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Nullity invariance for pivot and the interlace polynomial

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ABSTRACT

We show that the effect of principal pivot transform on the nullity values of the principal submatrices of a given (square) matrix is described by the symmetric difference operator (for sets). We consider its consequences for graphs, and in particular generalize the recursive relation of the interlace polynomial and simplify its proof.

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1. Introduction

Principal pivot transform (PPT, or simply pivot) is a matrix transformation operation capable of partially (component-wise) inverting a given matrix. Consider a $V \times V$ -matrix A (over some field) for some finite set V (the columns and rows are indexed by V), and $X \subseteq V$ such that $A[X]$ is nonsingular, where $A[X]$ is the principal submatrix of A w.r.t. X . Then the *principal pivot transform* of A on X , denoted by $A * X$, may be defined by the following relation:

$$A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \text{ iff } A * X \begin{pmatrix} y_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ y_2 \end{pmatrix}$$

where the vectors x_1 and y_1 correspond to the elements of X . Note that $A * V = A^{-1}$. The pivot operation is originally motivated by the well-known linear complementarity problem [20], and is applied in many other settings such as mathematical programming and numerical analysis, see [19] for an overview.

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A natural restriction of pivot is to graphs (with possibly loops), i.e., symmetric matrices over \mathbb{F}_2 . For graphs, each pivot operation can be decomposed into a sequence of elementary pivots. There are two types of elementary pivot operations, (frequently) called local complementation and edge complementation. These two graph operations are also (in fact, originally) defined for simple graphs, however, the definition of local complementation on simple graphs is less restrictive (unlike pivot, it is defined for all vertices). Local and edge complementation for simple graphs, introduced in [16] and [5] respectively, were originally motivated by the study of Euler circuits in 4-regular graphs and by the study of circle graphs (also called overlap graphs) as they model natural transformations of the underlying circle segments. Many other applications domains for these operations have since appeared, e.g., quantum computing [21], the formal theory of gene assembly in ciliates [11] (a research area within computational biology), and the study of interlace polynomials, initiated in [1]. In many contexts where local and edge complementation have been used, principal pivot transform has originally appeared in disguise (we briefly discuss some examples in the paper).

In this paper we show that the pivot operation fulfills the following property, which we refer to as the *nullity invariant* of pivot. We denote the nullity of a matrix A by $n(A)$ and denote the symmetric difference of sets X and Y by $X \oplus Y$.

Theorem 5. *Let A be a $V \times V$ -matrix (over some field), and let $X \subseteq V$ be such that $A[X]$ is nonsingular. Then, for all $Y \subseteq V$, $n((A * X)[Y]) = n(A[X \oplus Y])$.*

Hence we find that symmetric difference and pivot play a “similar role” w.r.t. nullity. We subsequently apply the nullity invariant to the interlace polynomial. The interlace polynomial for a graph G is defined as

$$q(G) = \sum_{S \subseteq V} (y - 1)^{n(G[S])}.$$

It was shown in [3] that $q(G)$ fulfills a characteristic recursive relation. Using Theorem 5, we generalize the notion of interlace polynomial and its recursive relation to square matrices in general. We show that the *interlace polynomial* for a $V \times V$ -matrix A defined by

$$q(A) = \sum_{S \subseteq V} (y - 1)^{n(A[S])}$$

is invariant under pivot, i.e., $q(A) = q(A * X)$ when $A * X$ is defined, and moreover satisfies the following recursive relation (we let $A \setminus u = A[V \setminus \{u\}]$).

Theorem 14. *Let A be a $V \times V$ -matrix (over some field), let $X \subseteq V$ with $A[X]$ nonsingular, and let $u \in X$. We have $q(A) = q(A \setminus u) + q(A * X \setminus u)$.*

The recursive relation of $q(G)$ in [3] is easily obtained from Theorem 14, see Proposition 16. As a consequence, we not only generalize the interlace polynomial and its recursive relation, but also simplify the proof of the (original) recursive relation for interlace polynomials for graphs. Also, in Section 3 we recall a motivation of pivot applied to overlap graphs, and relate it to the nullity invariant.

2. Notation and terminology

A *set system* (over V) is a tuple $M = (V, D)$ with V a finite set, called the *ground set* of M , and $D \subseteq 2^V$ a family of subsets of V . To simplify notation we often write $X \in M$ to denote $X \in D$. Moreover, we often simply write V to denote the ground set of the set system under consideration. We denote by \oplus the logical exclusive-or (i.e., addition in \mathbb{F}_2 , the field having two elements), and we carry this operator over to sets, where it is called symmetric difference.

We consider matrices and vectors indexed by a finite set V . For a vector v indexed by V , we denote the element of v corresponding to $i \in V$ by $v[i]$. Also, we denote the nullity (dimension of the null

space) and the determinant of a matrix A by $n(A)$ and $\det(A)$ respectively. For $X \subseteq V$, the principal submatrix of A w.r.t. X is denoted by $A[X]$. Moreover, for $Y \subseteq V$, we define $A \setminus Y = A[V \setminus Y]$. In case $Y = \{v\}$ is a singleton, to simplify notation, we also write $A \setminus Y = A \setminus v$.

