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THE ACYCLIC POLYNOMIAL OF A GRAPH

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In this paper we shall consider graphs without loops and multiple edges. Let the vertices of a graph G be denoted by $v_1, v_2, \ldots, v_n$ and the edges by $e_1, e_2, \ldots, e_m$. By e we shall denote an arbitrary edge of G.

The adjacency matrix of G is the matrix $A = \left\| a_{ij} \right\|_1^n$, where $a_{ij}=1$ if the vertices v_i and v_j are adjacent and $a_{ij}=0$ otherwise. The characteristic polynomial of this matrix, $\Phi(G)=\Phi(G, \lambda)=\det(\lambda I - A)$ is called the characteristic polynomial of the graph G.

If the graph G has n vertices, m edges and c components, its cyclomatic number $\nu=\nu(G)$ is given by $\nu=m-n+c$. Graphs with $\nu=0$ are called forests. The set of all graphs with n vertices and with the cyclomatic number not greater than ν will be denoted by $\Gamma_{n,\nu}$ ($\Gamma_{n,\nu} \subset \Gamma_{n,\nu+1}$). Hence, $\Gamma_{n,0}$ is the set of all forests with n vertices.

Let further $p(G, j)$ be the number of ways in which j mutually non-incident edges can be selected in G. It is both consistent and convenient to define $p(G, 0)=1$ for all graphs. It is known [10, 9, 8] that the characteristic polynomial of G can be presented in the form

$$\Phi(G) = \sum_{j=0}^{[n/2]} (-1)^j p(G, j) \lambda^{n-2j} \tag{1}$$

if and only if $\nu(G)=0$.

In a number of recent papers [7, 1, 5], a polynomial of the form (1) was considered also for the case of graphs having cycles. This was the motivation to introduce the following notion

Definition. The polynomial

$$\alpha(G) = \alpha(G, \lambda) = \sum_{j=0}^{[n/2]} (-1)^j p(G, j) \lambda^{n-2j} \tag{2}$$

will be called the acyclic polynomial of the graph G.

Hence, in the case of G being a forest, $\alpha(G)$ coincides with $\Phi(G)$. Accordingly, in the present work we shall focus our interest mainly on the graphs having cycles, i.e. graphs with $\nu(G)>0$, for which $\alpha(G)\neq\Phi(G)$.

There exist nonisomorphic graphs having cycles with equal acyclic polynomials. The smallest example of this kind is the pair G_1, G_2 with 5 vertices and with $\alpha(G_1)=\alpha(G_2)=\lambda^5-5\lambda^3+4\lambda$.

G_1 G_2

Let us firstly list some simple properties of the numbers $p(G, j)$, which can be proved without difficulty.

$$p(G, 1)=m;\ p(G, 2)=m(m+1)/2-(d_1^2+d_2^2+\cdots+d_n^2)/2,$$

where d_i is the degree of the vertex v_i. If n is even, $p(G, n/2)$ is equal to the number of 1-factors in G. From $p(G, j)=0$ or $p(G, j)=1$ it follows $p(G, j+1)=0$. Let the graph G possess k $(k\geqslant 0)$ isolated vertices $v_1, \ldots, v_k$, and let $G_0=G-v_1-\cdots-v_k$. Then from $p(G, j)=1$ it follows $j=(n-k)/2$ and the graph G_0 has a unique 1-factor. Further properties of the numbers $p(G, j)$ for regular graphs can be found in [10].

Let $G-e$ be the graph obtained by deletion of the edge e from G. Furthermore, $G-(e)$ is the graph obtained from G by deletion of the edge e and the both vertices incident to it. Then the recurrence relation $\Phi(G)=\Phi(G-e)-\Phi(G-(e))$, which is valid for forests [3] can be generalized to all graphs.

Theorem 1. *If G is a graph with at least one edge, then*

$$\alpha(G)=\alpha(G-e)-\alpha(G-(e)) \tag{3}$$

Proof. Let us consider the $p(G, j)$ distinct selections of mutually non-incident edges in G. There are $p(G-e, j)$ such selections which do not include the edge e. On the other hand, if the edge e is contained in a particular selection, then the edges incident to e are necessarily excluded. Hence, there are $p(G-(e), j-1)$ selections of j mutually non-incident edges which contain e. Therefore,

$$p(G, j)=p(G-e, j)+p(G-(e), j-1) \tag{4}$$

The substitution of (4) back into (2) results in eq. (3).//

By repeated application of eq. (3), one obtains the following conclusion.

