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GENERALIZATIONS OF A RECURRENCE RELATION FOR THE CHARACTERISTIC POLYNOMIALS OF TREES

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In this paper we shall consider digraphs G with finite number of vertices and arcs. G may possess loops.

Let A be the adjacency matrix of G. Then the characteristic polynomial of A

$$\Phi(G, \lambda) = \det(\lambda I - A) = \sum_{i=0}^{n} a_i(G)\lambda^{n-i} \tag{1}$$

is called the characteristic polynomial of the digraph G, where n is the number of vertices of G. For brevity we write $\Phi(G, \lambda) = \Phi(G)$.

The zeros of $\Phi(G)$ form the spectrum of G. Two digraphs G_1 and G_2 are called isospectral if they have the same spectrum.

Let $c(G)$ denote the number of components of G. If these components are $H_1, H_2, \ldots, H_{c(G)}$, we will write $G = H_1 \oplus H_2 \oplus \cdots \oplus H_{c(G)}$. Of course, $\Phi(G) = \Phi(H_1)\Phi(H_2)\cdots\Phi(H_{c(G)})$.

We denote by $\vec{E} = \vec{E}_{pq}$ the digraph containing (exactly) two vertices p and q and the arc $\vec{e} = \vec{e}_{pq}$ joining p with q. Analogously, $E = E_{pq}$ will denote the digraph containing the two vertices p and q and the two arcs $\vec{e}_{pq}$ and $\vec{e}_{qp}$. It is both convenient and consistent to replace the pair of arcs $\vec{e}_{pq}$ and $\vec{e}_{qp}$ by an edge $e = e_{pq}$. Accordingly, every (undirected) graph can be understood as being a digraph.

Let H be a subgraph of G. Then $G-(H)$ will denote the digraph obtained by deletion of all arcs contained in H from the digraph G. Further, $G-H$ will denote the digraph obtained by deletion of vertices of H and all arcs incident with them from the digraph G. If $c(G-(E)) = c(G)+1$, the edge e will be called a bridge.

A (directed) cycle $\vec{C}_k$ of the length k is a (strongly) connected digraph with k vertices, exactly one arc starting from and ending at every vertex. Note that E is a cycle of length 2. Moreover, every loop will be understood as a cycle of length 1. A digraph, the only components of which are cycles is called a linear digraph $\vec{L}$.

We define two classes $\boldsymbol{C}_k$ and $\boldsymbol{P}_k$ of digraphs.

A digraph G belongs to the class $\boldsymbol{C}_k$ if it contains a subgraph $\vec{C}_k$ such that $c(G-(\vec{C}_k))=c(G)+k$. The structure of a digraph $G \in \boldsymbol{C}_k$ can be presented as in Fig, 1, with $H_1, H_2, \ldots, H_k$ being arbitrary digraphs. Obviously, $G-(\vec{C}_k)= =H_1 \oplus H_2 \oplus \cdots \oplus H_k$. Hence, the members of $\boldsymbol{C}_1$ possess a loop, while the members of $\boldsymbol{C}_2$ possess a bridge. Note also that $\vec{C}_k \in \boldsymbol{C}_k$.

A digraph G belongs to the class $\boldsymbol{P}_k$ $(k \geqslant 3)$ if it contains two bridges e_1 and e_{k-1} such that $G-(E_1)-(E_{k-1})=H_1 \oplus H_2 \oplus P_{k-2}$, with H_1 and H_2 being arbitrary digraphs and P_n being the path with n vertices. The structure of the digraph $G \in \boldsymbol{P}_k$ can be represented as in Fig. 2. It is convenient to define also

