a μ -core vertex, then G is referred to as a μ -core-graph. For a one dimensional μ -eigenspace, a μ -core-graph is called a μ -nut-graph. Its μ -eigenspace is generated by a full vector, with no zero entries.

Theorem 3. [Interlacing Theorem] Let G be an n -vertex graph with vertex set \mathcal{V} and let $v \in \mathcal{V}$. If the monotonic non-increasing sequence of eigenvalues of G is $\lambda_1, \lambda_2, \dots, \lambda_n$ and that of $G - v$ is $\xi_1, \xi_2, \dots, \xi_{n-1}$, then

$$\lambda_1 \geq \xi_1 \geq \lambda_2 \geq \xi_2 \geq \dots \geq \xi_{n-1} \geq \lambda_n.$$

Proof. For a specific eigenvalue λ_0 , (2) above contains all the information regarding $\phi(G - v, \lambda)$ relative to the eigenspace \mathcal{E}_0 , corresponding to λ_0 . The RHS of (2) is a rational function $\psi(\lambda)$ with a number $m (\leq s)$ of poles and $m - 1$ zeros, where m depends on v . A zero ξ_i of ψ is an eigenvalue of $G - v$, lying strictly between two eigenvalues of G .

We distinguish three cases:

Case I: If v is a λ_0 -core-vertex, then the v th entry y_v^r of some eigenvector $\mathbf{y}^r \in \mathcal{E}_0$ is non-zero. Therefore, λ_0 is a pole in (2). Thus, the deletion of vertex v reduces the multiplicity of the eigenvalue λ_0 of G by one.

Now the remaining two cases deal with a λ_0 -core-forbidden-vertex v . By definition $y_v^r = 0$, for all eigenvectors $\mathbf{y}^r \in \mathcal{E}_0$. Then, λ_0 is not a pole in (2).

Case II: If λ_0 is not a zero of the RHS of (2), then the same holds for the LHS. Hence the multiplicity of the eigenvalue λ_0 of $G - v$ is the same as that of G . In this case v is a *middle λ_0 -core-forbidden vertex*

Case III: If λ_0 is a zero of the RHS of (2), then the multiplicity of the eigenvalue λ_0 of $G - v$ is one more than that of G and v is an *upper λ_0 -core-forbidden vertex*.

Thus, the deletion of a vertex causes a shift of the simple eigenvalues of the parent graph or changes the multiplicity of an eigenvalue by at most one. Therefore, eigenvalues of a daughter graph $G - v$ lie between those of the parent graph G . This proves the Interlacing Theorem. □

2.2. Eigenvalue-Based Invariant C_v^i of a Vertex

We now construct the graph invariant C_v^i for a vertex v . It is the contribution given by the entries v of the columns of \mathbf{P} associated with \mathcal{E}_i . This has a direct application in the estimate of the electronic charge distribution among the carbon atoms of a hydrocarbon.

Using the notation in the proof of Theorem 2, let $C_v^i = \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2$ be associated with vertex v . In the case when the multiplicity of the eigenvalue μ_i is 1, it is equal to $(y_v^i)^2$,

the square of entry v of the μ_i -eigenvector \mathbf{y}^i generating the one dimensional μ -eigenspace. We note that C_v^i is the contribution of v to η_i . Indeed, $\sum_{v=1}^n C_v^i = \eta_i$.

Theorem 4. Let $C_v^i = \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2$. Then,

$$\lim_{\lambda \rightarrow \mu_i} \frac{\phi(G - v, \lambda)}{\phi'(G, \lambda)} = \frac{C_v^i}{\eta_i} \tag{7}$$

Proof. As μ_i -core vertices exist for all μ_i , from Theorem 2, the multiplicity of $(\lambda - \mu_i)$ as a factor of the polynomial $\phi'(G, \lambda)$ is $\eta_i - 1$. By the Interlacing Theorem, the multiplicity of a μ_i -eigenvalue of $G - v$ differs from that of G by at most one. Therefore, we can write $\phi(G - v, \lambda) = \phi_{\mu_i}(G - v, \lambda)(\lambda - \mu_i)^{\eta_i - 1}$.

