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Immanantal invariants of graphs

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Abstract

Something between an expository note and an extended research problem, this article is an invitation to expand the existing literature on a family of graph invariants rooted in linear and multilinear algebra. There are a variety of ways to assign a real $n \times n$ matrix $K(G)$ to each n-vertex graph G, so that G and H are isomorphic if and only if $K(G)$ and $K(H)$ are permutation similar. It follows that G and H are isomorphic only if $K(G)$ and $K(H)$ are similar, i.e., that similarity invariants of $K(G)$ are graph theoretic invariants of G, an observation that helps to explain the enormous literature on *spectral* graph theory. The focus of this article is the *permutation* part, i.e., on matrix functions that are preserved under permutation similarity if not under all similarity.

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1. Introduction

Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \ldots, v_n\}$. The familiar adjacency matrix, $A(G)$, is the $n \times n$ matrix whose (i, j)-entry is 1 if $v_i v_j$ is an edge of G, and 0 otherwise. If $H = (W, F)$ is a graph with vertex set $W = \{w_1, w_2, \ldots, w_n\}$, then G and H are isomorphic if and only if there is a permutation $\sigma \in S_n$ such that

$$v_i v_j \in E \quad \text{if and only if} \quad w_{\sigma(i)} w_{\sigma(j)} \in F.$$

(The isomorphism $f : V \to W$ is defined by $f(v_i) = w_{\sigma(i)}$, $1 \leqslant i \leqslant n$.) In other words, G and H are isomorphic if and only if there is a $\sigma \in S_n$ such that

$$A(G) = P^{-1} A(H) P, \tag{1}$$

where the permutation matrix $P = P(\sigma) = (\delta_{i\sigma(j)})$. Thus, G and H are isomorphic if and only if $A(G)$ and $A(H)$ are *permutation* similar, only if $A(G)$ and $A(H)$ are similar, only if $\det(A(G)) = \det(A(H))$. It is natural to wonder whether determinant is the only matrix function that will fit in this last equation.

If $A = (a_{i,j})$ is any $n \times n$ matrix, then

$$\det(A) = (-1)^n \sum_{\tau \in S_n} (-1)^{c(\tau)} \prod_{i=1}^{n} a_{i,\tau(i)},$$

where $c(\tau)$ is the number of cycles (including cycles of length 1) in the disjoint cycle factorization of τ. Evidently, *any* real valued function f of the symmetric permutation group S_n induces a similar function of the $n \times n$ matrices, namely,

$$d_f(A) = \sum_{\tau \in S_n} f(\tau) \prod_{i=1}^{n} a_{i,\tau(i)}.$$

Moreover,

$$\begin{aligned} d_f(P(\sigma)^{-1} A P(\sigma)) &= \sum_{\tau \in S_n} f(\tau) \prod_{i=1}^{n} a_{\sigma(i),\sigma\tau(i)} \\ &= \sum_{\tau \in S_n} f(\tau) \prod_{j=1}^{n} a_{j,\sigma\tau\sigma^{-1}(j)} \\ &= \sum_{\tau \in S_n} f(\sigma^{-1}\tau\sigma) \prod_{j=1}^{n} a_{j,\tau(j)} \\ &= d_g(A), \end{aligned} \tag{2}$$

where $g(\tau) = f(\sigma^{-1}\tau\sigma)$, $\tau \in S_n$.

Recall that a real valued function f of S_n is a (conjugacy) *class function* if $f(\sigma^{-1}\tau\sigma) = f(\tau)$, for all $\sigma, \tau \in S_n$.

Proposition 1.1. *If f is class function of S_n then $d_f(A(G))$ is a graph invariant, i.e., G and H are isomorphic graphs only if $d_f(A(G)) = d_f(A(H))$.*

Proof. Immediate from Eq. (2) and the definitions. $\square$

Example 1.2. Recall that permutations $\mu, \nu \in S_n$ are conjugate if and only if they have the same cycle structure. In particular, $c(\tau)$, the number of cycles in the disjoint cycle factorization of τ, is a class function, as is $f : S_n \to \mathbb{R}$ defined by $f(\tau) = (-1)^{c(\tau)}$. Indeed, $d_f(A) = (-1)^n \det(A)$.

If $f(\tau) = 1$, $\tau \in S_n$, then $d_f(A) = \operatorname{per}(A)$, the *permanent* of A. Because it is (generically) preserved only under monomial similarities, the permanent might seem almost to have been designed with Eq. (1) in mind.

