Some analytical properties of the permanental polynomial of a graph

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Abstract

Let G be a graph and $\pi(G,x)$ its permanental polynomial. A vertex-deleted subgraph of G is a subgraph $G-v$ obtained by deleting from G vertex v and all edges incident to it. In this paper, we show that the derivative of permanental polynomial of G equals the sum of permanental polynomials of all vertex-deleted subgraphs of G. Furthermore, we discuss permanental polynomial version of Gutman's problem [Research problem 134, Discrete math. 88 (1991) 105-106], and give a solution.

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1 Introduction

By a graph G we mean a simple undirected graph, with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. For notation and terminologies not defined here, we refer the readers to [7].

The *permanent* of an $n \times n$ matrix M with entries m_{ij} $(i,j = 1, 2, \cdots, n)$ is defined by

$$\mathrm{per(M)} = \sum_{\sigma} \prod_{i=1}^{n} m_{i\sigma(i)},$$

where the sum is taken over all permutations σ of $\{1, 2, \cdots, n\}$. In contrast to determinants, computing permanents, even of matrices in which all entries are 0 or 1, is #P-complete [25].

Let $A(G)$ denote the adjacency matrix of G. The *characteristic polynomial* of G is defined by

$$\phi(G,x) = \det(xI - A(G) = \sum_{k=0}^{n} a_k(G) x^{n-k}, \qquad (1)$$

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where I is the unit matrix of order n. Analogously, one defines the *permanental polynomial* of G, $\pi(G,x)$, as

$$\pi(G,x) = \operatorname{per}(xI - A(G)) = \sum_{k=0}^{n} b_k(G)x^{n-k}. \tag{2}$$

A *Sachs graph* is a simple graph, each component of which is 1 or 2-regular. In other words, the components are single edges and cycles. Let H be a graph with k vertices. Denote by $\omega(H)$ the number of components in H and by $c(H)$ the number of cycles in H. Merris et al. obtained a modified Sachs theorem on the permanental polynomial of a graph as follows.

Theorem 1. *([22]) Let G be a graph with $\pi(G,x) = \sum_{k=0}^{n} b_k(G)x^{n-k}$. Then*

$$b_k(G) = (-1)^k \sum_{H} 2^{c(H)}, 1 \le k \le n, \tag{3}$$

where the sum is taken over all Sachs subgraphs H of G on k vertices.

Graph polynomials play an outstanding role in mathematical chemistry. The characteristic polynomials of graphs are extensively examined, see [7, 8, 9, 10, 23, 24]. The permanental polynomials of graphs were first systematically studied by Merris et al. [22], and the study of analogous objects in chemical literature were started by Kasum et al. [16]. Let G be a tree with n vertices, Merris et al. [22] proved that

$$\text{if } \phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{2k}x^{n-2k} \text{ then } \pi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k a_{2k}x^{n-2k}.$$

This result was generalized by Borowiechi [2] as follows. If G is a bipartite graph containing no cycle of length $4t$, $t \in \{1,2,\ldots\}$, and $\phi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} a_{2k}x^{n-2k}$, then $\pi(G,x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k a_{2k}x^{n-2k}$. Up to now, some papers about the permanental polynomial and its potential applications have been published [1, 3, 4, 5, 20, 17, 21, 26, 27, 28]. In general it is difficulty to compute the permanent $\operatorname{per}(xI - A)$.

For any graph polynomial, it is of interest to characterize its expression of the derivative. Clarke [6] first examined the derivative of the characteristic polynomial. Gutman and Hosoya [12] examined the derivative of the matching polynomial. Hoede and Li [15] gave the formulas of derivatives of the clique polynomial and the independence polynomial. Furthermore, Li and Gutman [18] introduced a general graph polynomial as follows. Let $f(\Lambda)$ be a complex-valued function defined on the set of all graphs Λ such that $\Lambda_1 \cong \Lambda_2$ implies $f(\Lambda_1) = f(\Lambda_2)$. Let G be a graph on n vertices and $S(G)$ the set of all subgraphs of G. Define $S_k(G) = \{\Lambda | \Lambda \in S(G) \text{ and } |V(\Lambda)| = k\}$ and $p(G,k) = \sum_{\Lambda \in S_k(G)} f(\Lambda)$. The general graph polynomial of G is defined as

$$P(G,x) = \sum_{k=0}^{n} p(G,k) x^{n-k}.$$

It is easy to verify that the characteristic, matching, clique and independence polynomials are just special cases of general graph polynomial. Additionally, Li and Gutman gave the formula of derivative of $P(G,x)$, which has the following expression:

$$\frac{d}{dx} P(G,x) = \sum_{v \in V(G)} p(G-v,x). \tag{4}$$

Let

$$f(\Lambda) = \begin{cases} (-1)^{|V(\Lambda)|} 2^{c(\Lambda)} & \text{if all components of } \Lambda \text{ are 1 or 2-regular,} \\ 0 & \text{otherwise.} \end{cases}$$

The resulting polynomial is the permanental polynomial. That is

$$P(G,x) = \pi(G,x),$$

which implies, by (4), that

Theorem 2. *Let G be a graph. Then*

$$\frac{d}{dx} \pi(G,x) = \sum_{v \in V(G)} \pi(G-v,x). \tag{5}$$

Gutman [13] proposed a research problem which is stated as follows.

