Discrete Applied Mathematics 46 (1993) 79–86
North-Holland

Note

On "The matching polynomial of a polygraph"

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Received 11 December 1990
Revised 25 January 1993

Abstract

In this note we give an explanation for two phenomena mentioned in the concluding remarks of "The matching polynomial of a polygraph" by Babić et al. The following results are obtained:

(1) Although three matrices for given polygraphs defined in the above article in general have different orders, they determine the same recurrence relations for the matching polynomial of these polygraphs.

(2) Under certain symmetry conditions, the order of the recurrence relations can be reduced by almost a half.

Keywords. Polygraph, matching polynomial, recurrence relation.

1. Terminology

For notation and terminology not defined here we refer to [1] and [4, 11].

Let $G = (V, E)$ be a graph on n vertices, that is, with $|V| = n$. Then the *matching polynomial* of G, denoted by $\alpha(G; x)$, is defined by

$$\alpha(G;x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k p(G,k) x^{n-2k},$$

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where $p(G,k)$ denotes the number of k-matchings of G, i.e., the number of ways we can choose k independent edges in G, and $p(G,0) := 1$. If $E = \emptyset$, then $\alpha(G;x) = x^n$. The sum of the absolute values of all coefficients of $\alpha(G;x)$ is the so-called *Hosoya index* of G.

For a subset F of E, $M(F)$ denotes the set of all matchings in F, i.e., the set of all independent subsets of F.

Let $G_1, G_2, \ldots, G_m$ be a set of mutually disjoint graphs, and let $X_1, X_2, \ldots, X_m$ be a set of binary relations such that $X_i \subseteq V(G_i) \times V(G_{i+1})$ $(1 \le i \le m-1)$ and $X_m \subseteq V(G_m) \times V(G_1)$. Then the *polygraph* Ω_m is defined as follows:

$$\begin{cases} V(\Omega_m) = V(G_1) \cup V(G_2) \cup \cdots \cup V(G_m), \\ E(\Omega_m) = E(G_1) \cup X_1 \cup E(G_2) \cup X_2 \cup \cdots \cup E(G_m) \cup X_m. \end{cases}$$

Denote by Γ_i the subgraph of Ω_m with $V(\Gamma_i) = V(G_1) \cup \cdots \cup V(G_i)$ and $E(\Gamma_i) = E(G_1) \cup X_1 \cup \cdots \cup E(G_i)$ $(i \in \{1, 2, \ldots, m\})$. If $G_1 = G_2 = \cdots = G_m = G$ and $X_1 = X_2 = \cdots = X_m = X$, we denote Ω_m by ω_m and Γ_i by γ_i; ω_m and γ_m are called a *rotagraph* and a *fasciagraph*, respectively.

2. Introduction

Hosoya's index has many applications, e.g., in physical chemistry, statistical physics and thermodynamics. The computation of this index is a very difficult problem (# P-complete).

Recently, many authors (see [6–10]) gave explicit expressions or recurrence relations for matching polynomials of some polygraphs. Furthermore, Babić et al. [1] obtained a systematic method to compute matching polynomials for polygraphs. Many of the known results can be regarded as special cases of their results. In [1], they introduced three types of matrices to obtain recurrence relations for the matching polynomials of ω_m and γ_m by using the Cayley–Hamilton Theorem from linear algebra (see [4, 11]). We repeat some of the definitions in [1]. By $M(X)$ we denote the set of all matchings in X, with a matching viewed as a subset of independent edges, including the empty set. To distinguish between the elements of $M(X)$ we use a one-to-one mapping of the set $M(X)$ onto the set of indices $\{1, 2, \ldots, |M(X)|\}$ and denote the elements of $M(X)$ with the assigned index j by W_j. The matching W_j can also be viewed as a binary relation with domain $D(W_j) \subseteq V(G_i)$ and range

$$R(W_j) \subseteq \begin{cases} V(G_{i+1}) & \text{for } i = 1, 2, \ldots, m-1, \\ V(G_1) & \text{for } i = m. \end{cases}$$

The three types of matrices are defined as follows (see [1, p. 18]):

$$[T_1]_{jk} := (-1)^{|W_k|} \alpha(G - R(W_j) - D(W_k); x),$$

where W_j and W_k are elements of $M(X)$ with range $R(W_j)$ and domain $D(W_k)$, respectively.

$$[T_2]_{jk} := (-1)^{|W_k|} \sum_{W|D(W)=D(W_j)} \alpha(G - R(W) - D(W_k); x),$$

where j runs through only those values with different $D(W_j)$.

$$[T_3]_{jk} := (-1)^{|W_k|} \sum_{W|R(W)=R(W_j)} \alpha(G - R(W_j) - D(W); x),$$

where k runs through only those values with different $R(W_k)$.

