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Computing the Permanental Polynomial of a Matrix from a Combinatorial Viewpoint

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Dedicated to Enzo M. Li Marzi on occasion of his 65-th birthday.

Abstract

Recently, in the book [A Combinatorial Approach to Matrix Theory and Its Applications, CRC Press (2009)] the authors proposed a combinatorial approach to matrix theory by means of graph theory. In fact, if A is a square matrix over any field, then it is possible to associate to A a weighted digraph G_A, called Coates digraph. Through G_A (hence by graph theory) it is possible to express and prove results given for the matrix theory. In this paper we express the permanental polynomial of any matrix A in terms of permanental polynomials of some digraphs related to G_A.

1 Introduction

Let $A = (a_{i,j})$ be a square matrix of order n (over any field). The permanent of A is defined as

$$\mathrm{per}(A) = \sum_{\sigma \in \mathcal{S}_n} \prod_{i=1}^{n} a_{i\,\sigma(i)},$$

where $\mathcal{S}_n$ denotes the symmetric group over n elements. In general, permanents have important combinatorial meaning, in particular the permanents of $(0, 1)$ matrices enumerate matchings in bipartite graphs (see, for example [16]). Permanents also have applications in physics of interacting Bose particles [25]. A brief but concise introduction into properties of permanents can be found, for example, in [20]. If we consider the *characteristic* *matrix* of A, that is $xI - A$, then $\mathrm{per}(xI - A) = \pi(A, x)$ is the *permanental polynomial* of A. Besides the permanental polynomial of A, we will consider also the *characteristic polynomial* $\phi(A, x) = \det(xI - A)$, which depends on the more common notion of determinant.

If A is a symmetric $\{0, 1\}$-matrix then A can be interpreted as the adjacency matrix of a simple graph, and such a graph can eventually represent the skeleton of a hydrocarbon molecule in the, so called, Chemical Graph Theory. Permanental polynomial is one of the graph polynomials mostly considered in chemical graph theory. However, it is hard to be computed and due to the latter reason, the literature on permanental polynomial is far less than that on matching and characteristic polynomials. In fact, permanental polynomials were initially studied only for smaller fullerenes (see [6, 7]). Later, more attention has been paid to this problem [8–12, 18, 21, 26].

Here, following the papers [1,2], we give some formulas which express the permanental polynomial of any square matrix (over any field) in terms of the permanental polynomial of weighted digraphs. Before doing the latter we need to introduce some mathematical definitions and notations.

Let $G = (\mathcal{V}_G, \mathcal{A}_G)$ be a digraph with vertex set $\mathcal{V}_G = \{v_1, v_2, \ldots, v_n\}$ and arc set $\mathcal{A}_G = \{a_1, a_2, \ldots, a_m\}$. Recall, if $a \in \mathcal{A}_G$ is an arc then $a = \overrightarrow{uv}$ for some vertices $u, v \in \mathcal{V}_G$; we also assume that it is oriented from u to v. Usually, an arc $\overrightarrow{vv}$, whose end-vertices coincide, is called a *loop* (for loops the orientation is unimportant). We say that G is a *weighted digraph*, if to each edge is assigned a scalar in some field $\mathbb{K}$. Let $\mathcal{W}_G \subset \mathbb{K}$ be the set of arc weights of G (here $\mathbb{K}$ is any field). The function $\omega_G : \mathcal{A}_G \to \mathcal{W}_G$ is the weight function of G. Usually, we assume that an arc a with zero weight does not belong to $\mathcal{A}_G$, or equivalently, that a non-arc a belongs to $\mathcal{A}_G$ but with zero weight; so $\mathcal{A}_G$ can be naturally reduced, or extended if necessary. It is also clear that to each weighted digraph there corresponds a weight function, and vice versa. If $\mathcal{W}_G$ consists of nonnegative integers then G is called a multi-digraph (then each arc of weight k can be substituted with k parallel arcs with weight one); in particular, if $\mathcal{W}_G = \{0, 1\}$ then G is a digraph.

Coates in [13] (see also [5]) defined a bijection between matrices and weighted digraphs. Indeed consider the $n \times n$ matrix $A = (a_{ij})$ (over a field $\mathbb{K}$), then the *Coates digraph* G_A is a weighted digraph defined as follows (cf. also Fig. 1):

- the vertex set of G_A is equal to $\{1, 2, \ldots, n\}$, where the i-th vertex $(1 \le i \le n)$

corresponds to the i-th row (or equivalently, to the i-th column) of A;

- the arc set of G_A consists of all arcs of the form $\overrightarrow{ij}$ with weight a_{ij} $(1 \leq i, j \leq n)$; for $i = j$ the corresponding arc is a loop. If the weight of some arc is zero, then it can be ignored (as already noted).

$$A = \begin{bmatrix} 1 & -1 & 0 & 2 \\ 1 & -1 & -1 & 0 \\ 2 & 0 & 2 & -1 \\ -1 & 0 & 0 & 0 \end{bmatrix}$$

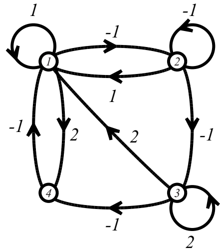

Fig. 1: A matrix A and its corresponding Coates digraph G_A.