Corollary 1. 1. The acyclic polynomial of a graph can be expressed as a linear combination of characteristic polynomials of its subforests.

Corollary 1. 2. Let C_n and P_n be the cycle and the path, respectively, with n vertices. Then,

(5) $$\alpha(C_n)=\Phi(P_n)-\Phi(P_{n-2})$$

Substituting $\lambda=2\cos t$, it can be shown [3] that $\Phi(P_n)=\frac{\sin(n+1)t}{\sin t}$. Therefrom, $\alpha(C_n)=2\cos nt$, and the zeros of $\alpha(C_n)$ are $2\cos\frac{(2j+1)\pi}{2n}$, $j=1,\ldots,n$.

Corollary 1. 3. Let the graphs P_n^k and C_n^k be obtained by joining k $(k\geqslant 1)$ new vertices to each vertex of P_n and C_n, respectively. Hence, P_n^k and C_n^k contain $(k+1)n$ vertices. Then from Theorem 1, $\alpha(C_n^k)=\Phi(P_n^k)-\lambda^{2k}\Phi(P_{n-2}^k)$. On the other hand [2], $\Phi(P_n^k,\ \lambda)=\lambda^{nk}\Phi\left(P_n,\ \lambda-\frac{k}{\lambda}\right)$. Substituting $\lambda-\frac{k}{\lambda}=$ $=2\cos u$, we obtain $\alpha(C_n^k)=2\lambda^{nk}\cos nu$, from which the zeros of $\alpha(C_n^k)$ can be easily determined: $\cos\frac{(2j+1)\pi}{2n}\pm\sqrt{\cos^2\frac{(2j+1)\pi}{2n}+k}$, $j=1,\ldots,n$ and 0, $(k-1)n$ times.

Corollary. 4. Let among the n vertices of the graph G_k be k $(k\geqslant 0)$ vertices $v_1,\ldots,v_k$ of degree two, such that the vertex v_i is adjacent to v_{i-1} and v_{i+1} $(i=2,\ldots,k-1)$. Then,

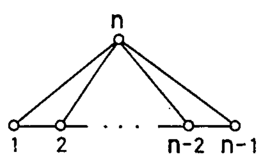
(6) $$\alpha(G_k)=\lambda\alpha(G_{k-1})-\alpha(G_{k-2})$$

In particular, $\alpha(C_n)=\lambda\alpha(C_{n-1})-\alpha(C_{n-2})$.

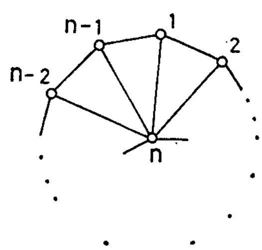
Proof is completely analogous to that of Theorem 3 in [3] and will not be reproduced here. In [3] is also shown that the recurrence relation (6) can be transformed into

$$\alpha(G_k)=\alpha(G_1)\Phi(P_{k-1})-\alpha(G_0)\Phi(P_{k-2})$$

Let the graphs $V_n(n\geqslant 2)$ and $W_n(n\geqslant 4)$ be obtained by joining all vertices $v_1, v_2,\ldots,v_{n-1}$ of P_{n-1} and C_{n-1}, respectively, to a new vertex v_n.



V_n



W_n

Theorem 2.

$$\alpha(V_n)=\Phi(P_n)-\sum_{j=0}^{n-3}\Phi(P_{n-2-j})\,\Phi(P_j) \tag{7}$$

$$\alpha(W_n)=\alpha(C_n)-\sum_{j=0}^{n-3}\alpha(C_{n-2-j})\,\Phi(P_j) \tag{8}$$

where by definition, $\alpha(C_1)=\Phi(P_1)$ *and* $\alpha(C_2)=\Phi(P_2)$.

