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# SOME COMMENTS ON THE EIGENSPACES OF GRAPHS

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**Abstract.** We continue the investigations on the relations between eigenvalues, eigenspaces and the structure of graphs. The angles between eigenspaces and the axes of a standard basis of $\mathbf{R}^n$ play an important role. A general problem is how to construct graphs with the given eigenvalues and angles. In particular, we treat connectivity and metric properties, reconstruction of unicyclic and bicyclic graphs, etc. The results are mostly of an algorithmic character rather than in form of explicit characterization theorems. Therefore we propose to treat these problems with the aid of a computer using artificial intelligence means.

## 1. Introduction

Let $G$ be a graph on $n$ vertices. Let $\mu_1, \mu_2, \dots, \mu_m$ ($\mu_1 > \mu_2 > \dots > \mu_m$) be the distinct eigenvalues of (the adjacency matrix $A$) of $G$ with the corresponding eigenspaces $S_1, S_2, \dots, S_m$. Let $e_1, e_2, \dots, e_n$ be an orthonormal basis of $\mathbf{R}^n$. The quantities $\alpha_{ij} = \cos \beta_{ij}$ ($i = 1, 2, \dots, m$; $j = 1, 2, \dots, n$), where $\beta_{ij}$ is the angle between $S_i$ and $e_j$, are called *angles* of $G$. The matrix $\mathcal{A} = \|\alpha_{ij}\|_{m,n}$ is called the angle matrix of $G$. We understand that the columns of $\mathcal{A}$ are ordered lexicographically so that $\mathcal{A}$ is a graph invariant. The rows of $\mathcal{A}$ are associated with the eigenvalues and are called *eigenvalue angle sequences* while the columns of $\mathcal{A}$ are associated with the vertices and are called *vertex angle sequences*.

If a graph (vertex) invariant or property or subgraph can be determined provided the eigenvalues and angles of the graph are known, then this object is called EA-reconstructible.

Let $P(\lambda) = \det(\lambda I - A)$ be the characteristic polynomial of $G$ and let $P_i(\lambda)$ $i = 1, 2, \dots, n$ be the characteristic polynomials of vertex deleted subgraphs $G - i$ of $G$. We have (c.f. [**4**])

$$P_j(\lambda) = P(\lambda) \sum_{i=1}^{m} \frac{\alpha_{ij}^2}{\lambda - \mu_i} \qquad (j = 1, 2, \dots, n). \tag{1}$$

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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

$$H_i(t) = \frac{P_i(1/t)}{tP(1/t)}. \tag{2}$$

Formulas (1) and (2) show that the polynomials $P_i(\lambda)$ and the functions $H_i(t)$ are EA-reconstructible. From (2) we see also that the vertex degrees are EA-reconstructible.

In this paper we are primarily interested in EA-reconstructibility of graphs [**6**], [**8**], [**10**], [**11**]. See [**7**] for relations to Ulam's graph reconstruction conjecture.

## 2. Connectedness and angles

Given the eigenvalues and the angle of a graph $G$, we can establish:

1° whether or not $G$ is connected [**6**],

2° separate vertices in components having the same largest eigenvalue [**8**],

3° the number of components [**8**],

4° the sizes of regular components,

5° sometimes separate groups of regular components.

To show 4° and 5° we assume that we have already separated components having the same largest eigenvalue by 2°. Consider a group of components having the largest eigenvalue $r$ ($r$ being an integer). We are looking for components being regular graphs of degree $r$. Consider the eigenvalue angle sequence belonging to $r$. The coordinates corresponding to vertices belonging to a regular component on $s$ vertices are equal to $1/\sqrt{s}$. We can recognize the case when all components are regular by looking at vertex degrees. In this case we readily establish the sizes of the components. If the components are of different sizes we can recognize vertices in each component.

However, the components are not uniquely determined, as the following example shows.

*Example* 1. Let $G \triangledown H$ denote the graph obtained from the graphs $G$ and $H$ by joining each vertex of $G$ to each vertex of $H$. The graphs $G_1 = (C_6 \triangledown C_6) \cup (2C_3 \triangledown 2C_3)$ and $G_2 = (C_6 \triangledown 2C_3) \cup (C_6 \triangledown 2C_3)$ are cospectral. They are regular of degree 12 and can be obtained one from the other by the (Seidel) switching with respect to vertices from a copy of $C_6$ and a copy of $2C_3$. Since switching in regular graphs does not change angles [**3**], the graphs $G_1$ and $G_2$ have the same angles. However, the graphs $G_1$ and $G_2$ have nonisomorphic components with different spectra.

