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On eigenvalues and eigenvectors of graphs*

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It is known that there exists an equivalence relation between the adjacency matrix of graph theory and the Hückel matrix of Hückel molecular orbital theory. This paper presents some useful methods which allow us to systematically find eigenvalues and eigenvectors of various classes of graphs without calculating characteristic polynomials. Results obtained from this study give insight into the topological studies of molecular orbitals.

1. Introduction

In this paper, we treat ordinary graphs (i.e. finite, undirected, at most one edge joining a pair of vertices, and no edge joining a vertex to itself). Since an ordinary graph has no loops or undirected edges, its adjacency matrix A is a symmetric matrix and has real eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$, which are called the spectrum of G [1]. There is an immediate one-to-one correspondence between labeled graphs on n nodes and $n \times n$ symmetric binary matrices with zero diagonal elements. The row sums of $A(G)$ are the degrees of the nodes in G. If A_1 and A_2 are adjacency matrices which arise from two differentt labelings of the same graph G, then for some permutation matrix P, $A_1 = P^{-1}A_2P$. According to the following theorem [1], the spectrum of G is invariant under relabeling.

THEOREM 1

The characteristic polynomial of matrix A and, hence, the eigenvalues, are the same as those of $B^{-1}AB$, where B is any non-singular matrix.

*Dedicated to Professor Frank Harary on the occasion of his 70th birthday.

Clearly, the spectrum of G yields some information about G. There has been much work done on the question of relating geometric and combinatorial properties of G to the eigenvalues of G. Related concepts include the coloring number $k(G)$ [2], the girth number $g(G)$ [3,4], the line graph of G [3,5], and the embedding problem [3]. It is known that there exists a relation between the adjacency matrix of graph theory and the Hückel matrix of Hückel molecular orbital theory [6,7]. Topological analysis of molecular orbitals of chemical compounds [8,9] can be performed using the newly proposed net sign approach by Lee et al. [10,11]. The values of net signs of molecular orbital graphs of model chemical compounds can be calculated from the eigenvectors of the adjacency matrix. This paper presents some methods which can systematically derive eigenvalues and eigenvectors of various classes of graphs with minimal calculation. Graphs such as the annulus, cone, cycle, hypercube, path, spider, sun, torus, five kinds of regular polyhedra, etc. will be considered to illustrate the utility of our approach.

In section 2, some concepts and results of linear algebra and operations on graphs are reviewed and discussed. Also in section 2, we derive eigenvectors and eigenvalues of circulant graphs (e.g. cycles, complete graphs), hypercube, path, ladder, annulus, torus, grid, cylinder, etc. from the characteristics of circulant matrix and the product operation of graphs. In section 3, similar procedures are applied to graphs whose adjacency matrices can be expressed in partitioned form. Classes of graphs belonging to this type, such as the k-level-circulant graph, regular polyhedra, etc. are considered. In section 4, eigenvectors and eigenvalues of a full complete binary tree and a full complete m-ary tree are discussed. Conclusions are given in section 5.

Notation

Let ρ_n denote the value $e^{2i\pi/n} = \cos 2\pi/n + i \sin 2\pi/n$, where $i^2 = -1$. Let I_n denote the identity matrix of order n, 0_{mn} denote the zero matrix of dimension $m \times n$, and J_{mn} denote the matrix of dimension $m \times n$ of 1's. CSET(A) is denoted as a complete set of eigenvectors of matrix A which contains n independent eigenvectors of A.

2. Linear algebra and operations of graphs

In this section, we discuss and describe some observations connecting operations of matrices and the corresponding operations of graphs. It would be useful if we could generate the eigenvalues and eigenvectors of various classes of graphs from well-studied graphs, say paths, cycles and small graphs, with the help of those operations on graphs.

We will follow Harary [12,13] and Marcus and Minc [14] for any graph-theoretic and matrix terminologies which are not defined in this paper. Let G_1 and G_2 have disjoint node sets V_1 and V_2 and edge sets E_1 and E_2, respectively. To define their *Kronecker product* [15] $G_1 \otimes G_2$, consider any two nodes $u = (u_1, u_2)$ and $v = (v_1, v_2)$. Then, u and v are adjacent in $G_1 \otimes G_2$ whenever $u_2 v_2 \in E(G_2)$ and $u_1 v_1 \in E(G_1)$. Let $A = [a_{ij}]$ and $B = [b_{ij}]$ be two square matrices of order m and n, respectively. Their join $A \oplus B$ is defined as the square matrix of order $m + n$,

$$A \oplus B = \begin{bmatrix} A & J_{mn} \\ J_{nm} & B \end{bmatrix}.$$

Their *Cartesian product* $A \times B$ is defined as the square matrix of order mn,

$$A \times B = I_n \otimes A + B \otimes I_m.$$

The relations between these operations on matrices and the corresponding operations on graphs are described in the following proposition:

PROPOSITION 1

Let G and H be two graphs. Then

(1) $A(G \cup H) = A(G) \cup A(H)$;
(2) $A(G \oplus H) = A(G) \oplus A(H)$;
(3) $A(G \otimes H) = A(G) \otimes A(H)$;
(4) $A(G \times H) = A(G) \times A(H)$.

According to the following proposition, we can easily find the eigenvalues and eigenvectors of graph $G \cup H$, $G \otimes H$, $G \times H$ if we have already found them for graphs G and H.