We consider undirected graphs without parallel edges, however we do allow loops. Hence a graph $G = (V, E)$ can be represented by a symmetric $V \times V$ -matrix $A = (a_{u,v})$ over \mathbb{F}_2 : for $u \in V$, $\{u\} \in E$ (i.e., u has a loop in G) iff $a_{u,u} = 1$, and for $u, v \in V$ with $u \neq v$, $\{u, v\} \in E$ iff $a_{u,v} = 1$. We denote the set of edges of G by $E(G)$. We often make no distinction between G and its matrix representation A . Thus, e.g., we write $n(G) = n(A)$, and, for $X \subseteq V$, $G[X] = A[X]$, which consequently is the subgraph of G induced by X . Note that as G is represented by a matrix A over \mathbb{F}_2 , $n(G)$ is computed over \mathbb{F}_2 . Similar as for set systems, we often write V to denote the vertex set of the graph under consideration.

3. Background: nullity and counting closed walks

In this section we briefly and informally discuss an application of principal pivot transform where nullity plays an important role. As the rest of this paper does not depend on this application, the hasty reader may safely skip this section. In [9] a first connection between counting cycles and the nullity of a suitable matrix was established. It is shown in that paper that the number of cycles obtained as the result of applying disjoint transpositions to a cyclic permutation is described by the nullity of a corresponding “interlace matrix”.

It has been recognized in [18] that the result of [9] has an interpretation in terms of 2-in, 2-out digraphs (i.e., directed graphs with 2 incoming and 2 outgoing edges for each vertex), linking it to the interlace polynomial [2]. We discuss now this interpretation in terms of 2-in, 2-out digraphs and subsequently show the connection to the pivot operation.

Let $V = \{1, 2, 3, 4, 5, 6\}$ be an alphabet and let $s = 146543625123$ be a double occurrence string (i.e., each letter of the string occurs precisely twice) over V . The *overlap graph* O_s corresponding to s has the letters of s as the set of vertices and an edge $\{u, v\}$ precisely when u and v overlap: the vertices u and v appear either in order u, v, u, v or in order v, u, v, u in s . The overlap graph O_s is given in Fig. 1. One may verify that the nullity of O_s is $n(O_s) = 0$. Consider now the subgraph $O_s[X]$ of O_s induced by $X = \{3, 4, 5, 6\}$. Then it can be verified that $n(O_s[X]) = 2$.

We discuss now the link with connected 2-in, 2-out digraphs (only in this section we consider digraphs). Let G be the 2-in, 2-out digraph of Fig. 2 with $V = \{1, 2, 3, 4, 5, 6\}$ as the set of vertices.

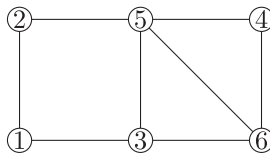


Fig. 1. The overlap graph of $s = 146543625123$.

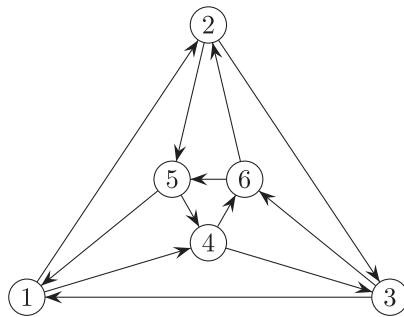


Fig. 2. A 2-in, 2-out digraph.

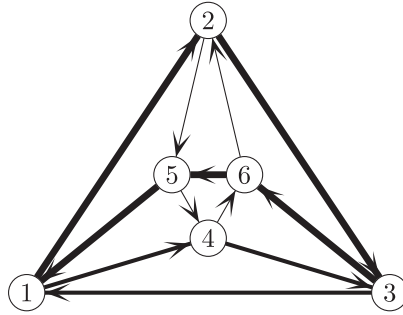


Fig. 3. Partition of the edges of a 2-in, 2-out digraph into three closed walks.

Although our example graph does not have loops or parallel edges, there is no objection to consider such “2-in, 2-out multidigraphs”. Notice that the double occurrence string $s = 146543625123$ considered earlier corresponds to an Euler circuit C of G . We now consider partitions P of the edges of G into closed walks (i.e., cycles where repeated vertices are allowed). Note that there are $2^{|V|}$ such partitions: if in a walk passing through vertex v we go from incoming edge e of v to outgoing edge e' of v , then necessarily we also walk in P from the other incoming edge of v to the other outgoing edge of v . Hence for each vertex there are two “routes”. Let P now be the partition of the edges of G into 3 closed walks as indicated by Fig. 3 using three types of line thicknesses. Then P follows the same route as the Euler circuit (corresponding to) s in vertices $\{1, 2\}$, while in the other vertices $X = \{3, 4, 5, 6\}$ it follows the other route. We say that P is induced by X in s .

Theorem 1 in [9] now states (applying it to the context of connected 2-in, 2-out digraphs) that the number of closed walks of a partition P of edges induced by X in s is $n(O_s[X]) + 1$. In our case we have indeed $|P| = 3$ and $n(O_s[X]) = 2$.