Recall that a nonincreasing sequence $\pi = [\pi_1, \pi_2, \ldots, \pi_k]$ of positive integers is a *partition* of n, denoted $\pi \vdash n$, provided

$$\pi_1 + \pi_2 + \cdots + \pi_k = n.$$

The integers π_j, $1 \leqslant j \leqslant k$, are the *parts* of π. The *cycle type* of permutation $\tau \in S_n$ is the partition $\pi \vdash n$ whose parts are the lengths of the cycles of τ. If $\pi \vdash n$, denote by $f_\pi : S_n \to \mathbb{R}$ the function defined by $f_\pi(\tau) = 1$, if π is the cycle type of τ, and $f_\pi(\tau) = 0$, otherwise. Then f_π is the *characteristic function* of the conjugacy class of S_n consisting of the permutations of cycle type π. In fact, $\{f_\pi : \pi \vdash n\}$ is a basis for the vector space of class functions of S_n.

2. Invariants and graph structure

While invariants of the form $d_f(A(G))$ may seem natural enough from an algebraic perspective, their ultimate value depends on what they reveal about graph structure. The case of $\det(A(G))$, e.g., extends naturally to $\eta(G)$, the *nullity* of $A(G)$, about which articles continue to appear. (See, e.g., [23].) One of the nicest results about $\eta(G)$ emerges from the coincidence of the adjacency characteristic polynomial of a tree with its *matching polynomial*. Let $\mu(G)$ be the *matching number* of G, i.e., the maximum number of mutually nonadjacent edges.

Theorem 2.1. *If T is a tree with n vertices, then $\eta(T) = n - 2\mu(T)$. In particular,* $\det(A(T)) \neq 0$ *if and only if T has a perfect matching.*

In the chemistry literature, perfect matchings are known as Kekulé structures, the number of which, $K(G)$, is related to chemical stability. The following result is a classic. (See, e.g., [21] or [12].)

Theorem 2.2. *If G is a graph, then* $\operatorname{per}(A(G)) \geqslant K(G)^2$, *with equality if and only if G is bipartite. In particular, if G is bipartite, then* $\operatorname{per}(A(G)) \neq 0$ *if and only if G has a perfect matching.*

What about invariants induced by characteristic functions?

A graph is *hamiltonian* if it has a cycle that contains all of its vertices. (Among the classical NP-Complete problems is to determine whether a given graph is hamiltonian.) Denote by $h(G)$ the number of hamiltonian cycles in G.

Theorem 2.3. *Suppose G is a graph on $n \geqslant 3$ vertices. Let $f = f_{[n]}$ where $[n]$ is the unique one-part partition of n. Then $d_f(A(G)) = 2h(G)$. In particular, $d_f(A(G)) \neq 0$ if and only if G is hamiltonian.*

Proof. If $C_{[n]}$ is the conjugacy class of S_n consisting of all $(n-1)!$ full n-cycles then

$$d_f(A(G)) = \sum_{\tau \in C_{[n]}} \prod_{i=1}^{n} a_{i,\tau(i)}, \tag{3}$$

where $A(G) = (a_{i,j})$. For a fixed but arbitrary $\tau \in C_{[n]}$

$$\prod_{i=1}^{n} a_{i,\tau(i)} = \begin{cases} 1, & \text{if } \langle v_{\tau(1)}, v_{\tau^2(1)}, \ldots, v_{\tau^n(1)} \rangle \text{ is a cycle of G,} \\ 0, & \text{otherwise.} \end{cases}$$

Now, $\langle v_{\tau(1)}, v_{\tau^2(1)}, \ldots, v_{\tau^n(1)} \rangle$ cycle of G if and only if $\langle v_{\tau^{-1}(1)}, v_{\tau^{-2}(1)}, \ldots, v_{\tau^{-n}(1)} \rangle = \langle v_{\tau^n(1)}, v_{\tau^{n-1}(1)}, \ldots, v_{\tau(1)} \rangle$ is a cycle; indeed, if and only if it is the *same* cycle with the order reversed. In particular, Eq. (3) counts every hamiltonian cycle of G exactly twice. □

3. Immanants

Corresponding to each partition $\pi \vdash n$ is an *irreducible character* χ_π of S_n. For our purposes, the irreducible characters may be viewed as certain integer valued class functions given by tables such as the one in Fig. 1, where C_π denotes the conjugacy class of cycle type π. The set $\mathrm{Irr}(S_n) = \{\chi_\pi : \pi \vdash n\}$ is another basis of the vector space of class functions of S_n. (Details can be found, e.g., in [24], or [18, Chapter 4].)