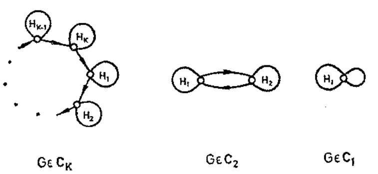

Fig. 1

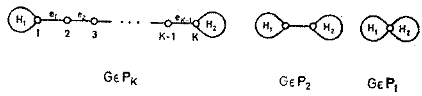

Fig. 2

the classes $\boldsymbol{P}_2$ and $\boldsymbol{P}_1$. A digraph G belongs to $\boldsymbol{P}_2$ if it contains a bridge and belongs to $\boldsymbol{P}_1$ if it contains a cutpoint. Of course, $\boldsymbol{P}_2=\boldsymbol{C}_2$ and $\boldsymbol{P}_{k-1} \subset \boldsymbol{P}_k$. Note also that $P_k \in \boldsymbol{P}_k$.

If e is a bridge, the following relation exists between the characteristic polynomials of G, $G-(E)$ and $G-E$.

T h e o r e m 1.

$$\Phi(G)=\Phi(G-(E))-\Phi(G-E). \tag{2}$$

Formula (2) has been first used by Coulson and Longuet-Higgins [1], but without proof. In chemical [2] and mathematical literature [3,4] the proofs of Theorem 1 have been given independently. It is worth mentioning that (2) is of some importance in theoretical chemistry (e.g. see [5]).

Since all edges of a tree (or more general of a forest) are bridges, we have

C o r o l l a r y 1.1. *Eq.* (2) *applies to an arbitrary edge of a tree.*

If q is a vertex of degree one, adjacent to the vertex p, the application Theorem 1. gives

C o r o l l a r y 1.2.

$$\Phi(G)=\lambda \Phi(G-q)=\Phi(G-p-q).$$

In particular, for a path P_n we have,

$$\Phi(P_n)=\lambda \Phi(P_{n-1})-\Phi(P_{n-2}). \tag{3}$$

In the present paper we offer generalizations of both (2) and (3).

Theorem 2. *If* $G \in C_k$,

$$\Phi(G) = \Phi(G - (\vec{C}_k)) - \Phi(G - \vec{C}_k). \tag{4}$$

Proof. According to a theorem of Sachs [6], the coefficient $a_i(G)$ of the characteristic polynomial (1) can be calculated from the equation

$$a_i(G) = \sum_{\vec{L} \in L_i(G)} (-1)^{c(\vec{L})} \tag{5}$$

where the summation goes over the set $L_i(G)$ of all linear digraphs $\vec{L}$ with i vertices, which are contained as subgraphs in G. Now, from the definition of the class C_k it follows that the vertices belonging to $\vec{C}_k$ appear in a linear subgraph of G only if the cycle $\vec{C}_k$ is a component of this linear subgraph. Let us, therefore, divide the set $L_i(G)$ into two subsets $L_{i1}(G)$ and $L_{i2}(G)$, where $\vec{L} \in L_{i1}(G)$ if $\vec{C}_k$ is a component of $\vec{L}$ and $\vec{L} \in L_{i2}(G)$ if $\vec{C}_k$ is not a component of $\vec{L}$. But then $L_{i2}(G) = L_i(G - (\vec{C}_k))$. Moreover, there is a one-to--one correspondence between the elements of $L_{i1}(G)$ and $L_{i-k}(G - \vec{C}_k)$. Namely, if $\vec{L} \in L_{i-k}(G - \vec{C}_k)$, then $\vec{L} \oplus \vec{C}_k \in L_{i1}(G)$. Substituting these relations back into eq. (5) we have

$$a_i(G) = \sum_{\vec{L} \in L_i(G - (\vec{C}_k))} (-1)^{c(L)} + \sum_{\vec{L} \in L_{i-k}(G - \vec{C}_k)} (-1)^{c(L)+1} =$$

$$= a_i(G - (\vec{C}_k)) - a_{i-k}(G - \vec{C}_k).$$

Theorem 2 follows now immediately from (1).

Corollary 2.1. *For* $k = 2$, *Theorem* 2 *becomes Theorem* 1. *For* $k = 1$, *namely if* G *has a loop, say on the vertex* p, *we have*

$$\Phi(G) = \Phi(G^\circ) - \Phi(G - p)$$

with G° *being the digraph obtained after the deletion of the loop from the vertex* p *of* G.