Proof. Applying Theorem 1 first to the edge between the vertices v_n and v_{n-1} of the graph V_n and thereafter to the edge between v_{n-1} and v_{n-2}, we obtain the recursion relation $\alpha(V_n)=\lambda\alpha(V_{n-1})=\alpha(V_{n-2})-\Phi(P_{n-2})$. Eq. (7) follows then from the initial conditions $V_1=P_1$ and $V_2=P_2$.

Applying the Theorem 1 to the edge between the vertices v_1 and v_{n-1} of the graph W_n, we get $\alpha(W_n)=\alpha(V_n)-\alpha(V_{n-2})$. The combination of this equation with (7) and (5) results in eq. (8).//

Theorem 3. *The acyclic polynomial of the complete graph* K_n *is given by*

$$\alpha(K_n)=\sum_{j=0}^{[n/2]}(-1)^j\frac{(2j)!}{2^j j!}\binom{n}{2j}\lambda^{n-2j} \tag{9}$$

or by a recursion relation

$$\alpha(K_n)=\lambda\alpha(K_{n-1})-(n-1)\,\alpha(K_{n-2}) \tag{10}$$

Proof. The recursion formula (10) can be verified directly by eq. (9). In order to prove (9), it is sufficient to show that

$$p(K_n,\ j)=\frac{(2j)!}{2^j j!}\binom{n}{2j}$$

There are $\binom{n}{2j}$ ways to select $2j$ vertices in the graph K_n. Every such a selection induces a distinct subgraph K_{2j}. Hence, $p(K_n,\ j)=\binom{n}{2j}\ p(K_{2j},\ j)$. But $p(K_{2j},\ j)$ is just the number of 1-factors in K_{2j}, which is known (see, for example, [6], p. 92) to be equal to $(2j)!/(2^j\ j!)$.//

Theorem 4. *The acyclic polynomial of the bicomplete graph* $K_{n_1,\,n_2}$ $(n_1+$ $+n_2=n,\ n_1\geqslant n_2)$ *is given by*

$$\alpha(K_{n_1,\,n_2})=\sum_{j=0}^{n_2}(-1)^j j!\binom{n_1}{j}\binom{n_2}{j}\lambda^{n-2j} \tag{11}$$

and satisfies the recursion formula

$$\alpha(K_{n_1,\,n_2})=\lambda\alpha(K_{n_1,\,n_2-1})-n_1\,\alpha(K_{n_1-1,\,n_2-1}) \tag{12}$$

P r o o f. The n_1+n_2 vertices of K_{n_1,n_2} can be partitioned into two classes, such that neither the n_1 vertices from the first class, nor the n_2 vertices from the second class are mutually adjacent. There are $\binom{n_1}{j}\binom{n_2}{j}$ ways to select j vertices from the first class and j vertices from the second class. Every such a selection induces a distinct subgraph $K_{j,j}$ of K_{n_1,n_2}. Therefore, $p(K_{n_1,n_2}\, j)=$ $=\binom{n_1}{j}\binom{n_2}{j}\, p(K_{j,j},\, j)$. Since $p(K_{j,j},\, j)$ is just the number of 1-factors in $K_{j,j}$, which is equal to $j!$, we have

$$p(K_{n_1,n_2},\, j)=j!\binom{n_1}{j}\binom{n_2}{j}$$

and eq. (11) follows. Eq. (12) can be verified directly by eq. (11).//

Let the edges of G be labeled so that $F=G-e_1-\cdots-e_\nu$ is a (maximal) spanning forest of G.

T h e o r e m 5. *If the cyclomatic number of the graph G is ν and F is a (maximal) spanning forest of G, then for all $j=1,\ldots,[n/2]$,*

$$0\leqslant p(G,\, j)-p(F,\, j)\leqslant \nu\cdot\max\{p(H,\, j-1)\mid H\in\Gamma_{n-2,\,\nu-1}\}$$

P r o o f. A repeated application of Theorem 1 gives

$$\alpha(G)=\alpha(G-e_1-\cdots-e_\nu)-\sum_{t=1}^{\nu}\alpha(G-e_1-\cdots-e_{t-1}-(e_t))$$

Now, the graphs $G-e_1-\cdots e_{t-1}-(e_t)$ have $n-2$ vertices and their cyclomatic numbers are not greater than $\nu-t$ $(t=1,\ldots,\nu)$, hence are not greater than $\nu-1$.//

C o r o l l a r y 5. 1. For all $j=1,\ldots,[n/2]$,

$$p(G,\, j)\leqslant p(F,\, j)+\sum_{t=1}^{\nu}\max\{p(H,\, j-1)\mid H\in\Gamma_{n-2,\,\nu-t}\}$$

If G is composed of two disjoint components H_1 and H_2, we write $G=H_1\oplus H_2$.