On the other hand, to a weighted digraph G, we can associate the *adjacency (or weight) matrix* of G, that is the $n \times n$ matrix $A = A_G = (a_{ij})$, where $a_{ij} = \omega_G(\overrightarrow{v_iv_j})$ if $\overrightarrow{v_iv_j} \in \mathcal{A}_G$, and $a_{ij} = 0$ otherwise. Clearly, given a weighted digraph G, if $A = A_G$ is its adjacency matrix then $G = G_A$. Conversely, given a matrix A, if $G = G_A$ then $A = A_G$. So, weighted digraphs and square matrices can be considered as same objects, and this will be used later interchangeably. Similarly, we will consider $\pi(G, x)$ and $\phi(G, x)$, namely the permanental polynomial and the characteristic polynomial of G, respectively, as those of its adjacency matrix $A = A_G$.

If A is symmetric then the arcs $\overrightarrow{uv}, \overrightarrow{vu} \in \mathcal{A}_G$ have the same weights and represent the edge $e = uv$ of G with common weight. Then, instead of the arc set, we can consider the edge set of G denoted by $\mathcal{E}_G = \{e_1, e_2, \ldots, e_m\}$, and G becomes a (weighted) graph, or a multi-graph if the weights are (nonnegative) integers; in addition, G is a simple graph if it has no multiple edges, nor loops. Then we write $u \sim v$ to indicate that vertices u and v are adjacent. Finally, note that each weighted graph can be interpreted as a weighted digraph obtained by substituting each edge by two parallel arcs with opposite directions, and weights equal to the weight of the corresponding edge. In what follows we shall suppress graph names in our notation if it is understood from the context.

If X is a subset of the vertex set of G, then $G - X$ denotes the weighted digraph induced by the vertex set $\mathcal{V} \setminus X$. If $X = \{v\}$ then we abbreviate the latter to $G - v$. Similarly, if Y is a subset of the arc (or edge) set of G, then $G - Y$ denotes the spanning subgraph of

G whose arc (edge) set is equal to $\mathcal{A} \setminus Y$ (resp. $\mathcal{E} \setminus Y$). If $Y = \{a\}$ ($Y = \{e\}$) then we use $G - a$ (resp. $G - e$) instead. This notation is naturally extended if two or more vertices, or arcs, or edges are deleted from G. Needless to say, in all these situations the weight functions are the restrictions of the original ones. Given two vertex disjoint weighted (di)graphs G and H, we denote by $G\dot{\cup}H$ their disjoint union (then, their vertex sets, and also arc (or edge) sets, are joined together, and weight functions naturally combined).

Now, we state the *Coates permanent formula* of any square matrix A. In order to do that, we first need to introduce *factors* of G_A. They are defined as follows:

> a factor of G_A is a spanning (weighted) sub-digraph whose all vertices have in-degrees and out-degrees equal to 1; so it is a disjoint union of (weighted) directed cycles. The set of all factors of G_A, i.e. its *factor space*, is denoted by $\mathcal{F}_{G_A}$ (or by $\mathcal{F}_G$, or $\mathcal{F}_A$).

If $F \in \mathcal{F}_A$ then $c(F)$ is a number of components (i.e. cycles) of F, whereas $\omega_G(F)$ is the weight of F, equal to the product of weights of all arcs of F. More generally, if H is any weighted sub-digraph of G then $\omega_G(H)$ $(= \omega_A(H))$ is a product of weights of its arcs (or edges for sub-graphs).

We are now in position to introduce the Coates permament formula, which is a simple variant of the Coates determinant formula (see [13], or [5] p. 65). It reads:

$$\mathrm{per}(A) = \sum_{F \in \mathcal{F}_A} \omega(F). \tag{1}$$

Note that the determinat variant of the above formula is

$$\det(A) = (-1)^n \sum_{F \in \mathcal{F}_A} (-1)^{c(F)} \omega(F).$$

In [1, 2], the authors made use of the latter formula (i.e. in the determinant variant) to obtain the characteristic polynomial of any matrix in terms of some weighted digraphs. In this paper, by making use of (1) we will essentially give the same formulas reported in [2] but in the, permanent variant. Clearly proofs are almost the same, so we will omit most of them and we refer the readers to read [2] in order to reproduce the proofs in its permanent variant. For all other notation, or definitions not given here, see [19] or [14, 15] for graph spectra.

This paper has three main goals. First, to promote a combinatorial approach to linear algebra in the spirit of the book [5], which just recently appeared. Secondly, to extend some formulas related to permanental polynomials in the spectral graph theory [3] to weighted graphs and/or digraphs (with natural interpretation to matrices). Thirdly, the formulas given here can be of some help in the problem of computing the permanental polynomial of matrices. Indeed, in strong contrast to determinants, Valiant in [24] showed that computing permanents is a $\#P$-complete problem for $\{0,1\}$-matrices. Due to the latter reason, a considerable effort was spent by several authors on developing various approximation methods (see, for example, [17] and references therein).