The pivot operation, which is recalled in the next section, has the property that it can map O_{s_1} into O_{s_2} for any two double occurrence strings s_1 and s_2 that correspond to Euler circuits of a 2-in, 2-out digraph G , see, e.g., the survey section of [6]. For example, the partition of edges induced by $\{1, 3\}$ in s corresponds to a single closed walk which may be described by the double occurrence string $s' = 123625146543$. It then holds that $O_{s'}$ is obtained from O_s by pivot on $\{1, 3\}$, denoted by $O_{s'} = O_s * \{1, 3\}$. We notice that the partition induced by $\{1, 3\} \oplus \{3, 4, 5, 6\} = \{1, 4, 5, 6\}$ in s' is equal to the partition P induced by $\{3, 4, 5, 6\}$ in s depicted in Fig. 3. Hence $n(O_{s'} * Y[Y \oplus X]) = n(O_s[X])$ for $X = \{3, 4, 5, 6\}$ and $Y = \{1, 3\}$. In Theorem 5 below we prove this property for arbitrary X and Y and for arbitrary square matrices (over some field) instead of restricting to overlap graphs O_s .

4. Pivot

In this section we recall principal pivot transform (pivot for short) for square matrices over an arbitrary field in general, see also [19].

Let A be a $V \times V$ -matrix (over an arbitrary field), and let $X \subseteq V$ be such that the corresponding principal submatrix $A[X]$ is nonsingular, i.e., $\det A[X] \neq 0$. The pivot of A on X , denoted by $A * X$, is defined as follows. Let $A = \begin{pmatrix} P & Q \\ R & S \end{pmatrix}$ with $P = A[X]$. Then

$$A * X = \begin{pmatrix} P^{-1} & -P^{-1}Q \\ RP^{-1} & S - RP^{-1}Q \end{pmatrix}. \tag{1}$$

Matrix $S - RP^{-1}Q$ is called the Schur complement of P in A .

The pivot can be considered a partial inverse, as A and $A * X$ are related by the following equality, where the vectors x_1 and y_1 correspond to the elements of X .

$$A \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \text{ iff } A * X \begin{pmatrix} y_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ y_2 \end{pmatrix}. \tag{2}$$

Eq. (2) is sufficient to define the pivot operation, see [19, Theorem 3.1]. Note that if $\det A \neq 0$, then $A * V = A^{-1}$. Also note by Eq. (2) that the pivot operation is an involution (operation of order 2), and more generally, if $(A * X) * Y$ is defined, then it is equal to $A * (X \oplus Y)$.

5. Nullity invariant

It is well known that any Schur complement in a matrix A has the same nullity as A itself, see, e.g., [22, Section 6.0.1]. See moreover [22, Chapter 0] for a detailed historical account of the Schur complement. We can rephrase the nullity property of the Schur complement in terms of pivot as follows.

Proposition 1 (Nullity of Schur complement). *Let A be a $V \times V$ -matrix, and let $X \subseteq V$ such that $A[X]$ is nonsingular. Then $n(A * X[V \setminus X]) = n(A)$.*

The following result is from [20, Theorem 3] and [17, Theorem 1] (the latter strengthened the original result of the former), see also [10, Theorem 4.1.2].

Proposition 2. *Let A be a $V \times V$ -matrix, and let $X \subseteq V$ be such that $A[X]$ is nonsingular. Then, for all $Y \subseteq V$, $\det(A * X)[Y] = \det A[X \oplus Y] / \det A[X]$.*

As a consequence of Proposition 2 we have the following result.

Corollary 3. *Let A be a $V \times V$ -matrix, and let $X \subseteq V$ be such that $A[X]$ is nonsingular. Then, for all $Y \subseteq V$, $(A * X)[Y]$ is nonsingular iff $A[X \oplus Y]$ is nonsingular.*

We will now combine and generalize Proposition 1 and Corollary 3 to obtain Theorem 5 below.

We denote by $A\sharp X$ the matrix obtained from A by replacing every row v_x^t of A belonging to $x \in V \setminus X$ by i_x^t where i_x is the vector having value 1 at element x and 0 elsewhere.

Lemma 4. *Let A be a $V \times V$ -matrix and $X \subseteq V$. Then $n(A\sharp X) = n(A[X])$.*

Proof. By rearranging the elements of V , A is of the following form $\begin{pmatrix} P & Q \\ R & S \end{pmatrix}$ where $A[X] = P$. Now

$A\sharp X$ is $\begin{pmatrix} P & Q \\ 0 & I \end{pmatrix}$ where I is the identity matrix of suitable size. We have $n(P) = n(A\sharp X)$. \square

We are now ready to prove the following result, which we refer to as the *nullity invariant*.

Theorem 5. *Let A be a $V \times V$ -matrix (over some field), and let $X \subseteq V$ be such that $A[X]$ is nonsingular. Then, for all $Y \subseteq V$, $n((A * X)[Y]) = n(A[X \oplus Y])$.*

Proof. We follow the same line of reasoning as the proof in [17] of Proposition 2 (see also [10, Theorem 4.1.1]). Let $Ax = y$. Then

$$((A\sharp X)x)[i] = \begin{cases} y[i] & \text{if } i \in X, \\ x[i] & \text{otherwise.} \end{cases}$$

As, by Eq. (2),

$$((A * X)(A\#X)x)[i] = \begin{cases} x[i] & \text{if } i \in X, \\ y[i] & \text{otherwise,} \end{cases}$$

we have, by considering each of the four cases depending on whether or not i in X and i in Y separately,

$$(((A * X)\#Y)(A\#X)x)[i] = \begin{cases} y[i] & \text{if } i \in X \oplus Y, \\ x[i] & \text{otherwise.} \end{cases}$$

Thus we have $((A * X)\#Y)(A\#X) = A\#(X \oplus Y)$. By Lemma 4, $n(A\#X) = n(A[X]) = 0$, and therefore $A\#X$ is invertible. Therefore $n(((A * X)\#Y)(A\#X)) = n(A\#(X \oplus Y))$, and the result follows by Lemma 4. \square

By Theorem 5, we see that the pivot operator $*X$ on matrices and the symmetric difference operator $\oplus X$ on sets have an equivalent effect on the nullity values of principal submatrices.