PROPOSITION 2 ([16])

Let $\mathrm{CSET}(A) = \{U_1, U_2, \ldots, U_m\}$ with $AU_k = \alpha_k U_k$ for $k = 1, 2, \ldots, m$ and $\mathrm{CSET}(B) = \{V_1, V_2, \ldots, V_n\}$ with $BV_j = \beta_j V_j$ for $j = 1, 2, \ldots, n$. Then

(1) $\mathrm{CSET}(A \cup B) = \{W_1, W_2, \ldots, W_{mn}\}$, where $W_k^{\mathrm{T}} = [U_k^{\mathrm{T}}\, 0_n]$ for $1 \le k \le m$ and $W_{k+j}^{\mathrm{T}} = [0_m V_j^{\mathrm{T}}]$ for $1 \le j \le n$. The corresponding eigenvalue $\lambda_k = \alpha_k$ for $1 \le k \le m$ and $\lambda_{k+j} = \beta_j$ for $1 \le j \le n$.

(2) $\mathrm{CSET}(A \otimes B) = \{W_1, W_2, \ldots, W_{mn}\}$, where $W_{(k-1)n+j}^{\mathrm{T}} = U_k^{\mathrm{T}} \otimes V_j^{\mathrm{T}}$ for $1 \le k \le m$ and $1 \le j \le n$. The corresponding eigenvalue $\lambda_{(k-1)n+j} = \alpha_k \beta_j$ for $1 \le k \le m$ and $1 \le j \le n$.

(3) $\mathrm{CSET}(A \times B) = \{W_1, W_2, \ldots, W_{mn}\}$, where $W_{(k-1)n+j} = V_j \oplus U_k$ for $1 \le k \le m$ and $1 \le j \le n$. The corresponding eigenvalue $\lambda_{(k-1)n+j} = \alpha_k + \beta_j$ for $1 \le k \le m$ and $1 \le j \le n$.

A square matrix A is called a circulant matrix or a circulant if its successive rows are obtained by cyclic permutations of its first row. Thus,

$$A = \begin{bmatrix} a_1 & a_2 & a_3 & \cdots & a_n \\ a_n & a_1 & a_2 & \cdots & a_{(n-1)} \\ a_{(n-1)} & a_n & a_1 & \cdots & a_{(n-2)} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_2 & a_3 & a_4 & \cdots & a_1 \end{bmatrix}$$

is a circulant, denoted by $[[a_1, a_2, \ldots, a_n]]$. Eigenvectors and eigenvalues of a circulant matrix and a typical example, or path, are given in the following two propositions:

PROPOSITION 3 ([17])

Let square matrix A be a circulant matrix $[[a_1, a_2, \ldots, a_n]]$. Then CSET($A$) $= \{V_1, V_2, \ldots, V_n\}$, where $V_k^{\mathrm{T}} = [1\, \rho_n^k \rho_n^{2k} \ldots \rho_n^{(n-1)k}]$ for $1 \leq k \leq n$. The corresponding eigenvalue λ_k of eigenvector V_k is given by

$$\lambda_k = a_1 + a_2\rho_n^k + a_3\rho_n^{2k} + \ldots + a_n\rho_n^{(n-1)k}.$$

PROPOSITION 4 ([17])

Let $\delta_k = k\pi/(n+1)$ and let L_n be the graph of the path on n nodes. Then

(1) $$A(L_n) = [a_{ij}] = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 1 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{bmatrix},$$

where $a_{ij} = 1$ if $i = j \pm 1$; $a_{ij} = 0$ otherwise.

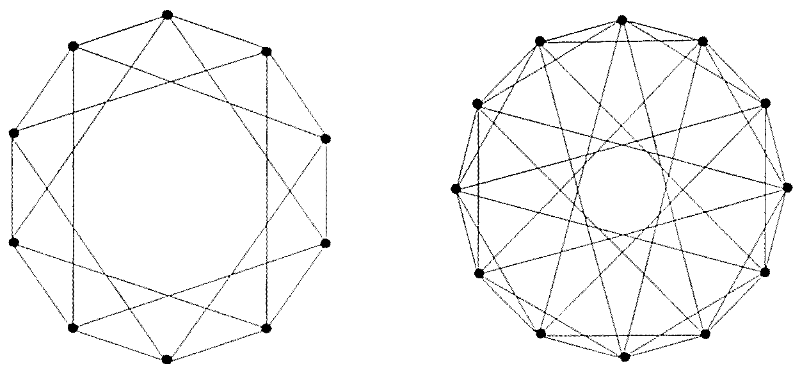
(2) CSET(L_n) $= \{V_1, V_2, \ldots, V_n\}$, where $V_k^{\mathrm{T}} = [x_{k1} x_{k2} \ldots x_{kn}]$ with $x_{kj} = \sin j\delta_k$ for $j, k = 1, 2, \ldots, n$.

(3) The corresponding eigenvalue λ_k of eigenvector V_k is given by $\lambda_k = 2\cos\delta_k$.

For a given positive integer, let $n_1, n_2, \ldots, n_k$ be a sequence of integers where

$$0 < n_1 < n_2 < \ldots < n_p \leq \tfrac{1}{2}n.$$

Then the circulant graph $C_n(n_1, n_2, \ldots, n_p)$ is the graph on n nodes $v_1, v_2, \ldots, v_n$ with vertex v_i adjacent to each vertex $v_{i \pm n_j (\mathrm{mod}\, n)}$. The values n_j are called *jump sizes*. The circulant graph $C_n(n_1, n_2, \ldots, n_p)$ is a d_A-regular graph, where $d_A = a_1 + a_2 + \ldots + a_m$. For example, the circulant graphs $C_{10}(1, 3)$ and $C_{12}(1, 2, 5)$ are displayed in fig. 1. The eigenvectors and eigenvalues of the multi-jump-size circulant are stated in corollary 5.



(a) $C_{10}(1,3)$ (b) $C_{12}(1,2,5)$

Fig. 1. Examples of multi-jump-size circulants.

