

A Study of Eigenspaces of Graphs

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ABSTRACT

We investigate the relationship between the structure of a graph and its eigenspaces. The angles between the eigenspaces and the vectors of the standard basis of \mathbb{R}^n play an important role. The key notion is that of a special basis for an eigenspace called a star basis. Star bases enable us to define a canonical bases of \mathbb{R}^n associated with a graph, and to formulate an algorithm for graph isomorphism.

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1. INTRODUCTION

Let G be a graph with vertices $1, \dots, n$. Let μ_1, \dots, μ_m ($\mu_1 > \dots > \mu_m$) be the distinct eigenvalues of [the $0, 1$ adjacency matrix $A = A(G)$ of] G , with corresponding eigenspaces $\mathcal{E}(\mu_1), \dots, \mathcal{E}(\mu_m)$. Let $\{e_1, \dots, e_n\}$ be the standard orthonormal basis of \mathbb{R}^n . The numbers $\alpha_{ij} = \cos \beta_{ij}$ ($i = 1, \dots, m$; $j = 1, \dots, n$), where β_{ij} is the angle between $\mathcal{E}(\mu_i)$ and e_j , are called *angles* of G . The $m \times n$ matrix $\mathcal{A} = (\alpha_{ij})$ is called the *angle matrix* of G . We may order the columns of \mathcal{A} lexicographically so that \mathcal{A} becomes a graph invariant. Rows of \mathcal{A} are associated with eigenvalues and are called *eigenvalue angle sequences*, while columns of \mathcal{A} are associated with vertices and are called *vertex angle sequences*.

A graph invariant, or property, or subgraph, is said to be *EA-reconstructible* if it can be determined once the eigenvalues and the angle matrix of the graph are known.

Let $\Phi(G, \lambda) [= \det(\lambda I - A)]$ be the characteristic polynomial of G , and let $G - i$ ($i = 1, \dots, n$) be the vertex-deleted subgraphs of G . We have (cf. [7])

$$\Phi(G - j, \lambda) = \Phi(G, \lambda) \sum_{i=1}^m \frac{\alpha_{ij}^2}{\lambda - \mu_i} \quad (j = 1, \dots, n). \quad (1.1)$$

Let N_k^i be the number of closed walks of length k starting and terminating at vertex i . For the generating function $H_i(t) = \sum_{k=0}^{\infty} N_k^i t^k$ we have

$$H_i(t) = \frac{\Phi(G - i, 1/t)}{t\Phi(G, 1/t)}. \quad (1.2)$$

Equations (1.1) and (1.2) show that the polynomials $\Phi(G - i, \lambda)$ and the functions $H_i(t)$ are EA-reconstructible. From Equation (1.2) we see also that vertex degrees are EA-reconstructible.

Let

$$A = \mu_1 P_1 + \dots + \mu_m P_m$$

be the usual spectral decomposition of the adjacency matrix A of a graph G ; the matrix $P_i = (p_{jk}^{[i]})$ represents the orthogonal projection onto the eigenspace $\mathcal{E}(\mu_i)$ ($i = 1, \dots, m$). We have $\alpha_{ij} = \|P_i e_j\|$ and (when $P_i e_j$,

$P_i e_k$ are nonzero)

$$p_{jk}^{[i]} = \alpha_{ij} \alpha_{ik} \cos \gamma_{jk}^{[i]},$$

where $\gamma_{jk}^{[i]}$ is the angle between $P_i e_j$ and $P_i e_k$. More generally, knowledge of α_{ij} , α_{ik} , and $p_{jk}^{[i]}$ is equivalent to the knowledge of $\|P_i e_j\|$, $\|P_i e_k\|$, and $\|P_i e_j + P_i e_k\|$.

Questions of EA-reconstructibility have been studied in the papers [3, 11, 4, 5]. See [10] for relations to Ulam's graph-reconstruction conjecture.

Since graphs are not EA-reconstructible in general [3, §5], we seek further algebraic invariants of graphs. In this paper we introduce special bases for eigenspaces defined by *eutactic stars* [19], obtained by projecting e_1, \dots, e_n to particular eigenspaces. Accordingly such bases are called *star bases*. Star bases enable us to define a *canonical* basis for \mathbb{R}^n and a *complete set* of graph invariants (i.e. a set determining the graph up to an isomorphism).

The plan of the paper is as follows. In Section 2 we study bases of eigenspaces and introduce star bases. Section 3 is devoted to the study of special vertex partitions induced by star bases and called *star partitions*. In Section 4 we derive a formula for the characteristic polynomial of a certain type of subgraph and consider other consequences. In Section 5 we introduce canonical star bases and relate them to the graph-isomorphism problem.

2. BASES OF EIGENSPACES

For a simple eigenvalue a basis of the corresponding eigenspace is of course determined uniquely to within a scalar factor. For a multiple eigenvalue the degree of freedom is such that it is desirable to identify natural choices for a basis of the corresponding eigenspace. Here we discuss two means of defining bases, related to our eventual construction of a canonical basis of \mathbb{R}^n .

2.1. Eutactic Stars and Star Bases

Let V be a Euclidean space. The span of the subset $\{v_1, \dots, v_k\}$ is denoted by $\langle v_i | i = 1, \dots, k \rangle$. Let (x, y) be the inner product of vectors $x, y \in V$, and let $\|x\|$ be the norm of x . A star in V is a finite set of vectors which span V . For a star $\mathcal{S} = \{v_1, \dots, v_k\}$,

- (1) \mathcal{S} is *orthogonal* if $(v_i, v_j) = 0$ ($i \neq j$);
- (2) \mathcal{S} is *spherical* if $\|v_i\| = \|v_j\|$ for all i, j .

DEFINITION 2.1 (See [19]). Let U be a nontrivial subspace of V . A *eutactic star* in U is the orthogonal projection onto U of an orthogonal spherical basis of V .