Corollary 2.2. *If two digraphs* G_1 *and* G_2 *from the class* C_k *fulfill the relations* $\Phi(G_1 - (\vec{C}_k)) = \Phi(G_2 - (\vec{C}_k))$ *and* $\Phi(G_1 - \vec{C}_k) = \Phi(G_2 - \vec{C}_k)$, *they are isospectral.*

As a consequence of this corollary, one is able to construct numerous multiplets of isospectral nonisomorphic digraphs. For example, the simplest pair of isospectral digraphs of this kind belongs to C_4. One should note, however, that the finding of isospectral digraphs presents no serious problem [3, 7, 8].

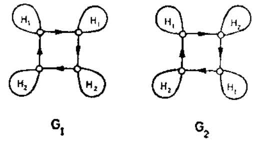

Fig. 3

As it is well known [9], the requirement that every two vertices of a graph are joined by a unique path can be taken as the definition of a tree. Let us extend this definition to digraphs. A ditree is a digraph with the property that every two vertices are joined by a unique directed path.

It is easily seen that a ditree is composed entirely from (directed) cycles. Two cycles $\vec{C}_a$ and $\vec{C}_b$ in a ditree are either disjoint or have exactly one common vertex. Therefore, every cycle of length k contained in a ditree fulfils the requirements for the class $\boldsymbol{C}_k$, and analogously to Corollary 1.1 we have

Corollary 2.3. *Eq.* (4) *applies to an arbitrary cycle of a ditree.*

Let us consider now a digraph $G_k \in \boldsymbol{P}_k$. According to the definition of the class $\boldsymbol{P}_k$, G_k contains a sequence of vertices $v_1, v_2, \ldots, v_k$ such that the vertices v_i and v_{i+1} are joined by a bridge e_i $(i=1, \ldots, k-1)$. By definition, the digraph $G_{k-1} \in \boldsymbol{P}_{k-1}$ is obtained from G_k by deleting the vertex v_i and joining the vertices v_{i-1} and v_{i+1} by a new edge.

We will show now that the validity of (3) is much wider and is not restricted to digraphs with a vertex of degree one.

Theorem 3. *For all* $G_k \in \boldsymbol{P}_k$,

$$\Phi(G_k) = \lambda \Phi(G_{k-1}) - \Phi(G_{k-2}). \tag{6}$$

Proof. Let $G_k - (E_i) = Q_i \oplus R_{k-i}$, where Q_i and R_{k-i} are digraphs obtained by joining of the end vertex of P_{i-1} to an arbitrary digraph H_1 and of P_{k-i-1} to an arbitrary digraph H_2, respectively. Then it is also $G_k - E_i' = Q_{i-1} \oplus R_{k-i-1}$, and by Theorem 1,

$$\Phi(G_k) = \Phi(Q_i)\,\Phi(R_{k-i}) - \Phi\,Q_{i-1})\,(\Phi(R_{k-i-1}).$$

Besides, since R_i contains a vertex of degree one,

$$\Phi(R_{k-i}) = \lambda \Phi(R_{k-i-1}) - \Phi(R_{k-i-2}).$$

An analogous relation can be written also for $\Phi(R_{k-i-1})$. After appropriate transformations we get,

$$\Phi(G_k) = \lambda\,[\Phi(Q_i)\,\Phi(R_{k-i-1}) - \Phi(Q_{i-1})\,\Phi(R_{k-i-2})] -$$

$$-[\Phi(Q_i)\,\Phi(R_{k-i-2}) - \Phi(Q_{i-1})\,\Phi(R_{k-i-3})]$$

which immediately yields (6).