T h e o r e m 6. *If $G=H_1\oplus H_2$, then*

$$\alpha(G)=\alpha(H_1)\,\alpha(H_2) \tag{13}$$

P r o o f. j mutually non-incident edges in G can be selected so that k of them belong to H_1 and $j-k$ of them belong to H_2 (k = 0, 1, ..., j). There are $p(H_1,\, k)\,p(H_2,\, j-k)$ such selections. Therefore,

$$p(G,\, j)=\sum_{k=0}^{j}p(H_1,\, k)\,p(H_2,\, j-k)$$

which substituted back into (2) gives eq. (13).//

Corollary 6. 1. If $G=H_1\oplus H_2\oplus\cdots\oplus H_c$, then $\alpha(G)=\alpha(H_1)\alpha(H_2)\cdots\alpha(H_c)$.

In [4] is proved that the graphs $G\in\Gamma_{n,0}$ fulfil the inequalities

$$p(P_n, j)\geqslant p(G, j) \tag{14}$$

for all $j=1, \ldots, [n/2]$. This result can be generalized for graphs with cyclomatic number not greater than one.

Theorem 7. *If $G\in\Gamma_{n,1}$, then for all $j=1, \ldots, [n/2]$,*

$$p(C_n, j)\geqslant p(G, j)$$

Proof. Since P_n is a spanning tree of C_n, from Theorem 5 it follows that $p(C_n, j)\geqslant p(P_n, j)$. Because of (14), Theorem 7 holds for all $G\in\Gamma_{n,0}$. Thus we have to prove Theorem 7 only for graphs with $\nu(G)=1$.

Let the graph G^* with $\nu(G^*)=1$ has the property $p(G^*, j)\geqslant p(G, j)$ for all $G\in\Gamma_{n,1}$. We prove that $G^*=C_n$.

In every graph G with $\nu(G)=1$, there exists an edge e_1 such that $G-e_1$ is a forest. Then $G-(e_1)$ is a forest too. From eq. (4). $p(G, j)=p(G-e_1, j)+p(G-(e_1), j-1)$. Now, $p(G, j)$ has to become maximal for $G=G^*$. According to (14), the right side of the expression for $p(G, j)$ is maximal if $G^*-e_1=P_n$ and $G^*-(e_1)=P_{n-2}$. But this is possible only if $G^*=C_n$.//

Let S_n be the star with n vertices. In [4] is proved that if G is any connected graph with n vertices and with $\nu=0$ (i. e. G is a tree), then for all $j=1, \ldots, [n/2]$, $p(S_n, j)\leqslant p(G, j)$. We present here a generalization of this result for $\nu=1$. Let S_n^* be obtained by introducing a new edge to S_n. Hence S_n^* contains a triangle.

S_n S_n^*

Theorem 8. *If G is any connected graph with n vertices and with $\nu=1$, then for all $j=1, \ldots, [n/2]$,*

$$p(S_n^*, j)\leqslant p(G, j)$$

Proof is straightforward, since $p(S_n^*, 1)=n$, $p(S_n^*, 2)=n-3$ and $p(S_n^*, 3)=0$. All connected graps with $\nu=1$ have $p(G, 1)=n$ but $p(G, 2)\geqslant n-3$, since the sum $d_1^2+d_2^2+\cdots+d_n^2$ is maximal for S_n^* and therefore $p(S_n^*, 2)$ is minimal.//

Concluding this paper we would like to point at a yet unproved property of the acyclic polynomials, which was tested in a large number of cases in [1, 5] and which is of some importance in chemistry.

Conjecture. The zeros of the acyclic polynomial are real.

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