Suppose now that A is a real symmetric matrix (for example, an adjacency matrix of the graph G) with (different) eigenvalues $\mu_1 > \dots > \mu_m$, and corresponding eigenspaces $\mathcal{E}(\mu_1), \dots, \mathcal{E}(\mu_m)$. Let $k_i [= \dim \mathcal{E}(\mu_i)]$ be the multiplicity of μ_i , and let $V = \mathbb{R}^n$ with $(x, y) = x^T y$. Denote by P_i the orthogonal projection of V onto $\mathcal{E}(\mu_i)$. Let \mathcal{E} be the standard basis $\{e_1, \dots, e_n\}$ of V , and let \mathcal{T}_i be the eutactic star $\{P_i e_1, \dots, P_i e_n\}$ obtained by projecting the star \mathcal{E} onto $\mathcal{E}(\mu_i)$. ($P_i e_j$ is one of the *arms* of the star \mathcal{T}_i , and the angle α_{ij} is the norm $\|P_i e_j\|$ of this arm.)

QUESTION 2.2. Given A , it is possible to find a basis \mathcal{B} of \mathbb{R}^n consisting of vectors from $\bigcup_{i=1}^m \mathcal{T}_i$ such that (for $P_i e_s, P_j e_t \in \mathcal{B}$) the condition

$$P_i e_s \neq P_j e_t \quad \Rightarrow \quad s \neq t$$

holds?

If such a basis \mathcal{B} exists, then there is a one-one correspondence between \mathcal{E} and \mathcal{B} . If a set X is partitioned into sets X_1, \dots, X_n , we write $X = X_1 \dot{\cup} \dots \dot{\cup} X_n$ and call X_1, \dots, X_n the *cells* of the partition. A cell X_i is called *nontrivial* if $|X_i| > 1$.

DEFINITION 2.3. A *star basis* of \mathbb{R}^n , corresponding to a symmetric matrix A , is a basis $\mathcal{B} = \{P_i e_s | s \in X_i, i = 1, \dots, m\}$, where P_i is defined as above, and $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a partition of the set $\{1, \dots, n\}$.

Now we proceed to prove that star bases do exist. The next theorem, concerning an arbitrary direct sum of two subspaces, plays a fundamental role in that respect.

THEOREM 2.4. Let V be a finite-dimensional vector space. If $V = U \oplus W$, let P (respectively, Q) be the projection of V on U along W (of V on W along U). If $\{e_1, \dots, e_n\}$ is a basis of V , then there exists a bipartition $I \dot{\cup} J$ of $\{1, \dots, n\}$ such that

$$U = \langle P e_i | i \in I \rangle \quad \text{and} \quad W = \langle Q e_j | j \in J \rangle.$$

Proof. Let U have basis $\{x_1, \dots, x_k\}$ and let W have basis $\{x_{k+1}, \dots, x_n\}$. Then $\{x_1, \dots, x_n\}$ is a basis of V , and we have a transition matrix $T = (t_{ij})$ from $\{x_1, \dots, x_n\}$ to $\{e_1, \dots, e_n\}$ given by

$$e_j = \sum_{i=1}^n t_{ij} x_i \quad (j = 1, \dots, n). \quad (2.1)$$

Consider the Laplacian development of $\det T$ determined by the first k rows of T . Since $\det T \neq 0$, there exists a bipartition $I \dot{\cup} J$ such that the matrices

$$(t_{ij})_{i \in \{1, \dots, k\}, j \in I}$$

and

$$(t_{ij})_{i \in \{k+1, \dots, n\}, j \in J}$$

are both invertible. Hence the vectors Pe_i ($i \in I$), and also Qe_j ($j \in J$), are linearly independent, and consequently $U = \langle Pe_i | i \in I \rangle$, $W = \langle Qe_j | j \in J \rangle$. ■

COROLLARY 2.5. *If $V = U_1 \oplus \dots \oplus U_m$, there exists a partition $X_1 \dot{\cup} \dots \dot{\cup} X_m$ of $\{1, \dots, n\}$ such that $U_i = \langle P_i e_j | j \in X_i \rangle$ ($i = 1, \dots, m$), where P_i is the projection of V onto U_i along $U_1 \oplus \dots \oplus U_{i-1} \oplus U_{i+1} \oplus \dots \oplus U_m$.*

Proof. By induction on m , making use of the previous theorem. ■

By putting $V = \mathbb{R}^n$ and $U_i = \mathcal{E}(\mu_i)$ ($i = 1, \dots, m$) in Corollary 2.5, it follows immediately that a star basis always exists.

Let us consider the case in which $\{x_1, \dots, x_n\}$ is an orthonormal basis of \mathbb{R}^n , ordered so that $\{x_j : j \in X_i\}$ is a basis of $\mathcal{E}(\mu_i)$ ($i = 1, \dots, m$). Then the orthogonal matrix U whose columns are x_1, \dots, x_n is the inverse of the transition matrix (t_{ij}) defined by (2.1). It follows that if U_{ii} denotes the principal submatrix of U determined by X_i , then U_{ii}^T is the transition matrix from the basis $\{P_i e_j : j \in X_i\}$ of $\mathcal{E}(\mu_i)$ to the basis $\{x_j : j \in X_i\}$ ($i = 1, \dots, m$).

2.2. Partial λ -Eigenvectors and Exit Values

Let A be an $n \times n$ matrix with real entries, and let $A_{i\bullet}$ ($A_{\bullet j}$) be the i th row (j th column) of A . Also let $\lambda \in \mathbb{R}$, and let $u \in \{1, \dots, n\}$. Following Neumaier [14], we say that $y = (y_1, \dots, y_n)^T \in \mathbb{R}^n$ is a *partial λ -eigenvector* of A with respect to u if $y_u = 1$ and y satisfies all eigenvalue equations

except the u th, i.e. if $y_u = 1$ and

$$A_{i \bullet} y = \lambda y_i \quad (2.2)$$

for all $i \neq u$. The corresponding *exit value* is defined by

$$\varphi_u(\lambda) = \lambda - A_{u \bullet} y. \quad (2.3)$$

Note that if $\varphi_u(\tilde{\lambda}) = 0$ then $\tilde{\lambda}$ is an eigenvalue of A .

