ON SPECTRAL STPUCTURE OF GRAPHS HAVING THE MAXIMAL EIGENVALUE NOT GREATER THAN TWO

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(Received August 26, 1974)

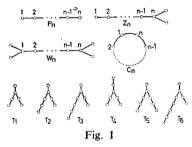
Let G be a graph with n vertices and the adjacency matrix A. The polynomial

(1)
$$P_G(\lambda) = \det(\lambda I - A) = \lambda^n + a_1 \lambda^{n-1} + \cdots + a_n$$

is called the characteristic polynomial of G. The roots $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $P_G(\lambda) = 0$ are called the eigenvalues of G. The "system of numbers" $[\lambda_1, \lambda_2, \ldots, \lambda_n]$ is called the spectrum of the graph G and will be denoted also by G. Note that some λ_i can be mutually equal.

Since A is a symmetric matrix, the eigenvalues of G are real. The maximal number in the spectrum of G is called the index of the graph G and is denoted by $\Lambda(G) = \Lambda$.

Relations between the structure of a graph and its index were the topic of several investigations [1-3]. In particular, J. H. Smith [1] was able to determine the set $\mathcal S$ of all graphs having $\Lambda \le 2$. The connected graphs from $\mathcal S$ are shown in Fig 1.



In this paper we shall study the properties of the spectra of graphs from $\mathcal S$. It will be shown that the condition $\Lambda \leqslant 2$ demands a particular algebraic form of the eigenvalues of these graphs. In addition, a procedure for deciding whether a system of numbers is a spectrum of a graph from $\mathcal S$ or not will be described. Moreover, all graphs, having the spectrum equal to a given system of numbers, can be determined by this procedure.

The spectrum of the union of two graphs (for definitions not given here see [4]) is obviously the union of their spectra (having in view the multiplicities of the eigenvalues). The expression $G_1 + G_2$ will denote the union of the graphs G_1 and G_2 and $G_1 + G_2$ the union of their spectra. kG(kG) denotes the union of k copies of G(G). If $G_2 \subset G_1$, the expression $G_1 - G_2$ denotes the difference of systems of numbers G_1 and G_2 .

The spectra of graphs from Fig. 1 can be easily obtained and so we have:

$$\mathbf{P}_{n} = \left[2\cos\frac{j\pi}{n+1} \middle| j=1, 2, \dots, n \right],$$

$$\mathbf{Z}_{n} = \left[2\cos\frac{(2j+1)\pi}{2(n+1)} \middle| j=0, 1, \dots, n \right] + [0],$$

$$\mathbf{W}_{n} = \left[2\cos\frac{j\pi}{n+1} \middle| j=1, 2, \dots, n \right] + [2, 0, 0, -2],$$

$$\mathbf{C}_{n} = \left[2\cos\frac{2j\pi}{n} \middle| j=1, 2, \dots, n \right],$$

$$\mathbf{T}_{1} = \left[2\cos\frac{j\pi}{12} \middle| j=1, 4, 5, 7, 8, 11 \right],$$

$$\mathbf{T}_{2} = \left[2\cos\frac{j\pi}{18} \middle| 1=1, 5, 7, 9, 11, 13, 17 \right],$$

$$\mathbf{T}_{3} = \left[2\cos\frac{j\pi}{30} \middle| j=1, 7, 11, 13, 17, 19, 23, 29 \right],$$

$$\mathbf{T}_{4} = \left[2\cos\frac{j\pi}{6} \middle| j=1, 2, 3, 4, 5, 6 \right] + [0],$$

$$\mathbf{T}_{5} = \left[2\cos\frac{j\pi}{4} \middle| j=1, 2, 3 \right] + [2, 1, 0, -1, -2],$$

$$\mathbf{T}_{6} = \left[2\cos\frac{j\pi}{5} \middle| j=1, 2, 3, 4 \right] + [2, 1, 0, -1, -2].$$

Spectra of the path P_n and the circuit C_n are well known [5], while the spectra of Z_n and W_n can be easily obtained and are given in [6] and [7]. The validity of the given spectra for $T_1 - T_6$ can be checked by direct calculation, although this is not simple in all cases.

From the quoted facts the following theorem is evident.