For a fixed but arbitrary $\chi \in \mathrm{Irr}(S_n)$, the corresponding matrix function d_χ is called an *immanant* [13]. It will be convenient to abbreviate the notation and denote

	$C_{[1^5]}$	$C_{[2,1^3]}$	$C_{[2^2,1]}$	$C_{[3,1^2]}$	$C_{[3,2]}$	$C_{[4,1]}$	$C_{[5]}$
$\chi_{[1^5]}$	1	-1	1	1	-1	-1	1
$\chi_{[2,1^3]}$	4	-2	0	1	1	0	-1
$\chi_{[2^2,1]}$	5	-1	1	-1	-1	1	0
$\chi_{[3,1^2]}$	6	0	-2	0	0	0	1
$\chi_{[3,2]}$	5	1	1	-1	1	-1	0
$\chi_{[4,1]}$	4	2	0	1	-1	0	-1
$\chi_{[5]}$	1	1	1	1	1	1	1

Fig. 1. Character table for S_5.

by d_r the immanant corresponding to $[r, 1^{n-r}] \vdash n$. Thus, d_1 is another name for the determinant and d_n for the permanent.

Because $\chi \in \mathrm{Irr}(S_n)$ is a class function, it follows from Proposition 1.1 that $d_\chi(A(G))$ is an invariant for n-vertex graphs. Indeed, transcribing Theorem 2.3 for immanants yields the following.

Theorem 3.1 [15]. *Let G be a graph on n vertices. Then the number of hamiltonian cycles in G is*

$$h(G) = \frac{1}{2n} \sum_{r=\eta+1}^{n} (-1)^{n-r} d_r(A(G)),$$

where η is the nullity of $A(G)$.

If $D(G) = \mathrm{diag}(d(v_1), d(v_2), \ldots, d(v_n))$ is the diagonal matrix of its vertex degrees, the *Laplacian matrix* of G is $L(G) = D(G) - A(G)$. The Laplacian analog of Eq. (1) is that G and H are isomorphic graphs if and only if there is a permutation matrix P such that $L(G) = P^{-1}L(H)P$. In particular, $d_f(L(G))$ is (also) a graph invariant for every class function f.

Because $L(G)$ is *positive semidefinite* symmetric, $d_\chi(L(G))$ is the norm of a certain "decomposable symmetrized tensor". (See, e.g., [20, Theorem 1.4] or [18, Theorem 7.26].) In particular, $d_\chi(L(G)) \geqslant 0$ for every $\chi \in \mathrm{Irr}(S_n)$ and every n-vertex graph G. For this and other reasons, Laplacian matrices and immanants seem well fitted to each other.

Recall that $H = (W, F)$ is a *spanning subgraph* of $G = (V, E)$ if $W = V$ and $F \subset E$. A *spanning tree* of G is a spanning subgraph that is a tree. The number, $t(G)$, of spanning trees of G is a well known graph invariant.

Theorem 3.2. *Let G be a graph with $n \geqslant 3$ vertices and m edges. Then $d_2(L(G)) = 2mt(G)$.*

This well known result follows from the Matrix-Tree Theorem (see, e.g., [19, Theorem 9.19]) and the fact [16, Eq. (5)] that for any $n \times n$ matrix $B = (b_{i,j})$,

$$d_2(B) = \sum_{i=1}^{n} b_{ii} \det(B_i) - \det(B),$$

where B_i is the $(n-1)$-square submatrix of B obtained by deleting its i*th* row and column.

In 1947, Harry Wiener introduced what has come to be known as the *Wiener Index* [27].[1] If u and v are vertices of some tree T on n vertices, denote by $\ell(u, v)$

[1] Wiener discovered a remarkable correlation between his index and the boiling point of alkanes (also known as paraffins), hence between the index and such properties as surface tension and viscosity.

the *distance* from u to v, i.e., the length of the unique path in T from u to v. The Wiener Index of an *alkane*, with *chemical graph* T, is

$$W(T) = \sum \ell(u, v),$$

where the sum is over all $C(n, 2)$ pairs of vertices of T.