Now assume that A is the adjacency matrix of a graph G , and let u be some specified vertex of G . If (2.2) and (2.3) are interpreted in G , we have

$$\sum_{j \sim i} y_j = \lambda y_i \quad (i \neq u),$$

where $p \sim q$ means that vertex p is adjacent to vertex q , and for $i = u$

$$\varphi_u(\lambda) = \lambda - \sum_{j \sim u} j_i.$$

We now proceed to find the partial λ -eigenvectors of a graph G (i.e. of its adjacency matrix) corresponding to vertex u . Without loss at generality, let $u = n$. Starting from the system

$$\begin{aligned} (\lambda - a_{11})x_1(\lambda) & - a_{12}x_2(\lambda) - \cdots & - a_{1n}x_n(\lambda) &= 0, \\ -a_{21}x_1(\lambda) & + (\lambda - a_{22})x_2(\lambda) - \cdots & - a_{2n}x_n(\lambda) &= 0, \\ & & \vdots & \\ -a_{n1}x_1(\lambda) & - a_{n2}x_2(\lambda) - \cdots + (\lambda - a_{nn})x_n(\lambda) &= 0 \end{aligned} \quad (2.4)$$

it immediately follows [by ignoring the last equation and applying Cramer's rule to the system in $x_1(\lambda), \dots, x_{n-1}(\lambda)$] that

$$\Phi(G - n, \lambda)x_i(\lambda) = x_n(\lambda)\theta_{ni}(\lambda I - A) \quad (i = 1, \dots, n-1),$$

where $\theta_{st}(X)$ denotes the (s, t) cofactor of a matrix X . By [17] we get

$$\begin{aligned} \theta_{ni}(\lambda I - A) \\ = \begin{cases} \frac{1}{2}[\Phi(G - in, \lambda) + \Phi(G - i - n, \lambda) - \Phi(G, \lambda)] & \text{if } i \sim n, \\ \frac{1}{2}[\Phi(G, \lambda) - \Phi(G - i - n, \lambda) - \Phi(G + in, \lambda)] & \text{if } i \not\sim n. \end{cases} \end{aligned}$$

Assuming $\Phi(G - n, \lambda) \neq 0$, and letting $x_n(\lambda) = 2\Phi(G - n, \lambda)$, we obtain (for any u , not necessarily $u = n$)

$$\begin{aligned} x_i(\lambda) &= x_i(G; u, \lambda) \\ &= \begin{cases} \Phi(G - iu, \lambda) + \Phi(G - i - u, \lambda) - \Phi(G, \lambda) & \text{if } i \sim u, \\ \Phi(G, \lambda) - \Phi(G - i - u, \lambda) - \Phi(G + iu, \lambda) & \text{if } i \not\sim u, \\ 2\Phi(G - u, \lambda) & \text{if } i = u. \end{cases} \end{aligned} \quad (2.5)$$

For the partial λ -eigenvector y we have $y_i(\lambda) = x_i(\lambda)/x_u(\lambda)$ ($i = 1, \dots, n$). According to [14], for the exit value we have

$$\varphi_u(\lambda) = \frac{\Phi(G, \lambda)}{\Phi(G - u, \lambda)}. \quad (2.6)$$

Now we first make use of formulas from (2.5) to compute the eigenvectors of G corresponding to an eigenvalue μ_s .

Case 1: μ_s is a simple eigenvalue of G ($k_s = 1$). By

$$\Phi'(G, \lambda) = \sum_{i=1}^n \Phi(G - i, \lambda), \quad (2.7)$$

we have that $\Phi(G - u, \mu_s) \neq 0$ for at least one u . Now let $x^{(u)} = (x_1, \dots, x_n)^T$, where

$$x_i = x_i(G; u, \mu_s) \quad (i = 1, \dots, n). \quad (2.8)$$

Then $x^{(u)}$ is an eigenvector of G corresponding to the vertex u .

Case 2: μ_s is a multiple eigenvalue of G ($k_s > 1$). Then $\Phi(G - U, \mu_s) \neq 0$ for at least one U , where $U \subseteq V(G)$ and $|U| = k_s$ [otherwise, $\Phi^{(k_s)}(G; \mu_s) = 0$ by repeated use of Equation (2.7)]. Making use of (2.8) for the subgraph H_u induced by the vertex set $\{u\} \cup (V(G) \setminus U)$ ($u \in U$), we

let $x^{(u)} = (x_1, \dots, x_n)^T$, where

$$x_i = \begin{cases} 0, & i \notin V(H_u), \\ x_i(H_u; u, \mu_s), & i \in V(H_u) \end{cases} \quad (i = 1, \dots, n). \quad (2.9)$$

Then $x^{(u)}$ is an eigenvector of G corresponding to any vertex u from the vertex set U .

REMARK 2.6. For a fixed eigenvalue μ_s , the k_s vectors $x^{(u)}$ ($u \in U$) specified by Equation (2.9) are linearly independent. They are indeed eigenvectors of A , i.e. of G . To see this, observe that each $x^{(u)}$ represents a solution of the $n - k_s$ equations of the system (2.4) indexed by $V(G) \setminus U$. Since $\mu_s I - A$ has rank $n - k_s$ and $\Phi(G - U, \mu_s) \neq 0$, these $n - k_s$ equations are equivalent to (2.4). Thus the above set of vectors constitute a basis for the corresponding eigenspace $\mathcal{E}(\mu_s)$.

The above conclusions can be summarized in the next theorem.

THEOREM 2.7. *Let μ_s be an eigenvalue of G with multiplicity k_s . Suppose that U is a vertex subset of G of cardinality k_s . If $\Phi(G - U, \mu_s) \neq 0$, then the k_s vectors $x^{(u)} = (x_1, \dots, x_n)^T$ with components given by (2.9) constitute a basis of the eigenspace $\mathcal{E}(\mu_s)$.*

REMARK 2.8. From (2.9) we see that the components of $x^{(u)}$ ($u \in U$) do not depend on the structure of the subgraph induced by vertices from U . This phenomenon is explained in Theorem 4.6.

QUESTION 2.9. Is there a partition $X_1 \dot{\cup} \dots \dot{\cup} X_m$ of the vertex set of a graph G such that $\Phi(G - X_i, \mu_i) \neq 0$ for each $i = 1, \dots, m$?

An affirmative answer to the above question is given in the next section (Theorems 3.9 and 3.11), and an alternative argument appears in Section 4 (see Remark 4.4). As a consequence there exists a square matrix of eigenvectors of the form

$$\begin{bmatrix} I_{k_1} & * & & * \\ * & I_{k_2} & & * \\ & & \ddots & \\ * & * & & I_{k_m} \end{bmatrix},$$

where $*$ denotes a block of an appropriate size. The converse is also true (to be proved in a forthcoming article).