## 3. Metric properties

Let $A = \mu_1 P_1 + \mu_2 P_2 + \cdots + \mu_m P_m$ be the usual spectral decomposition of the adjacency matrix $A$ of a graph $G$, where $P_i$ ($i = 1, 2, \ldots, m$) is the projector onto eigenspace $S_i$. Let $P_i = \|p^i_{jk}\|$. We have $p^i_{jk} = \alpha_{ij}\alpha_{ik}\cos\gamma^i_{jk}$ where $\gamma^i_{jk}$ is the angle between $P_ie_j$ and $P_ie_k$. If $A^s = \|a^{(s)}_{jk}\|$, we have

$$a^{(s)}_{jk} = \sum_{i=1}^{m} \mu_i^s p^i_{jk} = \sum_{i=1}^{m} \mu_i^s \alpha_{ij}\alpha_{ik}\cos\gamma^i_{jk}, \qquad |a^{(s)}_{jk}| \le \sum_{i=1}^{m} |\mu_i|^s \alpha_{ij}\alpha_{ik}.$$

Let $d(j,k)$ be the distance between the vertices $j$ and $k$.

PROPOSITION 1. *If* $g = \min_s\bigl(\sum_{i=1}^m |\mu_i|^s\alpha_{ij}\alpha_{ik} \ge 1\bigr)$, *then* $d(j,k) \ge g$.

*Proof*. From the assumption we get $|a^{(s)}_{jk}| = 0$ for $s < g$. Hence there is no walk of length $s$ $(s < g)$ between $j$ and $k$. □

COROLLARY 1. *If* $\sum_{i=1}^m |\mu_i|\alpha_{ij}\alpha_{ik} < 1$, *then* $j$ *and* $k$ *are not adjacent.*

This corollary provides a necessary condition for two vertices to be adjacent, an alternative to the edge condition of [**11**].

Finally, we can formulate the following

THEOREM 2. *Let* $G$ *be a graph on* $n$ *vertices with distinct eigenvalues* $\mu_1, \mu_2, \dots, \mu_m$ *and let* $\alpha_{ij}$ $(i = 1,2,\dots,m\,;\ j = 1,2,\dots,n)$ *be angles of* $G$. *Let*

$$d = \max_{j,k}\min_{s}\left(\sum_{i=1}^{m} |\mu_i|^s\alpha_{ij}\alpha_{ik} \ge 1\right).$$

*Then the diameter of* $G$ *is at least* $d$.

## 4. Unicyclic graphs

It was shown in [**6**] that for trees the angles and the eigenvalues, "almost" suffice for the graph structure reconstruction. Although we have nonisomorphic trees with the same eigenvalues and angles, even although this happens "almost" always, we are still in the position to construct easily all trees with given eigenvalues and angles. Treating the vertices from leaves towards the centre we can "calculate" the remaining neighbour of each particular vertex by the use of a reconstruction lemma given below.

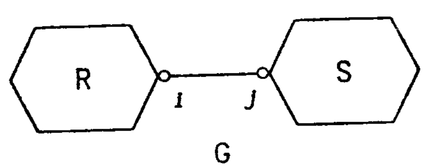


Fig. 1

Suppose there is a bridge $i - j$ in the graph $G$ (see Fig. 1). Suppose further that we know completely the structure of the subgraph $R$ including the fact that the bridge starts at vertex $i$. Now the problem is how to cross the bridge, i.e. to identify vertex $j$. Let $P_X(\lambda)$ denote the characteristic polynomial of the graph $X$. We have [**6**] the following

Reconstruction Lemma. *Given the subgraph $R$ and the vertex $i$ (see Fig. 1), the vertex $j$ is among those vertices $k$ for which*

$$P_k(\lambda) = P_R(\lambda)(P_{R-i}(\lambda))^{-2}\big(P_R(\lambda)P_i(\lambda) - P_{R-i}(\lambda)P_G(\lambda)\big). \tag{3}$$

A connected graph with $n$ vertices and $n$ edges is called a unicyclic graph. The following lemma is straightforward.

