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THE LAPACIAN PERMANENTAL POLYNOMIAL: FORMULAS AND ALGORITHMS

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Abstract

This study extends relationships previously demonstrated (Gutman, MATCH Commun. Math. Comput. Chem. **47** (2003) 133-140) between the ordinary and Laplacian characteristic polynomials to the ordinary and Laplacian permanental polynomials. Various formulas relating the ordinary and Laplacian permanental polynomials are evaluated for their efficiency as algorithms for calculating the Laplacian permanental polynomials of chemical graphs.

INTRODUCTION

Let G be a graph on n vertices and $A(G)$ be its adjacency matrix. Further, let $D(G)$ be a diagonal matrix with elements equal to the vertex degrees of G, with the vertices taken in the same order as in $A(G)$. Then, $L(G) = D(G) - A(G)$ is the Laplacian matrix of G. In some earlier literature, this matrix is called the matrix of admittance, a term taken from the theory of electrical networks [1]. In the same context, the term Kirchhoff matrix is sometimes encountered [2].

Adopting and extending notation previously used [3-5], we call the characteristic polynomials of these matrices $\phi^-(G) = \phi^-(G,\lambda) = \det[\lambda I_n - A(G)]$ and $\psi^-(G) = \psi^-(G,\lambda) = \det[\lambda I_n - L(G)]$, and the permanental polynomials $\phi^+(G) = \phi^+(G,\lambda) = \mathrm{per}[\lambda I_n - A(G)]$ and $\psi^+(G) = \psi^+(G,\lambda) = \mathrm{per}[\lambda I_n - L(G)]$. We express the characteristic polynomials in coefficient form, as in [5]:

$$\phi^-(G,\lambda) = \sum_j a_j(G)\,\lambda^{n-j} \quad ; \quad \psi^-(G,\lambda) = \sum_j (-1)^j c_j(G)\,\lambda^{n-j} \tag{1}$$

and by extension,

$$\phi^+(G,\lambda) = \sum_j p_j(G)\,\lambda^{n-j} \quad ; \quad \psi^+(G,\lambda) = \sum_j (-1)^j q_j(G)\,\lambda^{n-j} \tag{2}$$

In this notation, all the coefficient c_j and q_j are non-negative, while the a_j and p_j may take on any integer value. As noted in [5], an immediate consequence of (1) is

$$(-1)^n \psi^-(G,-\lambda) = \sum_j c_j(G)\,\lambda^{n-j}. \tag{3}$$

By extension,

$$(-1)^n \psi^+(G,-\lambda) = \sum_j q_j(G)\,\lambda^{n-j}. \tag{4}$$

In the discussion below, we will describe subgraphs of G in the following way. Let k distinct vertices of G be $v_{r_1}, v_{r_2}, \ldots, v_{r_k}$. Then the $(n-k)$-vertex subgraph obtained by deleting these vertices from G is denoted by $G_{r_1 r_2 \ldots r_k}$. More specifically, G_r is the $(n-1)$-vertex

subgraph obtained from G by deleting the vertex v_r, $G_{r,s}$ is the (n – 2)-vertex subgraph obtained by deleting v_r and v_s, etc. Additionally, we denote by $G[h_r]$ the graph G which has been modified by adding a loop of weight h_r to vertex v_r, and, more generally, by $G[h_1, h_2, h_3, \ldots, h_n]$ the graph obtained by adding a loop of weight h_k, to each vertex v_k, $k = 1,2,3,\ldots,n$. This notation may represent any general graph, since some or all of the h_k may be zero.

An established result [5] in this notation is

$$\phi^-(G[h_r]) = \phi^-(G) - h_r\,\phi^-(G_r). \tag{5}$$

The characteristic polynomial of the graph containing the loop is the *difference* between the two characteristic polynomials on the right, because of the alteration of sign in expanding the determinant. The equivalent expression for permanental polynomials is the *sum*

$$\phi^+(G[h_r]) = \phi^+(G) + h_r\,\phi^+(G_r). \tag{6}$$

By applying another iteration to (6), one obtains

$$\phi^+(G[h_r,h_s]) = \phi^+(G[h_r]) + h_s\,\phi^+(G_s[h_r]) = \{\phi^+(G) + h_r\phi^+(G_r)\} + h_s\{\phi^+(G_s) + h_r\,\phi^+(G_{r,s})\},$$

which rearranges to

$$\phi^+(G[h_r,h_s]) = \phi^+(G) + h_r\,\phi^+(G_r) + h_s\,\phi^+(G_s) + h_r\ h_s\,\phi^+(G_{r,s}). \tag{7}$$

Since there is no alteration of sign in expanding the permanent, there is no alteration of signs in Eq. (7). Additional iterations can be made to take into account loops on additional vertices. For loops on all n vertices, the expression becomes

$$\phi^+(G[h_1,h_2,\ldots,h_n]) = \phi^+(G) + \sum_{k=1}^{n} \sum_{r_1<\cdots<r_k} h_{r_1}\cdots h_{r_k}\,\phi^+(G_{r_1\cdots r_k}). \tag{8}$$

Note that the second summation in Eq. (8) is over *all possible combinations* of k vertices.