Finally, we give a new recursive formula for computing the characteristic polynomial of a graph. It is worth mentioning that the graphs involved in our formula are rather local modifications of the graph in question, in contrast to the formulas of A. J. Schwenk (see, for example [9, p. 78] or [18]). For some other formulas see the monographs [9, 8] and the papers [16, 5, 18, 20].

THEOREM 2.11. *Let G be a graph, and u a vertex of G whose degree differs from 2, i.e. $\deg u \neq 2$. Then*

$$\Phi(G, \lambda) = \frac{1}{\deg u - 2} \left(\sum_{i \sim u} \Phi(G - iu, \lambda) + \sum_{i \sim r} \Phi(G - i - u, \lambda) - 2\lambda \Phi(G - u, \lambda) \right). \quad (2.10)$$

Proof. From (2.3) and (2.6) we immediately get

$$\Phi(G, \lambda) = \lambda \Phi(G - u, \lambda) - \frac{1}{2} \sum_{i \sim u} x_i(\lambda).$$

Next, by (2.5), we obtain

$$\begin{aligned} (\deg u - 2)\Phi(G, \lambda) &= \sum_{i \sim u} \Phi(G - iu, \lambda) \\ &\quad + \sum_{i \sim u} \Phi(G - i - u, \lambda) - 2\lambda \Phi(G - u, \lambda), \end{aligned}$$

and hence the theorem. ■

REMARK 2.12. The formula (2.10) can also be derived by combining the aforementioned formulas of A. J. Schwenk. Note also that if $\deg u = 2$, (2.10) reduces to a simple consequence of Heilbronner's formulas (see, for example, [9, p. 59]).

3. STAR PARTITIONS

The fact that star bases do exist enables us to partition the vertex set $V(G)$ of an arbitrary graph G as follows:

DEFINITION 3.1. For a graph G , the partition $X_1 \dot{\cup} \cdots \dot{\cup} X_m$ of $V(G)$ is a star partition if

$$\mathcal{E}(\mu_i) = \langle P_i e_s \mid s \in X_i \rangle \quad (i = 1, \dots, m).$$

REMARK 3.2. Since $|X_i| \geq k_i [= \dim \mathcal{E}(\mu_i)]$ for each i , we have $|X_i| = k_i$ ($i = 1, \dots, m$). In what follows any partition $Y_1 \dot{\cup} \dots \dot{\cup} Y_m$ of $V(G)$ with $|Y_i| = k_i$ for each i is called a *feasible* partition.

THEOREM 3.3. *Let $X_1 \dot{\cup} \dots \dot{\cup} X_m$ be a star partition of $V(G)$, and let $s \in X_i$. Then, either s is adjacent to some vertex $t \in \bar{X}_i (= V(G) \setminus X_i)$, or s is isolated and moreover $\mu_i = 0$.*

Proof. Since $\mu_i P_i e_s = A P_i e_s = P_i A e_s = P_i \sum_{t \sim s} e_t = \sum_{t \sim s} P_i e_t$, we have: if s is not isolated, the vectors $\{P_i e_s\} \cup \{P_i e_t | t \sim s\}$ are linearly dependent and so not every $t \sim s$ can be in X_i . On the other hand, if s is isolated then $\mu_i = 0$, since $P_i e_s \neq 0$. ■

From the above theorem, it follows that feasible partitions are not necessarily star partitions. To see this, observe that for any nonisolated vertex u of a graph, its closed neighborhood $\Delta^*(u) [= \{u\} \cup \Delta(u); \Delta(u) = \{v | v \sim u\}]$ is not included in any cell X_i , i.e., $\Delta^*(u)$ is *forbidden* as a subset of any X_i . Moreover, all isolated vertices lie within the same cell. For some graphs, these restrictions are sufficient to determine the form of star partitions; for example, if $G = K_{m,n}$ ($m, n \geq 3$), then a star partition necessarily has the form $\{u\} \dot{\cup} (V(G) \setminus \{u, v\}) \dot{\cup} \{v\}$, where $u \sim v$. Some further restrictions can be obtained by extending the argument of Theorem 3.3.

EXAMPLE 3.4. The argument of Theorem 3.3 extends to any polynomial f in A , since $f(\mu_i) P_i e_s = P_i f(A) e_s$. In particular, if $f(A) = A^2$ and s is nonisolated, then we find that the vertices in $W_2(s)$ (those reachable from s by walks of length 2) form a forbidden set unless $W_2(s) = \{s\}$. If $\{s\} \subset W_2(s)$ and $\mu_i^2 = \deg s$, then $W_2(s) \setminus \{s\}$ is forbidden.

EXAMPLE 3.5. Consider $\mu_i (P_i e_s - P_i e_t)$. If $s \rightsquigarrow t$, then we find that the symmetric difference $\Delta^*(s) + \Delta^*(t)$ is forbidden. If $s \sim t$, then $\Delta(s) + \Delta(t)$ is forbidden unless $\mu_i = -1$. If $s \sim t$ and $\mu_i = -1$, then $\Delta^*(s) + \Delta^*(t)$ is forbidden unless $\Delta^*(s) = \Delta^*(t)$. If $s \sim t$ and $\Delta(s) + \Delta(t) \subseteq X_i$, then $\mu_i = -1$ and either $\Delta^*(s) = \Delta^*(t)$ or $\Delta^*(s) + \Delta^*(t) \not\subseteq X_i$.

THEOREM 3.6. *Let $X_1 \dot{\cup} \dots \dot{\cup} X_m$ be a star partition of a graph G , and let k'_i (possibly zero) be the multiplicity of μ_i as an eigenvalue of $G - \bar{X}_i$. Then the number of vertices in \bar{X}_i which are adjacent to some vertex of X_i is at least $k_i - k'_i$.*

Proof. For $u \in X_i$, let $\Gamma(u) = \Delta(u) \cap X_i$ and $\bar{\Gamma}(u) = \Delta(u) \cap \bar{X}_i$. Let $\bar{\Gamma}(X_i) = \bigcup_{u \in X_i} \bar{\Gamma}(u)$, and let $A_i = A(G - \bar{X}_i)$.