Lemma 1. *The property of being unicyclic is EA-reconstructible.*

It was noted in [**6**] that the algorithm for reconstructing trees can be applied to unicyclic graphs. We reconstruct trees attached to the circuit until the subgraph not yet reconstructed has all vertex degrees equal to 2. Now we have the following problems:

1° How to reconstruct the circuit?

2° Is the vertex set of the circuit uniquely determined?

We shall use several times in this paper the well known fact (see e.g. [**2**, p. 87]) that a graph $G$ on $n$ vertices is bipartite if and only if the characteristic polynomial $P_G(\lambda)$ of $G$ has the property

$$P_G(-\lambda) = (-1)^n P_G(\lambda). \tag{4}$$

If $P_G(\lambda)$ satisfies (4) we shall say that $P_G(\lambda)$ is a symmetric polynomial.

1° In the case the graph is reduced to a circuit we have a lot of reconstructions (any hamiltonian circuit in the complete graph). In other cases vertices generally have their individualities and one can try to find the details.

2° If the circuit is odd its vertex set is uniquely reconstructed as $\{i \mid P_{G-i}(\lambda)$ is symmetric$\}$. To handle the even case one can use: bridge condition [**11**], constant term of the characteristic polynomial [**9**], multiplicity of the eigenvalue 0 in polynomial $P_{G-i}(\lambda)$ [**2**, p. 233], etc.

## 5. Bicyclic graphs

A connected graph with $n$ vertices and $n+1$ edges is called a bicyclic graph.

Bicyclic graphs without vertices of degree 1 are of types $P(m,p,n)$, $C(m,n)$ and $B(m,p,n)$ as presented in Fig. 2 following [**12**]. In general, bicyclic graphs consist of a part (which we call the *central part*) of the type either $P(m,p,n)$ or $C(m,n)$ or $B(m,p,n)$ and a number of trees (*tails*) attached to the central part.

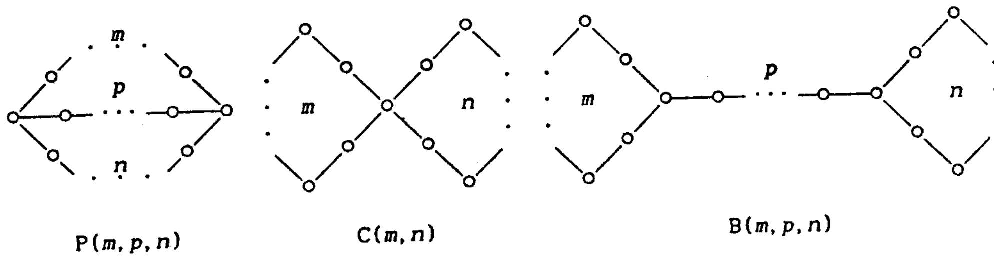


Fig. 2

LEMMA 2. *The property of being bicyclic is EA-reconstructible.*

The proof is obvious.

As in the case of unicyclic graphs we can apply algorithm from [**6**] to bicyclic graphs. Tails can be reconstructed and we have the problem of reconstructing the central part of a bicyclic graph.

PROBLEM. *Is the vertex set of the central part od a bicyclic graph uniquely reconstructed?*

We treat here a more modest problem: reconstructing details provided the vertex set of the central part is already reconstructed.

Let $X$ be the vertex set of the central part of a bicyclic graph $G$. A reduced degree of vertex $x$ from $X$ is the number of vertices of $X$ which are adjacent to $x$ in $G$.

1° Suppose first that $G$ is *not bipartite.*

Consider the set $K = \{i \mid P_{G-i}(\lambda) \text{ is symmetric}\}$.

In the sequel we shall also use the well-known fact that the length and the number of shortest odd circuits in a graph can be determined from the coefficients of its characteristic polynomial (see e.g. [**2**, p. 87]).

PROPOSITION 2. *If $G$ is not bipartite and $K = \varnothing$, then the central part of $G$ is isomorphic to $B(m, p, n)$ for some uniquely determined integers $m$, $p$, $n$.*

*Proof*. Since $G$ is not bipartite, $G$ contains odd circuits. Since $K = \varnothing$, deletion of no vertex destroys all odd circuits. Hence $G$ has two disjoint odd circuits. The lengths $m$, $n$ of the two odd circuits can be determined from the coefficients of polynomials $P_G(\lambda)$ and $P_{G-i}(\lambda)$ $(i = 1, 2, \ldots, n)$ and $p = |X| - m - n$. □

The vertices belonging to odd circuits are precisely those vertices $i$ for which $G - i$ contains only one circuit. If $m = n$ we find the set of all such vertices and if $m \neq n$ we can specify the vertex set of each circuit.