Corollary 3.1.

$$\Phi(G_k) = \Phi(G_2)\,\Phi(P_{k-2}) - \Phi(G_1)\,\Phi(P_{k-3}).$$

Proof. From (6) it follows straightforwardly that

$$\Phi(G_k) = \alpha\left[\frac{\lambda + \sqrt{\lambda^2-4}}{2}\right]^k + \beta\left[\frac{\lambda - \sqrt{\lambda^2-4}}{2}\right]^k$$

where α and β are to be determined from the knowledge of, say, $\Phi(G_1)$ and $\Phi(G_2)$. Substituting $\lambda = 2\cos t$, one obtains

$$\Phi(G_k) = \alpha \exp(ikt) + \beta \exp(-ikt)$$

which yields

$$\Phi(G_k) = \Phi(G_2) \cdot \frac{\sin(k-1)t}{\sin t} - \Phi(G_1) \cdot \frac{\sin(k-2)t}{\sin t}.$$

If we set $G_k = P_k$, $\Phi(P_1) = \lambda$, $\Phi(P_2) = \lambda^2 - 1$, we obtain $\Phi(P_k) = \frac{\sin(k+1)t}{\sin t}$, from which the Corollary 3.1 follows straightforwardly.

Corollary 3.2. *The characteristic polynomials of the graphs* $G_1, \ldots, G_5$ (see Fig. 4) *are given by*

$$\Phi(G_1) = \frac{\cos[(2k+1)t/2]}{\cos(t/2)},$$

$$\Phi(G_2) = 2(\cos t - 1)\frac{\sin(kt)}{\sin t},$$

$$\Phi(G_3) = 4\cos t \cos(k+1)t,$$

$$\Phi(G_4) = -8\cos t \sin(t/2)\sin[(2k+1)t/2],$$

$$\Phi(G_5) = 16\cos^2 t(\cos^2 t - 1)\frac{\sin(k+1)t}{\sin t},$$

where $\lambda = 2\cos t$.

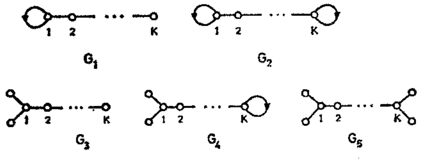

Fig. 4

From these expressions the spectra of $G_1, \ldots, G_5$ can be deduced without difficulty. The spectra of G_3 and G_5 have been obtained earlier [10].

REFERENCES

[1] C. A. Coulson, H. C. Longuet-Higgins, *The electronic structure of conjugated systems. V. The interaction of two conjugated systems,* Proc. Roy. Soc. (London) **A 195** (1948) 188—197.

[2] E. Heilbronner, *Das Kompositions-Prinzip,* Helv. Chim. Acta **36.** (1953) 170—188.

[3] F. Harary, C. King, A. Mowshowitz, R. C. Read, *Cospectral graphs and digraphs,* Bull. London Math. Soc. **3** (1971) 321—328.

[4] L. Lovász, J. Pelikán, *On eigenvalues of trees*, Periodica Math. Hung. **3** (1973) 175—182.

[5] T. Živković, N. Trinajstić, M. Randić, *On conjugated molecules with identical topological spectra*, Mol. Phys. **30** (1975) 517-532.

[6] H. Sachs, *Beziehungen zwischen den in einem Graphen enthaltenen Kreisen und seinem characteristischen Polynom*, Publ. Math. (Debrecen) **11** (1963) 119—134.

[7] V. Krishnamoorthy, K. R. Parthasarathy, *A note on nonisomorphic cospectral digraphs*, J. Comb. Theory (B) **17** (1974) 39—40.

[8] V. Krishnamoorthy, K. R. Parthasarathy, *Cospectral graphs and digraphs with given automorphism group*, J. Comb. Theory (B] **19** (1975) 204—214.

[9] F. Harary, *Graph theory*, Addison-Wesley, 1969, p. 32.

[10] D. M. Cvetković, I. Gutman, *On spectral structure of graphs having the maximal eigenvalue not greater than two*, Publ. Inst. Math. (Beograd) **18** (32) (1975) 39—45.