From

$$\mu_i P_i e_u = A P_i e_u = P_i A_i e_u = \sum_{v \sim u} P_i e_v = \sum_{v \in \Gamma(u)} P_i e_v + \sum_{v \in \bar{\Gamma}(u)} P_i e_v,$$

we obtain

$$\mu_i P_i e_u - \sum_{v \in \Gamma(u)} P_i e_v = \sum_{v \in \bar{\Gamma}(u)} P_i e_v.$$

On the other hand $\mu_i I - A_i$ is the matrix with respect to the basis $\{P_i e_u | u \in X_i\}$ of the linear transformation of $\mathcal{E}(\mu_i)$ defined by

$$P_i e_u \mapsto \mu_i P_i e_u - \sum_{v \in \Gamma(u)} P_i e_v.$$

Since the rank of $\mu_i I - A_i$ is $k_i - k'_i$, the vectors $\sum_{v \in \bar{\Gamma}(u)} P_i e_v$ span a $(k_i - k'_i)$ -dimensional subspace of the space $\langle P_i e_j | j \in \bar{\Gamma}(X_i) \rangle$. This space has dimension at most $|\bar{\Gamma}(X_i)|$, and so we have $|\bar{\Gamma}(X_i)| \geq k_i - k'_i$, as required. ■

COROLLARY 3.7. *If μ_i is not an eigenvalue of $G - \bar{X}_i$, then there are at least k_i vertices of \bar{X}_i which are adjacent to some vertex of X_i .*

In the sequel we prove some nontrivial properties of star partitions.

LEMMA 3.8. *If $X_1 \dot{\cup} \cdots \dot{\cup} X_m$ is a star partition, then $\mathbb{R}^n = \mathcal{E}(\mu_i) \oplus V_i$, where $V_i = \langle e_s | s \notin X_i \rangle$ ($i = 1, \dots, m$).*

Proof. Since $\dim \mathcal{E}(\mu_i) = k_i$ and $\dim V_i = n - k_i$, it suffices to show that $\mathcal{E}(\mu_i) \cap V_i = \{0\}$. Let $x \in \mathcal{E}(\mu_i) \cap V_i$. Then $x = P_i x$ and $x^T e_s = 0$ for all $s \in X_i$. Hence, $x^T (P_i e_s) = x^T (P_i^T e_s) = (P_i x)^T e_s = 0$ for all $s \in X_i$. Thus $x \in \langle P_i e_s | s \in X_i \rangle^\perp = \mathcal{E}(\mu_i)^\perp$ and $x = 0$. ■

THEOREM 3.9. *If $X_1 \dot{\cup} \cdots \dot{\cup} X_m$ is a star partition of a graph G , then μ_i is not an eigenvalue of $G - X_i$ ($i = 1, \dots, m$).*

Proof. Without loss of generality, take $i = 1$, and let H be the subgraph $G - X_1$. Also, let A' be the adjacency matrix of H . Suppose that $A'x' =$

$\mu_1 x'$. If $y = [0 \ x']^T$, then

$$Ay = \begin{bmatrix} * & * \\ * & A' \end{bmatrix} \begin{bmatrix} 0 \\ x' \end{bmatrix} = \begin{bmatrix} * \\ \mu_1 x' \end{bmatrix}.$$

Now if $x \in V_1 (= \langle e_s | s \notin X_1 \rangle)$, then

$$x^T Ay = \begin{bmatrix} 0 \\ z \end{bmatrix}^T \begin{bmatrix} * \\ \mu_1 x' \end{bmatrix} = \mu_1 z^T x' = \mu_1 x^T y$$

and so $(A - \mu_1 I)y \in V_1^\perp$. On the other hand, if $x \in \mathcal{E}(\mu_1)$, then $x^T Ay = x^T A^T y = (Ax)^T y = (\mu_1 x)^T y = \mu_1 x^T y$ and so $(A - \mu_1 I)y \in \mathcal{E}(\mu_1)^\perp$. Hence $(A - \mu_1 I)y \in V_1^\perp \cap \mathcal{E}(\mu_1)^\perp = [\mathcal{E}(\mu_1) + V_1]^\perp$, which is zero by Lemma 3.8. Hence $y \in \mathcal{E}(\mu_1)$. But $y \in V_1$, and since $\mathcal{E}(\mu_1) \cap V_1 = \{0\}$ by Lemma 3.8, we have $y = 0$, and hence $x' = 0$. Thus μ_1 is not an eigenvalue of $G - X_1$. ■

COROLLARY 3.10. *If $S \subset X_i$, then μ_i is an eigenvalue of $G - S$ with multiplicity $k_i - |S|$.*

Proof. Removal of a vertex always reduces the multiplicity of μ_i at most by 1; but after the k_i vertices of X_i are removed, μ_i has multiplicity 0. Hence the multiplicity of μ_i is reduced by 1 on removal of any vertex of X_i (in any order). ■

THEOREM 3.11. *If $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a partition of $V(G)$ such that μ_i is not an eigenvalue of $G - X_i$ ($i = 1, \dots, m$), then $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a star partition.*

Proof. Without loss of generality, take $i = 1$. It suffices to prove that $\langle P_1 e_s | s \in X_1 \rangle = \mathcal{E}(\mu_1)$. Suppose to the contrary that $\langle P_1 e_s | s \in X_1 \rangle \subset \mathcal{E}(\mu_1)$. Then there is a nonzero vector $x \in \mathcal{E}(\mu_1) \cap \langle P_1 e_s | s \in X_1 \rangle^\perp$. Thus $x^T P_1 e_s = 0$ for all $s \in X_1$. Hence $(P_1 x)^T e_s = (x^T P_1) e_s = 0$ for all $s \in X_1$. Consequently $P_1 x \in \langle e_s | s \in X_1 \rangle^\perp = \langle e_s | s \notin X_1 \rangle = V_1$. But $x = P_1 x$, and so we have nonzero $x \in \mathcal{E}(\mu_1) \cap V_1$. Since $x = [0 \ x']^T$ with $x' \neq 0$, it follows that x' is an eigenvector of $G - X_1$, a contradiction. ■

Theorems 3.9 and 3.11 show that the star partitions are just the same partitions as required by Question 2.9. In the next section (see Remark 4.4) we shall give an alternative proof of this result.