If v is a μ_i -core-forbidden vertex, then for each ℓ , $1 \leq \ell \leq \eta_i$, the entry $y_{v,\ell}^i = 0$ and thus $C_v^i = 0$. In this case, the multiplicity of $(\lambda - \mu_i)$ in $\phi(G - v, \lambda)$ is at least $\eta_i \geq 1$. Therefore, the limit in (7) is zero and (7) holds.

If on the other hand, v is a μ_i -core vertex, then the multiplicity of $(\lambda - \mu_i)$ in $\phi(G - v, \lambda)$ is $\eta_i - 1$. The characteristic polynomial $\phi(G, \lambda) = \prod_{i=1}^s (\lambda - \mu_i)^{\eta_i}$. Its derivative $\phi'(G, \lambda) = \sum_{r=1}^s \eta_r (\lambda - \mu_r)^{\eta_r - 1} \prod_{\mu_k \neq \mu_r} (\lambda - \mu_k)^{\eta_k}$. Then,

$$\lim_{\lambda \rightarrow \mu_i} \frac{(\lambda - \mu_i)\phi'(G, \lambda)}{\phi(G, \lambda)} = \eta_i \tag{8}$$

As λ approaches μ_i , only one term does not vanish in the left hand side of (3). Thus,

$$\lim_{\lambda \rightarrow \mu_i} \frac{(\lambda - \mu_i)\phi(G - v, \lambda)}{\phi(G, \lambda)} = C_v^i \tag{9}$$

From (8) and (9), it follows that $\lim_{\lambda \rightarrow \mu_i} \frac{\phi(G - v, \lambda)}{\phi'(G, \lambda)} = \frac{C_v^i}{\eta_i}$ \square

Theorem 4 establishes minimal data from which the parameter C_v^i can be calculated. The polynomials $\phi(G - v, \lambda)$ and $\phi(G, v)$ suffice to derive it. Note that $C_v^i = 0$ if and only if v is a core-forbidden vertex.

Corollary 4. The invariant C_v^i of a graph G can be constructed from (i) the entries v of orthonormal vectors generating \mathcal{E}_i or (ii) μ_i together with the spectra of G and of $G - v$.

For an eigenspace of dimension one, the entries of an eigenvector can be obtained up to sign from the spectrum of G and of $G - v$, $1 \leq v \leq n$. From (7) the following result is immediate.

Lemma 4. Let μ_i be a simple eigenvalue of a graph G . Then, the spectrum of G and $G - v$ alone suffices to yield each entry of the associated eigenvector up to sign.

For a graph whose eigenvalues are all simple the spectrum suffices to obtain all the eigenvector entries up to sign.

Theorem 5. If G has distinct eigenvalues, then the v -entries of the μ_i -eigenvector of length one can be obtained for all i , $1 \leq i \leq n$, up to sign, from the spectrum of G and $G - v$.

Proof. If G has distinct eigenvalues, then the multiplicity η_i of each eigenvalue μ_i is one. Therefore, $C_v^i = (y_{v,1}^i)^2$, the square of the entry v of the unit μ_i -eigenvector is obtained from (7). \square

Note that for certain applications the square of the entry of a unit eigenvector suffices. For instance, $C_v^i = \sum_{\ell=1}^{\eta_i} (y_{v,\ell}^i)^2$ is the fractional electronic charge of the atom positioned at

v at the energy level μ_i of the molecule with adjacency matrix \mathbf{A} . If the molecular graph has distinct eigenvalues, the fractional charge of an electron for energy μ_i at the v th carbon atom of an unsaturated hydrocarbon or all-carbon molecule is given by $(y_{v,1}^i)^2$.

3. Approaches to the Resolution of the PRP

From the p-deck and Corollary 2, we can determine immediately, for the parent graph H , the order n , the degree sequence, the number of edges, and the number of triangles. The p-deck even supplies the information required to obtain all the non-constant terms of $\phi(H, \lambda)$, but fails however to give a direct way of determining $\text{Det}(\mathbf{A}(H))$ from which the constant term a_0 of the characteristic polynomial of H is derived.