COROLLARY 5

Let $C_n(n_1, n_2, \ldots, n_p)$ be a circulant graph on n nodes. Then

(1) $A(C_n(n_1, n_2, \ldots, n_p)) = [[a_1, a_2, \ldots, a_n]]$, where $a_i = 1$ if $i = 1 + n_j$ or $i = n + 1 - n_j$ for some j; $a_i = 0$ otherwise.

(2) $\mathrm{CSET}(C_n(n_1, n_2, \ldots, n_p)) = \{V_1, V_2, \ldots, V_n\}$, where $V_k^{\mathrm{T}} = [1\, \rho_n^k \rho_n^{2k} \ldots \rho_n^{(n-1)k}]$ for $k = 1, 2, \ldots, n$.

(3) The corresponding eigenvalue λ_k of eigenvector V_k is

$$\lambda_k = 2 \sum_{1 \le i \le p} \cos 2n_i k\pi/n \quad \text{if} \quad n_p \neq \tfrac{1}{2}n$$

and

$$\lambda_k = (-1)^k + 2 \sum_{1 \le i < p} \cos 2n_i k\pi/n \quad \text{if} \quad n_p = \tfrac{1}{2}n.$$

The graph of cycle C_n on n nodes is $C_n(j)$, where $\gcd(n, j) = 1$ and the complete graph K_n on n nodes is $C_n(1, 2, \ldots, x)$, where $x = \frac{1}{2}n$ if n is even; $x = \frac{1}{2}(n-1)$ otherwise. A complete set of eigenvectors and eigenvalues of these two classes of graphs above are easily calculated by corollary 5.

Several classes of graphs can be generated by the Cartesian product of L_n, C_n and K_2. For example, Ladder$(n) = L_n \times K_2$, Annulus$(n) = C_n \times K_2$, Torus(m, n)

$= C_m \times C_n$, Grid$(m, n) = L_m \times L_n$, Cylinder$(m, n) = L_m \times C_n$. The class of cross graphs Cross(n, m) (see fig. 2) is the Kronecker product of L_m and L_n. The eigenvalues and eigenvectors of the above six classes of graphs can also be easily found by propositions 2, 3 and 4.

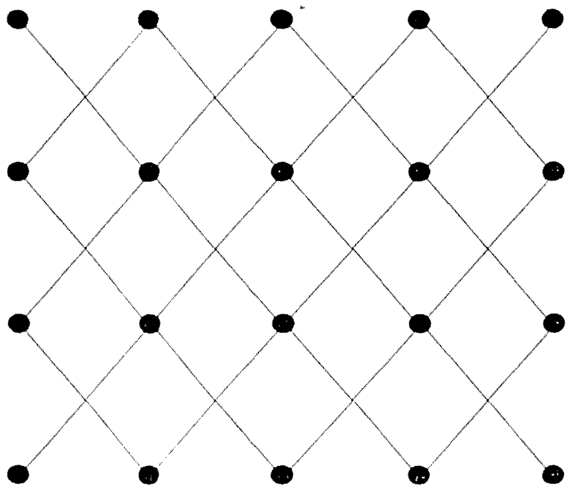


Fig. 2. $L_4 \otimes L_5$.

The hypercube of order n, H_n, is defined by

$H_0 = K_1$ and $H_n = K_2 \times K_2 \times \ldots \times K_2 (n \text{ times})$ if $n > 0$.

Obviously, CSET$(H_0) = \{[1]\}$ and the eigenvalue is 0. CSET(H_n) can be recurrently constructed in the manner stated in corollary 6.

COROLLARY 6

Let H_n be the graph of the hypercube of order n. Then

(1) $A(H_n) = \begin{bmatrix} A(H_{n-1}) & I_{2^{(n-1)}} \\ I_{2^{(n-1)}} & A(H_{n-1}) \end{bmatrix}.$

(2) CSET$(H_n) = \{W_1^{(n)}, W_2^{(n)}, \ldots, W_{2^n}^{(n)}\}$, where $\{W_{2k-1}^{(n)^{\mathrm{T}}}, W_{2k}^{(n)^{\mathrm{T}}}\} = \{[W_k^{(n-1)^{\mathrm{T}}} \pm W_k^{(n-1)^{\mathrm{T}}}] \mid W_k^{(n-1)^{\mathrm{T}}} \in \text{CSET}(H_{n-1})\}$ for $k = 1, 2, \ldots, 2^{(n-1)}$.

(3) The corresponding eigenvalue $\lambda_k^{(n)}$ of eigenvector $W_k^{(n)}$ is $n - 2i$, where i is the number of sign changes in the process of constructing $W_k^{(n)}$, i.e. where i is the number of -1's appearing in the $2^j + 1$ position, $1 \leq j \leq (n-1)$, in the vector $W_k^{(n)}$.

3. k-level circulant graph and regular polyhedra

Consider graphs whose adjacency matrices can be expressed in partitioned form. Every block is a square matrix of order m and has the same complete set of eigenvectors. Examples of such graphs include generalized sun, generalized combs, dodecahedron and icosahedron. A lemma and a theorem which are useful for finding the eigenvectors and eigenvalues of these graphs are given below.

LEMMA 1 ([16])

Any number of commuting real symmetric matrices can be diagonalized by the same real orthogonal matrix.

