Laplacian Matrices of Graphs: A Survey

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Dedicated to Miroslav Fiedler in commemoration of his retirement.

Submitted by Jose A. Dias da Silva

ABSTRACT

Let G be a graph on n vertices. Its Laplacian matrix is the n-by-n matrix $L(G) = D(G) - A(G)$, where $A(G)$ is the familiar (0, 1) adjacency matrix, and $D(G)$ is the diagonal matrix of vertex degrees. This is primarily an expository article surveying some of the many results known for Laplacian matrices. Its six sections are: Introduction, The Spectrum, The Algebraic Connectivity, Congruence and Equivalence, Chemical Applications, and Immanants.

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1. INTRODUCTION

Let $G = (V, E)$ be a graph with vertex set $V = V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E = E(G) = \{e_1, e_2, \dots, e_m\}$. For each edge $e_j = \{v_i, v_k\}$, choose one of v_i, v_k to be the positive "end" of e_j and the other to be the negative "end." Thus G is given an *orientation* [11]. The vertex-edge *incidence matrix* (or "cross-linking matrix" [33]) afforded by an orientation of G is the n-by-m matrix $Q = Q(G) = (q_{ij})$, where $q_{ij} = +1$ if v_i is the positive end of e_j, -1 if it is the negative end, and 0 otherwise.

*This article was prepared in conjunction with the author's lecture at the 1992 conference of the International Linear Algebra Society in Lisbon. Its preparation was supported by the National Security Agency under Grant MDA904-90-H-4024.

655 Avenue of the Americas, New York, NY 10010 0024-3795/94/$7.00

It turns out that the *Laplacian matrix*, $L(G) = QQ^t$, is independent of the orientation. In fact, $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees and $A(G)$ is the $(0, 1)$ adjacency matrix. One may also describe $L(G)$ by means of its quadratic form

$$xL(G)x^t = \sum (x_i - x_j)^2,$$

where $x = (x_1, x_2, \ldots, x_n)$, and the sum is over the pairs $i < j$ for which $\{v_i, v_j\} \in E$. So $L(G)$ is a symmetric, positive semidefinite, singular M-matrix.

We are primarily interested in nondirected graphs without loops or multiple edges. However, many of the results we discuss have extensions to edge weighted graphs. A *C-edge-weighted graph*, G_C, is a pair consisting of a graph G and a positive real-valued function C of its edges. The function C is most conveniently described as an n-by-n, symmetric, nonnegative matrix $C = (c_{ij})$ with the property that $c_{ij} > 0$ if and only if $\{v_i, v_j\} \in E$. With r_i denoting the ith row sum of C, define $L(G_C) = \operatorname{diag}(r_1, r_2, \ldots, r_n) - C$. Another way to describe $L(G_C)$ is by means of its quadratic form:

$$xL(G_C)x^t = \sum c_{ij}(x_i - x_j)^2,$$

where, as before, the sum is over the pairs $i < j$ for which $\{v_i, v_j\} \in E$.

Forsman [47] and Gutman [66] have shown how the connection between $L(G)$ and $K(G) = Q^tQ$ simultaneously explains the statistical and dynamic properties of flexible branched polymer molecules. Unlike its vertex counterpart, the entries of $K(G)$ depend on the orientation. However, if G is bipartite, an orientation can always be chosen so that $K(G) = 2I_m + A(G^*)$, where G^* is the line graph of G. (It follows that the minimum eigenvalue of $A(G^*)$ is at least -2. This observation, first made by Alan Hoffman, leads to a connection with *root systems* [29, 145].)

One may view $K(G)$ as an *edge version* of the Laplacian. For graphs without isolated vertices, there are other versions, e.g., the *doubly stochastic matrix* $I_n - d_1^{-1}L(G)$, where d_1 is the maximum vertex degree, and the *correlation matrix* $M(G) = D(G)^{-1/2}L(G)D(G)^{-1/2}$. (A symmetric positive semidefinite matrix is a *correlation matrix* if each of its diagonal entries is 1.) Note that $M(G)$ is similar to $D(G)^{-1}L(G) = I_n - R(G)$, where $R(G)$ is the *random-walk matrix*. The first recognizable appearance of $L(G)$ occurs in what has come to be known as *Kirchhoff's matrix tree theorem* [77]:

THEOREM 1.1. *Denote by $L(i|j)$ the $(n-1)$-by-$(n-1)$ submatrix of $L(G)$ obtained by deleting its ith row and jth column. Then $(-1)^{i+j} \det L(i|j)$ is the number of spanning trees in G.*

(Variations, extensions and generalizations of Theorem 1.1 appear, e.g., in [8, 16, 17, 25, 26, 51, 78, 94, 97, 127, 132, 149, 150].)

In view of this result, it is not surprising to find $L(G)$ referred to as a *Kirchhoff matrix* or *matrix of admittance* (admittance = conductivity, the reciprocal of impedance). Reflecting its independent discovery in other contexts, $L(G)$ has also been called an *information matrix* [25], a *Zimm matrix* [47], a *Rouse-Zimm matrix* [130], a *connectivity matrix* [35], and a *vertex-vertex incidence matrix* [153]. Perhaps the best place to begin is with a justification of the name "Laplacian matrix."

In a seminal article, Mark Kac posed the question whether one could "hear the shape of a drum" [74, 115]. Consider an elastic plane membrane whose boundary is fixed. If small vibrations are induced in the membrane, it is not unreasonable to expect a point (x, y, z) on its surface to move only vertically. Thus, we assume $z = z(x, y, t)$. If the effects of damping are ignored, the motion of the point is given (at least approximately) by the *wave equation*

$$\nabla^2 z = z_{tt}/c^2,$$

where $\nabla^2 z = z_{xx} + z_{yy}$ is the *Laplacian* of z. Since we are assuming the membrane is elastic and the vibrations are small, the restoring force is linear (Hooke's law), i.e., $z_{tt} = -kz$, where $k > 0$ encompasses mass and "spring constant." Combining these equations, we obtain

$$z_{xx} + z_{yy} = -kz/c^2. \tag{1}$$

The classical solution to this "Dirichlet problem" involves a countable sequence of eigenvalues that manifest themselves in audible tones. An alternate version of Kac's question is this: can nonisometric drums afford the same eigenvalues? (The recently announced answer is yes [146, 148].)

To produce a finite analog, suppress the variable t and use differential approximation to obtain the estimates

$$z(x-h, y) \doteq z(x, y) - z_x(x, y)h,$$
$$z(x, y) \doteq z(x+h, y) - z_x(x+h, y)h.$$

Subtracting the second of these equations from the first and rearranging terms, we find

$$h[z_x(x+h, y) - z_x(x, y)] \doteq z(x+h, y) + z(x-h, y) - 2z(x, y). \tag{2}$$

Another approximation by differentials leads to

$$z_x(x+h, y) \doteq z_x(x, y) + z_{xx}(x, y)h.$$

Putting this into (2) gives

$$h^2 z_{xx} \doteq z(x+h, y) + z(x-h, y) - 2z(x, y).$$

Similarly,

$$h^2 z_{yy} \doteq z(x, y+h) + z(x, y-h) - 2z(x, y).$$

Substituting these estimates into (1), we obtain

$$4z(x, y) - z(x+h, y) - z(x-h, y) - z(x, y+h) - z(x, y-h) \doteq \lambda z(x, y), \tag{3}$$

where $\lambda = kh^2/c^2$. But (3) is the equation $L(G)z = \lambda z$, where G is the "grid graph" of Figure 1. So the eigenvalue problem for $L(G)$ is, arguably at least, a finite analog of the continuous problem (1). (M. E. Fischer suggested that discrepancies between discrete models like (3) and continuous models like (1) may well reflect the "lumpy nature of physical matter" [46].) The first examples of nonisomorphic graphs G_1 and G_2 such that $L(G_1)$ and $L(G_2)$ have the same spectra were found in [31, 69, 147]. In fact, as we will see in Theorem 5.2, below, there is a plentiful supply of nonisomorphic, Laplacian cospectral graphs.