Note that Theorem 5 generalizes Corollary 3 as a matrix is nonsingular iff the nullity of that matrix is 0 (the empty matrix is nonsingular by convention). One can immediately see that Theorem 5 generalizes Proposition 1.

Also note that by replacing Y by $V \setminus Y$ in Theorem 5, we also have, equivalently, $n((A * X)[X \oplus Y]) = n(A[Y])$.

The “Nullity Theorem” [13, Theorem 2], restricted to *square* principal submatrices, states that if A is an invertible $V \times V$ -matrix, then, for $Y \subseteq V$, $n(A^{-1}[Y]) = n(A[V \setminus Y])$. Note that this is implied by Theorem 5 as $A * V = A^{-1}$.

Example 6. Let $V = \{a, b, c\}$ and let A be the $V \times V$ -matrix $\begin{matrix} & a & b & c \\ a & \begin{pmatrix} 1 & 2 & 5 \\ 1 & 4 & 2 \\ 3 & 2 & 1 \end{pmatrix} \end{matrix}$ over \mathbb{Q} . We see that

$A[\{b, c\}] = \begin{matrix} & b & c \\ b & \begin{pmatrix} 4 & 2 \\ 2 & 1 \end{pmatrix} \\ c & \end{matrix}$ and therefore $n(A[\{b, c\}]) = 1$. Moreover, for $X = \{a, b\}$, the columns of $A[X]$ are independent and thus $n(A[X]) = 0$. We have therefore that $A * X$ is defined, and it is given below.

$$A * X = \begin{matrix} & a & b & c \\ a & \begin{pmatrix} 2 & -1 & -8 \\ -\frac{1}{2} & \frac{1}{2} & \frac{3}{2} \\ 5 & -2 & -20 \end{pmatrix} \\ b & \\ c & \end{matrix}$$

By Theorem 5, we have $n(A[\{b, c\}]) = n(A * X[X \oplus \{b, c\}]) = n(A * X[\{a, c\}])$. Therefore $n(A * X[\{a, c\}]) = 1$. This can easily be verified given $A * X[\{a, c\}] = \begin{matrix} & a & c \\ a & \begin{pmatrix} 2 & -8 \\ 5 & -20 \end{pmatrix} \\ c & \end{matrix}$.

It is easy to verify from the definition of pivot that $A * X$ is skew-symmetric whenever A is. In particular, if G is a graph (i.e., a symmetric matrix over \mathbb{F}_2), then $G * X$ is also a graph. Recall that for graphs, all matrix computations, including the determinant, will be over \mathbb{F}_2 .

Example 7. Let G be the graph given on the left-hand side of Fig. 4. Let $X = \{1, 2, 3\}$. Then the $X \times X$ -

matrix belonging to $G[X]$ is $\begin{matrix} & 1 & 2 & 3 \\ 1 & \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 3 & 1 & 1 \end{pmatrix} \\ 2 & \\ 3 & \end{matrix}$. We see that the columns of $G[X]$ are independent (over \mathbb{F}_2)

and therefore $\det G[X] = 1$. Consequently $G * X$ is defined and the graph is given on the right-hand

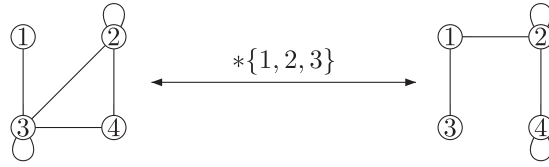


Fig. 4. Graphs G and $G * X$ of Example 7.

side of Fig. 4. Let now $Y = \{1, 4\}$. We see that $G[Y]$ is a discrete graph (i.e., the graph has no edges). Therefore $n(G[Y]) = 2$. Now by Theorem 5, we have $n(G[Y]) = n(G * X[X \oplus Y]) = n(G * X[\{2, 3, 4\}])$. One may verify that removing vertex 1 from $G * X$ indeed obtains a graph of nullity 2.

6. Set systems

Let A be a $V \times V$ -matrix. Let $\mathcal{M}_A = (V, D)$ be the set system with $X \in D$ iff $A[X]$ is nonsingular. Set system \mathcal{M}_A turns out to fulfill a specific exchange axiom if A is (skew-)symmetric, making it in this case a delta-matroid [4] (we will not recall its definition here as we do not use this notion explicitly).