The following proposition is staightforward.

PROPOSITION 3. *Let $G$ be nonbipartite and $K \neq \varnothing$. The central part of $G$ is isomorphic to*:

i) $C(m,n)$ *if $X$ contains a vertex of reduced degree* 4;

ii) $P(m,p,n)$ *if $X$ contains two vertices of reduced degree* 3 *and both belong to $K$*;

iii) $B(m,p,n)$ *if $X$ contains two vertices of reduced degree* 3 *and exactly one belongs to $K$.*

In case i) we can reconstruct the circuit vertex sets. If $|K| = 1$ both $m$, $n$ are odd and can be determined by looking at $P_{G-i}(\lambda)$ for $i \in K$. In this way we determine also the circuit vertex sets. If $|K| > 1$, then $K$ is just the odd circuit vertex set.

In case ii) the set $K$ is just the set of vertices belonging to the two odd circuits.

In case iii) the odd circuit vertex set is $K$. We could use the bridge condition from [**11**] to distinguish between bridges and nonbridges in the remaining central part of the graph.

2° Suppose now $G$ is *bipartite*. The reconstruction is now more difficult and we note only a couple of observations.

If $X$ contains a vertex of degree 4, then central part of $G$ is isomorphic to $C(m,n)$ with $m$, $n$ even.

If $X$ contains two vertices of degree 3, then we have $P(m,p,n)$ with $m$, $p$, $n$ of the same parity or $B(m,p,n)$ with $m$, $n$ even and $p \equiv |X| (\mathrm{mod}\, 2)$.

## 6. Reconstructing the characteristic polynomial

The result from [**6**] on constructing trees with given eigenvalues and angles has been strengthen in [**10**]. We can suppose that instead of eigenvalues and angles we are given only the characteristic polynomials $P_i(\lambda)$, $(i = 1, 2, \dots, n)$ of the vertex deleted subgraphs $G - i$ of a graph $G$. We can still construct all trees $G$.

Since $P'(\lambda) = \sum_{i=1}^{n} P_i(\lambda)$ we can readily calculate the characteristic polynomial $P(\lambda) = \sum_{k=0}^{n} a_k \lambda^{n-k}$ except for the constant term $a_n$. If we determine $a_n$ anyhow, we can calculate eigenvalues and angles of $G$ and proceed with the construction of $G$ in the same way as in [**6**].

The problem of a unique reconstruction of the characteristic polynomial $P(\lambda)$ of a graph $G$ from the collection of characteristic polynomials $P_i(\lambda)$ $(i = 1, 2, \dots, n)$ of vertex deleted subgraphs $G - i$ of $G$ has been treated in [**1**]. If we know an eigenvalue of $G$, the constant term $a_n$ is uniquely determined. In particular any multiple root of any of the polynomials $P_i(\lambda)$ would cause (by interlacing theorem) the existence of the same eigenvalue in the spectrum of $G$. It was shown in [**1**] that for many trees $a_n$ is uniquely reconstructible. The only trees for which this reconstruction is perhaps not unique are trees having a 1-factor. Note [**1**] that in this case we have $a_n = (-1)^{n/2}$.

It can be shown that if $a_n$ is not unique then the other graphs $H$ are bipartite disconnected graphs, at least one component being a tree; further all components have an even number of vertices, zero is not an eigenvalue and all components have simple eigenvalues [**10**]. Any automorphism of each component is an involution. The largest eigenvalue is equal to the maximal largest eigenvalue of the vertex deleted subgraphs.

We go a step further.

Let $G$ be a tree having a 1-factor. Let $i$ be a vertex of $G$ of degree 1 and let $j$ be the vertex adjacent to $i$.

Let $H$ be a graph such that $G$ and $H$ have the same collection of characteristic polynomials of vertex deleted subgraphs with $P_G(\lambda) \neq P_H(\lambda)$ (i.e. with different constant terms).