2. THE SPECTRUM

Strictly speaking $L(G)$ depends not only G but on some (arbitrary) ordering of its vertices. However, Laplacian matrices afforded by different vertex orderings of the same graph are permutation-similar. Indeed, graphs G_1 and G_2 are isomorphic if and only if there exists a permutation matrix P such that

$$L(G_2) = P^t L(G_1) P. \tag{4}$$

Thus, one is not so much interested in $L(G)$ as in permutation-similarity invariants of $L(G)$. Of course, two matrices cannot be permutation-similar if

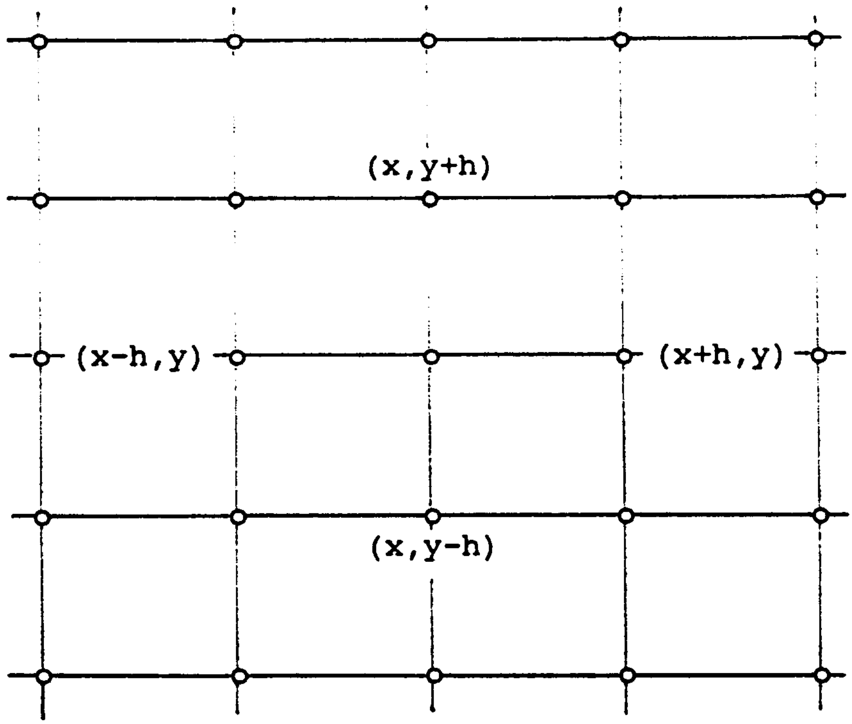

FIG. 1. Grid graph.

they are not similar, and two real symmetric matrices are similar if and only if they have the same eigenvalues. Denote the spectrum of $L(G)$ by

$$S(G) = (\lambda_1, \lambda_2, \dots, \lambda_n),$$

where we assume the eigenvalues to be arranged in nonincreasing order: $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n = 0$. When more than one graph is under discussion, we may write $\lambda_i(G)$ instead of λ_i. It follows, e.g. from the matrix-tree theorem, that the rank of $L(G)$ is $n - w(G)$, where $w(G)$ is the *number of connected components* of G. In particular, $\lambda_{n-1} \neq 0$ if and only if G is connected. (Already, we see graph structure reflected in the spectrum.) This observation led M. Fiedler [37, 40–43] to define the *algebraic connectivity* of G by $a(G) = \lambda_{n-1}(G)$, viewing it as a quantitative measure of connectivity. In the next section we will discuss the algebraic connectivity and some of its many applications.

Denote the complement of G (in K_n) by G^c, and let J_n be the n-by-n matrix each of whose entries is 1. Then, as observed in [5], $L(G) + L(G^c) = L(K_n) = nI_n - J_n$. It follows that

$$S(G^c) = (n - \lambda_{n-1}(G), n - \lambda_{n-2}(G), \dots, n - \lambda_1(G), 0). \tag{5}$$

Letting $m_G(\lambda)$ denote the multiplicity of λ as an eigenvalue of $L(G)$, one may deduce from (5) that $\lambda_1(G) \leqslant n$ and $m_G(n) = w(G^c) - 1$. (See [65] for another interpretation.)

In Section 1, we defined $D(G)$ to be the diagonal matrix of vertex degrees. We now abuse the language by also using $D(G)$ to denote the nonincreasing *degree sequence*

$$D(G) = (d_1, d_2, \dots, d_n),$$

$d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$. (We do not necessarily assume that $d_i = d(v_i)$, the *degree of vertex i*.) It follows from the Geršgorin circle theorem [applied to $K(G)$] that $\lambda_1 \leqslant \max[d(u) + d(v)]$, where the maximum is taken over all $\{u, v\} \in E$. (Also see [5].) In particular,

$$d_1 + d_2 \geqslant \lambda_1. \tag{6}$$

[Note that (6) improves the bound $2d_1 \geqslant \lambda_1$ obtained by applying Geršgorin's theorem directly to $L(G)$.]

If $(a) = (a_1, a_2, \dots, a_r)$ and $(b) = (b_1, b_2, \dots, b_s)$ are nonincreasing sequences of real numbers, then (a) *majorizes* (b) if

$$\sum_{i=1}^{k} a_i \geqslant \sum_{i=1}^{k} b_i, \qquad k = 1, 2, \dots, \min\{r, s\},$$

and

$$\sum_{i=1}^{r} a_i = \sum_{i=1}^{s} b_i.$$

THEOREM 2.1. *For any graph G, $S(G)$ majorizes $D(G)$.*

Proof. It was proved in [125] (see, e.g., [84, p. 218]) that the spectrum of a positive semidefinite Hermitian matrix majorizes its main diagonal (when both are rearranged in nonincreasing order). ■

Majorization techniques have been widely used in graph-theoretic investigations ranging from degree sequences to the chemical "Balaban index." (See, e.g., [121, 122].) In its intersection with algebraic graph theory, this work has often been impeded by a stubborn reliance on the adjacency matrix. (See, e.g., [100].) In fact, it is the Laplacian matrix that affords a natural vehicle for majorization.

The first inequality arising from Theorem 2.1 is $\lambda_1 \geqslant d_1$. It is not surprising that a result holding for all positive semidefinite Hermitian matrices should be subject to some improvement upon restriction to the class of Laplacian matrices. Indeed [62], if G has at least one edge, then

$$\lambda_1 \geqslant d_1 + 1. \tag{7}$$

For G a connected graph on $n > 1$ vertices, equality holds in (7) if and only if $d_1 = n - 1$. In fact, (7) is the beginning of a chain of inequalities that include $\lambda_1 + \lambda_2 \geqslant d_1 + d_2 + 1$ and $\lambda_1 + \lambda_2 + \lambda_3 \geqslant d_1 + d_2 + d_3 + 1$. These suggest the following:

CONJECTURE 2.2 [62]. Let G be a connected graph on $n \geqslant 2$ vertices. Then the sequence $(d_1 + 1, d_2, d_3, \ldots, d_{n-1}, d_n - 1)$ is majorized by $S(G)$.

Nonincreasing *integer* sequences are frequently pictured by means of so-called Ferrers-Sylvester (or Young) diagrams. For example, the diagram for $(a) = (5, 5, 5, 4, 4, 4, 3)$ is pictured on the left in Figure 2. Its transpose is the diagram on the right corresponding to the *conjugate* sequence $(a)^* =$

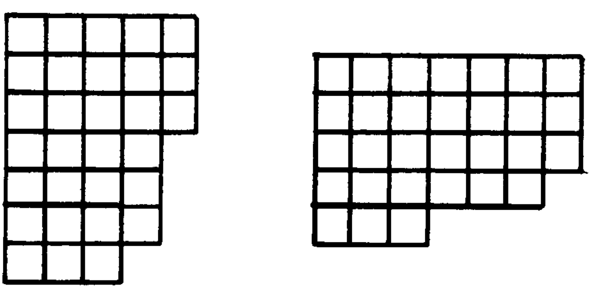

FIG. 2. Ferrers-Sylvester diagrams.