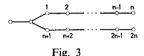
Theorem 1. 1° All eigenvalues of any graph from $\mathcal S$ are of the form $2\cos\frac{p}{q}\pi$, where p and q are integers and $q\neq 0$. The index of a graph from $\mathcal S$

is either equal to 2 or is of the form $2\cos\frac{\pi}{q}$ where q is a natural number. Only graphs from $\mathcal S$ have these two properties.

2° The set of eigenvalues of all graphs from $\mathcal S$ is equal to the set of all numbers of the form $2\cos\frac{p}{q}\pi$, where p and q are integers and $q\neq 0$.

Since $|2\cos\theta| < 2$, it is clear that the result which is summarized in Theorem 1 is intimately related to the condition $\Lambda < 2$. It is to be expected that in the spectra of graphs with the property $\Lambda < 2 + \varepsilon$ for any $\varepsilon > 0$, numbers are contained having a different (probably much more complicated) algebraic form. In connection to this we mention that graphs P_n , Z_n and W_n are the only three graphs of the form from Fig. 2 the spectrum of which is known in a closed

analytical form. According to the results obtained by Hoffman [2], the spectrum of the graph from Fig. 3 would be of a special interest.



If graphs G_1 and G_2 have the same spectra, we shall write $\mathbf{G}_1 = \mathbf{G}_2$. Thus G_1 and G_2 are isospectral. A pair of isospectral nonisomorphic graphs will be called a PING. Now we shall list some PING's from the set \mathcal{S} . As it will be shown later, the following relations enable the generation of all PING's contained in \mathcal{S} . We have

(2a)
$$Z_n + P_n = P_{2n+1} + P_1$$
,

$$\mathbf{W}_{n} = \mathbf{C}_{4} + \mathbf{P}_{n},$$

(2c)
$$\mathbf{C}_{2n} + 2\mathbf{P}_1 = \mathbf{C}_4 + 2\mathbf{P}_{n-1}$$

(2d)
$$T_1 + P_3 + P_5 = P_1 + P_2 + P_{11}$$

(2e)
$$T_2 + P_5 + P_8 = P_{17} + P_2 + P_1$$
,

(2f)
$$T_3 + P_{14} + P_9 + P_5 = P_{29} + P_4 + P_2 + P_1$$

(2g)
$$T_4 + P_1 = C_4 + 2 P_2$$
,

(2h)
$$T_5 + P_1 = C_4 + P_3 + P_2$$
,

(2i)
$$T_6 + P_1 = C_4 + P_4 + P_2$$
.

For n = 1 relation (2b) yields the PING shown in Fig. 4. This is the unique PING with graphs with 5 vertices. There is no PING with graphs with less than 5 vertices [8].

$$\sum_{W_1} \qquad \qquad \bigcup_{C_4+P_1} \circ$$

Fig. 4

Let S_1, S_2, \ldots, S_m be some systems of numbers and $\sigma_1, \sigma_2, \ldots, \sigma_m$ integers such that the expression

(3)
$$\sigma_1 \mathbf{S}_1 + \sigma_2 \mathbf{S}_2 + \cdots + \sigma_m \mathbf{S}_m$$

can be calculated in at least one way by successive performing the quoted operations. Then (3) defines a systems S and we shall say that S is a linear combination of S_1, S_2, \ldots, S_m .

Theorem 2. The spectrum of any bipartite graph from $\mathcal G$ can be represented in a unique way as a linear combination of the form

(4)
$$\sigma_0 \mathbf{C}_4 + \sigma_1 \mathbf{P}_1 + \sigma_2 \mathbf{P}_2 + \cdots + \sigma_m \mathbf{P}_m.$$

The number m is bounded by a function of the number of vertices. σ_0 is always nonnegative and the non-vanishing coefficient σ_i with the greatest i is positive.

Proof. From the relations (2) we see that the spectrum of each connected bipartite graph from $\mathcal G$ can be expressed as a linear combination of C_4 , P_1 , P_2 , P_3 , Since the spectrum of a disconnected graph is a linear combination of spectra of some connected graphs, the last statement can be immediately extendend to every bipartite graph from S. For example, we have

$$\mathbf{Z}_n = \mathbf{P}_{2n-1} - \mathbf{P}_n + \mathbf{P}_1,$$

 $\mathbf{T}_3 = \mathbf{P}_{29} - \mathbf{P}_{14} - \mathbf{P}_9 - \mathbf{P}_5 + \mathbf{P}_4 + \mathbf{P}_2 + \mathbf{P}_1.$