THEOREM 7

Let A_{ij}, $1 \le i, j \le n$, be square matrices of order n and have the same complete set of eigenvectors $\{U_1, U_2, \ldots, U_m\}$ with $A_{ij}U_k = \alpha_{ij}^{(k)}U_k$. Let $B_k = [\alpha_{ij}^{(k)}]$ be square matrices of order n and have a complete set of eigenvectors $\{V_1^{(k)}, V_2^{(k)}, \ldots, V_n^{(k)}\}$ with $B_kV_j^{(k)} = \beta_j^{(k)}V_j^{(k)}$ for $1 \le k \le m$ and $1 \le j \le n$. Then a complete set of eigenvectors $\{W_1, W_2, \ldots, W_{mm}\}$ of the square matrix

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{bmatrix}$$

is given by $W_{(k-1)n+j}^{\mathrm{T}} = V_j^{(k)^{\mathrm{T}}} \otimes U_k^{\mathrm{T}}$ for $k = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. The corresponding eigenvalue $\lambda_{(k-1)n+j}$ is $\beta_j^{(k)}$.

Interesting applications of this theorem can be found if the A_{ij} are circulant matrices. For a given positive integer, let $\{\mathcal{N}_1\} = \{n_{11}, n_{12}, \ldots, n_{1p_1}\}$, $\{\mathcal{N}_2\} = \{n_{21}, n_{22}, \ldots, n_{2p_2}\}$ and $\{\mathcal{M}\} = \{m_{11}, m_{12}, \ldots, m_{1q_1}\}$ be three sequences of integers, where

$$0 < n_{11} < n_{12} < \ldots < n_{1p_1} \le \tfrac{1}{2}n,$$

$$0 < n_{21} < n_{22} < \ldots < n_{2p_2} \le \tfrac{1}{2}n,$$

$$0 < m_{11} < m_{12} < \ldots < m_{1q_1} \le n.$$

Then the two-level-circulant graph, denoted as $C_n(\{n_{11}, n_{12}, \ldots, n_{1p_1}\}, \{n_{21}, n_{22}, \ldots, n_{2p_2}\}; \{m_{11}, m_{12}, \ldots, m_{1q_2}\})$, is the graph defined on $2n$ nodes $v_{11}, v_{12}, \ldots, v_{1n}, v_{21}, v_{22}, \ldots, v_{2n}$ with vertex v_{ab} adjacent to vertex v_{cd} whenever

[$a = c$ and $b = c + n_{aj}(\text{mod } n)$ for some j] or [$a = 1, c = 2, d = b + m_{1j}(\text{mod } n)$ for some j]. The Annulus(n) is $C_n(\{j\}, \{j\}; \{0\})$, where $\gcd(n, j) = 1$.

Let $a_1, a_2, \ldots, a_n$ be a sequence with $a_i = 1$ if $i = 1 + m_{1j}$ for some j; $a_i = 0$ otherwise. Let $V_k = [1\, \rho_n^k \rho_n^{2k} \ldots \rho_n^{(n-1)k}]$. By corollary 5, $\{V_k | k = 1, 2, \ldots, n\}$ is a complete set of eigenvectors of any circulant graph on n nodes. Let $B = [[a_1, a_2, \ldots, a_n]]$, $A_1 = A(C_n(n_{11}, n_{12}, \ldots, n_{1p_1}))$ and $A_2 = A(C_n(n_{21}, n_{22}, \ldots, n_{2p_2}))$ be three circulant matrices with $V_k B = y_k V_k$, $V_k B^{\mathrm{T}} = z_k V_k$ and $V_k A_j = \sigma_{jk} V_k$ for $k = 1, 2, \ldots, n$ and $j = 1, 2$.

COROLLARY 8

Let A_1, A_2, B, V_k, $\{\mathcal{N}_1\}$, $\{\mathcal{N}_2\}$, $\{\mathcal{M}\}$, y_k, z_k, σ_{ik} and a_k, $k = 1, 2, \ldots, n$ and $i = 1, 2$, be defined as above. Let $C_n(\{\mathcal{N}_1\}, \{\mathcal{N}_2\}; \{\mathcal{M}\})$ be a two-level-circulant graph. Then

(1)
$$C_n(\{\mathcal{N}_1\}, \{\mathcal{N}_2\}; \{\mathcal{M}\}) = \begin{bmatrix} A_1 & B \\ B^{\mathrm{T}} & A_2 \end{bmatrix}.$$

(2) $\mathrm{CSET}(C_n(\{\mathcal{N}_1\}, \{\mathcal{N}_2\}; \{\mathcal{M}\})) = \{W_1, W_2, \ldots, W_{2n}\}$, where $\{W_{2k-1}^{\mathrm{T}}, W_{2k}^{\mathrm{T}}\} = \{[V_k^{\mathrm{T}}\ \alpha V_k^{\mathrm{T}}] \,|\, y_k\alpha^2 + (\sigma_{1k} - \sigma_{2k})\alpha - z_k = 0\}$ for $k = 1, 2, \ldots, n$.

(3) The corresponding eigenvalues are given by $\{\lambda_{2k-1}, \lambda_{2k}\} = \{\sigma_{1k} + y_k\alpha \,|\, y_k\alpha^2 + (\sigma_{1k} - \sigma_{2k})\alpha - z_k = 0\}$.

The graphs $C_5(\{1\}, \{1\}; \{0, 1\})$, $C_5(\{0\}, \{1\}; \{0, 1\})$ and $C_8(\{0\}, \{1\}; \{0\})$ are given in fig. 3.