The rest of the paper is organized as follows: in Section 2 we will report the formulas obtained in [2] for the determinant variant; in Section 3 we give the formulas reported in Section 2 in their permanent variant; in Section 4 we give some examples for the formulas obtained in this paper.

2 Determinant variant

There are several formulas which express the permanental polynomial of a simple graph in terms of the permanental polynomial of its subgraphs. These formulas are mostly due to Borowiecki et al. [3, 4]. In the latter papers the authors considered the proofs of the corresponding determinant variant (based on the Coefficient Theorem of Sachs, see [14] for example). We will follow the same strategy but instead of Sachs' formula, we will rely on the Coates formula (1). We now report the determinant variant of the formulas that will be next given in the permanental variant. All these formulas are proved in [2].

The following formulas have been given by Schwenk in [23] in their simplest variant, i.e. for simple graphs. So we say that they are *Schwenk-like formulas* (cf. Section 3 in [2]). To keep formulas shorter, we omit the variable if its presence is clear from the context.

Theorem 2.1. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. If v is a fixed vertex of G then*

$$\phi(G) = (x - a_{vv})\phi(G - v) - \sum_{\overrightarrow{C} \in \mathcal{C}_v} \omega_A(\overrightarrow{C})\phi(G - \mathcal{V}(\overrightarrow{C})),$$

where $\mathcal{C}_v$ is the set of directed cycles of G of length ≥ 2 passing through v, while $\omega_A(\overrightarrow{C}) = \prod_{\overrightarrow{ij} \in \mathcal{A}(\overrightarrow{C})} a_{ij}$.

Theorem 2.2. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. If $\overrightarrow{uv}$ $(u \neq v)$ is a fixed arc of G then*

$$\phi(G) = \phi(G - \overrightarrow{uv}) - (a_{uv}a_{vu})\phi(G - u - v) - \sum_{\overrightarrow{C} \in \mathcal{C}_{\overrightarrow{uv}}} \omega_A(\overrightarrow{C})\phi(G - \mathcal{V}(\overrightarrow{C})),$$

where $\mathcal{C}_{\overrightarrow{uv}}$ is the set of all directed cycles of G of length ≥ 3 passing through $\overrightarrow{uv}$, while $\omega_A(\overrightarrow{C}) = \prod_{\overrightarrow{ij} \in \mathcal{A}(\overrightarrow{C})} a_{ij}$.

The above formulas have an easier expression in the case that matrix A is symmetric.

Theorem 2.3. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. If v is a fixed vertex of G then*

$$\phi(G) = (x - a_{vv})\phi(G - v) - \sum_{u \neq v} a_{uv}^2 \phi(G - u - v) - 2\sum_{C \in \mathcal{C}_v} \omega_A(C)\phi(G - \mathcal{V}(C)),$$

where $\mathcal{C}_v$ is a set of all undirected cycles of G of length ≥ 3 passing through v, while $\omega_A(C) = \prod_{ij \in \mathcal{E}(C)} a_{ij}$.

Theorem 2.4. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. If uv $(u \neq v)$ is a fixed edge of G then*

$$\phi(G) = \phi(G - uv) - a_{uv}^2 \phi(G - u - v) - 2\sum_{C \in \mathcal{C}_{uv}} \omega_A(C)\phi(G - \mathcal{V}(C)),$$

where $\mathcal{C}_{uv}$ is the set of all undirected cycles of G of length ≥ 3 passing through uv, while $\omega_A(C) = \prod_{ij \in \mathcal{E}(C)} a_{ij}$.

The coalescence of two rooted graphs G and H (with roots u and v, respectively), given for simple graphs in Section 2, can be naturally extended to weighted digraphs (including weighted graphs). At this place it is only noteworthy to add that loops at u and v give rise to a loop at w $(= u = v)$ in $G \cdot H$ after identification, and that its weight is equal to the sum of weights of the former two loops (of G and H).

Theorem 2.5. *Let $G \cdot H$ be the coalescence of two rooted weighted digraphs G and H whose roots are u and v, respectively. Then*

$$\phi(G \cdot H) = \phi(G)\phi(H - v) + \phi(G - u)\phi(H) - x\phi(G - u)\phi(H - v).$$

Next formulas are similar in principle to one given by Rowlinson in [22] for the contraction-deletion algorithm, so we called them *Rowlinson-like formulas* (cf. Section

4 in [2]). In fact, for Rowlinson-like formulas we contract two vertices and (some) edges incident to them, so the digraphs involved in those formulas are not (in general) subdigraphs of the graph under consideration.

In order to state them we need some further definitions. If u and v are two vertices of some digraph, say G, then $G[uv]$ denotes the digraph obtained from $G - \{\overrightarrow{uv}, \overrightarrow{vu}\}$ by contracting u and v. More precisely, we have: u and v are identified (giving rise to a new vertex, say w); all arcs which were previously in-incident (or out-incident) to u, or to v, are now in-incident (resp. out-incident) to w; if parallel arcs of the same direction occur, they are substituted by a single arc (of the same direction) with resulting weight obtained by summing the weights of former arcs; the same applies for parallel loops at w. This is illustrated in Fig. 2 (the weights of the arcs not involved in the contraction are not depicted).