There exists no PING whose graphs contain only paths and circuits C_4 as components. This follows from the fact that no two graphs C_4 , P_1 , P_2 , P_3 , ... have the same index. According to this, two linear combinations $\sigma_0 C_4 + \sigma_1 P_1 + \sigma_2 P_2 + \cdots + \sigma_m P_m$ and $\sigma_0 C_4 + \sigma_1 P_1 + \sigma_2 P_2 + \cdots + \sigma_m P_m$ are equal if, and only if $\sigma_0 = \sigma_0, \ \sigma_1 = \sigma_1, \ \sigma_2 = \sigma_2, \dots, \ \sigma_m = \sigma_m.$ This completes the proof of the Theorem 2.

One of the fundamental problems in the spectral graph theory is the following one. Let a system of numbers be given. The question arises whether there exists a graph (from a given class of graphs) or not, the spectrum of which is equal to the given system of numbers.

Of course, for a given system S, containing n numbers one can check all graphs with n vertices in order to answer the above question. Nevertheless, we would like to present a more effective procedure which enables the determination of all graphs having the spectrum equal to a given system of numbers of the form $2\cos\frac{p}{\pi}$.

Let first consider only bipartite graphs from \mathcal{S} . As it is well known, bipartite graphs have a symmetric spectrum with respect to the zero point. Given a symmetric system S of numbers* of the form $2\cos\frac{p}{\pi}\pi$, we try to represent it as a linear combination of C_4 , P_1 , P_2 , If this is not possible,

^{*} This means that if a number α belongs to S with the multiplicity p, then $-\alpha$ also belongs to S with the same multiplicity p.

S is not a spectrum of any graph (according to Theorems 1 and 2). In the case such a representation is possible, the mentioned linear combination is unique. Principles of finding the corresponding coefficients are clear since among C_4 , P_1 , P_2 , ... no two systems have the same greatest element.

Let now S be represented as

(5)
$$\mathbf{S} = \sigma_0 \, \mathbf{C}_4 + \sigma_1 \, \mathbf{P}_1 + \sigma_2 \, \mathbf{P}_2 + \cdots + \sigma_m \, \mathbf{P}_m.$$

Suppose that S is the spectrum of a graph. Presenting it as a linear combination of spectra of the components we get

(6)
$$\mathbf{S} = p_1 \, \mathbf{P}_1 + p_2 \, \mathbf{P}_2 + p_3 \, \mathbf{P}_3 + \cdots + z_1 \, \mathbf{Z}_1 + z_2 \, \mathbf{Z}_2 + z_3 \, \mathbf{Z}_3 + \cdots + w_1 \, \mathbf{W}_1 + w_2 \, \mathbf{W}_2 + w_3 \, \mathbf{W}_3 + \cdots + c_2 \, \mathbf{C}_4 + c_3 \, \mathbf{C}_6 + \cdots + t_1 \, \mathbf{T}_1 + t_2 \, \mathbf{T}_2 + t_3 \, \mathbf{T}_3 + t_4 \, \mathbf{T}_4 + t_5 \, \mathbf{T}_5 + t_6 \, \mathbf{T}_6$$

for some non-negative integers

(7)
$$p_1, p_2, p_3, \ldots, z_1, z_2, z_3, \ldots, w_1, w_2, w_3, \ldots, c_2, c_3, \ldots, t_1, t_2, t_3, t_4, t_5, t_6.$$

Using the relations (2) one can express the eq. (6) in the form

(8)
$$S = F_0 C_4 + F_1 P_1 + F_2 P_2 + \cdots,$$

where the coefficients F_i (i = 0, 1, ...) in (8) are functions of variables (7). Hence,

(9a)
$$F_0 = (w_1 + w_2 + w_3 + \cdots) + (c_2 + c_3 + \cdots) + t_A + t_S + t_S$$