Let $M = (V, D)$ be a set system. We define for $X \subseteq V$, the *pivot* (often called *twist*) of M on X , denoted $M * X$, by $(V, D * X)$ where $D * X = \{Y \oplus X \mid Y \in M\}$. By Corollary 3 it is easy to verify, see [14], that the operations of pivot on set systems and matrices match, i.e., $\mathcal{M}_A * X = \mathcal{M}_{A * X}$ if the right-hand side is defined (i.e., if $X \in \mathcal{M}_A$).

Theorem 5 allows now for a generalization of this result from the set system \mathcal{M}_A of nullity 0 to a “sequence of set systems” \mathcal{P}_A for each possible nullity i . We formalize this as follows.

For a finite set V , we call a sequence $P = (P_0, P_1, \dots, P_n)$ with $n = |V|$ and $P_i \subseteq 2^V$ for all $i \in \{0, \dots, n\}$ a *partition sequence* (over V) if the nonempty P_i ’s form a partition of 2^V . Regarding P as a vector indexed by $\{0, \dots, n\}$, we denote P_i by $P[i]$. Moreover, we define for partition sequence P and $X \subseteq V$, the *pivot* of P on X , denoted by $P * X$, to be the partition sequence $(P_0 * X, P_1 * X, \dots, P_n * X)$. Also, we call the vector $(|P_0|, |P_1|, \dots, |P_n|)$ of dimension $n + 1$, denoted by $\|P\|$, the *norm* of P . Clearly, $\|P\| = \|P * X\|$, i.e., the norm of P is invariant under pivot.

For a $V \times V$ -matrix A we denote by \mathcal{P}_A the partition sequence over V where $X \in \mathcal{P}_A[i]$ iff $n(A[X]) = i$. As nullity 0 corresponds to a non-zero determinant (this holds also for \emptyset as $\det A[\emptyset] = 1$ by convention), we have $\mathcal{M}_A = (V, \mathcal{P}_A[0])$.

We now have the following consequence of Theorem 5. Note that $X \in \mathcal{P}_A[0]$ iff $A * X$ is defined.

Theorem 8. *Let A be a $V \times V$ -matrix, and $X \in \mathcal{P}_A[0]$. Then $\mathcal{P}_{A * X} = \mathcal{P}_A * X$.*

Proof. By Theorem 5 we have for all $i \in \{0, \dots, n\}$, $Y \in \mathcal{P}_{A * X}[i]$ iff $n((A * X)[Y]) = i$ iff $n(A[X \oplus Y]) = i$ iff $X \oplus Y \in \mathcal{P}_A[i]$ iff $Y \in \mathcal{P}_A[i] * X$. \square

Since the norm of a partition sequence is invariant under pivot, we have by Theorem 8, $\|P_A\| = \|\mathcal{P}_{A * X}\|$. Therefore, for each $i \in \{0, \dots, n\}$, the number of principal submatrices of A of nullity i is equal to the number of principal submatrices of $A * X$ of nullity i .

For $X \subseteq V$, it is easy to see that $\mathcal{P}_{A[X]}$ is obtained from \mathcal{P}_A by removing all $Y \in \mathcal{P}_A[i]$ containing at least one element outside X : $\mathcal{P}_{A[X]}[i] = \{Z \subseteq X \mid Z \in \mathcal{P}_A[i]\}$ for all $i \in \{0, \dots, |X|\}$.

Example 9. For matrix A from Example 6, we have $\mathcal{P}_A = (P_0, P_1, P_2, P_3)$ with $P_0 = 2^V \setminus \{\{b, c\}\}$, $P_1 = \{\{b, c\}\}$, and $P_2 = P_3 = \emptyset$.

Example 10. For graph G from Example 7, depicted on the left-hand side of Fig. 4, we have $\mathcal{P}_G = (P_0, P_1, P_2, P_3, P_4)$ with

- $P_0 = \{\emptyset, \{2\}, \{3\}, \{1, 3\}, \{2, 4\}, \{3, 4\}, \{1, 2, 3\}, \{1, 2, 3, 4\}\}$,
- $P_1 = \{\{1\}, \{4\}, \{1, 2\}, \{2, 3\}, \{1, 2, 4\}, \{1, 3, 4\}, \{2, 3, 4\}\}$,
- $P_2 = \{\{1, 4\}\}, P_3 = P_4 = \emptyset$.

By Theorem 8 we have for $G * X$ with $X = \{1, 2, 3\}$, depicted on the right-hand side of Fig. 4, $\mathcal{P}_{G*X} = (P'_0, P'_1, P'_2, P'_3, P'_4)$ where

$$\begin{aligned} P'_0 &= \{\emptyset, \{2\}, \{4\}, \{1, 2\}, \{1, 3\}, \{1, 2, 3\}, \{1, 2, 4\}, \{1, 3, 4\}\}, \\ P'_1 &= \{\{1\}, \{3\}, \{1, 4\}, \{2, 3\}, \{2, 4\}, \{3, 4\}, \{1, 2, 3, 4\}\}, \\ P'_2 &= \{\{2, 3, 4\}\}, P'_3 = P'_4 = \emptyset. \end{aligned}$$

We have $\|\mathcal{P}_G\| = \|\mathcal{P}_{G*X}\| = (8, 7, 1, 0, 0)$.