Theorem 3.3 [7]. *If T is a tree on n vertices, then $d_3(L(T)) = 4W(T) - 2n(n - 1)$.*

4. Immanantal polynomials

Suppose K is a function from the graphs on n vertices to the $n \times n$ matrices. Suppose further, that G is isomorphic to H if and only if there is a permutation matrix $P = P(\sigma)$ such that $K(G) = P^{-1}K(H)P$. Then, for any class function f of S_n,

$$\begin{aligned} d_f[xI_n - K(H)] &= d_f(P^{-1}[xI_n - K(H)]P) \\ &= d_f(xI_n - [P^{-1}K(H)P]) \\ &= d_f[xI_n - K(G)]. \end{aligned} \tag{4}$$

In particular, the *immanantal polynomials* $d_\chi[xI_n - A(G)]$ and $d_\chi[xI_n - L(G)]$ are graph invariants.

Definition 4.1. Suppose $n \geqslant 3$. If G is a graph with n vertices and m edges, write

$$d_2[xI_n - L(G)] = \sum_{k=0}^{n} (-1)^k c_k(G) x^{n-k}. \tag{5}$$

It follows from Eq. (4) that the coefficients $c_k(G)$ on the right-hand side of Eq. (5) are all graph invariants. It is not hard to give formulas for the first few, e.g., $c_0(G) = n - 1$ and $c_1(G) = 2m(n - 1)$. Moreover, from Theorem 3.2, $c_n(G) = 2mt(G)$. What about the other coefficients? A special case of the general answer [16, Theorem 5] can be found in Theorem 4.3.

Definition 4.2. If $T = (V, E)$ is a tree, the *moment* at vertex $u \in V$ is

$$M(u) = \sum_{w \in V} d(w)\ell(u, w),$$

where, recall, $d(w)$ is the degree of vertex w and $\ell(u, w)$ is the distance in T from u to w.

Theorem 4.3. *Let $T = (V, E)$ be a tree on n vertices. Denote by $c_{n-1}(T)$ the coefficient of $(-1)^{n-1}x$ in the immanantal polynomial $d_2[xI_n - L(G)]$. Then $c_{n-1}(T)$ is the moment sum, i.e.,*

$$c_{n-1}(T) = \sum_{u \in V} M(u).$$

With appropriate modifications, Theorem 4.3 can be extended to graphs that are not trees. More interesting, perhaps, is the relation between the moment sum and the Wiener Index. For trees, at least, $c_{n-1}(T)$ is equal to the *Schultz molecular topological index* which, in turn, is $4W(T) - n(n-1)$ [11]. (Also see [4,7,8,25].)

5. The graph isomorphism problem

Might immanantal polynomials, taken all together, suffice to distinguish nonisomorphic graphs?

Theorem 5.1 [1]. *Denote by t_n the number of nonisomorphic trees on n vertices and by s_n the number of such trees T for which there exists a nonisomorphic tree T' such that, simultaneously,*

(a) $d_{\chi_\pi}[xI_n - A(T)] = d_{\chi_\pi}[xI_n - A(T')], \pi \vdash n$, *and*
(b) $d_{\chi_\pi}[xI_n - L(T)] = d_{\chi_\pi}[xI_n - L(T')], \pi \vdash n$.

Then $\lim(s_n/t_n) = 1$.

6. Open problems

It will no doubt be a long time before the spectra of $A(G)$ and $L(G)$ are fully understood, graph theoretically. Thus, even in the case $d_\chi = \det$, questions involving $d_\chi[xI_n - A(G)]$ and $d_\chi[xI_n - L(G)]$ remain open. However, as the main thrust of this article involves matrix functions preserved generically not under all similarities, but only under monomial similarities, we will discuss spectral graph theory no further.

Some illustrative results for $d_r[xI_n - L(G)]$ and $d_r[A(G)]$ appeared in Sections 4 and 3. What about $d_\chi[xI_n - L(G)]$ when $\chi = \chi_\pi$ corresponds to a partition $\pi \neq [r, 1^{n-r}]$? What about the coefficients of $d_\chi[xI_n - A(G)]$? Good questions! While some results have appeared (see, e.g., [2,10,14,22,26]) and various applications suggested (see, e.g., [3,9]), it seems likely that many more results about these graph invariants remain to be discovered.