THEOREM 3.12. *Let G be the disjoint union of graphs H and K . Then X_i is a star cell in $V(G)$ if and only if $X_i = Y_i \dot{\cup} Z_i$, where Y_i and Z_i (one of them possibly empty) are star cells of $V(H)$ and $V(K)$, respectively.*

Proof. Suppose that k_i is the multiplicity of an eigenvalue μ_i of G (corresponding to a star cell X_i). Then μ_i is an eigenvalue of H and K of multiplicities a_i and b_i respectively (possibly $a_i = 0$ or $b_i = 0$). Let $Y_i = X_i \cap V(H)$ and $Z_i = X_i \cap V(K)$. Then $|Y_i| \geq a_i$ and $|Z_i| \geq b_i$; otherwise μ_i is an eigenvalue of $H - Y_i$ or $K - Z_i$, and thus of $G - X_i$ (contrary to Theorem 3.10). Since $a_i + b_i = k_i$, we must have $|Y_i| = a_i$ and $|Z_i| = b_i$. Now, by Theorem 3.11, since μ_i is not an eigenvalue of $H - Y_i$ or $K - Z_i$ for any i , Y_i and Z_i (if nonempty) are star cells in H and K , respectively.

To prove the converse, let $X_i = Y_i \dot{\cup} Z_i$, where Y_i and Z_i (one of them possibly empty) are the star cells corresponding to μ_i in H and K respectively. Making use of Theorem 3.11, we have immediately that each X_i is a star cell in $V(G)$. ■

4. SOME FURTHER CONSIDERATIONS

One of the most natural questions regarding any structure concerns the relation between it and some of its substructures. Let us first rewrite (1.1) in the form

$$\Phi(G - j, \lambda) = \Phi(G, \lambda) \sum_{i=1}^m \frac{\|P_i e_j\|^2}{\lambda - \mu_i}. \quad (4.1)$$

In this section we first generalize this formula and take advantage of the generalization. Next we discuss certain types of spectral reconstruction problems.

THEOREM 4.1. *If $S \subset V(G)$, then*

$$\Phi(G - S, \lambda) = \Phi(G, \lambda) \det \left(\sum_{i=1}^m (\lambda - \mu_i)^{-1} P_i^S \right), \quad (4.2)$$

where P_i^S denotes the principal submatrix of P_i determined by S .

Proof. From the spectral form of A we have $(\lambda I - A)^{-1} = \sum_{i=1}^m (\lambda - \mu_i)^{-1} P_i$. On the other hand, by Jacobi's ratio theorem (see, for

example, [12, p. 21]) the principal submatrix of $(\lambda I - A)^{-1}$ determined by S has $\Phi(G - S, \lambda)/\Phi(G, \lambda)$ as its determinant. Thus (4.2) follows at once. ■

In particular, if $S = \{u, v\}$ with $u \neq v$, then (4.2) yields an affirmative answer to the following question which arises from [17, §2.7].

QUESTION 4.2. If u, v are distinct vertices of the graph G , is $\Phi(G - u - v, \lambda)$ determined by $\Phi(G, \lambda)$ and $\|P_i e_u\|, \|P_i e_v\|, \|P_i e_u + P_i e_v\|$ ($i = 1, \dots, m$)? (It was proved in [17, §2.5] that this is indeed the case when u, v are nonadjacent.)

Some further corollaries of Theorem 4.1 related to the problems considered in the previous section are given below.

COROLLARY 4.3. If $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a feasible partition of $V(G)$, then

$$\Phi(G - X_i, \mu_i) = \prod_{s \neq i} (\mu_i - \mu_s)^{k_s} \det P_i^{X_i}. \quad (4.3)$$

Proof. By applying (4.2) and determinant multilinearity with respect to rows (or columns), we get (4.3) when taking the limit of $\Phi(G - X_i, \lambda)$ as $\lambda \rightarrow \mu_i$. ■

REMARK 4.4. Since $P_i^2 = P_i = P_i^T$ for each i , $\sqrt{\det P_i^{X_i}}$ can be interpreted as the volume of the parallelepiped generated by vectors $P_i e_s$, $s \in X_i$. Thus $\det P_i^{X_i} \neq 0$ if and only if the vectors $P_i e_s$ with $s \in X_i$ are linearly independent. Since $\prod_{s \neq i} (\mu_i - \mu_s)^{k_s} \neq 0$, we have that the feasible partition $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a star partition if and only if $\Phi(G - X_i, \mu_i) \neq 0$ for all i (another proof of the results from Theorems 3.9 and 3.11).

COROLLARY 4.5. If $X_1 \dot{\cup} \dots \dot{\cup} X_m$ is a feasible partition for the graph G , then the volume $V(X_1, \dots, X_m)$ of the parallelepiped generated by the vectors $P_i e_s$ ($i = 1, \dots, m$, $s \in X_i$) is given by

$$V(X_1, \dots, X_m) = \sqrt{C \prod_{i=1}^m \Phi(G - X_i, \mu_i)}, \quad (4.4)$$

where C depends only on the spectrum of G and not on the particular partition.

Proof. Since $P_i^2 = P_i = P_i^T$ for each i , the Gram matrix of the vectors $P_i e_s$ ($i = 1, \dots, m; s \in X_i$) has the form

$$M = P_1^{X_1} + \dots + P_m^{X_m},$$

where $+$ denotes the direct sum of matrices. Now, since $V(X_1, \dots, X_m) = \sqrt{\det M}$, we easily get (4.4) by making use of (4.3). ■

In what follows we discuss some spectral-reconstruction problems. The first problem is contained implicitly in Remark 2.8.