Example 11. In the context of Section 3, where matrix A an overlap graph O_s for some double occurrence string s , we have that $\|\mathcal{P}_{O_s}\| [i]$ is the number of partitions of the edges of the 2-in, 2-out digraph D corresponding to s into closed walks of D , such that the number of closed walks is precisely $i + 1$. The value $\|\mathcal{P}_{O_s}\| [0]$ is therefore the number of Euler circuits in D .

7. Elementary pivots on graphs

In this section we consider pivot on graphs (i.e., symmetric $V \times V$ -matrices over \mathbb{F}_2), and thus all matrix computations will be over \mathbb{F}_2 . Hence for graph G , $\mathcal{M}_G = (V, D_G)$ is the set system with $X \in D_G$ iff $\det(G[X]) = 1$. Also, G can be (re)constructed given \mathcal{M}_G . Indeed, $\{u\}$ is a loop in G iff $\{u\} \in D_G$, and $\{u, v\}$ is an edge in G iff $(\{u, v\} \in D_G) \oplus ((\{u\} \in D_G) \wedge (\{v\} \in D_G))$, see [7, Property 3.1]. Therefore, the function $\mathcal{M}_{(\cdot)}$ assigning to each graph G the set system \mathcal{M}_G is an injective function from the family of graphs to the family of set systems. In this way the family of graphs may be regarded as a subclass of the family of set systems. Note that $\mathcal{M}_G * X$ is defined for all $X \subseteq V$, while pivot on graphs $G * X$ is defined only if $X \in \mathcal{M}_G$ (or equivalently, $\emptyset \in \mathcal{M}_G * X$).

In this section we recall from [14] that the pivot operation on graphs can be defined as compositions of two graph operations: local complementation and edge complementation.

The pivots $G * X$ where X is a minimal element of $\mathcal{M}_G \setminus \{\emptyset\}$ w.r.t. inclusion are called *elementary*. It is noted in [14] that an elementary pivot X on graphs corresponds to either a loop, $X = \{u\} \in E(G)$, or to an edge, $X = \{u, v\} \in E(G)$, where both vertices u and v are non-loops. Thus for $Y \in \mathcal{M}_G$, if $G[Y]$ has elementary pivot X_1 , then $Y \setminus X_1 = Y \oplus X_1 \in \mathcal{M}_{G*X_1}$. In this way, each $Y \in \mathcal{M}_G$ can be partitioned $Y = X_1 \cup \dots \cup X_n$ such that $G * Y = G * (X_1 \oplus \dots \oplus X_n) = (\dots (G * X_1) \dots * X_n)$ is a composition of elementary pivots. Consequently, a direct definition of the elementary pivots on graphs G is sufficient to define the (general) pivot operation on graphs.

The elementary pivot $G * \{u\}$ on a loop $\{u\}$ is called *local complementation*. It is the graph obtained from G by complementing the edges in the neighbourhood $N_G(u) = \{v \in V \mid \{u, v\} \in E(G), u \neq v\}$ of u in G : for each $v, w \in N_G(u)$, $\{v, w\} \in E(G)$ iff $\{v, w\} \notin E(G * \{u\})$, and $\{v\} \in E(G)$ iff $\{v\} \notin E(G * \{u\})$ (the case $v = w$). The other edges are left unchanged.

The elementary pivot $G * \{u, v\}$ on an edge $\{u, v\}$ between distinct non-loop vertices u and v is called *edge complementation*. For a vertex x consider its closed neighbourhood $N'_G(x) = N_G(x) \cup \{x\}$. The edge $\{u, v\}$ partitions the vertices of G connected to u or v into three sets $V_1 = N'_G(u) \setminus N'_G(v)$, $V_2 = N'_G(v) \setminus N'_G(u)$, $V_3 = N'_G(u) \cap N'_G(v)$. Note that $u, v \in V_3$.

The graph $G * \{u, v\}$ is constructed by “toggling” all edges between different V_i and V_j : for $\{x, y\}$ with $x \in V_i, y \in V_j$ and $i \neq j$: $\{x, y\} \in E(G)$ iff $\{x, y\} \notin E(G[\{u, v\}])$, see Fig. 5. The other edges remain unchanged. Note that, as a result of this operation, the neighbours of u and v are interchanged.

Example 12. Fig. 6 depicts an orbit of graphs under pivot. The figure also shows the applicable elementary pivots (i.e., local and edge complementation) of the graphs within the orbit.

Interestingly, in many contexts, principal pivot transform originally appeared in disguise. For example, PPT was recognized in [15] as the operation underlying the recursive definition of the interlace polynomial, introduced in [1]. We will consider the interlace polynomial in the next section. Also, e.g., the graph model defined in [12] within the formal theory of (intramolecular) gene assembly in ciliates

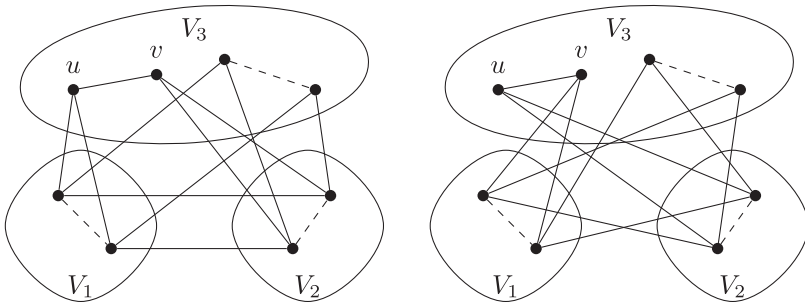


Fig. 5. Pivoting on an edge $\{u, v\}$ in a graph with both u and v non-loops. Connection $\{x, y\}$ is toggled iff $x \in V_i$ and $y \in V_j$ with $i \neq j$. Note u and v are connected to all vertices in V_3 , these edges are omitted in the diagram. The operation does not affect edges adjacent to vertices outside the sets V_1, V_2, V_3 , nor does it change any of the loops.

