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ON THE MATCHING POLYNOMIAL OF THE GRAPH $G\{R_1,R_2,...,R_n\}$

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__Abstract__: A formula for the matching polynomial of the graph $G\{R_1,R_2,...,R_n\}$ is derived, which is fully analogous to the Godsil-McKay's expression for the characteristic polynomial of $G\{R_1,R_2,...,R_n\}$.

In the preceding paper [1] the characteristic and matching polynomials of various special cases of the graph $G\{R_1,R_2,...,R_n\}$ have been examined. While a general expression exists for $\Phi(G\{R_1,...,R_n\})$ - the Godsil-McKay formula [2], an analogous statement for $\alpha(G\{R_1,...,R_n\})$ was not known. In this note we shall derive such a result.

We will use here the same notation and terminology as in [1], with the only difference that here G will denote an arbitrary (not necessarily bipartite) graph.

According to [2],

$$\Phi(G\{R_1,R_2,...,R_n\}) = \det \underset{\sim}{B} \tag{1}$$

where $\underset{\sim}{B}$ is a square matrix of order n, the elements of which are given as

$$B_{ij} = \begin{cases} \Phi(R_j) & i=j \\ -A_{ij}\Phi(R_j^*) & i\neq j \end{cases} \tag{2}$$

$\underset{\sim}{A} = \underset{\sim}{A}(G) = ||A_{ij}||$ is the adjacency matrix of the graph G. Combining (1) and (2) we straightforwardly deduce

$$\Phi(G\{R_1,R_2,...,R_n\}) =$$

$$= [\prod_{j=1}^{n} \Phi(R_j^*)] \det[\mathrm{diag}(\Phi(R_1)/\Phi(R_1^*),\Phi(R_2)/\Phi(R_2^*),...$$

$$...,\Phi(R_n)/\Phi(R_n^*)) - \underset{\sim}{A}], \tag{3}$$

with $\mathrm{diag}(M_1,M_2,...,M_n)$ denoting a diagonal matrix, whose diagonal elements are $M_1,M_2,...,M_n$.

Let $G\{h_1,h_2,...,h_n\}$ be the graph obtained from G by joining to each of its vertices v_j, $j=1,2,...,n$, a self-loop of the weight h_j. For the following consideration it will be important that the weights h_j can be not only arbitrary numbers, but also arbitrary functions.

Note that $h_j=0$ means that there is no loop on v_j. Thus $G\{0,0,...,0\}=G$.

The adjacency matrix of $G\{h_1,h_2,...,h_n\}$ has the following form:

$$\underset{\sim}{A}(G\{h_1,h_2,...,h_n\}) = \mathrm{diag}(h_1,h_2,...,h_n) + \underset{\sim}{A}(G). \qquad (4)$$

Consequently,

$$\Phi(G\{h_1,h_2,...,h_n\}) = \det(x\,\underset{\sim}{I}_n - \mathrm{diag}(h_1,h_2,...,h_n) - \underset{\sim}{A}(G)).$$

If the weights h_j are adjusted to satisfy the conditions

$$\Phi(R_j)/\Phi(R_j^*) = x-h_j \ , \ j=1,2,...,n, \qquad (5)$$

then the substitution of (5) and (4) back into (3) gives

$$\Phi(G\{R_1,R_2,...,R_n\}) = $$
$$= \Phi(G\{h_1,h_2,...,h_n\}) \prod_{j=1}^{n} \Phi(R_j^*) \qquad (6)$$

Eq. (6) is, of course, only a suitable reformulation of the Godsil-McKay's result (1).

Before presenting our formula for $\alpha(G\{R_1,R_2,\ldots,R_n\})$, we need some preparations. The original definition [3] of the matching polynomial applies only to graphs without self--loops. If a graph contains self-loops, then one has to properly extend the concept of matching polynomial. The following definition is consistent with the previous work on the topological resonance energy of heteroconjugated molecules [4], where the computation of the matching polynomial of graphs with self-loops was necessary.

Let $G\{h_1,h_2,\ldots,h_n\}$ possesses an edge e which connects the vertices v and w.

<u>Definition 4</u>: The matching polynomial of $G\{h_1,h_2,\ldots,h_n\}$ is determined recursively by

$$\alpha(G\{h_1,\ldots,h_n\}) = \alpha(G\{h_1,\ldots,h_n\}-e) - \alpha(G\{h_1,\ldots,h_n\}-v-w) \qquad (7)$$

with the initial conditions

$$\alpha(O_n\{h_1,\ldots,h_n\}) = \prod_{j=1}^{n} (x-h_j)$$

for the graph O_n without edges and with n vertices, and

$$\alpha(P_2\{h_1,h_2\}) = (x-h_1)(x-h_2)-1$$

for the path P_2 with two vertices and one edge.