$(7,7,7,6,3)$. In general, the conjugate of a nonincreasing integer sequence $(a) = (a_1, a_2, \ldots, a_r)$ is $(a)^* = (a_1^*, a_2^*, \ldots, a_s^*)$, where a_i^* is the cardinality of the set $\{j : a_j \geqslant i\}$.

THEOREM 2.3 [62]. *Let $D(G)$ be the degree sequence of a graph. Then $D(G)^*$ majorizes $D(G)$.*

Theorems 2.1 and 2.3 raise the natural question whether $S(G)$ and $D(G)^*$ are majorization-comparable.

CONJECTURE 2.4 [62]. Let G be a connected graph. Then $D(G)^*$ majorizes $S(G)$.

One consequence of Conjecture 2.4 would be

$$\lambda_{n-1} \geqslant d_{n-1}^*, \tag{8}$$

i.e., the number of vertices of G of degree $n-1$ is no larger than the algebraic connectivity, $a(G)$. Since $a(K_n) = n$, (8) is true for $G = K_n$. Otherwise, if G has exactly k vertices of degree $n-1$, then G^c has at least $k+1$ components, the largest of which has at most $n-k$ vertices, so $\lambda_1(G^c) \leqslant n-k$ and $a(G) = n - \lambda_1(G^c) \geqslant k = d_{n-1}^*$.

There is, of course, an enormous literature on the adjacency spectra of graphs, and much of it concerns regular graphs. (See, e.g., [28–30].) If G is r-regular, $L(G) + A(G) = rI_n$, so λ is an eigenvalue of $L(G)$ if and only if $r - \lambda$ is an eigenvalue of $A(G)$. Similarly, since $L(G)$ and its edge counterpart, $K(G)$, share the same nonzero eigenvalues, any results about the adjacency spectra of line graphs of bipartite graphs can be carried over to the Laplacian by means of the equation $K(G) = 2I_m + A(G^*)$. These connections with the adjacency literature lead easily to many results for the Laplacian that we won't even try to describe here. There are some other results about $A(G)$ whose Laplacian counterparts do not follow for the reasons just given, but whose proofs consist of relatively straightforward modifications of adjacency arguments. Three results of this type are presented in Theorems 2.5–2.7.

THEOREM 2.5. *Let G be a connected graph with diameter d. Suppose $L(G)$ has exactly k distinct eigenvalues. Then $d + 1 \leqslant k$.*

Let $\Gamma(G)$ denote the automorphism group of G, regarded as a group of permutations on $V = \{v_1, v_2, \ldots, v_n\}$.

THEOREM 2.6. *Let G be a connected graph. If some permutation in $\Gamma(G)$ has s odd cycles and t even cycles, then $L(G)$ has at most $s + 2t$ simple eigenvalues.*

If some permutation in $\Gamma(G)$ has a cycle of length 3 or more, we see immediately from Theorem 2.6 that the eigenvalues of $L(G)$ are not distinct; if the eigenvalues of $L(G)$ are all distinct, then $\Gamma(G)$ must be Abelian (as each of its elements has order 2).

Denote by $V_1, V_2, \ldots, V_t$ the orbits of $\Gamma(G)$ in V, and let $n_i = o(V_i)$ be the cardinality of V_i, $1 \leqslant i \leqslant t$. Assume V ordered so that

$$V_1 = \{v_1, v_2, \ldots, v_{n_1}\},$$

$$V_2 = \{v_{n_1+1}, v_{n_1+2}, \ldots, v_{n_1+n_2}\},$$

etc. Partitioning $L(G)$ in the same way, we obtain a t-by-t block matrix (L_{ij}), where L_{ij} is the n_i-by-n_j submatrix of $L(G)$ whose rows correspond to the vertices in V_i and whose columns are indexed by the vertices in V_j.

THEOREM 2.7 [58]. *Let $L(G) = (L_{ij})$ be the block matrix partitioned by $\Gamma(G)$ as described above. Let $A = (a_{ij})$ be the t-by-t matrix defined by $a_{ij} = (n_i n_j)^{-1/2}$ times the sum of the entries in L_{ij}. Then the characteristic polynomial of A is a factor of the characteristic polynomial of $L(G)$.*

The eigenvalues of the matrix A in Theorem 2.7, multiplicities included, constitute the *symmetric part* of the spectrum of $L(G)$. The remaining eigenvalues of $L(G)$, multiplicities included, constitute the *alternating part*. If $\Gamma(G) = \{e\}$, then the alternating part of the spectrum is empty. On the other hand, it may happen that some multiple eigenvalue of $L(G)$ belongs to both parts.

We now discuss some results directly relating $S(G)$ to various structural properties of G.

THEOREM 2.8 [62]. *Let u be a cut vertex of the connected graph G. If the largest component of G-u contains k vertices, then $k + 1 \geqslant \lambda_2(G)$.*

A *pendant* vertex of G is a vertex of degree 1. A *pendant neighbor* is a vertex adjacent to a pendant vertex. We suppose G has $p(G)$ pendant vertices and $q(G)$ pendant neighbors.

THEOREM 2.9 [36]. *Let G be a graph. Then $p(G) - q(G) \leqslant m_G(1)$.*

See Theorem 6.1 (below) for the permanental analog of this result. Extensions of Theorem 2.9 can be found in [59]. The correlation between $m_G(1)$ and the viscosity of polydimethylsiloxane is discussed in [110]. If I is an interval of the real line, denote by $m_G(I)$ the number of eigenvalues of $L(G)$, multiplicities included, that belong to I. Then $m_G(I)$ is a natural extension of $m_G(\lambda)$.

THEOREM 2.10 [63]. *Let G be a graph. Then $q(G) \leqslant m_G[0, 1)$.*

It is immediate from Theorems 2.9 and 2.10 that $p(G) \leqslant m_G[0, 1]$. (The relevance of $m_G(0, 1)$ to long relaxation times in elastic networks is discussed in [110, p. 885; 130, p. 5184]. Also see [35, Section J].)

THEOREM 2.11 [96]. *Let G be a connected graph satisfying $2q(G) < n$. Then $q(G) \leqslant m_G(2, n]$.*

A subset S of $V(G)$ is said to be *stable* or *independent* if no two vertices of S are adjacent. The maximum size of an independent set is called the *interior stability number* or the *point independence number* and is denoted by $\alpha(G)$.

THEOREM 2.12. *Let G be a graph. Then $m_G[d_n, n] \geqslant \alpha(G)$ and $m_G[0, d_1] \geqslant \alpha(G)$.*

Proof. We require the following well-known fact from matrix theory: Suppose that B is a principal submatrix of the symmetric matrix A. Then the number of nonnegative (respectively, nonpositive) eigenvalues of B is a lower bound for the number of nonnegative (respectively, nonpositive) eigenvalues of A. Suppose $S = \{v_1, v_2, \dots, v_k\}$ is an independent set of vertices. Let B be the leading k-by-k principal submatrix of $L(G) - d_n I_n$. Then B is a diagonal matrix, each of whose eigenvalues is nonnegative. Therefore, k is a lower bound for the number of nonnegative eigenvalues of $L(G) - d_n I_n$. The argument for $m_G[0, d_1]$ is similar. ∎

If G is r-regular, then Theorem 2.12 becomes

$$m_G[r, n] \geqslant \alpha(G) \leqslant m_G[0, r],$$

from which one may recover the regular case of an analogous result for the adjacency matrix [30, Theorem 3.14].

THEOREM 2.13 [63]. *If T is a tree with diameter d, then $m_T(0, 2) \geqslant [d/2]$, the greatest integer in $d/2$, and $m_T(2, n] \geqslant [d/2]$.*

It follows, of course, that $m_{P_n}(2) = 1$ if and only if n is even. In fact [63, Theorem 2.5], $m_T(2) = 1$ for any tree T with a perfect matching.