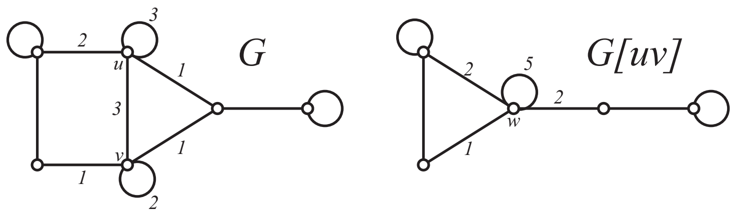

Fig. 2: A multi-graph G and the graph $G[uv]$.

A similar approach is used to define $G\langle uv\rangle$. Denote by $\overrightarrow{u*}$ ($\overrightarrow{*v}$) the set of arcs (including loops) out-coming from u (resp. in-coming to v). Let $G^*_{uv} = G - \overrightarrow{u*} - \overrightarrow{*v} - \overrightarrow{vu}$. So G^*_{uv} does not have arcs between u and v, nor loops at u and v. Let $G\langle uv\rangle$ be the digraph obtained from G^*_{uv} by contracting u and v. So $G\langle uv\rangle = G^*_{uv}[uv]$. Similarly we define $G\langle vu\rangle$. In Fig. 3 we depict a weighted digraph G and the digraph $G\langle uv\rangle$ (the weight of arcs not involved in the contraction are not depicted).

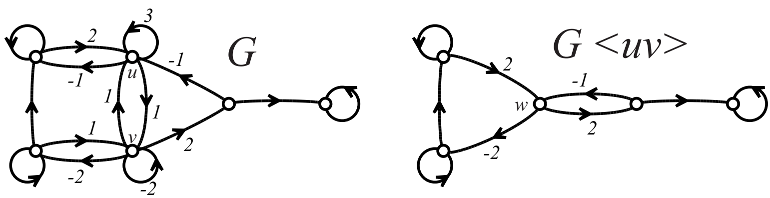

Fig. 3: A weighted digraph G and the graph $G\langle uv\rangle$.

Theorem 2.6. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. Let $\overrightarrow{uv}$ $(u \neq v)$ be a fixed arc of G. Then*

$$\phi(G) = \phi(G - \overrightarrow{uv}) + a_{uv}\phi(G\langle uv\rangle) - a_{uv}(x + a_{vu})\phi(G - u - v),$$

where all graphs in question are defined as above.

Theorem 2.7. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. Let $\overrightarrow{uv}$ and $\overrightarrow{vu}$ $(u \neq v)$ two arcs of G. Then*

$$\begin{aligned}\phi(G) &= \phi(G - \overrightarrow{uv} - \overrightarrow{vu}) + a_{uv}\phi(G\langle uv\rangle) + a_{vu}\phi(G\langle vu\rangle) \\ &\quad -[(a_{uv} + a_{vu})x + a_{vu}a_{vu}]\phi(G - u - v),\end{aligned}$$

where all graphs in question are defined as above.

Theorem 2.8. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. Let uv $(u \neq v)$ be a fixed edge of G of weight ω $(= a_{uv} = a_{vu})$. Then*

$$\phi(G) = \phi(G - uv) + 2\omega\phi(G\langle uv\rangle) - (2\omega x + \omega^2)\phi(G - u - v),$$

where all graphs in question are defined as above.

Theorem 2.9. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. Let uv $(u \neq v)$ be a fixed edge of G, and ω $(= a_{uv} = a_{vu})$. Then*

$$\phi(G) = \phi(G - uv) + \omega\phi(G[uv]) + \omega(x - \omega)\phi(G - u - v) - \omega\phi(G - u) - \omega\phi(G - v),$$

where all graphs in question are defined as above.

3 Permanent variant

In this section we finally give the permanent variant of the formulas reported in Section 2. Note that these formulas can be also considered as matrix formulas. As already noted, we will give just few proofs and we refer the reader to follow [2] in order to reproduce the remaining ones.

In sequel we assume that $\pi(G) = \pi(A) = \mathrm{per}(xI - A)$, where $G = G_A$. Let $B = xI - A$ (so $\mathrm{per}(B) = \mathrm{per}(xI - A)$). Then G_B has a loop of weight $x - a_{ii}$ at vertex i, and an arc of weight $-a_{ij}$ between vertices i and j (directed from i to j).

We next assume that $\dot{\bigcup}_{i=1}^{k}\mathcal{F}_i$ is a partition of $\mathcal{F}_B$. Then from (1) we get

$$\pi(G) = \mathrm{per}(B) = \sum_{i=1}^{k}\sum_{F\in\mathcal{F}_i}\omega_B(F). \tag{2}$$

This simple observation leads to the following results.

Theorem 3.1. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. If v is a fixed vertex of G then*

$$\pi(G) = (x - a_{vv})\pi(G - v) + \sum_{\overrightarrow{C}\in\mathcal{C}_v}(-1)^{l(\overrightarrow{C})}\omega_A(\overrightarrow{C})\pi(G - \mathcal{V}(\overrightarrow{C})),$$

where $\mathcal{C}_v$ is the set of directed cycles of G of length ≥ 2 passing through v, while $\omega_A(\overrightarrow{C}) = \prod_{\overrightarrow{ij}\in\mathcal{A}(\overrightarrow{C})} a_{ij}$.