By $m(G,k)$ we denote the number of k-matchings of the graph G. The *matching polynomial* of the graph G is defined as

$$\alpha(G,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(G,k) x^{n-2k}.$$

Define

$$\alpha(G,x,y) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(G,k) x^{n-2k} y^k.$$

It is not difficult to determine that

$$\frac{\partial \alpha(G,x,y)}{\partial y} = - \sum_{uv\in E(G)} \alpha(G-u-v,x,y). \tag{6}$$

If G is a bipartite graph, then the characteristic polynomial of G can be written as

$$\phi(G,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k a(G,k) x^{n-2k}.$$

Define

$$\phi(G,x,y) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k a(G,k) x^{n-2k} y^k.$$

Is there a formula for $\partial\phi(G,x,y)/\partial y$ analogous to (6)? Li and Zhang [19] gave a solution to the above problem. Additionally, Gutman et al. [14] used a different method to answer the above problem for an arbitrary graph. The solution is demonstrated as follows.

$$\begin{aligned} \frac{\partial \phi(G,x,y)}{\partial y} &= - \sum_{uv\in E(G)} \phi(G-u-v,x,y) \\ &\quad - \sum_{C\in \mathscr{C}(G)} |C| y^{\frac{|C|-2}{2}} \phi(G-V(C),x,y). \end{aligned} \tag{7}$$

Note that $\alpha(G,x,y) = y^{n/2}\alpha(G,xy^{-1/2})$. For any graph G, we may define the permanental-polynomial-equivalent of $\alpha(G,x,y)$ as:

$$\pi(G,x,y) = \sum_{k=0}^{n} b_k(G) x^{n-k} y^{k/2}.$$

Is there a formula for $\partial\pi(G,x,y)/\partial y$ analogous to (6) or (7)?

In this paper, we answer the above problem, and give an expression of $\partial\pi(G,x,y)/\partial y$ as follows.

Theorem 3. *Let $\mathscr{C}(G)$ be the set consisting of all cycles in G. Then*

$$\begin{aligned} \frac{\partial \pi(G,x,y)}{\partial y} &= \sum_{uv\in E(G)} \pi(G-u-v,x,y) \\ &\quad + \sum_{C\in \mathscr{C}(G)} (-1)^{|C|} |C| y^{\frac{|C|-2}{2}} \pi(G-V(C),x,y). \end{aligned} \tag{8}$$

2 Proof of Theorem 3

We will prove it by comparing the coefficients of $x^{n-k}y^{k/2-1}$ on the two sides of Eq. (8). By Theorem 1, we know that the coefficient on the left-hand side of Eq. (8) is

$$\frac{k}{2}b_k(G) = \frac{k}{2}(-1)^k \sum_H 2^{c(H)},$$

where the sum is taken over all Sachs subgraphs H of G on k vertices.

Let $|C|$ be the number of edges or vertices in C. By checking Eq. (8), we can obtain that the coefficient in the first sum on the right-hand side of Eq. (8) is

$$\sum_{uv \in E(G)} b_{k-2}(G-u-v),$$

and the coefficient in the second sum on the right-hand side of Eq. (8) is

$$\sum_{C \in \mathscr{G}(G)} (-1)^{|C|}|C| b_{k-|C|}(G-V(C)).$$

Thus, we know that the coefficient on the right-hand side of Eq. (8) is

$$\begin{aligned} &\sum_{uv \in E(G)} b_{k-2}(G-u-v) + \sum_{C \in \mathscr{G}(G)} (-1)^{|C|}|C| b_{k-|C|}(G-V(C)) \\ = &\sum_{uv \in E(G)} (-1)^{k-2} \sum_{H'} 2^{c(H')} + \sum_{C \in \mathscr{G}(G)} (-1)^{|C|}|C|(-1)^{k-|C|} \sum_{H''} 2^{c(H'')}, \quad (9) \end{aligned}$$

where H' takes over all Sachs subgraphs of $G-u-v$ with $k-2$ vertices, and H'' over all Sachs subgraphs of $G-V(C)$ with $k-|C|$ vertices. Therefore, (9) can be written as

$$\sum_{uv \in E(G)} (-1)^k \sum_H 2^{c(H)} + \sum_{C \in \mathscr{G}(G)} (-1)^{|C|}|C|(-1)^{k-|C|} \sum_H 2^{c(H)-1}, \quad (10)$$

where the first sum H takes over all Sachs subgraphs of G with k vertices containing the single edge uv as a componment, and the second sum H runs over all Sachs subgraphs of G which has k vertices and contains cycle C. Since uv takes over all edges of G, and C runs over the set $\mathscr{G}(G)$, (10) can be written as

$$
\begin{aligned}
&\sum_{uv\in E(G)}(-1)^k\sum_H 2^{c(H)}+\sum_{C\in\mathscr{C}(G)}(-1)^{|C|}|C|(-1)^{k-|C|}\sum_H 2^{c(H)-1}\\
=&\sum_H(-1)^k\sum_{uv\subset H}2^{c(H)}+\sum_H\frac{|C|}{2}(-1)^k\sum_{C\subset H}2^{c(H)}\\
=&(-1)^k\sum_H 2^{c(H)}\left(\sum_{uv\subset H}1+\sum_{C\subset H}\frac{|C|}{2}\right)\\
=&(-1)^k\sum_H 2^{c(H)}\left(\omega(H)-c(H)+\sum_{C\subset H}\frac{|C|}{2}\right), \qquad (11)
\end{aligned}
$$

where H runs over all Sachs subgraphs of G with k vertices. Since H contains $\omega(H)-c(H)$ single edges and $c(H)$ cycles, we have that

$$\frac{k}{2}=\omega(H)-c(H)+\sum_{C\subset H}\frac{|C|}{2}. \qquad (12)$$

By (11) and (12), we obtain that the coefficient on the right-hand side of (8) is

$$\frac{k}{2}(-1)^k\sum_H 2^{c(H)}.$$

This completes the proof of Theorem 3.

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