In the above formulas, $\alpha(G - A - B; x) = 0$ if $A \cap B \neq \emptyset$.

Let T be one of the matrices T_1, T_2 or T_3. Then, by [1, Corollary 10],

$$\begin{cases} \alpha(\omega_m; x) = \operatorname{tr}(T) \text{ and} \\ \alpha(\gamma_m - R(W_j) - D(W_k); x) = (-1)^{|W_k|} [T^m]_{jk}. \end{cases}$$

Let the characteristic polynomial of T be

$$\phi(T; \lambda) := \det(\lambda I_N - T) = \sum_{i=0}^{N} a_i(x) \lambda^{N-i},$$

where N is the order of T and $a_0(x) := 1$. Then, by [1, Corollary 11], the recurrence relations for the matching polynomials of ω_m and γ_m are given by

$$\begin{cases} \sum_{i=0}^{N} a_i(x) \alpha(\omega_{m-i}; x) = 0, \\ \sum_{i=0}^{N} a_i(x) \alpha(\gamma_{m-i} - R(W_j) - D(W_k); x) = 0 \end{cases} \quad (*)$$

where $m \geq N$, $\alpha(\omega_0; x) := N$ and $\alpha(\gamma_0 - R(W_j) - D(W_k); x) := (-1)^{|W_k|} \delta_{jk}$ (δ_{jk} is Kronecker's symbol).

It is obvious from the above results that the order of the recurrence relations is closely related to the rank of T: the higher the rank of T, the higher the order of (*).

In the concluding remarks of [1], Babić et al. proposed two problems with regard to the order of (*).

Problem 1. In [1, Example 14], three matrices with different orders give rise to three recurrence relations with the same order and coefficients. Is this a general phenomenon?

In the next section we prove that the answer is affirmative.

Problem 2. In [1, Example 13], it is possible to obtain another matrix T' with lower order than T for the special case when γ_m is constructed from a graph G and a 1–1 binary relation X that are both symmetric (in a sense to be defined in Section 4). What is the role of the symmetry of G and X in a possible reduction of the order?

We answer this question in Section 4 and show that the order of the recurrence relation of $\alpha(\gamma_m; x)$ in this special case can be reduced from $2^{2p}+1$ to $2^{2p-1}+2^{p-1}+1$, where $p = |X|/2$.

3. Answer to Problem 1

We claim that, although in general T_1, T_2 and T_3 have different orders (especially when X is not 1–1), they determine the same recurrence relations $(*)$.

Before we prove this, we introduce the following matrix transformation. Let A be an $n \times n$ matrix with entries from a commutative ring. Denote by α_i the ith row of A and by A_j the jth column of A. Two columns are said to be in the same class if and only if they are equal. Assume that the columns of A are classified into s classes. Let A^* be the $n \times s$ matrix obtained from A by deleting all columns except for those with minimum index in every class. Now, two rows α_i^* and α_j^* of A^* are said to be in the same class if and only if A_i and A_j are in the same class. Obviously, the rows of A^* also fall into s classes. Let B be the $s \times s$ matrix obtained from A^* by replacing the rows with minimum index in every class by the sum of all rows in that class and by deleting the other rows.

Lemma 3.1. $\det(\lambda I_n - A) = \lambda^{n-s}\det(\lambda I_s - B)$.

Proof. From linear algebra (see [4, 11]), we know that the coefficient a_i of x^{n-i} $(0 \le i \le n)$ in the characteristic polynomial $\det(\lambda I_n - A) = \sum_{i=0}^{n} a_i x^{n-i}$ of A is equal to $(-1)^i$ times the sum of all main minors of A with order i. It is clear that all minors with order $> s$ are zero. Hence, $a_n = a_{n-1} = \cdots = a_{s+1} = 0$. It remains to prove that the sum of all main minors of A with order i $(0 \le i \le s)$ is equal to that of B. This is an easy consequence of the following property $|A_1 \cdots A_i + A_i' \cdots A_n| = |A_1 \cdots A_i \cdots A_n| + |A_1 \cdots A_i' \cdots A_n|$ and other elementary properties of determinants. □

Theorem 3.2. *The recurrence relations $(*)$ for the matching polynomials of ω_m and γ_m determined by T_1, T_2 and T_3, respectively, have the same order and coefficients.*

Proof. It is not difficult to check that T_2 is obtained from T_1 by applying the above transformation, and that T_3 is obtained by applying this transformation to the transpose T_1^{T} of T_1. Let the orders of T_1, T_2 and T_3 be n, s and t, respectively. Then, by Lemma 3.1, we have

$$\det(\lambda I_n - T_1) = \lambda^{n-s}\det(\lambda I_s - T_2)$$

and

$$\det(\lambda I_n - T_1) = \det(\lambda I_n - T_1^{\mathrm{T}}) = \lambda^{n-t}\det(\lambda I_t - T_3).$$

As a consequence, T_1, T_2 and T_3 yield three recurrence relations $(*)$ with the same order and coefficients. □

4. Answer to Problem 2

Throughout this section we assume X is a 1–1 binary relation, implying that $T_1 = T_2 = T_3 = T$.