RESULTS AND DISCUSSION

By combining Eq. (4) with the definitions of the permanental polynomials for the adjacency and Laplacian matrices, we obtain

$$\begin{aligned}(-1)^n \psi^+(G,-\lambda) &= (-1)^n \operatorname{per}[-\lambda I_n - D(G) + A(G)] \\ &= \operatorname{per}[\lambda I_n - A(G) + D(G)] \\ &= \operatorname{per}[\lambda I_n - A(G^*)] = \phi^+(G^*,\lambda),\end{aligned}$$

where $A(G^*) = A(G) - D(G)$, the adjacency matrix of some graph G^*. $A(G)$ and $A(G^*)$ differ only in their diagonal elements, these being all zero in $A(G)$ and equal to the negative vertex degrees, $-d_1, -d_2,\ldots,-d_n$, in $A(G^*)$. Thus, $A(G^*)$ may be viewed as the adjacency matrix of a graph obtained from G by adding to each vertex v_r a loop of weight $-d_r$. In the notation developed above, $G^* \equiv G[-d_1, -d_2,\ldots,-d_n]$, and consequently

$$\phi^+(G[-d_1,-d_2,\ldots,-d_n],\lambda) = (-1)^n \psi^+(G,-\lambda). \tag{9}$$

Combining Eqs. (8) and (9), we have an expression relating the permanental polynomial of the Laplacian matrix of G to the sum of permanental polynomials of all vertex-deleted subgraphs of G:

$$(-1)^n \psi^+(G,-\lambda) = \phi^+(G) + \sum_{k=1}^{n} \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\, \phi^+(G_{r_1\cdots r_k}). \tag{10}$$

In view of the formula (2) for $\phi^+(G,\lambda)$, Eq. (10) may be transformed into

$$(-1)^n \psi^+(G,-\lambda) = \sum_j [p_j(G) + \sum_{k=1}^{j} \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\, p_{j-k}(G_{r_1\cdots r_k})], \tag{11}$$

which, in view of (4), implies

$$q_j(G) = p_j(G) + \sum_{k=1}^{j} \sum_{r_1<\cdots<r_k} d_{r_1}\cdots d_{r_k}\, p_{j-k}(G_{r_1\cdots r_k}). \tag{12}$$

Note that Eqs. (12) and (10) are fully equivalent.

If m is the number of edges in G, then $p_0(G) = 1$, $p_1(G) = 0$, $p_2(G) = m$, and the sum of vertex degrees is $2m$. For $j = 0, 1, 2$, from Eq. (12) we obtain:

$$q_0(G) = p_0(G) = 1$$

$$q_1(G) = p_1(G) + \sum_r d_r\, a_0(G_r) = 0 + \sum_r d_r = 2m$$

$$q_2(G) = p_2(G) + \sum_r d_r\, a_1(G_r) + \sum_{r<s} d_r\, d_s\, a_0(G_{r,s}) = m + 0 + \sum_{r<s} d_r\, d_s$$

$$= m + \left(\frac{1}{2} \sum_r \sum_s d_r\, d_s - \sum_r (d_r)^2 \right) = m + \frac{1}{2}(2m)^2 - \frac{1}{2} \sum_r (d_r)^2$$

$$= 2m^2 + m - \frac{1}{2} \sum_r (d_r)^2$$

Except for signs, these results are analogous to those for characteristic polynomials, reported in in [5]. Note, however, that $q_2(G) - c_2(G) = 2m$. The fact that $q_1(G) = 2m$ was also noticed by Merris [6].

Since all graphs possess a zero Laplacian eigenvalue [2], $c_n(G) = 0$. It has also long been known that $c_{n-1}(G)/n$ equals the number of spanning trees in G. No similar statements apply to $q_n(G)$ and $q_{n-1}(G)$, so formulas for $q_n(G)$ and $q_{n-1}(G)$, analogous to those in [5] for $c_n(G)$ and $c_{n-1}(G)$, based on these equalities cannot be set forth.