(9b)
$$F_1 = p_1 - z_1 + w_1 + 2c_2 + (z_1 + z_2 + z_3 + \cdots) - 2(c_2 + c_3 + \cdots) + t_1 + t_2 + t_3 - t_4 - t_5 - t_6$$

and for i>1 and $i\neq 2, 3, 4, 5, 8, 9, 11, 14, 17, 29$

$$(9c) F_i = \tilde{F}_i,$$

where

(9d)
$$\tilde{F}_{i} = \begin{cases} p_{i} - z_{i} + w_{i} + 2 c_{i+1}, & i \text{ even} \\ p_{i} + z_{i-1} - z_{i} + w_{i} + 2 c_{i+1}, & i \text{ odd} \end{cases}$$

for the excluded values of i

(9e)
$$F_i = \tilde{F}_i + h_i,$$

where

(9f)
$$h_2 = t_1 + t_2 + t_3 + 2 t_4 + t_5 + t_6,$$

$$h_3 = -t_1 + t_5, \quad h_4 = t_3 + t_6,$$

$$h_5 = -t_1 - t_2 - t_3, \quad h_8 = -t_2, \quad h_9 = -t_3,$$

$$h_{11} = t_1, \quad h_{14} = -t_3, \quad h_{17} = t_2, \quad h_{29} = t_3.$$

Comparing (5) and (8) we get the following system of linear algebraic equations in unknowns (7):

(10)
$$F_i = \sigma_i \qquad i = 0, 1, 2, \ldots, m.$$

Now we can formulate the following theorem.

Theorem 3. Let S be a symmetric system of numbers of the form $2\cos\frac{p}{q}\pi$ where p, q, are integers and $q\neq 0$. A necessary condition for S to be a graph spectrum is that S can be represented in the form (5). In this case, to every solution of the system of equations (10) in unknowns (7), these quantities being non-negative integers, a graph corresponds, the spectrum of which is S. All graphs having the spectrum equal to S can be obtained in this way.

If S is not symmetric and is the spectrum of a graph, this graph necessarily contains some circuits of odd lengths as components. According to a theorem due to H. Sachs [9], the length of the shortest odd circuit in a graph is equal to the index f of the first non-vanishing coefficient among a_1, a_3, a_5, \ldots from the correspoding characteristic polynomial (1) and the number of shortest odd circuits is equal to $-a_r/2$.

Hence, we have to determine the polynomial whose zeros are the numbers from S. The coefficients of this polynomial must be integers. If so, we find f and $-a_f/2=k$, (k must be an integer), and S must contain k times the spectrum of a circuit C_f . If this is not true, S is not a graph spectrum. In the other case we remove from S all eigenvalues belonging to k circuits C_f and get a new system S'. If S' is symmetric, we apply Theorem 3. If not, the above described procedure is to be applied on S' etc.

Theorem 4. Let S be a non-symmetric system of numbers of the form $2\cos\frac{p}{q}\pi$, where p, q are integers and $q\neq 0$. A necessary condition for S to be a graph spectrum is that S can be represented as a union of a symmetric system and a linear combination of spectra of some circuits of odd lengths. This linear combination (if it exists) can be uniquely determined from S.

Theorems 3 and 4 solve entirely the problem of deciding whether or not is a given system of numbers of the form $2\cos\frac{p}{q}\pi$ equal to the spectrum of some graph. Moreover, using these theorems all graphs having the spectrum equal to S can be determined

Corollary. All PING's from \mathcal{S} can be generated using relation (2).

REFERENCES

- [1] J. H. Smith, Some properties of the spectrum of a graph, Combinatorial structures and their applications, New York London Paris 1970, 403—406.
- [2] A. J. Hoffman, On limit points of spectral radii of non-negative symmetric integral matrices, Graph theory and applications, Berlin—Heidelberg—New York 1972, 165—172.
- [3] L. Lovász, J. Pelikán, On the eigenvalues of trees, Periodica Math. Hungarica 3 (1-2) (1973), 175-182.

- [4] F. Harary, Graph theory, Reading 1969.
- [5] L. Collatz. U. Sinogowitz, Spektren endlicher Graphen, Abh. Math. Sem. Univ. Hamburg 21 (1957), 63—77.
- [6] I. Gutman, N. Trinajstić, Violation of the Dewar-Longuet-Higgins Conjecture, Z. Naturforsch. 29 a (1974), 1238.
- [7] D. Cvetković, I. Gutman, N. Trinajstić, Conjugated molecules having integral graph spectra, Chem. Phys. Letters, 29 (1974), 65-68.
- [8] D. M. Cvetković, Graphs and their spectra, Univ. Beograd, Publ. Elektrotehn. Fak. Ser. Mat. Fiz. № 354—356 (1971), 1—50.
- [9] H. Sachs, Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem charakteristischen Polynom, Publ. Math. (Debrecen) 11 (1963), 119-134.