Definition 4.1. Let G be a graph with vertex set $V(G) = \{1, 2, \ldots, m\} \cup \{1', 2', \ldots, m'\}$ and X a relation on $V(G)$. Then G and X are said to be *symmetric* if

(i) the mapping φ defined by $\varphi(i) = i'$ and $\varphi(i') = i$ $(i = 1, 2, \ldots, m)$ is an automorphism of G, and

(ii) $X = \{(i_1, j_1), \ldots, (i_p, j_p)\} \cup \{(i'_1, j'_1), \ldots, (i'_p, j'_p)\}$, where $i'_r = i$ if $i_r = i'$ and $j'_r = j$ if $j_r = j'$.

The following facts are obvious and stated without proofs.

Proposition 4.2. *Let G and X be as in Definition* 4.1. *Then*:

(1) *$R(W_j)$ is an r-subset $(r = 0, 1, \ldots, 2p)$ of $\{j_1, j'_1, \ldots, j_p, j'_p\}$ and thus there are 2^{2p} different $R(W_j)$. Similarly, there are 2^{2p} different $D(W_k)$;*

(2) *T is a matrix of order 2^{2p}, and the recurrence relation $(*)$ for γ_m determined by T has $2^{2p} + 1$ terms;*

(3) *let $S = \{v_1, v_2, \ldots, v_s\} \cup \{w'_1, w'_2, \ldots, w'_t\} \subseteq V(G)$. Then $S' := \{v'_1, v'_2, \ldots, v'_s\} \cup (w_1, w_2, \ldots, w_t) \subseteq V(G)$ and $G[V(G) - S] \cong G[V(G) - S']$, where $G[U]$ denotes the subgraph of G induced by a subset U of $V(G)$;*

(4) *for every $D(W_k)$ there exists a W_j such that $\varphi(D(W_k)) = D(W_j)$ and $\varphi(R(W_k)) = R(W_j)$ and such that $D(W_k) = D(W_j)$ if and only if $R(W_k) = R(W_j)$.*

By arranging T in a proper way it is possible to reduce the order of $(*)$ for γ_m from $2^{2p} + 1$ to $2^{2p-1} + 2^{p-1} + 1$. Before we prove this, we need some more terminology.

Definition 4.3. Let $Y = (y_1, y_2, \ldots, y_n)$ and $Z = (z_1, z_2, \ldots, z_n)$ be two n-dimensional vectors. We call Y and Z a pair of *associated vectors* if, for all $i \in \{1, 2, \ldots, n\}$, either $y_i = z_i$ or $y_i = z_{i+1}$ and $y_{i+1} = z_i$; an index i for which $y_i = z_i$ is called an *E-index*, an index i for which $y_i = z_{i+1}$ and $y_{i+1} = z_i$ is called an *F-index*.

Definition 4.4. Let P be an $n \times n$ matrix. Denote by p_i the ith row of P and by P_j the jth column of P. If P satisfies the following conditions:

(i) P_{i_k} and p_{i_k+1} are associated vectors, where $k = 1, 2, \ldots, r$, and $|i_t - i_s| \geq 2$ for all $s, t \in \{1, 2, \ldots, r\}$, $s \neq t$;

(ii) $i_1, i_2, \ldots, i_r$ are precisely all the F-indices of p_{i_k} and p_{i_k+1} (for all $k = 1, 2, \ldots, r$), then we define the *associate* $(n - r) \times (n - r)$ *matrix* P^a of P as follows:

First, we construct an $n \times (n - r)$ matrix P^* from P by replacing P_{i_k} by $P_{i_k} + P_{i_k+1}$ and deleting P_{i_k+1} for all $k \in \{1, 2, \ldots, r\}$. Now P^a is obtained from P^* by deleting the

(i_k+1)th row for all $k \in \{1,2,\ldots,r\}$. We call $i_1, i_2, \ldots, i_r$ the *associate indices* of P and P^{a}.

If the $n \times n$ matrix P satisfies (i) and (ii) above, then pairs of associated row vectors of P share no vectors, and for all associated vectors $p_{i_k} = (y_1, \ldots, y_n)$ and $p_{i_k+1} = (z_1, \ldots, z_n)$ $(k \in \{1,2,\ldots,r\})$ we have:

$$\begin{cases} y_i = z_i & \text{for } i \neq i_1, \ldots, i_r, \\ y_i = z_{i+1},\ y_{i+1} = z_i & \text{for } i = i_1, \ldots, i_r. \end{cases}$$

This implies that, replacing column P_{i_k} by $P_{i_k} + P_{i_k+1}$ and deleting P_{i_k+1} for all $k \in \{1,2,\ldots,r\}$, yields an $n \times (n-r)$ matrix P^* in which every i_kth and (i_k+1)th row are identical $(k = 1, \ldots, r)$.