Proof. Let $B = xI - A$, and consider G_B, the Coates digraph of B, so $\pi(G) = \mathrm{per}(B)$. To apply (2), we first partition $\mathcal{F}_B$. Let $F \in \mathcal{F}_B$. Then $F = \overrightarrow{C_v}\dot{\cup}\hat{F}$, where $\overrightarrow{C_v}$ is a cycle passing through v, while $\hat{F}$ a factor in $G - \mathcal{V}(\overrightarrow{C_v})$. Let $l(\overrightarrow{C})$ be the length of corresponding cycle. Then we distinguish the following subsets (partition cells) of $\mathcal{F}_B$:

- $\mathcal{F}_1 = \{F : l(\overrightarrow{C_v}) = 1\}$;
- $\mathcal{F}_2 = \{F : l(\overrightarrow{C_v}) \geq 2\}$.

Given $F = \overrightarrow{C_v}\dot{\cup}\hat{F}$, then $\omega_B(F) = \omega_B(\overrightarrow{C_v})\omega_B(\hat{F})$. Therefore we have:

(i) $\sum_{F\in\mathcal{F}_1}\omega_B(F) = (x - a_{vv})\sum_{\hat{F}\in\mathcal{F}_{\hat{B}}}\omega_{\hat{B}}(\hat{F})$, where $\hat{B} = B - v$ is obtained from B by deleting its v-th row and column. So we have

$$\sum_{F\in\mathcal{F}_1}\omega_B(F) = (x - a_{vv})\pi(G - v).$$

(ii) $\sum_{F\in\mathcal{F}_2}\omega_B(F) = \sum_{\overrightarrow{C}\in\mathcal{C}_v}(-1)^{l(\overrightarrow{C})}\omega_A(\overrightarrow{C})\sum_{\hat{F}\in\mathcal{F}_{\hat{B}}}\omega_{\hat{B}}(\hat{F})$,
where $\hat{B} = B - \mathcal{V}(\overrightarrow{C})$ is obtained from B by deleting the rows and columns indexed by vertices from $\mathcal{V}(\overrightarrow{C})$ (note, $\omega_B(\overrightarrow{C}) = (-1)^{l(\overrightarrow{C})}\omega_A(\overrightarrow{C})$). So we have

$$\sum_{F\in\mathcal{F}_2}\omega_B(F) = \sum_{\overrightarrow{C}\in\mathcal{C}_v}(-1)^{l(\overrightarrow{C})}\omega_A(\overrightarrow{C})\pi(G - \mathcal{V}(\overrightarrow{C})).$$

The rest of the proof easily follows. $\square$

In the case of symmetric matrices we easily deduce the following result:

Theorem 3.2. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. If v is a fixed vertex of G then*

$$\begin{aligned}\pi(G) &= (x - a_{vv})\pi(G - v) + \sum_{u \neq v} a_{uv}^2 \pi(G - u - v) \\ &+ 2 \sum_{C \in \mathcal{C}_v} (-1)^{l(\overrightarrow{C})} \omega_A(C) \pi(G - \mathcal{V}(C)),\end{aligned}$$

where $\mathcal{C}_v$ is a set of all undirected cycles of G of length ≥ 3 passing through v, while $\omega_A(C) = \prod_{ij \in \mathcal{E}(C)} a_{ij}$.

Theorem 3.3. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. If $\overrightarrow{uv}$ $(u \neq v)$ is a fixed arc of G then*

$$\pi(G) = \pi(G - \overrightarrow{uv}) + (a_{uv}a_{vu})\pi(G - u - v) + \sum_{\overrightarrow{C} \in \mathcal{C}_{\overrightarrow{uv}}} (-1)^{l(\overrightarrow{C})} \omega_A(\overrightarrow{C}) \pi(G - \mathcal{V}(\overrightarrow{C})),$$

where $\mathcal{C}_{\overrightarrow{uv}}$ is the set of all directed cycles of G of length ≥ 3 passing through $\overrightarrow{uv}$, while $\omega_A(\overrightarrow{C}) = \prod_{\overrightarrow{ij} \in \mathcal{A}(\overrightarrow{C})} a_{ij}$.

Theorem 3.4. *Let $G \cdot H$ be the coalescence of two rooted weighted digraphs G and H whose roots are u and v, respectively. Then*

$$\pi(G \cdot H) = \pi(G)\pi(H - v) + \pi(G - u)\pi(H) - x\pi(G - u)\pi(H - v).$$

We now consider the permanental variant of Rowlinson-like formulas given in Section 2. We will prove just the first one and we again refer the readers to [2] to reproduce the remaining ones. Let $a = \overrightarrow{uv}$ be an arc in A, so we consider the following partition for the factor space of $B = xI - A$:

(i) $\mathcal{F}_1$ with $F \in \mathcal{F}_1$ if F does not contain a;

(ii) $\mathcal{F}_2$ with $F \in \mathcal{F}_2$ if F contains a and a';

(iii) $\mathcal{F}_3$ with $F \in \mathcal{F}_3$ if F contains a, but not a'.