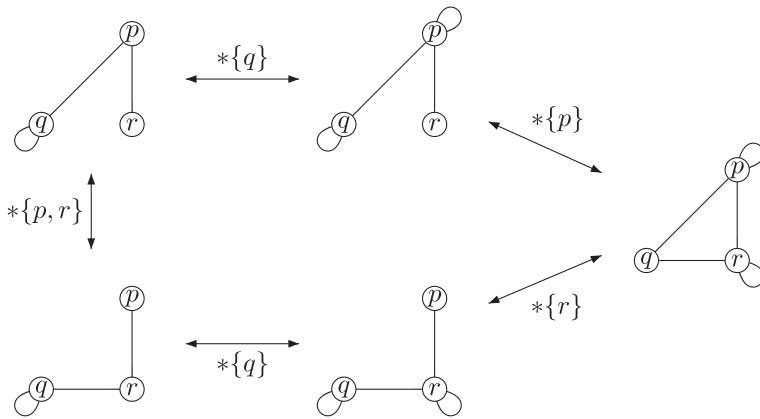


Fig. 6. The orbit of a graph under pivot. Only the elementary pivots are shown.

turns out to be exactly the elementary pivots, as noted in [8]. Furthermore, the proof of the result from [9], connecting nullity to the number of cycles in permutations, as mentioned in Section 3, implicitly uses the Schur complement (which is an essential part of PPT).

8. The interlace polynomial

The interlace polynomial is a graph polynomial introduced in [1,2]. We follow the terminology of [3]. The single-variable interlace polynomial (simply called interlace polynomial in [2]) for a graph G (with possibly loops) is defined by

$$q(G) = \sum_{S \subseteq V} (y - 1)^{n(G[S])}.$$

It is shown in [3] that the interlace polynomial fulfills an interesting recursive relation, cf. Proposition 16 below, which involves local and edge complementation. As we consider here principal pivot transform, which generalizes local and edge complementation, it makes sense now to define the interlace polynomial for $V \times V$ -matrices (over some arbitrary field) in general. Therefore, we define the *interlace polynomial* for $V \times V$ -matrix A as

$$q(A) = \sum_{S \subseteq V} (y - 1)^{n(A[S])}.$$

We may (without loss of information) change variables $y := y - 1$ in the definition of the interlace polynomial to obtain

$$q'(A) = \sum_{S \subseteq V} y^{n(A[S])}.$$

As $q(A)$ (and $q'(A)$) deals with nullity values for (square) matrices in general, one can argue that the *nullity polynomial* is a more appropriate name for these polynomials.

We see that the coefficient a_i of term $a_i y^i$ of $q'(A)$ is equal to $\|\mathcal{P}_A\| [i]$ (the element of $\|\mathcal{P}_A\|$ corresponding to i) for all $i \in \{0, \dots, n\}$. Therefore, we have for matrices A and A' , $q(A) = q(A')$ iff $q'(A) = q'(A')$ iff $\|\mathcal{P}_A\| = \|\mathcal{P}_{A'}\|$.

Example 13. Let O_s be the overlap graph for some double occurrence string s , and let a_i be the coefficient a_i of term $a_i y^i$ of $q'(O_s)$. We have, see Example 11, that a_i is equal to the number of partitions of the edges of the 2-in, 2-out digraph D corresponding to s into closed walks of D , such that the number of closed walks is precisely $i + 1$. More specifically, a_0 is the number of Euler circuits in D . The interlace polynomial is originally motivated by the computation of these coefficients a_i of 2-in, 2-out digraphs, see [2].

It is shown in [2] that the interlace polynomial (for graphs) is invariant under edge complementation. Moreover, by it may be easily deduced from [3, Theorem 6] that the interlace polynomial is invariant under local complementation as well. Theorem 8 generalizes invariance under edge and local complementation to invariance under pivot: $\|\mathcal{P}_{A * X}\| = \|\mathcal{P}_A\|$ and equivalently $q(A * X) = q(A)$.

Furthermore, we show that $q(A)$ fulfills the following recursive relation.

Theorem 14. Let A be a $V \times V$ -matrix (over some field), let $X \subseteq V$ with $A[X]$ nonsingular, and let $u \in X$. We have $q(A) = q(A \setminus u) + q(A * X \setminus u)$.