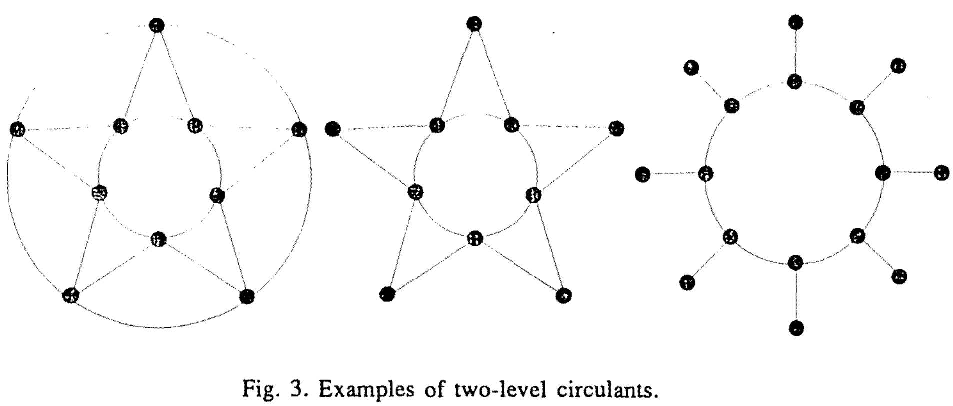


Fig. 3. Examples of two-level circulants.

The graph of generalized sun (generalized comb, respectively), Gsun(n, m) (Gcomb(n, m), respectively) on mn nodes $V_{11}, V_{12}, \ldots, V_{mn}$ with V_{ik} is adjacent to vertex V_{jk} for all k and all distinct i, j and the nodes $\{V_{11}, V_{12}, \ldots, V_{1n}\}$ form a cycle

C_n (path L_n, respectively). Then, eigenvectors and eigenvalues of these two classes of graphs can be obtained by theorem 7.

$C_n(\{\mathcal{N}_1\}, \{\mathcal{N}_2\}, \ldots, \{\mathcal{N}_k\}; \{\mathcal{M}_{12}\}, \{\mathcal{M}_{13}\}, \ldots, \{\mathcal{M}_{k(k-1)}\})$, where n_i's stand for intra-circulant jump sizes in the ith circulant and m_{ij}'s stand for inter-circulant jump sizes between ith and jth circulants. There are many classes of graphs which can be included in this category, such as the graphs in fig. 4.

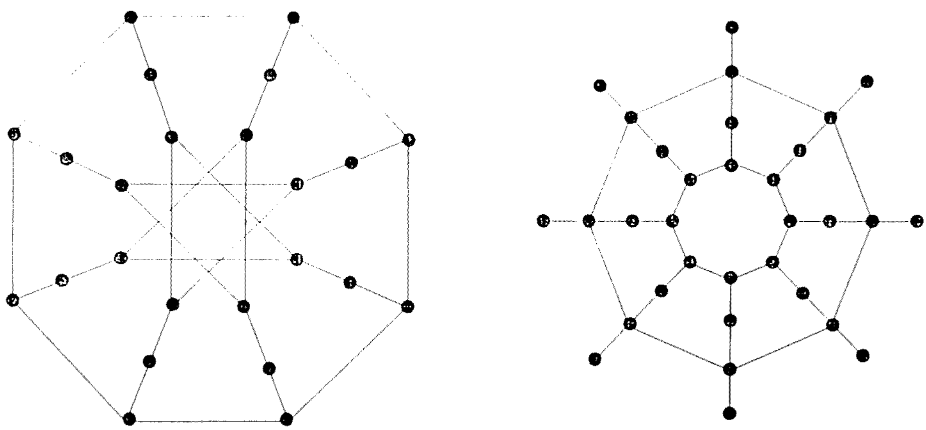


Fig. 4. Three-level and four-level circulants.

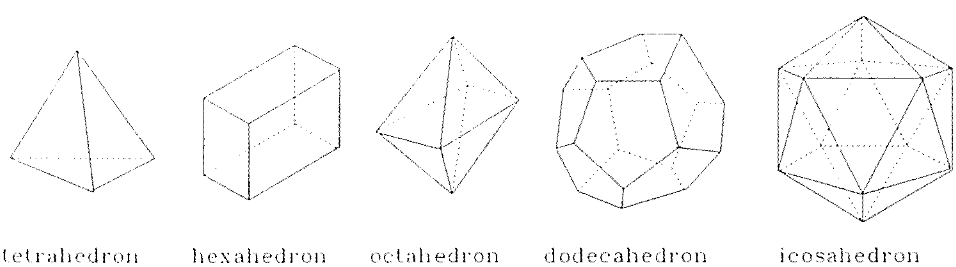


Fig. 5. Five regular polyhedra.

There are exactly five kinds of regular polyhedra (see fig. 5): tetrahedron (K_4), hexahedron (H_3), octahedron ($K_2 + C_4$), dodecahedron and icosahedron. The eigenvectors and eigenvalues of the dodecahedron can be derived by applying theorem 7 and the following lemma. The results are stated in corollary 9.

LEMMA 2

Given the matrix

$$M = \begin{bmatrix} a & 1 & 0 & 0 \\ 1 & 0 & b & 0 \\ 0 & c & 0 & 1 \\ 0 & 0 & 1 & a \end{bmatrix}.$$

Then:

(1) $\mathrm{CSET}(M) = \{[1\ \alpha\ \alpha\beta\ \beta] \mid c\beta^2 = b$ and $\alpha^2 + (a - c\beta)\alpha - 1 = 0\}$, and

(2) The corresponding eigenvalues are $\{\alpha + a \mid c\beta^2 = b$ and $\alpha^2 + (a - c\beta)\alpha - 1 = 0\}$.