$\mathcal{F}_3$ is the term which gives rise to sum over all cycles passing through a in A. In next lemma we can express the contribution of $\mathcal{F}_3$ by the permanental polynomial of some graphs in which the arc a is contracted.

Lemma 3.5. *Let A be any square matrix. Under the above notation we have*

$$\sum_{F\in\mathcal{F}_3}\omega_B(F) = -a_{uv}\pi(G\langle uv\rangle) + a_{uv}x\pi(G-u-v).$$

Proof. Let $B = xI - A$, and consider G_B, the Coates digraph of B, so $\pi(G) = \mathrm{per}(B)$. Next, let $a = \overrightarrow{uv}$. If $F \in \mathcal{F}_3$ then $F = \overrightarrow{C_a}\dot{\cup}\hat{F}$, where $\overrightarrow{C_a}$ is a cycle (of length ≥ 3) passing through a. Observe first that the arcs $\overrightarrow{ut}$ $(t \neq v)$, $\overrightarrow{sv}$ $(s \neq u)$ and $\overrightarrow{vu}$ do not belong to F. So, they can be ignored, or equivalently, we can assume that F is a factor of $G^*_{uv} + \overrightarrow{uv}$ (note, G^*_{uv} has no loops at u and v). Let $G\langle uv\rangle$ be the digraph obtained from G^*_{uv} by contracting u and v. Note, that after this contraction arcs in-coming to w were those in-coming to u, and arcs out-coming from w were those out-coming from v; in addition, there are no loops at w $(= u = v)$. After this contraction, F becomes $F' = \overrightarrow{C'_w}\dot{\cup}\hat{F}$, where $\overrightarrow{C'_w}$ is a cycle passing through w resulting from $\overrightarrow{C_a}$ by a contraction (note that its length is ≥ 2). Let A' be the adjacency matrix of $G\langle uv\rangle$ and $B' = xI - A'$. So F' runs over all factors of B' containing a cycle at w of length at least two. Then we have

$$\sum_{F\in\mathcal{F}_3}\omega_B(F) = -a_{uv}\sum_{F'\in\mathcal{F}'_2}\omega_{B'}(F'),$$

where $\mathcal{F}'_2 = \{F' : F \in \mathcal{F}_3\}$ in view of bijection $F \leftrightarrow F'$ (note, $F' \in \mathcal{F}_{B'}$ and $l(\overrightarrow{C'_w}) \geq 2$; in addition $\omega_B(F) = -a_{uv}\omega_{B'}(F')$). On the other hand (cf. Theorem 3.1) we have

$$\pi(G\langle uv\rangle) = x\pi(G\langle uv\rangle - w) + \sum_{F'\in\mathcal{F}'_2}\omega_{B'}(F').$$

Since $G\langle uv\rangle - w = G - u - v$, we have

$$\pi(G\langle uv\rangle) = x\pi(G-u-v) + \sum_{F'\in\mathcal{F}'_2}\omega_{B'}(F').$$

Therefore we have

$$\sum_{F\in\mathcal{F}_3}\omega_B(F) = -a_{uv}\sum_{F'\in\mathcal{F}'_2}\omega_{B'}(F') = -a_{uv}[\pi(G\langle uv\rangle) - x\pi(G-u-v)],$$

as required. □

We can now prove the formula given in the following theorem:

Theorem 3.6. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. Let $\overrightarrow{uv}$ $(u \neq v)$ be a fixed arc of G. Then*

$$\pi(G) = \pi(G - \overrightarrow{uv}) - a_{uv}\pi(G\langle uv\rangle) + a_{uv}(x + a_{vu})\pi(G-u-v),$$

where all graphs in question are defined as above.

Proof. Consider the matrix $B = xI - A$ and apply (2) to subsets $\mathcal{F}_1$, $\mathcal{F}_2$ and $\mathcal{F}_3$, (see items (i)–(iii) from above). So we have (for item (iii) cf. Lemma 3.5):

(i) $\sum_{F\in\mathcal{F}_1} \omega_B(F) = \pi(G - \overrightarrow{uv});$

(ii) $\sum_{F\in\mathcal{F}_2} \omega_B(F) = a_{uv}a_{vu}\pi(G - u - v);$

(iii) $\sum_{F\in\mathcal{F}_3} \omega_B(F) = -a_{uv}[\pi(G\langle uv\rangle) - x\pi(G - u - v)].$

The rest of the proof easily follows. $\square$

The following corollary easily follows from two consecutive applications of Theorem 3.6: first to G (with respect to arc $\overrightarrow{uv}$), and next to $G - \overrightarrow{uv}$ (with respect to arc $\overrightarrow{vu}$).

Corollary 3.7. *Let A be any square matrix, and let G $(= G_A)$ be its Coates digraph. Let $\overrightarrow{uv}$ and $\overrightarrow{vu}$ $(u \neq v)$ two arcs of G. Then*

$$\begin{aligned}\pi(G) \;&=\; \pi(G - \overrightarrow{uv} - \overrightarrow{vu}) - a_{uv}\pi(G\langle uv\rangle) - a_{vu}\pi(G\langle vu\rangle)\\ &\quad +[(a_{uv} + a_{vu})x + a_{vu}a_{vu}]\pi(G - u - v),\end{aligned}$$

where all graphs in question are defined as above.