In this section, we focus on counter examples to the positive resolution of the PRP among disconnected graphs with a common eigenvalue deck. One such graph could have the same p-deck as a connected graph G . If the graphs in a pair (H, G) , of graphs with the same p-deck have different characteristic polynomial, the pair would be a counter example to the positive resolution of the PRP.

Note that graphs with an eigenvalue μ and an upper μ -core-forbidden-vertex have a repeated eigenvalue in a card of the p-deck and are therefore p-reconstructible. In this section, our ultimate aim is to seek potential candidates among disconnected simple graphs that could be counter examples to the positive solution of the PRP. From cited results, mostly from the work in [16], we deduce Corollary 6 in which the scope for further investigation is narrowed down to just two subclasses of disconnected graphs. We show, in Theorem 8, that a graph not having eigenvalue μ is reconstructible from a μ -eigenvector deck. We then consider the special case of a disconnected graph with two components, on the same number of vertices, having the eigenvalue μ and with each card of the deck showing μ of multiplicity one. We characterize the two components as μ -nut graphs in Theorem 10.

3.1. The Counter Example Technique

First, let us suppose that a graph H is not uniquely polynomial reconstructible. Then there exists a graph G such that H and G form a counter example pair to the PRP. Thus G is not co-spectral to H and $\phi(G, \lambda)$ is a reconstruction from $\mathcal{PD}(H)$. This technique reveals classes of graphs that are polynomial reconstructible without deriving the characteristic polynomial explicitly.

From Corollary 2, we deduce that the characteristic polynomials of H and of G differ only in the constant term a_0 . We shall assume that $a_0(H) = a_0(G) + \Delta a_0$ where $\Delta a_0 > 0$.

Immediate deductions are

- i $\phi(H, \lambda) \neq \phi(G, \lambda)$.
- ii As $a_0(H)$ is equal to $\text{Det}(-\mathbf{A}(H))$ and $a_0(G)$ is different, it follows that $\mathbf{A}(H) \neq \mathbf{A}(G)$ and that H and G are *not* isomorphic.
- iii G and H have no eigenvalue μ in common; otherwise, $\phi(G, \mu) = \phi(H, \mu) = 0$. This implies that the constant term of $\phi(G, \lambda)$ is the same as that of $\phi(H, \lambda)$.
- iv No polynomial in the p-deck $\mathcal{PD}(H)$ has a repeated eigenvalue μ . Otherwise, interlacing forces each of the graphs G and H to have the eigenvalue μ . By iii., this implies that G and H would be co-spectral.

3.2. A Disconnected Graph in a Counter Example Pair

We proceed to consider the PRP for disconnected graphs. Whether connectivity of G can be recognized from the p-deck $\{\phi(G - v, \lambda)\}_v$ or not is an open problem to date. We settle the problem for all subclasses of disconnected graphs except two, specified in Corollary 6.

If a graph H is known to be disconnected, then its spectrum is recoverable from the p-deck. This follows as the maximum eigenvalue in the p-deck is also an eigenvalue of H . Recognizing that a graph is disconnected from the p-deck is proving to be hard to show.

We shall use the counter example approach to obtain subclasses of disconnected graphs that are polynomial reconstructible.

If a disconnected graph H is not uniquely polynomial reconstructible and (G, H) is a counter example pair to the PRP, then the two graphs H and G are not both disconnected. Henceforth, we shall assume that G is connected and that H is disconnected in a counter example pair (G, H) to the positive solution of the PRP. This is consistent with the condition $a_0(H) = a_0(G) + \Delta a_0$ where $\Delta a_0 > 0$.

A graph H is polynomial reconstructible if and only if no other graph has the same p -deck as H . In [18], subclasses $\{H\}$ of the class of disconnected graphs that cannot share the same p -deck with any other graph are given.