THEOREM 4.6. *If X_i is the cell of a star partition that corresponds to the eigenvalue μ_i , then G is reconstructible from the graph $G - E(X_i)$ (the graph obtained by deleting the edges of the subgraph induced by X_i).*

Proof. Without loss of generality, take $i = 1$. By Lemma 3.8, there exists a basis $\{x_1, \dots, x_k\}$ of $\mathcal{E}(\mu_1)$ such that the matrix $[x_1, \dots, x_k]$ has the form

$$X = \begin{bmatrix} I \\ X' \end{bmatrix}.$$

By taking

$$A = \begin{bmatrix} A_1 & B_1^T \\ B_1 & C_1 \end{bmatrix},$$

it follows from $(\mu_1 I - A)X = 0$ that

$$\begin{aligned} \mu_1 I - A_1 - B_1^T X' &= 0, \\ -B_1 + (\mu_1 I - C_1) X' &= 0. \end{aligned}$$

Since $\mu_1 I - C_1$ is invertible by Theorem 3.9, we have

$$A_1 = \mu_1 I - B_1^T (\mu_1 I - C_1)^{-1} B_1,$$

where B_1 and C_1 are known. ■

COROLLARY 4.7. *Let G, H be graphs with star cells X, Y corresponding to a common eigenvalue. If there is a bijection $\varphi: V(G) \rightarrow V(H)$ such that*

- (i) $\varphi(X) = Y$,
- (ii) φ reduces to an isomorphism $G - E(X)$ to $H - E(Y)$,

then φ is an isomorphism from G to H .

Finally, suppose that $X_1 \dot{\cup} \cdots \dot{\cup} X_m$ and $Y_1 \dot{\cup} \cdots \dot{\cup} Y_m$ are feasible partitions of G and H , respectively.

QUESTION 4.8. If for each i ($i = 1, \dots, m$) one has $\Phi(G - X_i, \lambda) = \Phi(H - Y_i, \lambda)$, does it follow that $\Phi(G, \lambda) = \Phi(H, \lambda)$?

This question seems to be intractable in general. To see this, consider the case when the eigenvalues of G and H are all simple. Then the problem becomes the nontrivial case of the polynomial-reconstruction problem from [13, 6], i.e. the problem of reconstructing the characteristic polynomial of a graph from the collection of the characteristic polynomials of its vertex-deleted subgraphs.

Suppose now that $X_1 \dot{\cup} \cdots \dot{\cup} X_m$ is a star partition of a graph G , and $P_1^{X_1}, \dots, P_m^{X_m}$ are the principal submatrices of the projection matrices P_1, \dots, P_m corresponding to cells X_1, \dots, X_m , respectively.

QUESTION 4.9. To what extent is the graph G determined by its characteristic polynomial (or equivalently, by its eigenvalues) and the submatrices $P_1^{X_1}, \dots, P_m^{X_m}$?

5. CANONICAL STAR BASES AND GRAPH ORDERINGS

Throughout this section, we allow our graphs to have loops. It remains the case that star bases exist, because this notion extends to any symmetric matrix with real entries.

Given a graph G on n vertices, we use the notion of a star basis to define a unique canonical basis of eigenvectors for \mathbb{R}^n . To construct this basis we introduce a total order of graphs, called CGO (*canonical graph ordering*), together with a quasiorder of vertices called CVO (*canonical vertex ordering*). Recall that a quasiorder is reflexive and transitive but not necessarily antisymmetric. Both CGO and CVO are defined recursively in terms of graphs with fewer than n vertices.

Our canonical basis together with the spectrum of G constitutes a *complete set* of invariants for G , i.e. it determines G to within isomorphism. Of course G has as a complete invariant the first (or least) matrix in a lexicographical ordering of adjacency matrices corresponding to all $n!$ orderings of vertices. (Instead of adjacency matrices we can consider binary numbers obtained by concatenation of rows [or rows of the upper triangle] of

adjacency matrices and characterize the graph by the largest [or least] such number; see, for example, [15].) However, the algorithmic complexity of finding this matrix (or the largest associated binary number) is an exponential function of n . No complete set of invariants computable in polynomial time is known, but since eigenvalues and eigenvectors are polynomially computable, it is reasonable to seek such sets of invariants among bases of eigenspaces.

5.1. Basis Images

All bases are considered as totally ordered sets. In particular, a star basis \mathcal{S} corresponding to an n -vertex graph G is a sequence of n linearly independent elements of \mathbb{R}^n , here ordered independently of the ordering of vertices of G .

DEFINITION 5.1. For $j = 1, \dots, n$ let e_j^* be the component vector of e_j with respect to \mathcal{S} . The set $\{e_1^*, \dots, e_n^*\}$ is called the *basis image* of \mathcal{S} , denoted by $I(\mathcal{S})$.

Thus $I(\mathcal{S})$ is the set of columns of the transition matrix T from (e_1, \dots, e_n) to \mathcal{S} .

Now suppose that π is a permutation of $\{1, \dots, n\}$ and that vertices $1, \dots, n$ are relabeled $\pi(1), \dots, \pi(n)$. If \mathcal{S} is determined by the star partition $X_1 \dot{\cup} \dots \dot{\cup} X_m$, then \mathcal{S} is transformed to a new star basis \mathcal{S}' with partition $\pi^{-1}(X_1) \dot{\cup} \dots \dot{\cup} \pi^{-1}(X_m)$. Moreover, the new transition matrix, that from (e_1, \dots, e_n) to \mathcal{S}' , is obtained from T by permuting the columns according to π . It follows that $I(\mathcal{S}) = I(\mathcal{S}')$, and so basis images are independent of vertex ordering in the above sense.

5.2. Ordering of Weighted Graphs

A *weighted graph* is a graph with a (real) weight assigned to each edge. Zero weights correspond to nonexistent edges. A weighted graph has *weight matrix* (w_{ij}) , where w_{ij} is the weight assigned to edge $\{i, j\}$; clearly, any symmetric matrix is the weight matrix of a weighted graph.

DEFINITION 5.2. The *weight* of a weighted graph is the family of its edge weights w_{ij} ordered in nondecreasing order.

DEFINITION 5.3. Let α be an edge weight in a weighted graph G . The (nonweighted) graph with vertices the vertices of G and edges the edges of G weighted α is called an α -graph or a *weight-generated graph*.

DEFINITION 5.4. Let $\alpha_1, \dots, \alpha_s$ be the distinct edge weights of G with $\alpha_1 < \dots < \alpha_s$. Let H_i be the associated α_i -graph for $i = 1, \dots, s$, and let $G_i = H_1 \cup \dots \cup H_i$ ($i = 1, \dots, s$). These graphs G_1, \dots, G_s are called *modified weight-generated graphs*.

Now suppose that G has n vertices and that CGO has been defined for graphs on n vertices.