Lemma 4.5. *Let A, B and C be three $n \times n$ matrices such that $A = BC$. Suppose C has an associate matrix C^{a} with associate indices $i_1, i_2, \ldots, i_r$. Construct A^{a} and B^{a} from A and B as if $i_1, i_2, \ldots, i_r$ were also associate indices of A and A^{a} and B and B^{a}, respectively. (Note that, in general, A^{a} and B^{a} are not associate matrices of A and B.) Then $A^{\mathrm{a}} = B^{\mathrm{a}} C^{\mathrm{a}}$.*

Proof. The result can be verified immediately by comparing the corresponding entries of $(BC)^{\mathrm{a}}$ and $B^{\mathrm{a}} C^{\mathrm{a}}$. □

Corollary 4.6. *Let G and X be as in Definition 4.1 and let $T = T_1$. Then T has an associate matrix T^{a} such that $(T^m)^{\mathrm{a}} = (T^{\mathrm{a}})^m$ for any positive integer m.*

Proof. By Proposition 4.2(4), we can arrange the elements of $M(X)$ in such a way that all pairs W_j, W_k with $j \neq k$ and $\varphi(D(W_k)) = D(W_j)$ (and $\varphi(R(W_k)) = R(W_j)$) are consecutive, i.e., $|k-j| = 1$. Except for such pairs, all elements W of $M(X)$ satisfy $\varphi(D(W)) = D(W)$ (and $\varphi(R(W)) = R(W)$).

Now consider a pair W_j, W_{j+1} with $\varphi(R(W_j)) = R(W_{j+1})$. If W_k is such that $\varphi(D(W_k)) = D(W_k)$, then, by Proposition 4.2(3),

$$\begin{aligned} [T]_{jk} &= (-1)^{|W_k|} \alpha(G - R(W_j) - D(W_k); x) \\ &= (-1)^{|W_k|} \alpha(G - R(W_{j+1}) - D(W_k); x) = [T]_{(j+1)k}. \end{aligned}$$

If W_k, W_{k+1} is a pair with $\varphi(D(W_k)) = D(W_{k+1})$, then

$$\begin{aligned} [T]_{jk} &= (-1)^{|W_k|} \alpha(G - R(W_j) - D(W_k); x) \\ &= (-1)^{|W_{k+1}|} \alpha(G - R(W_{j+1}) - D(W_{k+1}); x) = [T]_{(j+1)(k+1)}, \end{aligned}$$

and

$$\begin{aligned} [T]_{(j+1)k} &= (-1)^{|W_k|} \alpha(G - R(W_{j+1}) - D(W_k); x) \\ &= (-1)^{|W_{k+1}|} \alpha(G - R(W_j) - D(W_{k+1}); x) = [T]_{j(k+1)}. \end{aligned}$$

Clearly, by the above arrangement, the associated rows of T are consecutive. Let T^a be the associate matrix of T. Using Lemma 4.5 it is easy to prove, by induction on m, that $(T^m)^a = (T^a)^m$ for any positive integer m. □

Theorem 4.7. *Let G, X and T be as before. Then:*
(i) *T has $2^{2p-1} - 2^{p-1}$ associated pairs of rows;*
(ii) *the order of T^a is $2^{2p-1} + 2^{p-1}$;*
(iii) *the order of the recurrence relation $(*)$ for the matching polynomial of γ_m can be reduced from $2^{2p} + 1$ to $2^{2p-1} + 2^{p-1} + 1$, where $|X| = 2p$.*

Proof. Statements (i) and (ii) follow immediately from Proposition 4.2 (1), (2) and (4). For (iii), we use the characteristic polynomial of T^a and Cayley–Hamilton's Theorem to obtain

$$\sum_{i=0}^{N'} a_i'(x)(T^a)^{N'-i} = 0,$$

where $\sum_{i=0}^{N'} a_i'(x)\lambda^{N'-i}$ is the characteristic polynomial of T^a and N' is the order of T^a.

If $m \geq N'$, multiplying by $(T^a)^{m-N'}$ and applying Corollary 4.6 yields

$$\sum_{i=0}^{N'} a_i'(x)(T^{m-i})^a = 0 \quad (m \geq N').$$

From this formula and the definition of T, we can obtain the recurrence relation for the matching polynomial of γ_m (and of many subgraphs of γ_m). Since $N' = 2^{2p-1} + 2^{p-1}$, the order of the recurrence relation can be reduced to $N' + 1 = 2^{2p-1} + 2^{p-1} + 1$, where $p = |X|/2$. □

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