If $\chi = \chi_\pi$ an irreducible character of S_n of degree k (the value taken by χ at the identity permutation), the corresponding *normalized* immanant is defined by $\bar{d}_\chi(A) = d_\chi(A)/k$. In 1918, Schur proved that $\bar{d}_\chi(A) \geqslant \det(A)$ for every $\chi \in \mathrm{Irr}(S_n)$, and all $n \times n$ positive semidefinite symmetric matrices A. Perhaps the most famous open problem involving immanants is a sort of dual to Schur's result, namely, $\mathrm{per}(A) \geqslant \bar{d}_\chi(A)$. (See, e.g., [17].) Given the intractability of this *Permanental Dominance Conjecture*, it seems reasonable to consider special cases. It would be a significant achievement, e.g., to prove (or disprove) the following.

Conjecture 6.1. *If G is any graph on n vertices, then* $\mathrm{per}(L(G)) \geqslant \bar{d}_\chi(L(G))$ *for every irreducible character χ of S_n.*

Interesting result related to Conjecture 6.1 can be found in [5,6].

References

[1] P. Botti, R. Merris, Almost all trees share a complete set of immanantal polynomials, J. Graph Theory 17 (1993) 467–476.

[2] R.A. Brualdi, J.L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, Discrete Math. 48 (1984) 1–21.

[3] G.G. Cash, Immanants and immanantal polynomials of chemical graphs, J. Chem. Inf. Comput. Sci. 43 (2003) 1942–1946.

[4] O. Chan, I. Gutman, T.-K. Lam, R. Merris, Algebraic connections between topological indices, J. Chem. Inf. Comput. Sci. 38 (1998) 62–65.

[5] O. Chan, T.K. Lam, Hook immanantal inequalities for Laplacians of trees, Linear Algebra Appl. 261 (1997) 23–47.

[6] O. Chan, T.K. Lam, Hook immanantal inequalities for trees explained, Linear Algebra Appl. 273 (1998) 119–131.

[7] O. Chan, T.K. Lam, R. Merris, Wiener number as an immanant of the Laplacian of molecular graphs, J. Chem. Inf. Comput. Sci. 37 (1997) 762–765.

[8] A.A. Dobrynin, A.A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082–1086.

[9] R. Horaud, H. Sossa, Polyhedral object recognition by indexing, Pattern Recognition 28 (1995) 1855–1870.

[10] D. Kasum, N. Trinajstić, I. Gutman, Chemical graph theory III. On the permanental polynomial, Croat. Chem. Acta 54 (1991) 321–328.

[11] I. Gutman, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089.

[12] I. Gutman, Permanents of adjacency matrices and their dependence on molecular structure, Polycycl. Aromat. Compd. 12 (1998) 281–287.

[13] D.E. Littlewood, The Theory of Group Characters, Oxford University Press, London, 1958.

[14] R. Merris, K.R. Rebman, W. Watkins, Permanental polynomials of graphs, Linear Algebra Appl. 38 (1981) 273–288.

[15] R. Merris, Single-hook characters and Hamiltonian circuits, Linear Multilinear Algebra 14 (1983) 21–35.

[16] R. Merris, The second immanantal polynomial and the centroid of a graph, SIAM J. Algebr. Discrete Meth. 7 (1986) 484–503.

[17] R. Merris, The permanental dominance conjecture, in: R. Grone, F. Uhlig (Eds.), Current Trends in Matrix Theory, Elsevier, New York, 1987, pp. 213–223.

[18] R. Merris, Multilinear Algebra, Gordon & Breach, Amsterdam, 1997.

[19] R. Merris, Graph Theory, Wiley-Interscience, New York, 2001.

[20] G.N. de Oliveira, Generalized Matrix Functions, Estudos, Instituto Gulbenkian de Ciência, Oeiras, Portugal, 1973.

[21] O. Ore, Theory of Graphs, Amer. Math. Soc. Colloq. Publ. 38, Provicence, 1962.

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

[23] G.F. Royle, The rank of a cograph, Electron. J. Combin. 10 (2003), article 11.

[24] B.E. Sagan, The Symmetric Group, second ed., Springer, NY, 2001.

[25] I. Tomescu, Some extremal properties of the degree distance of a graph, Discrete Appl. Math. 98 (1999) 159–163.
[26] A. Vrba, The permanent of the Laplacian matrix of a bipartite graph, Czech. Math. J. 36 (1986) 7–17.
[27] H. Wiener, Structural determination of paraffin boiling points, J. Amer. Chem. Soc. 69 (1947) 17–20.