Note that

$$G\{h_1,h_2,\dots,h_n\}-e = (G-e)\{h_1,h_2,\dots,h_n\}$$

and

$$G\{h_1,h_2,\dots,h_n\}-v-w = (G-v-w)\{h_1,h_2,\dots,h_{n-2}\}.$$

Now we can formulate the following

<u>THEOREM 3</u>:

$$\alpha(G\{R_1,R_2,\dots,R_n\}) = \alpha(G\{k_1,k_2,\dots,k_n\}) \prod_{j=1}^{n} \alpha(R_j^*) \qquad (8)$$

with the parameters k_j being defined via

$$\alpha(R_j)/\alpha(R_j^*) = x-k_j. \qquad (9)$$

Note the close formal analogy between eqs. (6) and (8). According to (9), the weights k_j are certain functions of the variable x.

<u>Proof</u> follows by induction on the number of edges of the graph G. For $G=O_n$, Theorem 3 gives the correct result, since by Definition 4,

$$\alpha(O_n\{k_1,k_2,\dots,k_n\}) \prod_{j=1}^{n} \alpha(R_j^*) = \prod_{j=1}^{n} (x-k_j)\alpha(R_j^*) =$$

$$= \prod_{j=1}^{n} \alpha(R_j) = \alpha(O_n\{R_1,R_2,\dots,R_n\}). \qquad (10)$$

Therefore Theorem 3 is true for the graphs without edges.

From the hypothesis that Theorem 3 holds for all graphs with less than m edges we will deduce its validity also for the graphs with m edges.

Let G possesses m edges ($m > 0$). Without the loss of generality we may assume that the edge e connects the vertices $v=v_{n-1}$ and $w=v_n$. Then from eq. (4) from ref. [1],

$$\alpha(G\{R_1,\dots,R_n\}) = \alpha(G\{R_1,\dots,R_n\}-e)-\alpha(G\{R_1,\dots,R_n\}-v-w) =$$

$$= \alpha((G-e)\{R_1,\dots,R_n\})-\alpha(R^*_{n-1})\alpha(R^*_n)\alpha((G-v-w)\{R_1,\dots,R_{n-2}\}).$$

The graphs G-e and G-v-w have less than m edges. Therefore according to the induction hypothesis they satisfy eq. (8), i.e.

$$\alpha((G-e)\{R_1,\dots,R_n\}) = \alpha((G-e)\{k_1,\dots,k_n\}) \prod_{j=1}^{n} \alpha(R^*_j), \qquad (11)$$

$$\alpha((G-v-w)\{R_1,\dots,R_n\}) = \alpha((G-v-w)\{k_1,\dots,k_{n-2}\}) \prod_{j=1}^{n-2} \alpha(R^*_j). \qquad (12)$$

Substitution of (11) and (12) back into (10) yields

$$\alpha(G\{R_1,\dots,R_n\}) = [\alpha((G-e)\{k_1,\dots,k_n\})-$$

$$- \alpha((G-v-w)\{k_1,\dots,k_{n-2}\})] \prod_{j=1}^{n} \alpha(R^*_j).$$

Formula (8) follows now immediately from Definition 4. Q.E.D.

Let G be a bipartite graph with a+b vertices as defined in [1]. Then the special case of $G\{h_1,h_2,\dots,h_n\}$ when $h_1=h_2=\dots=h_a=k$ and $h_{a+1}=h_{a+2}=\dots=h_{a+b}=h$ is the previously [1] defined graph $G\{k,h\}$.

Lemma 2:

$$\alpha(G\{k,h\}) = \left(\frac{x-h}{x-k}\right)^{(b-a)/2} \alpha(G,\sqrt{(x-k)(x-h)}) \tag{13}$$

and

$$\alpha(G\{k,h\}) = (x-h)^{b-a} \prod_{j=1}^{a} [(x-k)(x-h)-y_j^2]. \tag{14}$$

This result is fully analogous to Lemma 1 of [1] and can be proved in a similar manner. Hence, (13) is proved by induction starting with the eq. (7). Formula (14) follows from (13), and eq. (3) from ref. [1].

Corollary 1: A combination of Lemma 2 and Theorem 3 results in Theorem 2 from [1].

Corollary 2: Let $G\{h\}$ denotes the graph obtained by attaching a self-loop of the weight h to each vertex of the graph G, i.e. $h_1=h_2=\ldots=h_n=h$. Then

$$\alpha(G\{h\}) = \alpha(G,x-h) = \prod_{j=1}^{n} (x-h-y_j).$$

Therefore, if $Sp_A(G) = \{y_1,y_2,\ldots,y_n\}$, then $Sp_A(G\{h\}) =$

$$= \{y_1+h,y_2+h,\ldots,y_n+h\}.$$

Corollary 2 holds also for nonbipartite graphs.

Corollary 3: If $R_1=R$, $R_2=R_3=\dots=R_n=P_1$, then $G\{R_1,R_2,\dots,R_n\} = G\cdot R$ is obtained by identifying the vertex v_1 of G with the root of R. Let us denote G-v by G^*. Then from (8),

$$\alpha(G\cdot R) = \alpha(G)\alpha(R^*)+\alpha(G^*)\alpha(R)-x\alpha(G^*)\alpha(R^*).$$

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