COROLLARY 9

Let $U_k^{\mathrm{T}} = [1\ \rho_n^k \rho_n^{2k} \ldots \rho_n^{(n-1)k}]$. Then we have

(1) $$A(\text{dodecahedron}) = \begin{bmatrix} A(C_5) & I_5 & 0_{55} & 0_{55} \\ I_5 & 0_{55} & B & 0_{55} \\ 0_{55} & B^{\mathrm{T}} & 0_{55} & I_5 \\ 0_{55} & 0_{55} & I_5 & A(C_5) \end{bmatrix},$$

where

$$B = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

(2) $\mathrm{CSET}(\text{dodecahedron}) = \{W_1, W_2, \ldots, W_{20}\}$. For $k = 1, 2, 3, 4, 5$,

$$\{W_{4k}^{\mathrm{T}}, W_{4k-1}^{\mathrm{T}}, W_{4k-2}^{\mathrm{T}}, W_{4k-3}^{\mathrm{T}}\} = \{[1\ \alpha\ \alpha\ \beta\ \beta] \otimes U_k \mid \alpha^2 + (2\cos(2k\pi/5) \pm 2^{1/2}(1 + \cos(k\pi/5))^{1/2})\alpha - 1 = 0\}.$$

(3) The corresponding eigenvalues are

$$\{\alpha + 2\cos(2k\pi/5) \mid \alpha^2 + (2\cos(k\pi/5) \pm 2^{1/2}(1 + \cos(k\pi/5))^{1/2}\alpha - 1 = 0, 1 \le k \le 5\}.$$

For the derivation of eigenvectors and eigenvalues of an icosahedron, it is necessary to learn the eigenproperties of graphs which can be obtained through the operation *direct sum* on two circulant graphs. A general theorem concerning the eigenproperties of *direct sum* on two circulants is stated below.

THEOREM 10

Let $U_k^{\mathrm{T}} = [1\ \rho_m^k \rho_m^{2k} \ldots \rho_m^{(m-1)k}]$ and $V_j^{\mathrm{T}} = [1\ \rho_n^j \rho_n^{2j} \ldots \rho_n^{(n-1)j}]$ for $k = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. Let square matrices $A = [[a_1, a_2, \ldots, a_m]]$ and $B = [[b_1, b_2, \ldots, b_n]]$ be two circulant matrices. Then

(1) $A \oplus B = \begin{bmatrix} A & J_{mn} \\ J_{nm} & B \end{bmatrix}$.

(2) $\mathrm{CSET}(A \oplus B) = \{W_1, W_2, \ldots, W_{m+n}\}$, where $W_k^{\mathrm{T}} = [0_{1m}\, V_k^{\mathrm{T}}]$ if $1 \le k \le n-1$; $W_{n+k}^{\mathrm{T}} = [U_k^{\mathrm{T}}\, 0_{1n}]$ if $1 \le k \le m-1$ and $\{W_n^{\mathrm{T}}, W_{n+m}^{\mathrm{T}}\} = \{[J_{1m}\, \alpha J_{1n}] \mid n\alpha^2 + \alpha(d_A - d_B) - m = 0\}$, where $d_A = a_1 + a_2 + \ldots + a_m$ and $d_B = b_1 + b_2 + \ldots + b_n$.

(3) The corresponding eigenvalue λ_k of eigenvector V_k is given by

$$\lambda_k = b_1 + b_2\rho_n^k + b_3\rho_n^{2k} + \ldots + b_n\rho_n^{(n-1)k} \qquad \text{if } 1 \le k \le n-1;$$

$$\lambda_{n+k} = a_1 + a_2\rho_m^k + a_3\rho_m^{2k} + \ldots a_m\rho_m^{(m-1)k} \qquad \text{if } 1 \le k \le m-1$$

and

$$\{\lambda_n, \lambda_{n+m}\} = \{n\alpha + d_A \mid n\alpha^2 + \alpha(d_A - d_B) - m = 0\}.$$

Let the generalized wheel graph $W_{m,n}$ be the graph $\overline{K}_m \oplus C_n$ and the complete bipartite graph $K_{m,n}$ be the graph $K_m \oplus K_n$. Then, $\mathrm{CSET}(W_{m,n})$, $\mathrm{CSET}(K_{m,n})$ and their corresponding eigenvalues can be obtained by theorem 10.

Now, we are able to develop the derivation for the case of an icosahedron and its generalization. The following theorem is essential in the derivation and the results are given in corollary 12.

THEOREM 11

Let $U_k^{\mathrm{T}} = [1\, \rho_m^k \rho_m^{2k} \ldots \rho_m^{(n-1)k}]$ for $k = 1, 2, \ldots, m$ and let P be the matrix

$$P = \begin{bmatrix} 0 & J_{1m} & 0 & 0_{1m} \\ J_{m1} & B & 0_{m1} & A \\ 0 & 0_{1m} & 0 & J_{1m} \\ 0_{m1} & A^{\mathrm{T}} & J_{m1} & B \end{bmatrix},$$

where square matrices $A = [[a_1, a_2, \ldots, a_m]]$ and $B = [[b_1, b_2, \ldots, b_n]]$ are two circulant maatrices. Then

(1) $\mathrm{CSET}(P) = \{W_1, W_2, \ldots, W_{2m+2}\}$, where $\{W_{2k-1}^{\mathrm{T}}, W_{2k}^{\mathrm{T}}\} = \{[0\, U_k^{\mathrm{T}}\, 0\, \alpha U_k^{\mathrm{T}}] \mid \alpha^2(\sum_{1<i\le m} a_{m+1-i}\rho_m^{ik}) = \sum_{1\le i\le m} a_i\rho_m^{(i-1)k}\}$ if $1 \le k \le m-1$; and $\{W_{2m-1}^{\mathrm{T}}, W_{2m}^{\mathrm{T}}, W_{2m+1}^{\mathrm{T}}, W_{2m+2}^{\mathrm{T}}\} = \{[\alpha\, J_m\, s\alpha\, sJ_m] \mid s = \pm 1, \alpha^2 + \alpha(d_A + sd_B) - m = 0\}$.