If A is a symmetric matrix, from the above corollary we can immediately the following formula:

Theorem 3.8. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. Let uv $(u \neq v)$ be a fixed edge of G of weight ω $(= a_{uv} = a_{vu})$. Then*

$$\pi(G) \;=\; \pi(G - uv) - 2\omega\pi(G\langle uv\rangle) + (2\omega x + \omega^2)\pi(G - u - v),$$

where all graphs in question are defined as above.

Proof. In the symmetric case we first put in the formula from Corollary 2.7 that $G-\overrightarrow{uv}-\overrightarrow{vu} = G - uv$, and next substitute a_{uv} and a_{vu} by ω. Then we observe that $G\langle uv\rangle$ and $G\langle vu\rangle$ are the converse digraphs. So their adjacency matrices are the transpose of each other. Therefore $\pi(G\langle uv\rangle) = \pi(G\langle vu\rangle)$, and the proof follows. $\square$

Theorem 3.9. *Let A be any symmetric matrix, and let G $(= G_A)$ be its Coates digraph. Let uv $(u \neq v)$ be a fixed edge of G, and ω $(= a_{uv} = a_{vu})$. Then*

$$\pi(G) \;=\; \pi(G - uv) - \omega\pi(G[uv]) + \omega(\omega - x)\pi(G - u - v) + \omega(\pi(G - u) + \pi(G - v)),$$

where all graphs in question are defined as above.

Remark 3.1. *Two facts deserve to be mentioned. First, if G is an empty graphs, i.e. without vertices, then $\pi(G) = 1$. Secondly, it is worth noting that now the Rowlinson-like formulas cannot be obtained alternatively by algebraic manipulations as it was the case for the characteristic polynomials, where elementary row and column transformations for determinants are allowed.*

4 Appendix

In this appendix we give some examples for the formulas shown in Section 3. In the figures, the vertices are labelled with letters so that $a = 1, b = 2, \ldots$, while the weights will be reported close to the corresponding arcs.

Example 4.1 Let A be the matrix in Fig. 1 and G be the corresponding Coates digraph associated to A. We now consider the formula from Theorem 3.3 and apply it to the arc $\overrightarrow{ab}$. The (oriented) cycles through $\overrightarrow{ab}$ of length ≥ 3 are $\overrightarrow{C_1} = \overrightarrow{abc}$ and $\overrightarrow{C_2} = \overrightarrow{abcd}$, with $(-1)^{l(\overrightarrow{C_1})}\omega(\overrightarrow{C_1}) = -2$ and $(-1)^{l(\overrightarrow{C_2})}\omega(\overrightarrow{C_2}) = 1$. Hence

$$\pi(G) \quad = \quad \pi(G - \overrightarrow{ab}) - \pi(G - a - b) - 2\pi(G - a - b - c) + \pi(\emptyset)$$

Since $\pi(G - \overrightarrow{ab}) = x^4 - 2x^3 - 3x^2 + 4x + 4$, $\pi(G - a - b) = x(x - 2)$, $\pi(G - a - b - c) = x$ and $\pi(\emptyset) = 1$, we get

$$\pi(G) = x^4 - 2x^3 - 4x^2 + 4x + 5,$$

that is the permanental polynomial of the matrix A. $\square$

Example 4.2 We consider the same matrix A from the latter example and we make use of the formula from Theorem 3.6 applied to the arc $\overrightarrow{ab}$. We now depict in Fig. 4 the graphs G and $G\langle ab\rangle$, in which w is the vertex arising from the contraction.

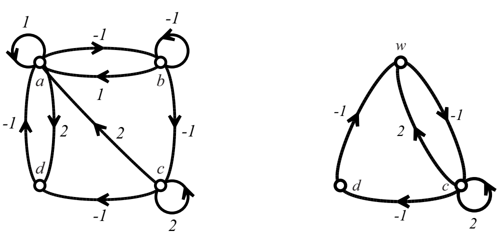

Fig. 4: The graphs G and $G\langle ab\rangle$.

It is easy to check that $\pi(G\langle ab\rangle) = x^3 - 2x^2 - 2x + 1$. We have:

$$\begin{aligned}\pi(G) &= \pi(G - \overrightarrow{ab}) + \pi(G\langle ab\rangle) - (x+1)\pi(G - a - b)\\ &= x^4 - 2x^3 - 4x^2 + 4x + 5,\end{aligned}$$

by Theorem 3.6. □

To conclude this paper, we give an example for the formula of Theorem 3.9 related to symmetric matrices, i.e. weighted undirected graphs.

Example 4.3 Let A, G and $G[ab]$ be defined as in Fig. 5.

$$A = \begin{bmatrix} 0 & 2 & -1 & -2 \\ 2 & -1 & 2 & 0 \\ -1 & 2 & 3 & 1 \\ -2 & 0 & 1 & -1 \end{bmatrix}$$

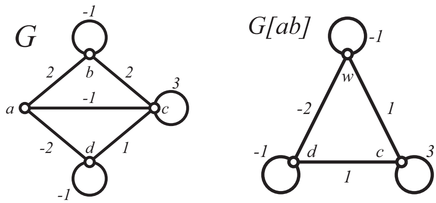

Fig. 5: The matrix A, its corresponding Coates digraph G and the graph $G[ab]$.