THEOREM 2.14 [62]. *Let G be a graph. If $m_G(2) > 0$, then $d(u) + d(v) \leqslant n$ for some pair of nonadjacent vertices u and v.*

THEOREM 2.15. *Let G be a connected graph. If t is the length of a longest path in G, then $m_G(2, n] \geqslant [t/2]$.*

Proof. If G is a tree, then t is the diameter and we use Theorem 2.13. Otherwise, the longest path in G is part of a spanning tree T. Since G may be obtained from T by adding edges, the result follows from Theorem 2.16. ■

The next result is part of the "Laplacian folklore" [63, 104].

THEOREM 2.16. *If u and w are nonadjacent vertices of G, let G^+ be the graph obtained from G by adding a new edge $e = \{u, w\}$. Then the $n - 1$ largest eigenvalues of $L(G)$ interlace the eigenvalues of $L(G^+)$.*

If $u \in V$, denote by $N(u)$ its set of *neighbors*, i.e.,

$$N(u) = \{v \in V : \{u, v\} \in E\}.$$

[If $X \subset V$, then $N(X)$ is the union over $u \in X$ of $N(u)$.]

Wasin So [131] found a nice addition to Theorem 2.16: If $N(u) = N(w)$, then the spectrum of $L(G^+)$ overlaps the spectrum of $L(G)$ in $n - 1$ places. That is, in passing from $L(G)$ to $L(G^+)$, one of the eigenvalues goes up by 2 and the rest are unchanged.

THEOREM 2.17 [63]. *If T is a tree and λ is any eigenvalue of $L(T)$, then $m_T(\lambda) \leqslant p(T) - 1$.*

Recall that $p(T) - 1$ is also an upper bound for the nullity of $A(T)$ [30, p. 258]. If G is connected and bipartite, then $L(G) = D(G) - A(G)$ is unitarily similar to the irreducible nonnegative matrix $D(G) + A(G)$, and $\lambda_1(G)$ is a simple eigenvalue.

THEOREM 2.18 [63, Theorem 2.1]. *Suppose T is tree. If $\lambda > 1$ is an integer eigenvalue of $L(T)$ with corresponding eigenvector u, then $\lambda \mid n$, $m_T(\lambda) = 1$, and no coordinate of u is 0.*

This may be a good time to recall a striking result of Fiedler [38]: Suppose $\lambda = 2$ is an eigenvalue of $L(T)$ for some tree $T = (V, E)$. Let $z = (z_1, z_2, \dots, z_n)$ be an eigenvector of $L(T)$ corresponding to $\lambda = 2$. Then the number of eigenvalues of $L(T)$ greater than 2 is equal to the number of edges $\{v_i, v_j\} \in E$ such that $z_i z_j > 0$.

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs on disjoint sets of vertices. Their *union* is $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. A *coalescence* of G_1 and G_2 is any graph on $o(V_1) + o(V_2) - 1$ vertices obtained from $G_1 + G_2$ by identifying (i.e., "coalescing" into a single vertex) a vertex of G_1

with a vertex of G_2. Denote by $G_1 \cdot G_2$ any of the $o(V_1)o(V_2)$ coalescences of G_1 and G_2.

THEOREM 2.19 [61]. *Let G_1 and G_2 be graphs. Then $S(G_1 \cdot G_2)$ majorizes $S(G_1 + G_2)$.*

The *join*, $G_1 \vee G_2$, of G_1 and G_2 is the graph obtained from $G_1 + G_2$ by adding new edges from each vertex of G_1 to every vertex of G_2. Thus, for example, $K_p^c \vee K_q^c = K_{p,q}$, the complete bipartite graph. Because $G_1 \vee G_2 = (G_1^c + G_2^c)^c$, the next result is an immediate consequence of (5):

THEOREM 2.20. *Let G_1 and G_2 be graphs on n_1 and n_2 vertices, respectively. Then the eigenvalues of $L(G_1 \vee G_2)$ are* 0; $n_1 + n_2$; $n_2 + \lambda_i(G_1)$, $1 \leqslant i < n_1$; *and* $n_1 + \lambda_i(G_2)$, $1 \leqslant i < n_2$.

The *product* of G_1 and G_2 is the graph $G_1 \times G_2$ whose vertex set is the Cartesian product $V(G_1) \times V(G_2)$. Suppose $v_1, v_2 \in V(G_1)$ and $u_1, u_2 \in V(G_2)$. Then (v_1, u_1) and (v_2, u_2) are adjacent in $G_1 \times G_2$ if and only if one of the following conditions is satisfied: (i) $v_1 = v_2$ and $\{u_1, u_2\} \in E(G_2)$, or (ii) $\{v_1, v_2\} \in E(G_1)$ and $u_1 = u_2$. For example, the line graph of $K_{p,q}$ is $K_p \times K_q$, and the "grid graph" is a product of paths.

THEOREM 2.21 [37, 104]. *Let G_1 and G_2 be graphs on n_1 and n_2 vertices, respectively. Then the eigenvalues of $L(G_1 \times G_2)$ are all possible sums $\lambda_i(G_1) + \lambda_j(G_2)$, $1 \leqslant i \leqslant n_1$ and $1 \leqslant j \leqslant n_2$.*

Majorization results involving products can be found in [24].

The study of graphs whose *adjacency* spectra consist entirely of integers was begun in [68]. Cvetković [27] proved that the set of connected, r-regular adjacency integral graphs is finite. When $r = 2$ there are three such graphs, C_3, C_4, and C_6; when $r = 3$ there are 13 [15, 129]. Of course, the theory of Laplacian integral graphs coincides with its adjacency counterpart for regular graphs. Elsewhere, there can be remarkable differences. Of the 112 connected graphs on $n = 6$ vertices, six are adjacency integral while 37 are Laplacian integral.

It is clear from (5) that the spectrum of $L(G)$ consists entirely of integers if and only if the spectrum of $L(G^c)$ is integral. From Theorems 2.20 and 2.21, we see that joins and products of Laplacian integral graphs are Laplacian integral. If T is a tree, then $a(T) < 1$ unless $T = K_{1,n-1}$ [37, 93]. Since $s(K_{1,n-1}) = (n, 1, 1, \ldots, 1, 0)$, the star is the only Laplacian integral tree on n vertices. Additional results on Laplacian integral graphs can be found in [62]. We conclude this section with a pair of results that guarantee the existence of certain particular integers in $S(G)$.

A *cluster* of G is an *independent* set of two or more vertices of G, each of which has the same set of neighbors. The *degree* of a cluster is the cardinality of its shared set of neighbors, i.e., the common degree of each vertex in the cluster. An *s-cluster* is a cluster of degree s. The number of vertices in a cluster is its *order*. A collection of two or more clusters is *independent* if the clusters are pairwise disjoint. (The neighbor sets of independent clusters need not be disjoint.) The next result is an extension of [36].

THEOREM 2.22 [154]. *Let G be a graph with k independent s-clusters of orders* $r_1, r_2, \dots, r_k$. *Then* $m_G(s) \geqslant r_1 + r_2 + \cdots + r_k - k$.

COROLLARY 2.23 [62]. *Let G be a graph with an r-clique,* $r \geqslant 2$. *Suppose every vertex of the clique has the same set of neighbors outside the clique. Let the degree of each vertex of the clique be s, so* $s - r + 1$ *is the number of vertices not belonging to the clique but adjacent to every member of the clique. Then* $m_G(s + 1) \geqslant r - 1$.

Proof. The clique corresponds to an $(n - s - 1)$-cluster of G^c of order r. ■

3. THE ALGEBRAIC CONNECTIVITY

Recall that the algebraic connectivity is $a(G) = \lambda_{n-1}(G)$. We begin this section with an early result of Fiedler.

THEOREM 3.1 [37]. *Let G be a graph (on n vertices) with vertex connectivity* $v(G)$ *and edge connectivity* $e(G)$. *Then* $2e(G)[1 - \cos(\pi/n)] \leqslant a(G)$. *If* $G \neq K_n$, *then* $a(G) \leqslant v(G)$.