Vertex degrees are reconstructible from the collection of characteristic polynomials of vertex deleted subgraphs [**1**]. Hence, the vertex $i$ has degree 1 also in $H$. However, we shall show that $i$ is not adjacent to $j$ in $H$. In fact we have the following

Proposition 4. *Let $a$ be the constant term of $P_H(\lambda)$. Let $k$ be the vertex of $H$ adjacent to $i$. Then*

$$a = -\lim_{\lambda \to 0} \frac{P_{G-k}(\lambda)}{\lambda}.$$

*Proof*. We have (c.f. [**2**, p. 59])

$$P_H(\lambda) = \lambda P_{H-i}(\lambda) - P_{H-i-k}(\lambda) = \lambda P_{H-i}(\lambda) - \lambda^{-1} P_{H-k}(\lambda).$$

Therefore

$$a = \lim_{\lambda \to 0} P_H(\lambda) = -\lim_{\lambda \to 0} \lambda^{-1} P_{H-k}(\lambda) = -\lim_{\lambda \to 0} \lambda^{-1} P_{G-k}(\lambda). \quad \square$$

Proposition 5. *We have $P_{G-j}(\lambda) - P_{G-k}(\lambda) = q\lambda$ for some integer $q$.*

*Proof*. We have

$$P_G(\lambda) = \lambda P_{G-i}(\lambda) - \lambda^{-1} P_{G-j}(\lambda), \tag{5}$$

$$P_H(\lambda) = \lambda P_{H-i}(\lambda) - \lambda^{-1} P_{H-k}(\lambda). \tag{6}$$

Since $P_G(\lambda)$ and $P_H(\lambda)$ differ only in constant term, we can write $P_H(\lambda) - P_G(\lambda) = q$ where $q$ is an integer. Having in mind that $P_{G-s}(\lambda) = P_{H-s}(\lambda)$ $(s = 1, 2, \dots, n)$, we get the assertion by subtracting (5) form (6). $\square$

Proposition 6. *The vertices $j$ and $k$ have the same degree.*

*Proof*. The coefficient of the term $\lambda^{n-3}$ in $P_{G-j}(\lambda)$ and $P_{G-k}(\lambda)$ determines the number of edges in $G - j$ and $G - k$ respectively. Now the assertion follows for $n \neq 4$. In the case $n = 4$ there are no exceptions. $\square$

In spite of knowing many properties of hypothetical graphs $H$ we are not aware of examples of their existence.

## 7. Graph reconstruction problem and artificial intelligence

A characterization of a graph up to an isomorphism by the graph spectrum is possible only in trivial or exceptional cases. To find all graphs having the given spectrum is a difficult task and generally we do not know any better procedure than to construct all graphs with the required number of vertices and edges, to calculate spectra of all these graphs and to select those ones we need.

By adding to the eigenvalues some invariants of the corresponding eigenspaces we come to a better position if we want to tell something about the graph structure. In particular, some attention has been paid to graph angles.

A general impression is that with eigenvalues only we can say very little while in case both eigenvalues and angles are known we are in position to reconstruct quite a lot about a graph. An exception represent the strongly regular graphs and other graphs of highly regular structure (see e.g. [**11**] where it is noted that the so called fuzzy image of a strongly regular graph is a complete graph with only "fuzzy" edges).

However, in studying to what extent graphs are determined by their eigenvalues and angles we come across many algorithmic results rather than explicit characterization theorems. This fact gives rise to a possible usage of computers in investigations.

It seems reasonable to implement an *artificial intelligence* computer program (an expert system) which would construct all graphs having a given spectrum, angles and possibly some other invariants. The reconstruction consists of many simple steps of a limited number of types. It would be difficult for a human to take care of all little details appearing in due course while the computer, provided by a sufficiently intelligent program, could cope with these difficulties. We have already expressed this idea in a less general context [**10**].

The expert system would be provided by a knowledge base consisting of a great number of theorems helping to reconstruct the details of a graph structure. These theorems have a limited application area and would be used selectively depending on the graph in question. The theorems would act as *production rules* in the expert system. If no production rule can be applied to a partially reconstructed graph the program should finish the graph reconstruction by a brute force. So besides artificial intelligence means the program should contain graph theoretical algorithms including a facility for searching through all possibilities such as, for example, backtracking.

Experiments with such a program could lead to new mathematical results in graph theory and to contribute to better understanding of the nature of discrete structures in general.

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