(2) The corresponding eigenvalues $\{\lambda_{2k-1}, \lambda_{2k}\} = \{(\sum_{1\le i\le m}(b_i + \alpha a_i)\rho_m^{(i-1)k}) \mid \alpha^2(\sum_{1\le i\le m} a_{m+1-i}\rho_m^{ik}) = \sum_{1\le i\le m} a_i\rho_m^{(i-1)k}\}$ if $1 \le k \le m-1$; and $\{\lambda_{2m-1}, \lambda_{2m}, \lambda_{2m+1}, \lambda_{2m+2}\} = \{m/\alpha \mid \alpha^2 + \alpha(d_B \pm d_A) - m = 0\}$.

COROLLARY 12

$$A(\text{icosahedron}) = \begin{bmatrix} 0 & J_{15} & 0 & 0_{15} \\ J_{51} & B & 0_{51} & A \\ 0 & 0_{15} & 0 & J_{15} \\ 0_{51} & A^{\mathrm{T}} & J_{51} & B \end{bmatrix},$$

where

$$B = \begin{bmatrix} 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$$

and

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

Then

(1) $\mathrm{CSET}(P) = \{W_1, W_2, \ldots, W_{12}\}$, where $\{W_{2k-1}^{\mathrm{T}}, W_{2k}^{\mathrm{T}}\} = \{[0\, U_k^{\mathrm{T}}\; 0\; \alpha U_k^{\mathrm{T}}] \mid \alpha^2(1+\rho_5^{4k}) = 1+\rho_5^k$ if $1 \le k \le 4$; $\{W_9^{\mathrm{T}}, W_{10}^{\mathrm{T}}\} = \{[V^{\mathrm{T}}\, V^{\mathrm{T}}] \mid V^{\mathrm{T}} = [1\;1\;1\;1\;1\;1]$ or $[-5\;1\;1\;1\;1\;1]\}$; and $\{W_{11}^{\mathrm{T}}, W_{12}^{\mathrm{T}}\} = \{[V^{\mathrm{T}} - V^{\mathrm{T}}] \mid V^{\mathrm{T}} = [5^{1/2}\;1\;1\;1\;1\;1]$ or $[-5^{1/2}\;1\;1\;1\;1\;1]\}$.

(2) The corresponding eigenvalues $\{\lambda_{2k-1}, \lambda_{2k}\} = \{(\alpha(1+\rho_5^k) + \rho_5^k + \rho_5^{4k}) \mid \alpha^2(1+\rho_5^{4k}) = 1+\rho_5^k\}$ if $1 \le k \le m-1$; and $\{\lambda_9, \lambda_{10}, \lambda_{11}, \lambda_{12}\} = \{5, -1, 5^{1/2}, -5^{1/2}\}$.

4. Full complete binary tree and full complete *m*-ary tree

A graph G in which a vertex is distinguished from other vertices is called a rooted graph and this distinct vertex is called the root of G. The complete binary tree is a rooted tree where each vertex has either 0 or 2 sons. The height of a rooted tree is the maximum level number of its external vertices. The full complete binary tree of height n, B_n (see fig. 6) is a complete binary tree where each external vertex has the same height.

The full complete binary tree is a special class which can be constructed recursively in the following way:

$$B_1 = K_1,$$

and let $p = 2^n - 1$ and $S_p = [s_1, s_2, \ldots, s_p]$, where $s_i = 1$ if $i = 1$; $s_i = 0$ otherwise. Then

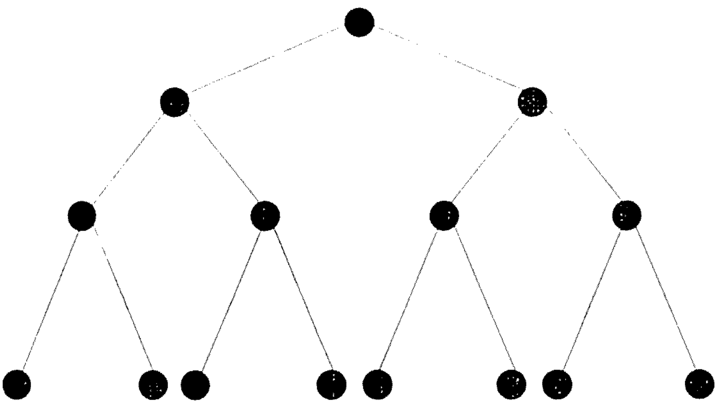


Fig. 6. Complete binary tree B_4.

$$A(B_{n+1}) = \begin{bmatrix} 0 & S_p & S_p \\ S_p^{\mathrm{T}} & B_n & 0 \\ S_p^{\mathrm{T}} & 0 & B_n \end{bmatrix} \quad \text{for} \quad n \geq 0.$$

Obviously, $\mathrm{CSET}(B_1) = \{[1]\}$ and the eigenvalue is 0. The complete set of eigenvectors and eigenvalues of B_n can be recurrently constructed according to theorem 13.

THEOREM 13

Let $p = 2^n - 1$, $q = 2^{n-1} - n$, $r = 2^{n-1} - 1$ and B_n be the graph of a full complete binary tree. Then

(1) $\mathrm{CSET}(B_n) = \{W_1^{(n)}, W_2^{(n)}, \ldots, W_p^{(n)}\}$, where $\{W_{2k-1}^{(n)^{\mathrm{T}}}, W_{2k}^{(n)^{\mathrm{T}}}\} = \{[0\, W_n^{(n-1)^{\mathrm{T}}} \pm W_k^{(n-1)^{\mathrm{T}}}] \mid W_k^{(n-1)} \in \mathrm{CSET}(B_{n-1})\}$ for $k = 1, 2, \ldots, q$; $W_{q+k}^{(n)^{\mathrm{T}}} = [0\, W_k^{(n-1)^{\mathrm{T}}} - W_k^{(n-1)^{\mathrm{T}}})]$ for $k = q+1, q+2, \ldots, r$; $W_{p-n+k}^{(n)^{\mathrm{T}}} = [1\, A_1^{(n,k)^{\mathrm{T}}}, A_2^{(n,k)^{\mathrm{T}}}]$ for $k = 1, 2, \ldots, n$, where $A_1^{(n,k)^{\mathrm{T}}} = A_2^{(n,k)^{\mathrm{T}}} = [a_1 a_2 \ldots a_r]$ with $a_{2^{(i-1)}} = \ldots = a_{2^i - 1} = 2^{(1-i)/2} \sin(i+1)\delta_k / \sin \delta_k$, where $\delta_k = k\pi/(n+1)$.