If $G \neq K_n$, one deduces that

$$a(G) \leqslant d_n, \tag{9}$$

the minimum vertex degree. An improvement on (9) can be found in [111]. It seems that $a(G)$ is related to the half-life of a certain "flowing process" in graphs [82]; its relevance to the theory of elasticity is discussed in [130]. The asymptotic behavior of $a(G)$ for random graphs is described, e.g., in [73, 87, 111, 130]. An inequality for the continuous analog of $a(G)$ in compact Riemannian manifolds was obtained by J. Cheeger [18].

Suppose X is a subset of $V(G)$ of cardinality $o(X)$. Define the *coboundary*, E_X, to be the edge cut consisting of those edges exactly one of whose vertices belong to X:

$$E_X = \{\{u, v\} \in E(G) : u \in X \text{ and } v \notin X\}.$$

The *isoperimetric number* of G is $i(G) = \min[o(E_X)/o(X)]$, where the minimum is over all $X \subset X(G)$ satisfying $1 \leqslant o(X) \leqslant n/2$.

THEOREM 3.2 [102, 103]. *If G is a graph on $n > 3$ vertices, then*

$$\frac{a(G)}{2} \leqslant i(G) \leqslant \{a(G)[2d_1 - a(G)]\}^{1/2}.$$

Related isoperimetric inequalities were established in [50, 151], and a continuous analog appeared in [57]. Graphs with large $a(G)$ are related to so-called expanders [2]. (See [3, 4, 10, 19, 20, 50, 104, 108].)

We now state, in terms of Laplacians, a result of M. Doob [30, p. 187].

THEOREM 3.3. *Let T be a tree on n vertices with diameter d. Then $a(T) \leqslant 2\{1 - \cos[\pi/(d + 1)]\}$.*

The next result, attributed to B. McKay [108], was proved in [105].

THEOREM 3.4. *Let G be a connected graph with diameter d. Then $a(G) \geqslant 4/dn$.*

Another bound involving $a(G)$ and the diameter of G was obtained by Alon and Milman:

THEOREM 3.5 [4]. *Let G be a connected graph with maximum vertex degree d_1. Then $[2d_1/a(G)]^{1/2} \log_2(n^2)$ is an upper bound for the diameter of G.*

Improvements on this result have been obtained by Mohar [105] and Chung, Faber, and Manteuffel [20]. (See [108].)

An upper bound for the diameter in terms of the number of 1's in the Smith normal form of $L(G)$ is given in Theorem 4.5 below.

We now consider eigenvectors corresponding to $a(G)$. (These eigenvectors play an interesting role in the study of random elastic networks [33] and in the solution of large, sparse, positive definite systems on parallel computers [114].) Denote by $\mathrm{Val}(G)$ the set of eigenvectors of $L(G)$ afforded by $a(G)$. Then $\mathrm{Val}(G)$ lacks only the zero vector to be a vector space. For our present purposes, it is useful to think of the elements of $\mathrm{Val}(G)$ as real-valued functions of $V = V(G)$. If, for example, $z = (z_1, z_2, \ldots, z_n)$ is an eigenvector of $L(G)$ afforded by $a(G)$, we write $f \in \mathrm{Val}(G)$ for the function defined by $f(v_i) = z_i$, $1 \leqslant i \leqslant n$. Fiedler has called the elements of $\mathrm{Val}(G)$ *characteristic valuations* of G.

THEOREM 3.6 [39]. *Let $T = (V, E)$ be a tree. Suppose $f \in \mathrm{Val}(T)$. Then two cases can occur.*

Case (i). If $f(v) \neq 0$ for all $v \in V$, then T contains exactly one edge $\{u, w\}$ such that $f(u) > 0$ and $f(w) < 0$. Moreover, the values of f along any path starting at u and not containing w increase, while the values of f along any path starting at w and not containing u decrease.

Case (ii). If $V_0 = \{v \in V : f(v) = 0\}$ is not empty, then the graph $T_0 = (V_0, E_0)$ induced by T on V_0 is connected and there is exactly one vertex $u \in V_0$ which is adjacent (in T) to a vertex not belonging to V_0. Moreover, the values of f along any path in T starting at u are increasing, decreasing, or identically zero.

Suppose $f \in \mathrm{Val}(T)$. A vertex $v \in V$ is a *characteristic vertex* of T defined by f if $v \in \{u, w\}$ in case (i), or if $v = u$ in case (ii), whichever applies to f. It turns out that characteristic vertices are independent of the characteristic valuation used to define them: If f, $g \in \mathrm{Val}(T)$, then $v \in V$ is a characteristic vertex of T defined by g if and only if it is a characteristic vertex of T defined by f [93]. Thus, every tree has a unique *characteristic center* consisting of either one or two characteristic vertices, and in the case of two, they are adjacent. (In spite of these similarities, the characteristic center of a tree need coincide with neither the center nor the centroid.) We say T is of *type I* if it has a single characteristic vertex [which must be a fixed point of $\Gamma(T)$]. Otherwise it is of *type II*. (The algebraic connectivity of a type-I tree is a unit in the ring of algebraic integers [58]. The algebraic connectivity of a type-II tree is a simple eigenvalue of $L(T)$ [38].)

Let T be a type-I tree with characteristic vertex u_T. A branch at u_T is a connected component of $T - u_T$. If B is a branch at u_T, denote by $r(B)$ the vertex of B adjacent (in T) to u_T. If $f \in \mathrm{Val}(T)$, then (Theorem 3.6) f is uniformly positive, uniformly negative, or identically zero on the vertices of B. We call B a *passive* branch if $f(r(B)) = 0$ for every $f \in \mathrm{Val}(T)$. Otherwise, B is *active*. In either case, denote by $L^+(B)$ the matrix obtained from $L(B)$ by adding 1 to its main-diagonal entry in the row corresponding to $r(B)$. Then the $(n-1)$-by-$(n-1)$ principal submatrix of $L(T)$ obtained by deleting the row and column corresponding to u_T is the direct sum of the $L^+(B)$ as B ranges over the branches of T at u_T. This leads to the following:

THEOREM 3.7 [58]. *Let T be a type-I tree with characteristic vertex u_T and algebraic connectivity $a(T)$. Then, for every branch B of T at u_T, $a(T) \leqslant$ the least eigenvalue of $L^+(B)$, with equality if and only if B is active, in which case $a(T)$ is a simple eigenvalue of $L^+(B)$.*

It is a consequence of Theorem 3.7 that exactly $m_T(a(T)) + 1$ of the branches at u_T are active. If $a(T)$ is a simple eigenvalue of $L(T)$, then u_T

and the passive branches "separate" the two active branches in the following sense: A subset $C \subset V(G)$ is said to *separate* vertex sets X and Y if (i) X, Y, and C partition $V(G)$, and (ii) no vertex of X is adjacent to a vertex of Y. It is of some interest to find separators with $o(C)$ small and $o(X)$ about equal to $o(Y)$.

THEOREM 3.8 [4, Lemma 2.1]. *Suppose C separates X and Y in the connected graph G. Let $x = o(X)$, $y = o(Y)$, z be the number of edges having at least one "end" in C, and d be the minimum distance between a vertex in X and a vertex in Y. Then $(x^{-1} + y^{-1})z/d^2 \geqslant a(G)$.*

See [114] for improvements on this result.

COROLLARY 3.9. *Let T be a type-I tree with characteristic vertex u_T and simple algebraic connectivity $a(T)$. If x and y are the numbers of vertices in the two active branches of T at u_T, then $a(T) \leqslant (x + y)/(2xy)$.*

Proof. Let T' be the subtree induced by T on u_T and the two active branches. It is proved in [93] that $a(T') = a(T)$. The result is an immediate consequence of Theorem 3.8. ∎

It is known [58] that $a(T)$ is in the alternating part of the spectrum if and only if at least two of the active branches at u_T are isomorphic. If T has just two isomorphic branches at u_T, then $a(T) \leqslant 2/(n-1)$ ($x = y$ in Corollary 3.9).