Theorem 6. [18] *A disconnected graph that satisfies one of the following sufficient conditions, is polynomial reconstructible:*

1. *if the number of components of H is more than two;*
or
2. *if $H = H_1 \dot{+} H_2$ and satisfies one of the following:*
 - (a) $n(H_1) \neq n(H_2)$;
 - (b) H_i and $H_j - v$, $i \neq j$, $i, j \in \{1, 2\}$ have a common eigenvalue.
 - (c) one of the components has a repeated eigenvalue;
 - (d) the second larger eigenvalue of one component H_i is greater than the maximum eigenvalue of H_j , $i \neq j$, $i, j \in \{1, 2\}$;
 - (e) $m(H_i) - m(H_j) \geq \rho_{min}$, $i, j \in \{1, 2\}$, where ρ_{min} is the minimum vertex degree of H .

An immediate consequence is that the PRP is still open for the disconnected graphs specified in the following result:

Corollary 6. *Let H be a disconnected graph with two components H_1 and H_2 on the same number of vertices. The graph H is reconstructible if H does not satisfy*

1. $H = H_1 \dot{+} H_2$ and $m(H_1) = m(H_2)$ or
2. $H = H_1 \dot{+} H_2$, $m(H_1) > m(H_2)$ and $0 < m(H_1) - m(H_2) < \rho_{min}$.

3.3. Common Eigenvalue Deck

Next, we consider \mathcal{G}_μ , which denotes the class of n vertex-labeled graphs G with a common simple eigenvalue μ -deck.

Lemma 6. *Let μ be a simple eigenvalue of each of the n subgraphs $G - v$, $1 \leq v \leq n$, of a graph G . Then, either μ is a repeated eigenvalue of G of multiplicity two or μ is not an eigenvalue of G .*

Proof. As the dimension of the μ -eigenspace of $G - v$ is 1, by interlacing, the multiplicity of μ for G lies between 0 and 2. Suppose $\phi(G, \lambda) = (\lambda - \mu)g(\lambda)$ and $g(\mu) \neq 0$. Then, $\phi'(G, \lambda) = (\lambda - \mu)g'(\lambda) + g(\lambda)$ and hence $\phi'(G, \mu) \neq 0$. For the given p -deck, this contradicts Theorem 2. Thus the multiplicity of μ as an eigenvalue of G is not 1. By interlacing, it must be 2 or 0. \square

Lemma 6 leads to a partition of \mathcal{G}_μ into two subclasses, for a particular eigenvalue μ : Class I includes those graphs with a common simple eigenvalue μ -deck and multiplicity $\eta_\mu = 0$; Class II contains those graphs with a common simple eigenvalue μ -deck and multiplicity $\eta_\mu = 2$.

In [16], it is shown that for $G \in \mathcal{G}_\mu$ in Class I, the associated μ -eigenspaces alone suffice to reconstruct a parent graph that does not have μ as an eigenvalue. We provide a sketch of the proof. The k th partial- μ -eigenvector \mathbf{y}_k of H is obtained from the μ -eigenvector \mathbf{z}_k of $H - v_k$ by inserting an entry 0 in the k th position. Reconstruction from eigenvectors demands that the parent graph be labeled. This follows since permutations of entries not of the same value need not remain eigenvectors.

Theorem 7 ([16]). Let μ be a real number. Consider a labeled parent graph G on $n > 2$ vertices whose deck consists of cards representing subgraphs each of which has the eigenvalue μ of multiplicity one. If the columns of matrix \mathbf{Q} are the n partial- μ -eigenvectors \mathbf{y}_i , $1 \leq i \leq n$, of G , then, depending on the invertibility of \mathbf{Q} , we have (i) if \mathbf{Q} is non-singular, then μ is not an eigenvalue of G . (ii) if \mathbf{Q} is singular, then $\text{rank}(\mathbf{Q}) = 2$ and μ is an eigenvalue of G with multiplicity two.

Proof. Let G be a labeled graph in \mathcal{G}_μ with 0–1 adjacency matrix \mathbf{A} and \mathbf{R}_i be the i -th row of $(\mathbf{A}(G) - \mu\mathbf{I})$. By definition of $\mathbf{z}_i = (z_{(\ell),i})$, $1 \leq \ell \leq n - 1$, $(\mathbf{A}(G - v_i) - \mu\mathbf{I})\mathbf{z}_i =$

$$(\mathbf{A}(G - v_i) - \mu\mathbf{I}) \begin{pmatrix} z_{(1)i} \\ z_{(2)i} \\ \vdots \\ \vdots \\ z_{(n-1)i} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}.$$