Now we have:

$$\begin{aligned}\pi(G) &= \pi(G - ab) - 2\pi(G[ab]) + 2(2-x)\pi(G - a - b) + 2(\pi(G-a) + \pi(G-b))\\ &= (x^4 - x^3 + 5x^2 - 8x + 1) - 2(x^3 - x^2 + x - 9) + 2(2-x)(x^2 - 2x - 2)\\ &\quad +2((x^3 - x^2 + 2) + (x^3 - 2x^2 + 3x - 15))\\ &= x^4 - x^3 + 9x^2 - 8x - 15,\end{aligned}$$

by Theorem 3.9. □

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References

[1] F. Belardo, E. M. Li Marzi, S. K. Simić, Schwenk-like formulas for weighted digraphs, in: T. E. Simos, G. Psihoyios, C. Tsitouras (Eds.), *Numerical Analysis and Applied Mathematics* **CP1168** vol. 2 (2009) 1251–1254.

[2] F. Belardo, E. M. Li Marzi, S. K. Simić, Combinatorial approach for computing the characteristic polynomial of a matrix, *Lin. Algebra Appl.* **433** (2010) 1513–1523.

[3] M. Borowiecki, T. Jóźwaik, Computing the characteristic polynomial of a multigraph, *Demonstr. Math.* **14** (1981) 361–370.

[4] M. Borowiecki, T. Jóźwaik, *On characteristic and permanental polynomials of multigraphs*, Report IF–3–80 WSInž, Inst. Mat. Finz., Zielona Góra, 1980.

[5] R. Brualdi, D. Cvetković, *A Combinatorial Approach to Matrix Theory and its Applications*, CRC Press, Boca Raton, 2008.

[6] G. G. Cash, The permanental polynomial, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1203–1206.

[7] G. G. Cash, Permanental polynomials of the smaller fullerenes, *J. Chem. Inf. Comput. Sci.* **40** (2000) 1207–1209.

[8] G. G. Cash, A fast computer algorithm for finding the permanent of adjacency matrices, *J. Math. Chem.* **18** (1995) 115–119.

[9] G. G. Cash, Permanents of adjacency matrices of fullerenes, *Polyc. Arom. Comp.* **12** (1997) 61–69.

[10] G. G. Cash, A differential–operator approach to the permanental polynomial, *J. Chem. Inf. Comput. Sci.* **42** (2002) 1132–1135.

[11] G. G. Cash, I. Gutman, The Lapacian permanental polynomial: formulas and algorithms, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 129–136.

[12] R. S. Chen, A note on the relations between the permanental and characteristic polynomials of coronoid hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 137–148.

[13] C. L. Coates, Flow-graph solutions of linear algebraic equations, in *IRE Trans. Circuit Theory* **CT-6** (1959) 170–187.

[14] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs - Theory and Applications*, Bart Verlag, Heidelberg, 1995.

[15] D. Cvetković, P. Rowlinson, S. Simić, *An Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.

[16] P. Diaconis, R. Graham, S. P. Holmes, *Statistical problems involving permutations with restricted positions* (1999), available at `http://www-stat.stanford.edu/cgates/PERSI/papers/perm8.ps`.

[17] S. Friedland, B. Rider, O. Zeitouni, Concentration of permanent estimators for certain large matrices, *Ann. Appl. Prob.* **14** (2004) 1559-1576.

[18] I. Gutman, G. G. Cash, Relations between the permanental and characteristic polynomials of fullerenes and benzenoid hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **45** (2002) 55–70.

[19] F. Harary, *Graph Theory*, Addison–Wesley, Reading, 1969.

[20] A. R. Kräuter, Permanenten – ein kurzer Überblick, Seminaire Lotharingien de Combinatoire, B09b (1983); available at `http://www.emis.ams.org/journals/SLC/opapers/s09kraeu.pdf`.

[21] V. R. Rosenfeld, I. Gutman, A novel approach to graph polynomials, *MATCH Commun. Math. Comput. Chem.* **24** (1989) 191–199.

[22] P. Rowlinson, A deletion-contraction algorithm for the characteristic polynomial of a multigraph, *Proc. Roy. Soc. Edinburgh* **105A** (1987) 153–160.

[23] A. J. Schwenk, Computing the characteristic polynomial of a graph, in: R. Bari, F. Harary (Eds.), *Graphs and Combinatorics*, Springer–Verlag, Berlin, 1974, pp. 153–172.

[24] L. G. Valiant, The complexity of computing the permanent, *Theor. Comput. Sci.* **8** (1979) 189–201

[25] J. Wosiek , A simple formula for Bose–Einstein corrections, *Phys. Lett. B* **399** (1997) 130–135.

[26] W. G. Yan, F. J. Zhang, On the permanental polynomials of some graphs, *J. Math. Chem.* **35** (2004) 175–188.