The algebraic connectivity for trees on n vertices ranges from $a(P_n) = 2[1 - \cos(\pi/n)]$ to $a(K_{1,n-1}) = 1$. Clearly, then, all trees are not equally connected. Some results explaining the partial ordering imposed on trees by $a(T)$ were obtained in [60]. (Also see [113].) Other approaches appear in Theorems 3.10 and 3.13. The first of these shows that graphs with large $a(G)$ do not contain small separators.

THEOREM 3.10 [108]. *Suppose C separates X and Y in the connected graph G. Let $x = o(X)$, $y = o(Y)$, and $c = o(C)$. Then $c \geqslant 4xya(G)/[nd_1 - a(G)(x + y)]$.*

In [104], Mohar investigated a *bandwidth*-type problem. For each edge $e = \{v_i, v_j\}$, he defined $\operatorname{jump}(e) = |i - j|$, and suggested that ordering the vertices, $v_1, v_2, \ldots, v_n$, by the values of a characteristic valuation comes close to minimizing

$$\operatorname{Jump}(G) = \sum_{e \in E(G)} [\operatorname{jump}(e)]^2.$$

THEOREM 3.11 [104]. $\operatorname{Jump}(G) \geqslant a(G)n(n^2 - 1)/12$.

If T_C is a C-edge weighted tree (see Section 1), denote by $a(T_C)$ the second smallest eigenvalue of $L(T_C)$. The *absolute algebraic connectivity* of the (unweighted) tree T is $\hat{a}(T) = \max a(T_C)$, where the maximum is over all positive real-valued functions C of $E(T)$ that satisfy $\sum_{i<j} c_{ij} = n - 1$.

Associated with T is a metric space T_m obtained by identifying each edge of T with the unit interval $[0, 1]$. The points of T_m are the vertices of T together with all points of the (unit interval) edges. The graph-theoretic distance between vertices in T extends naturally to a metric $d(x, y)$ between points x and y in T_m. The *variance* of T is

$$\operatorname{var}(T) = \min_{x \in T_m} \sum_{v \in V} \frac{d(x, v)^2}{n - 1}.$$

THEOREM 3.12 [43]. *Let T be a tree. Then $\hat{a}(T) = 1/\operatorname{var}(T)$.*

Let G_C be a C-edge-weighted graph. For $X \subset V(G)$, let E_X be its coboundary. Define the *max cut* of G_C by

$$\operatorname{MC}(G_C) = \max_{X \subset V(G)} \sum_{\{v_i, v_j\} \in E_X} c_{ij}.$$

THEOREM 3.13 [107]. *Let $\lambda_1(G_C)$ be the maximum eigenvalue of the C-edge weighted Laplacian $L(G_C)$. Then*

$$\operatorname{MC}(G_C) \leqslant \frac{n\lambda_1(G_C)}{4}.$$

The C-edge-weighted Laplacian is distantly related to the positive semidefinite symmetric matrices $B = (b_{ij})$ satisfying $\sum b_{ii} = 1$ and $b_{ij} = 0$ for $\{v_i, v_j\} \in E(G)$ that are used in [81] to study the Shannon capacity. Results involving chromatic numbers and multiplicities of eigenvalues of other matrices distantly related to C-edge-weighted Laplacians can be found in [136, 137].

4. CONGRUENCE AND EQUIVALENCE

As we have seen [Equation (4)], G_1 and G_2 are isomorphic if and only if there is a permutation matrix P such that $P^t L(G_1) P = L(G_2)$. Thus, one necessary condition for two graphs to be isomorphic is that they have similar

Laplacian matrices, partially explaining all the interest in the Laplacian spectrum. But there are other ways to view (4). Recall that an n-by-n integer matrix U is *unimodular* if $\det U = \pm 1$. So the unimodular matrices are precisely those integer matrices with integer inverses. Two integer matrices A and B are said to be *congruent* if there is a unimodular matrix U such that $U^tAU = B$. Because permutation matrices are unimodular, another interpretation of (4) is that two graphs are isomorphic only if they have unimodularly congruent Laplacian matrices. Henceforth, we will say G_1 and G_2 are *congruent* if there is a unimodular matrix U such that $U^tL(G_1)U = L(G_2)$. The first significant work on congruent graphs was done by William Watkins.

THEOREM 4.1 [140]. *Suppose G_1 and G_2 are graphs on n vertices. If the blocks of G_1 are isomorphic to the blocks of G_2, then G_1 and G_2 are congruent.*

Watkins showed that the converse of Theorem 4.1 *fails by exhibiting a pair of congruent, nonisomorphic* 2*-connected graphs. Two graphs, G_1 and G_2, are cycle-isomorphic* (*or* 2*-isomorphic* [144]) *if there is a bijection $f: E(G_1) \to E(G_2)$ with the property that Y is the set of edges constituting a cycle in G_1 if and only if $f(Y)$ is the set of edges constituting a cycle in G_2.*

THEOREM 4.2 [141]. *Let G_1 and G_2 be graphs with n vertices. Then G_1 and G_2 are congruent if and only if they are cycle-isomorphic.*

Denote the *chromatic polynomial* of G by

$$p_G(x) = \sum_{t=0}^{n-1} (-1)^t c_t(G) x^{n-t}. \tag{10}$$

Then $p_G(k)$ is the number of ways to color the vertices of G, using k colors, in which adjacent vertices are colored differently. Using either matroid theory or Whitney's theorem [143], one may easily deduce the following from Theorem 4.2:

COROLLARY 4.3 [97]. *Congruent graphs afford the same chromatic polynomial.*

The converse of Corollary 4.3 is false. R. C. Reed [116] produced the pair of "chromatically equivalent" graphs illustrated in Figure 3. Since they have 128 and 120 spanning trees, respectively, they are not even equivalent (see below), much less congruent.

Using another result of Whitney [144], one may draw a potentially more important conclusion from Theorem 4.2:

COROLLARY 4.4 [141]. *If G_1 is a 3-connected graph, then G_1 and G_2 are isomorphic if and only if they are congruent.*

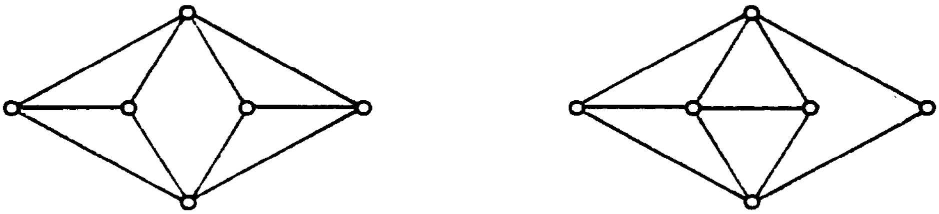

FIG. 3. Read's chromatically equivalent graphs.

The fact that there is no canonical form for congruence [49] places some practical limitations on the usefulness of Corollary 4.4. On the other hand, integer matrices cannot be congruent if they are not equivalent, and the question of unimodular equivalence is easily settled by means of the Smith normal form.

Recall that integer matrices A and B are *equivalent* if there exist unimodular matrices U_1 and U_2 such that $U_1 A U_2 = B$. So a third interpretation of (4) is that G_1 and G_2 are isomorphic only if their Laplacian matrices are equivalent. For the purpose of this article, we will say two graphs are equivalent if their Laplacian matrices are equivalent.