ALGORITHMS

While numerous chemical applications of the characteristic polynomial of $A(G)$ have been published (for a recent survey and an exhaustive bibliography see [7]), only in the last decade or so have a few papers on chemical applications of the characteristic polynomial of $L(G)$ begun to appear [2,8-18]. Similarly, and somewhat more recently, chemical applications of the permanental polynomial of $A(G)$ began to appear [19-22]. The permanental polynomial of $L(G)$, on the other hand, as received scant attention in the mathematics literature [6,23-27], and no specific applications to chemical graphs seem to have appeared at all. Merris [26] explicitly identified the difficulty in computing $\psi^*(G,\lambda)$ as a reason for the paucity of studies regarding its

properties. In the present study, we explored mathematical relationships between $\phi^+(G,\lambda)$ and $\psi^+(G,\lambda)$. Specifically, we modified the recently published [5] relationships between $\phi^-(G,\lambda)$ and $\psi^-(G,\lambda)$. Now, we examine the utility of these relationships as computer algorithms for calculating $\psi^+(G,\lambda)$ for graphs of chemical interest.

The fastest published algorithm for computing $\phi^+(G,\lambda)$ appears to be the one described by Cash in [21], which modified an approach by Rosenfeld and Gutman [4] based on applying differential operators to symbolic functions. A drawback to this algorithm is that it requires software capable of manipulating the symbolic functions, specifically, capable of taking partial derivatives with respect to symbolic variables without first assigning numerical values to the variables. Instead, the procedure generates a polynomial in λ by sequentially replacing a series of symbolic variables with the indeterminate λ at various points in the calculation. Using Eq. (9) above, it is straightforward to replace the symbolic variables at each step with $\lambda - d_r$ instead of λ for each vertex v_r. The reversal of sign, $\psi^+(G,-\lambda)$ in (9), is eliminated by using $d_r - \lambda$ in place of $\lambda - d_r$. Thus, the method described in [22] calculates $\psi^+(G,\lambda)$ as easily as $\phi^+(G,\lambda)$.

An earlier and slower method for calculating $\phi^+(G,\lambda)$, also published by Cash [19], basically evaluates Eq. (8) directly. In this algorithm, the problem of evaluating all 2^n possible vertex-deleted subgraphs is addressed by taking advantage of the sparseness of $A(G)$. All 2^n subgraphs are evaluated, but the evaluation tree is pruned as soon as it can be known that the contribution from a particular branch will be zero. The algorithm actually finds the *permanent* of $[A(G) + I]$, keeping count of the number of diagonal elements $a_{i,i}$ in each summation. Thus, a contribution to per$[A(G) + I]$ that contains k diagonal elements contributes to the coefficient of x^k in $\phi^+(G,\lambda)$. Unlike the algorithm in [22], the one in [19] performs only integer arithmetic and can be programmed in an ordinary language such as C or FORTRAN. One could alter the algorithm to keep track of the *product* of the various terms of the form $\lambda - d_r$ that contributed to each summation rather than simply keep a count. Each nonzero sum would contribute to several coefficients in $\psi^+(G,\lambda)$, but the various possible contributions could be calculated ahead of time and saved to disk, obviating the need to calculate them each time they are needed. Based on results in [19] and [22], this approach would be slower using current hardware and compilers, but it may not be *inherently* slower. A great increase in speed could probably be realized, for example, by coding the algorithm in assembler language.

Another consideration in calculating $\psi^{+}(G,\lambda)$ is that, even for modest values of n (20, for example), the coefficients can greatly exceed the capacity of the 32-bit integer registers normally found in desktop computers. There are several possible solutions to this problem, e. g., using a machine with 64-bit integer registers, storing the coefficients as double-precision floating-point variables (providing 52 unsigned bits), and using one of the widely available software workarounds for various programming languages. Some commercial software packages also retain all digits in integer calculations.

CONCLUSION

One of the present authors [5] recently identified mathematical relationships between the characteristic polynomials of the adjacency and Laplacian matrices of graphs. We have shown that most, but not all, of these relationships can be modified to apply to the permanental polynomials as well. Further, we evaluated the suitability of two such relationships as computer algorithms for application to chemical graphs. Virtually nothing about the properties of the Laplacian permanental polynomials of chemical graphs has appeared in the literature to date, and this is at least in part due to the difficulty of computing this polynomial for graphs large enough to be of chemical interest. We envision that the availability of the mathematical formulas and computer algorithms described here will help to facilitate these calculations.

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