(2) The corresponding eigenvalue λ_k of eigenvector $W_k^{(n)}$ is $\lambda_{2k-1}^{(n)} = \lambda_{2k}^{(n)} = \lambda_k^{(n-1)}$ for $k = 1, 2, \ldots, q$; $\lambda_{q+k}^{(n)} = \lambda_k^{(n-1)}$ for $k = q+1, q+2, \ldots, r$ and $\lambda_{p-n+k} = 2^{3/2} \cos \delta_k$ with $\delta_k = k\pi/(n+1)$ for $k = 1, 2, \ldots, n$.

The complete m-ary tree is a rooted tree where each vertex has either 0 or m sons. The full complete m-ary tree of height n, $B_n^{(m)}$, is a complete m-ary tree where each external vertex has the same height. Then

THEOREM 14

Let $p = m^{n-1} + m^{n-2} + \ldots + m + 1$, $q = m^{n-2} + m^{n-3} + \ldots + m + 1 - (n-1)$, $r = m^{n-2} + m^{n-3} + \ldots + m + 1$ and $B_n^{(m)}$ be the graph of the full complete m-ary tree. Then

$$A(B_{n+1}^{(m)}) = \begin{bmatrix} 0 & J_{1m} \otimes S_p \\ (J_{1m} \otimes S_p)^{\mathrm{T}} & 0 \end{bmatrix} = \begin{bmatrix} 0 & S_p & S_p & \cdots & S_p \\ S_p^{\mathrm{T}} & B_n^{(m)} & 0 & \cdots & 0 \\ S_p^{\mathrm{T}} & 0 & B_n^{(m)} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ S_p^{\mathrm{T}} & 0 & 0 & \cdots & B_n^{(m)} \end{bmatrix}$$

for $n \geq 0$.

(1) $\mathrm{CSET}(B_n^{(m)}) = \{W_1^{(n)}, W_2^{(n)}, \ldots, W_p^{(n)}\}$, where $\{W_{mk-m+1}^{(n)\mathrm{T}}, W_{mk-m+2}^{(n)\mathrm{T}}, \ldots, W_{mk}^{(n)\mathrm{T}}\}$ $= \{[0\, z_{mi} \otimes W_k^{(n-1)\mathrm{T}}] | W_k^{(n-1)\mathrm{T}} \in \mathrm{CSET}(B_{n-1}^{(m)}),\ 1 \leq i \leq m\}$ for $k = 1, 2, \ldots, q$; $\{W_{(m-1)k+q-(m-2)}^{(n)\mathrm{T}}, W_{(m-1)k+q-(m-3)}^{(n)\mathrm{T}}, \ldots, W_{(m-1)k+q}^{(n)\mathrm{T}}\} = \{[0\, z_{mi} \otimes W_k^{(n-1)\mathrm{T}}] | W_k^{(n-1)\mathrm{T}} \in \mathrm{CSET}(B_{n-1}^{(m)}),\ 2 \leq i \leq m\}$ for $k = q+1, q+2, \ldots, r$ and $W_{p-n+k}^{(n)\mathrm{T}}$ $= [1\, A_1^{(n,k)\mathrm{T}} A_2^{(n,k)\mathrm{T}} \ldots A_m^{(n,k)\mathrm{T}}]$ for $k = 1, 2, \ldots, q$, where $A_1^{(n,k)\mathrm{T}} = A_2^{(n,k)\mathrm{T}} = \ldots =$ $A_m^{(n,k)\mathrm{T}} = [a_1 a_2 \ldots a_r]$ with $a_{m^{i-2}+m^{i-3}+\ldots+m+1} = \ldots = a_{m^{i-1}+m^{i-2}+\ldots+m+1}$ $= 2^{(1-i)/2} \sin(i+1)\delta_k / \sin\delta_k$, where $\delta_k = k\pi/(n+1)$.

(2) The corresponding eigenvalue λ_k of eigenvector $W_k^{(n)}$ is $\lambda_{mk-m+1}^{(n)} = \lambda_{mk-m+2}^{(n)}$ $= \ldots = \lambda_{mk-m}^{(n)} = \lambda_k^{(n-1)}$ for $k = 1, 2, \ldots, q$; $\lambda_{(m-1)k+q-(m-2)}^{(n)} = \lambda_{(m-1)k+q-(m-3)}^{(n)}$ $= \ldots = \lambda_{(m-1)k+q}^{(n)} = \lambda_k^{(n-1)}$ for $k = q+1, q+2, \ldots, r$ and $\lambda_{p-n+k}^{(n)} = 2m^{1/2}\cos\delta_k$ with $\delta_k = k\pi/(n+1)$ for $k = 1, 2, \ldots, n$.

5. Conclusions

First of all, we investigate the general properties of eigenvectors and eigenvalues of circulant graphs and paths. By applying some graph operations, we can then easily derive the eigenvectors and eigenvalues for classes of graphs, which were built up from circulants and paths, without calculating the characteristic polynomial. Several classes of graphs such as generalized wheels, regular polyhedra, k-level-circulant graphs, etc., are given to demonstrate the application of our methods.

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