Denote by $d_k(G)$ (not to be confused with vertex degrees) the kth *determinantal divisor* of $L(G)$, i.e., the greatest common divisor of all the k-by-k determinantal minors of $L(G)$. [It follows from the matrix-tree theorem that $d_{n-1}(G)$ is the number of spanning trees in G; and $d_n(G) = 0$, because $L(G)$ is singular.] Of course, $d_k(G) \mid d_{k+1}(G)$, $0 < k < n$. The *invariant factors* of G are defined by $s_{k+1}(G) = d_{k+1}(G)/d_k(G)$, $0 \leqslant k < n$, where $d_0(G) = 1$. The *Smith normal form* of $L(G)$ is

$$F(G) = \operatorname{diag}(s_1(G), s_2(G), \dots, s_n(G)).$$

So G_1 and G_2 are equivalent if and only if $F(G_1) = F(G_2)$. In particular, if G_1 and G_2 are isomorphic, then $F(G_1) = F(G_2)$. Now, if *this* observation had a partial converse, e.g., for 3-connected graphs, it would have great computational significance because $F(G)$ can be obtained from $L(G)$ by a sequence of elementary row and column operations. However, the graphs in Figure 4 share the Smith normal form diag(1, 1, 1, 5, 15, 0), and the graph on the left ($P_2 \times C_3$) is 3-connected.

In spite of this discouraging example, $F(G)$ yields several bona fide graph-theoretic invariants and spawns a variety of applications: The *cycle space*, C_G (not to be confused with G_C), of the oriented graph G is the column null space of the vertex-edge incidence matrix $Q(G)$ [and hence the

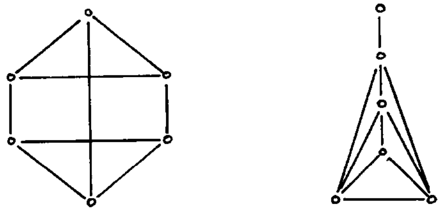

FIG. 4. Graphs with the same Smith normal form.

null space of the "edge version" $K(G)$]; the *cocycle space* or *bond space*, R_G, is the row space of $Q(G)$. As a subspace of real (or complex) m-space, the "bicycle" space, $B_G = C_G \cap R_G$, is trivially equal to $\{0\}$. When the coefficients come from Abelian groups, however, one obtains an analogous *bicycle group* which may be more interesting. K. A. Berman ([9], but see [85] and/or [97] for a clarifying discussion) used the invariant factors of $L(G)$ to completely characterize bicycle groups. Meanwhile, from another perspective, D. J. Lorenzini [79] investigated a similar application of $F(G)$ to the components of the Néron model of the Jacobian associated with a generic curve in algebraic geometry.

Denote by $b(G)$ the *multiplicity of* 1 *in* $F(G)$. Of course, $b(G) \geqslant n - 2$, for any graph G with a square-free number of spanning trees. Lorenzini [80] discusses a bound for $b(G)$ in terms of the number of independent cycles of G.

THEOREM 4.5 [64]. *Let G be a connected graph of diameter d. Then $b(G) \geqslant d$.*

At the present time, a clear understanding of the relation of the invariant factors, $s_i(G)$, $1 < i < n - 1$, to graph structure seems rather distant. In rather stark contrast, however, the Smith normal form of $K(G)$ has been described completely.

THEOREM 4.6 [97]. *Let G be a connected graph with n vertices and $m > 0$ edges. Then the Smith normal form of $K(G)$ is $I_{n-2} \dot{+} (n) \dot{+} 0_{m-n+1}$, where the identity (direct) summand is absent when $m = 1$, and the zero summand is missing when $m = n - 1$.*

Theorem 4.6 has applications to certain "flows" in directed graphs. Of these, the "0-flows," or "A-flows," have been counted by D. Welsh using the chromatic polynomial of the cocycle matroid [142].

The *elementary divisors* of $L(G)$ are the prime power factors of its invariant factors. Denote by $\mathrm{el}(G)$ the multiset of these elementary divisors.

THEOREM 4.7 [97, 140]. *Let $G_1 \cdot G_2$ be any coalescence of G_1 and G_2. Then* $\mathrm{el}(G_1 \cdot G_2) = \mathrm{el}(G_1 + G_2) = \mathrm{el}(G_1) \cup \mathrm{el}(G_2)$.

5. CHEMICAL APPLICATIONS

Modern organic chemists have synthesized and/or isolated several million different molecules [118]. Perhaps even more remarkable has been their ability to predict certain properties of chemical substances even before they have been synthesized. Among the tools used in such predictions are numerous "topological indices" (a term coined by Haruo Hosoya in 1971 [120]). A typical topological index is a number arising from the underlying graph of a chemical compound. (See, e.g., [6, 94, 101, 108, 109, 117–121].)

The *Wiener index*, introduced by Harry Wiener of Brooklyn College in 1947, has been used in a variety of ways from predicting antibacterial activity in drugs to correlating thermodynamic parameters in physical chemistry and modeling various solid-state phenomena [67]. It can be obtained by summing the entries in the upper triangular part of the "distance matrix" [133, p. 45].

The distance, $d(u, v)$, between vertices u and v in a connected graph G is the number of edges in a shortest path from u to v. The distance matrix $\Delta(G) = (d(v_i, v_j))$ is the n-by-n matrix whose (i, j) entry is the distance from v_i to v_j. So $\Delta(G)$ is a symmetric matrix with zeros along the main diagonal. Hosoya [70, 71] was among the first to study the distance matrix from a chemical perspective. It has since become a standard tool used in a variety of applications from investigating evolutionary distances in DNA sequences to predicting carcinogenicity in arene systems [119]. In the mathematical literature, distance matrices seem first to have appeared in [56], where the following remarkable result was proved:

THEOREM 5.1. *Let T be a tree on n vertices. Then* $\det \Delta(T) = (-1)^{n-1}(n-1)2^{n-2}$.

One surprising thing about Theorem 5.1 is that $\det \Delta(T)$ depends only on n and not at all on the structure of T. In any event, it follows that $\Delta(T)$ is an invertible matrix with exactly one positive eigenvalue. In spite of this elegant beginning, results about the distance matrix have not come easily. (See [21, 22, 32, 54, 55, 123].)

If there were a "Holy Grail" in graph theory, it would be a practical test for graph isomorphism. In the early days, it was incautiously conjectured that two graphs are isomorphic if and only if they have similar adjacency matrices, i.e., that two adjacency matrices could not be similar without being permutation-similar. The disproof of this conjecture began the study of adjacency cospectral graphs: G_1 and G_2 are *adjacency cospectral* if $A(G_1)$ and $A(G_2)$ have the same characteristic polynomial. One of the most dramatic results in algebraic graph theory is Allen Schwenk's "almost all trees are cospectral" theorem [128]: Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of such trees T for which there exists a nonisomorphic tree T' such that T and T' are adjacency cospectral. Then $\lim_{n\to\infty} r_n/t_n = 1$.

Perhaps $A(G)$ is just the wrong matrix. Maybe it is too sparse. What about the distance matrix, whose only zeros occur on the main diagonal? Not surprisingly, it was conjectured that two trees could not be distance-cospectral without being isomorphic [32, 71]. This conjecture eventually led to the following worthy successor of Schwenk's theorem.

THEOREM 5.2 [86]. *Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of such trees T for which there exists a nonisomorphic tree T' such that, simultaneously,*

(i) *T and T' are adjacency-cospectral,*
(ii) *T and T' are distance-cospectral, and*
(iii) *T and T' are Laplacian-cospectral.*

Then $\lim_{n\to\infty} r_n/t_n = 1$.

Additional simultaneous conditions will be added in Theorem 6.6. The next result [95] (also see [55]) further strengthens the spectral relationship between $L(T)$ and $\Delta(T)$.