$$\text{Thus, } (\mathbf{A}(G) - \mu\mathbf{I})\mathbf{y}_i = (\mathbf{A}(G) - \mu\mathbf{I}) \begin{pmatrix} z_{(1)i} \\ z_{(2)i} \\ \vdots \\ z_{(i-1)i} \\ 0 \\ z_{(i)i} \\ \vdots \\ z_{(n-1)i} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \mathbf{R}_i\mathbf{y}_i \\ \vdots \\ \vdots \\ 0 \end{pmatrix} \text{ and } (\mathbf{A}(G) - \mu\mathbf{I})\mathbf{Q} =$$

$\text{Diag}(\mathbf{R}_1\mathbf{y}_1, \mathbf{R}_2\mathbf{y}_2, \dots, \mathbf{R}_n\mathbf{y}_n)$.

If \mathbf{Q} is non-singular,

$$(\mathbf{A}(G) - \mu\mathbf{I}) = \text{Diag}(\mathbf{R}_1\mathbf{y}_1, \mathbf{R}_2\mathbf{y}_2, \dots, \mathbf{R}_n\mathbf{y}_n)\mathbf{Q}^{-1}, \quad (10)$$

$\mathbf{R}_i\mathbf{y}_i \neq \mathbf{0}$, $1 \leq i \leq n$ and μ is not an eigenvalue of G . This proves (i).

Now, if \mathbf{Q} is singular, then $\mathbf{R}_i\mathbf{y}_i = \mathbf{0}$, for some i . Thus, \mathbf{y}_i would be a μ -eigenvector of G . However, then the dimension of the μ -eigenspace of G is two and G is a μ -core graph. A fortiori, $\mathbf{R}_i\mathbf{y}_i = \mathbf{0}$, for all i . Moreover the rank of \mathbf{Q} is the dimension of the μ -eigenspace, which is less than n .

This completes the proof. \square

For a graph in Class I, Theorem 7 presents an algorithm that constructs, from the sequence of the generators of the μ -eigenvectors of the subgraphs in the deck, the labeled parent graph G directly. Moreover it gives also the value of μ .

Theorem 8. Let μ be a real number. For $n \geq 3$, let G be a n -vertex graph that does not have μ in its spectrum and has the simple eigenvalue μ in each card of its p -deck. From the sequence of the μ -eigenvectors of the vertex-deleted subgraphs in the deck, relative to some vertex-labeling of G ,

- (i.) the labeled graph G is reconstructible;
- (ii.) the unique eigenvalue μ can be obtained.

Proof. Using the notation of Theorem 7, since the graph G does not have the eigenvalue μ , then $(\mathbf{A}(G) - \mu\mathbf{I})^{-1}$ exists. In (10), the k -th column of $(\mathbf{A}(G) - \mu\mathbf{I})^{-1}$ is a scalar multiple of the k th partial- μ -eigenvector \mathbf{y}_k of H , obtained from the μ -eigenvector \mathbf{z}_k of $H - v_k$.

Thus, $\text{Diag}(\mathbf{R}_1\mathbf{y}_1, \mathbf{R}_2\mathbf{y}_2, \dots, \mathbf{R}_n\mathbf{y}_n) \neq \mathbf{0}$, that is, $\mathbf{R}_i\mathbf{y}_i \neq \mathbf{0}$, for all i ; otherwise, G would have the eigenvalue μ . As each entry of \mathbf{A} is 0 or 1, the i -th column of $(\mathbf{A}(G) - \mu\mathbf{I})^{-1}$ is $\frac{\mathbf{y}_i}{\mathbf{R}_i\mathbf{y}_i}$.

Thus \mathbf{A} can be obtained and hence the labeled graph G is reconstructible from (10). This proves (i.)