Proof. Let $\mathcal{P}_A = (P_0, P_1, \dots, P_n)$. Since X is nonempty and $A[X]$ is nonsingular, $P_n = \emptyset$. Let $R = (P_0, P_1, \dots, P_{n-1})$. Let $Z \in P_i$ for some $i \in \{0, 1, \dots, n - 1\}$. We have that Z does not appear in $\mathcal{P}_{A \setminus u}$ iff $u \in Z$ iff $u \notin Z \oplus X$ iff $Z \oplus X$ does appear in $\mathcal{P}_{A * X \setminus u}$. Hence $\|R\| = \|\mathcal{P}_{A \setminus u}\| + \|\mathcal{P}_{A * X \setminus u}\|$ (point-wise addition of the two vectors), and the statement holds. \square

Example 15. Consider again matrix A from Example 6. By Example 9, $\|\mathcal{P}_A\| = (7, 1, 0, 0)$. Hence $q(A) = (y - 1) + 7 = y + 6$.

Given Example 9, we have

$$\mathcal{P}_{A \setminus b} = (\{\emptyset, \{a\}, \{c\}, \{a, c\}\}, \emptyset, \emptyset).$$

Moreover, $\{a, b\} \in \mathcal{P}_A[0]$ and

$$\mathcal{P}_{A * \{a, b\} \setminus b} = (\{\emptyset, \{a\}, \{c\}\}, \{\{a, c\}\}, \emptyset).$$

We have thus $\|\mathcal{P}_{A \setminus b}\| + \|\mathcal{P}_{A * \{a, b\} \setminus b}\| = (4, 0, 0) + (3, 1, 0) = (7, 1, 0)$ which indeed corresponds to $\|\mathcal{P}_A\|$. Moreover, $q(A \setminus b) = 4$, and $q(A * \{a, b\} \setminus b) = y + 2$. Consequently, $q(A) = q(A \setminus b) + q(A * \{a, b\} \setminus b)$, as required.

The recursive relation for the single-variable interlace polynomial in [3] is now easily obtained from Theorem 14 by restricting to the case of elementary pivots on graphs.¹

Proposition 16 ([3]). Let G be a graph. Then $q(G)$ fulfills the following conditions.

¹ We use here the fact observed in [15] that the operations in the recursive relations of [3] are exactly the elementary pivots of Section 7, assuming that the neighbours of u and v are interchanged after applying the “pivot” operation of [3] on edge $\{u, v\}$.

1. $q(G) = q(G \setminus u) + q(G * \{u, v\} \setminus u)$ for edge $\{u, v\}$ in G where both u and v do not have a loop,
2. $q(G) = q(G \setminus u) + q(G * \{u\} \setminus u)$ if u has a loop in G , and
3. $q(G) = y^n$ if G is a discrete graph with n vertices.

Proof. Conditions (1) and (2) follow from Theorem 14 where A is a graph G , and X is an elementary pivot (i.e., $X = \{u\}$ is a loop in G or $X = \{u, v\}$ is an edge in G where both u and v do not have a loop, see Section 7). Finally, if G is a discrete graph with n vertices, then, for all $Y \subseteq V$, $Y \in P_{|Y|}$. Consequently, $|P_i| = \binom{n}{i}$. Thus, $q'(G) = (y + 1)^n$ and therefore $q(G) = y^n$. \square

Example 17. Consider again graph G depicted on the left-hand side of Fig. 4. By Example 10, $\|\mathcal{P}_G\| = (8, 7, 1, 0, 0)$ and hence $q(G) = (y - 1)^2 + 7(y - 1) + 8 = y^2 + 5y + 2$.

Vertex 2 of G has a loop. Therefore, we may apply local complementation on 2 to obtain graph $G * \{2\}$. The graph $G * \{2\} \setminus 2$ now has the following partition sequence

$$\mathcal{P}_{G*\{2\}\setminus 2} = (\{\emptyset, \{4\}, \{1, 3\}, \{1, 3, 4\}\}, \{\{1\}, \{3\}, \{1, 4\}, \{3, 4\}\}, \emptyset, \emptyset).$$

From \mathcal{P}_G given in Example 10, we find that

$$\mathcal{P}_{G\setminus 2} = (\{\emptyset, \{3\}, \{1, 3\}, \{3, 4\}\}, \{\{1\}, \{4\}, \{1, 3, 4\}\}, \{\{1, 4\}\}, \emptyset).$$

We have thus $\|\mathcal{P}_{G\setminus 2}\| + \|\mathcal{P}_{G*\{2\}\setminus 2}\| = (4, 3, 1, 0) + (4, 4, 0, 0) = (8, 7, 1, 0)$ which indeed corresponds to $\|\mathcal{P}_G\|$. Moreover, $q(G \setminus 2) = y^2 + y + 2$, and $q(G * \{2\} \setminus 2) = 4y$. Consequently, $q(G) = q(G \setminus 2) + q(G * \{2\} \setminus 2)$.

9. Discussion

We have shown that the pivot operator $*X$ on matrices A and the symmetric difference operator $\oplus X$ on sets Y have an equivalent effect w.r.t. the nullity value of the principal submatrices $A[Y]$ of A . This nullity invariant may be described in terms of partition sequences \mathcal{P}_A , where each set $Y \subseteq V$ is arranged according to the nullity value of $A[Y]$. We notice that interlace polynomial of a graph G corresponds to the norm $\|\mathcal{P}_G\|$ of the partition sequence of G (where G is considered as a matrix). Hence we (may) naturally consider interlace polynomials for square matrices in general, and obtain a recursive relation for these generalized interlace polynomials. As a consequence, we simplify the proof of the (original) recursive relation for interlace polynomials of graphs.

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