Weighted graphs on a prescribed number of vertices are ordered lexicographically by their weights. Weighted graphs with the same weight are ordered lexicographically using the sequence G_1, \dots, G_s of modified weight-generated graphs ordered by CGO.

5.3. Orthodox Star Bases

Let G be a graph with n vertices and distinct eigenvalues μ_1, \dots, μ_m . We define an ordering of the set of all star bases of \mathbb{R}^n determined by G . If \mathcal{S} is such a basis, then it determines a star basis \mathcal{S}_i of each eigenspace $\mathcal{E}(\mu_i)$ ($i = 1, \dots, m$). The Gram matrix of vectors from \mathcal{S}_i defines a weighted graph W_i ; and if $m > 1$, each W_i has fewer vertices than G . If $m = 1$, there is just one star basis of \mathbb{R}^n , namely (e_1, \dots, e_n) . (In this case either $G = \bar{K}_n$ or G consists solely of n loops.) Thus if CGO has been defined for graphs with fewer than n vertices, and if $m > 1$, we can order star bases of G lexicographically by the sequence W_1, \dots, W_m of weighted graphs using the ordering defined in Section 5.2.

DEFINITION 5.5. The smallest star bases in this lexicographic ordering are called *orthodox star bases*.

Note that for a given graph G , we may possibly have orthodox star bases with different basis images.

If CVO has been defined for graphs with fewer than n vertices, and if $m > 1$, then we can define a quasiorder on the elements of an orthodox star basis as follows. In each cell X_i of the corresponding partition we order vertices by CVO in the graph generated by the smallest weight in W_i . (This demonstrates the importance of star bases.) The cells X_1, \dots, X_m are ordered as usual by decreasing eigenvalues. The vertex ordering so obtained determines a corresponding quasiorder σ of the vectors in \mathcal{S} . Recall that our bases are to be totally ordered: the total orderings admitted are those compatible with σ . (If $m = 1$, then all $n!$ orderings are admissible.) Note that if vertices are relabeled, an orthodox basis is transformed to an orthodox basis, because the ordering of weighted graphs is independent of vertex ordering.

5.4. The Canonical Star Basis

For an orthodox star basis \mathcal{S} with $I(\mathcal{S}) = \{e_1^*, \dots, e_n^*\}$, define the corresponding *ordered basis image* $\text{OI}(\mathcal{S})$ by $\text{OI}(\mathcal{S}) = (e_{\pi(1)}^*, \dots, e_{\pi(n)}^*)$, where $e_{\pi(1)}^* > \dots > e_{\pi(n)}^*$ in the lexicographical ordering of vectors. For each \mathcal{S} for which $\text{OI}(\mathcal{S})$ is least, we reorder vertices according to π : the resulting basis is an orthodox basis \mathcal{S}' for which $\text{OI}(\mathcal{S}') = \text{OI}(\mathcal{S})$. A basis obtained in this way is called a *quasicanonical* star basis, and the corresponding vertex ordering is in general a quasiorder, because there may be several orthodox bases \mathcal{S} for which $\text{OI}(\mathcal{S})$ is least; indeed, similar vertices may be permuted.

DEFINITION 5.6. For a given graph G , we order quasicanonical star bases lexicographically: the smallest such basis is called the *canonical star basis* determined by G .

Note that the lexicographical ordering of star bases by ordered basis images can be performed efficiently only if vectors in a star basis are ordered in a prescribed way (by CVO for smaller graphs in our case). Otherwise, we would have to consider all possible orderings of the basis vectors in star bases. The situation would be very similar to that of lexicographical ordering of adjacency matrices as described at the beginning of Section 5.

Note that some quasicanonical bases can coincide up to ordering of graph vertices. For example, in complete graphs all quasicanonical bases are equal, but any ordering of vertices can be associated to them. In general, a permutation of vertices preserves a quasicanonical star basis if and only if it is an automorphism of the graph.

DEFINITION 5.7. The quasiorder of vertices corresponding to the canonical star basis is called the *canonical vertex ordering* (CVO) of the graph.

In this way we have recursively defined CVO (announced at the beginning of Section 5).

THEOREM 5.8. *Two graphs are isomorphic if and only if they have the same spectrum and determine the same canonical star basis.*

Proof. By construction, the canonical basis is a graph invariant. On the other hand, the elements of such a basis are eigenvectors which together with corresponding eigenvalues determine an adjacency matrix. ■

EXAMPLE 5.9. The graphs $C_4 \cup K_1$ and $K_{1,4}$ have the same spectrum, namely $2, 0, 0, 0, -2$, but different angle matrices (cf [11]):

$C_4 \cup K_1$ has angle matrix

$$\begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix};$$

$K_{1,4}$ has angle matrix

$$\begin{bmatrix} \sqrt{2}/2 & \sqrt{2}/4 & \sqrt{2}/4 & \sqrt{2}/4 & \sqrt{2}/4 \\ 0 & \sqrt{3}/2 & \sqrt{3}/2 & \sqrt{3}/2 & \sqrt{3}/2 \\ \sqrt{2}/2 & \sqrt{2}/4 & \sqrt{2}/4 & \sqrt{2}/4 & \sqrt{2}/4 \end{bmatrix}.$$

Norms of vectors from a star basis are graph angles. Hence, $C_4 \cup K_1$ and $K_{1,4}$ cannot have the same canonical bases and hence are nonisomorphic.

Now we define *canonical graph ordering* (CGO).

DEFINITION 5.10. Ordering graphs lexicographically by eigenvalues and canonical bases defines CGO.

Note that CGO is recursively defined.

We have not yet established the algorithmic complexity of finding a canonical star basis. It would also be interesting to relate our results to the results of L. Babai et al. [1]. They have proved that the isomorphism problem for graphs with bounded multiplicities of eigenvalues is solvable in polynomial time.

Strongly regular graphs always represent a difficult case for a graph-isomorphism algorithm. Therefore we emphasize the following simple consequence of the above ideas.

THEOREM 5.11. CVO in connected strongly regular graphs with at least five vertices is reduced to CVO in graphs induced by the two nontrivial cells of the star partition corresponding to the canonical star basis.

Proof. Connected strongly regular graphs with at least five vertices have exactly three distinct eigenvalues, only the largest one being simple. So we have exactly two nontrivial cells in any star partition; hence the theorem. ■

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