To prove (ii.), recalling that a diagonal entry of \mathbf{A} is 0, $\mu = -\mathbf{R}_i\mathbf{y}_i(\mathbf{Q}^{-1})_{ii}$. \square

3.4. Subclasses of Disconnected Graphs with a Common Eigenvalue Deck

Our ultimate objective is to determine the subclasses of the class of disconnected graphs which may not be polynomial reconstructible. From Corollary 6, we may assume in the sequel, that H is a disconnected graph $H_1 \dot{\cup} H_2$ with $|H_1| = |H_2|$. The maximum eigenvalue of H is also the maximum eigenvalue that appears in the p-deck. If (H, G) is a counter example pair to the positive resolution of the PRP, then G must be connected, as otherwise H and G would have a common eigenvalue. Let the multiplicity of μ in each card of the p-deck be 1. By Lemma 6, μ is an eigenvalue of H of multiplicity zero or two. We now consider the disconnected graphs $H = H_1 \dot{\cup} H_2$, with $|H_1| = |H_2|$, within Classes I and II.

Theorem 9. *Let the n vertex graph H be disconnected. Let $H = H_1 \dot{\cup} H_2$, with $|H_1| = |H_2|$ with a common simple eigenvalue μ -deck. Then, either (i) H belongs to Class I and every vertex of H is μ -upper core-forbidden, H does not have the eigenvalue μ . and can be reconstructed from the sequence of the n μ -eigenvectors of $H - v$, $1 \leq v \leq n$; or (ii) H belongs to Class II and every vertex of H is a μ -core vertex.*

Proof. (i) If μ is not an eigenvalue of H , then the multiplicity of the eigenvalue μ increased with a vertex-deletion from H . Hence each vertex of H is an upper μ -core forbidden vertex. In this case, from Theorem 8, the labeled graph H is reconstructible from a sequence of μ eigenvectors of $H - v$, $1 \leq v \leq n$.

(ii) By Lemma 6, there is only one remaining case. If μ is an eigenvalue of both H_1 and H_2 , then the multiplicity of the eigenvalue μ decreased with a vertex-deletion from H . Hence each vertex of H is a μ -core vertex. \square

A disconnected graph H in Class I and a partner graph G in a counter example pair to the positive resolution of the PRP are non-isomorphic and have different sequences of μ -eigenvectors of their respective p-decks. Moreover they are not co-spectral. To date we know of no such examples.

For graphs in Class II, there is a combinatorial characterization.

Theorem 10. *Let μ be a real number. For $n \geq 3$, let $H = H_1 \dot{\cup} H_2$, with $|H_1| = |H_2|$, and a common μ -eigenvalue deck. If $\eta_\mu(H) = 2$ and H is a graph in a counter example pair to the positive solution of the PRP, then each of the subgraphs H_1 and H_2 are μ -nut graphs, that is a μ -eigenvector in each subgraph has no entry zero.*

Proof. The graph H is in Class II. None of the components H_1 or H_2 can have μ of multiplicity two, as otherwise the repeated root μ would appear in the p-deck. Hence each of the subgraphs H_1 and H_2 has nullity one. As each vertex is a μ -core vertex, then H is a μ -core graph. Therefore, each of the subgraphs H_1 and H_2 is a μ -nut graphs, that is a μ -eigenvector in each subgraph has no entry zero. \square

3.5. Concluding Remarks

We have proved that potential counter examples to the PRP may occur in both Classes I and II. From a sequence of μ eigenvectors, graphs in Class I and μ can be reconstructed. A disconnected graph in Class II has a combinatorial characterization as the disjoint union of two μ -nut-graphs of the same order but has not been explicitly constructed. Note that μ -nut-graphs characterize the class of connected graphs and consist precisely of those graphs K that can be reconstructed from a single vertex-deleted subgraph together with the generator of the μ -eigenspace of K [19].

The PRP is also still open for disconnected graphs $H = H_1 \dot{\cup} H_2$, with $|H_1| = |H_2|$, without a common eigenvalue deck. Were such a graph to exist, it would have a connected graph as a partner in a counter example pair, with the same p-deck, which could give more than one polynomial reconstruction. These results could be seen in the context of the recognition of connectivity from the p-deck. The problem is therefore still open.

Methods to reconstruct the parameters of a parent graph based on data derived from the eigenspaces of vertex-deleted subgraphs are not only very attractive in spectral graph theory. They are also often at the cutting edge of applications in bioinformatics and mathematical chemistry.

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