THEOREM 5.3. *Let T be a tree. Then the eigenvalues of $-2K(T)^{-1}$ interlace the eigenvalues of $\Delta(T)$. That is, let $\delta_1 > 0 > \delta_2 \geqslant \cdots \geqslant \delta_n$ be the eigenvalues of $\Delta(T)$, and suppose $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1}$ are the nonzero eigenvalues of $L(T)$. Then*

$$0 > \frac{-2}{\lambda_1} \geqslant \delta_2 \geqslant \frac{-2}{\lambda_2} \geqslant \delta_3 \geqslant \cdots \geqslant \frac{-2}{\lambda_{n-1}} \geqslant \delta_n.$$

Theorem 5.3 makes it possible to transcribe some Laplacian spectral results for distance matrices. Suppose, for example, T is a tree with diameter d. Then $\delta_{[d/2]} > -1$. If T has p pendant vertices and q pendant neighbors, then $\delta_q > -1$ (provided $n > 2q$), $\delta_{n-q+2} < -2$, $\delta_p \geqslant -2$, and $\delta_{n-p+2} \leqslant$

-2. If δ is an eigenvalue of $\Delta(T)$ of multiplicity k, then $k \leqslant p$; among the eigenvalues of $\Delta(T)$, $\delta = -2$ occurs with multiplicity at least $p - q - 1$. (Karen Collins has improved this to $p - q$ [23].)

In a remarkable *tour de force*, M. Fiedler [44] placed Theorem 5.3 in a geometrical setting. One may view $L(G)$ as a Gram matrix based on n vectors, $y_1, y_2, \dots, y_n$ in $(n-1)$-dimensional real Euclidean space E_{n-1}. Let S be the unit sphere centered at the origin in E_{n-1}. Let P_i be the hyperplane tangent to S at its intersection with the ray generated by y_i. Let H_i be the half space, determined by P_i, that contains the origin. Then the intersection of the H_i produces a simplex. Let $A_1, A_2, \dots, A_n$ be the vertices of this simplex. Define e_{ij} to be the square of the Euclidean distance (in E_{n-1}) between A_i and A_j. The matrix $E(G) = (e_{ij})$ is called the (Cayley-)*Menger matrix* of the simplex [152].

THEOREM 5.4 [44, 150]. *If T is a tree, then $E(T) = \Delta(T)$, i.e., the distance matrix of a tree is the Menger matrix of the simplex arising from its Laplacian matrix.*

Returning to the Wiener index,

$$W(G) = \sum_{i<j} d(v_i, v_j),$$

we have the following result [88, 94, 95, 101, 105]:

THEOREM 5.5. *Let T be a tree with Laplacian eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} > 0 = \lambda_n$. Then $W(T)$ is given by*

$$\sum_{i=1}^{n-1} \frac{n}{\lambda_i}. \tag{11}$$

For a general graph, the Wiener index is not a function of its Laplacian spectrum [94]. This suggests that one might define $W_1(G) = W(G)$ and $W_2(G)$ by (11). Then $W_1(G) = W_2(G)$ if G is a tree, but the two indices may differ otherwise. Indeed, since the dominant contribution to $W_2(G)$ is n/λ_{n-1}, it may even be of interest to study $W_3(G) = n/a(G)$. Other possibilities are suggested in [101]. (Some ideas for computing $W(G)$ are contained in [106].)

The expression (11) has turned up in some other contexts. It is, for example, n^2 times the mean squared radius of gyration of a polymer molecule [33–35, 110]. If $S(n, m)$ denotes the set of all graphs on n vertices having at most m edges, then minimizing (11) over $S(n, m)$ corresponds to the A-optimality criterion in statistical design [25, p. 156].

6. IMMANANTS

Let $A = (a_{ij})$ be an n-by-n matrix. Then

$$\operatorname{per} A = \sum_{p \in S_n} \prod_{t=1}^{n} a_{tp(t)}, \tag{12}$$

where S_n is the symmetric permutation group. Permanents of adjacency matrices have received some attention, especially by chemists who use them to count "Kekulé structures" in chemical graphs [30, 124]. (August Kekulé von Stradonitz first proposed the hexagonal configuration for the benzene molecule [1, 133]. Arising from the alternating single and double bonding between carbon atoms in C_6H_6, a Kekulé structure corresponds to a perfect matching in the underlying carbon skeleton. The "Char postulate" [134] asserts that a benzenoid system with no Kekulé structure should be an unstable biradical. At the same time, aromatic compounds—characterized by benzene-like ring structures—"survive intact over geologic time and even persist in the harsh environment of nebulae" [1].)

The serious study of per $L(G)$ seems to have begun with the conjecture [98] that per $L(G) \geqslant 2(n-1)$, for all connected graphs on n vertices. This conjecture was established by R. Brualdi and J. L. Goldwasser [14] in the course of their study of the *Laplacian ratio*, per $L(G)/\prod d_i$. (Also see [7, 13, 52, 90, 138, 139]. It was suggested in [112] that $\min \operatorname{per} A = \operatorname{per} L(K_n)$, where the minimum is over the set of all singular correlation matrices.)

Now, per $L(G)$ is just the constant coefficient in the *Laplacian permanental polynomial*

$$f_G(x) = \operatorname{per}[xI - L(G)] = \sum_{t=0}^{n} (-1)^t a_t(G) x^{n-t}. \tag{13}$$

Since the permanent is invariant under permutation similarities, the coefficients and roots of $f_G(x)$ are graph-theoretic invariants. The following result is the permanental analog of Theorem 2.9.

THEOREM 6.1 [36]. *The multiplicity of* 1 *as a root of the permanental polynomial $f_G(x)$ is at least $p(G) - q(G)$.*

There are, of course, a number of obstacles to be overcome in the study of $f_G(x)$, not the least of which is the notorious computational intractability of the permanent function. (Only in some special cases, e.g. for trees, has this challenge been overcome [13, 83].) Another obstacle concerns the roots of

$f_G(x)$. For one thing, there is nothing resembling eigenvectors associated with them. For another, they need not all be real. [If, for example, A is an n-by-n correlation matrix, then the roots of $\operatorname{per}(xI - A)$ are all real if and only if $A = I_n$.] Say that a graph is *permanently real* if all roots of $f_G(x)$ are real. Then there is not a single permanently real graph among the 112 connected graphs on 6 vertices. But if $G = K_{1,n-1}$, then (Theorem 6.1) $(x-1)^{n-2}$ is a factor of $f_G(x)$. The other factor is $x^2 - nx + 2(n-1)$. Thus, $K_{1,n-1}$ is permanently real for all $n \geqslant 7$.

Denote the characteristic polynomial of $L(G)$ by

$$\det[xI - L(G)] = \sum_{t=0}^{n-1} (-1)^t b_t(G) x^{n-t}. \tag{14}$$

Graph-theoretic interpretations of the coefficients $b_t(G)$ were given in [30, 75, 76]. (See [45] for the edge-weighted version.)

THEOREM 6.2. *If G is a graph on n vertices, then*

$$b_t(G) = \sum P(F),$$

where the sum is over all $(n-t)$-edged spanning forests F of G, and $P(F)$ is the product of the numbers of vertices in each of the t components of F.

As in (10), denote the *chromatic polynomial* of G by

$$p_G(x) = \sum_{t=0}^{n-1} (-1)^t c_t(G) x^{n-t}.$$

THEOREM 6.3. *Let G be a connected graph on n vertices. Then $a_0(G) = b_0(G) = c_0(G) = 1$, $a_1(G) = b_1(G) = 2c_1(G) = 2m$, and*

$$a_t(G) \geqslant b_t(G) \geqslant (t+1)c_t(G), \qquad 1 < t < n. \tag{15}$$

In (15), the left-hand inequality is immediate from Schur's theorem [126]. In the right-hand inequality [93], equality holds for $t = n-1$ if and only if G is a tree; if $n \geqslant 4$, then equality holds for $t = n-2$ if and only if it holds for all t if and only if $G = K_{1,n-1}$.

Now, determinants and permanents are but two examples of matrix functions that have come to be known as *immanants*. If χ is an irreducible (characteristic 0) character of S_n, the corresponding *immanant*, d_χ, is defined by

$$d_\chi(A) = \sum_{p \in S_n} \chi(p) \prod_{t=1}^{n} a_{tp(t)} \tag{16}$$

for any n-by-n matrix $A = (a_{ij})$. If $\chi = \varepsilon$, the signum character, then $d_\chi = \det$. If $\chi = 1$, then $d_\chi = \text{per}$.

There is a natural one-to-one correspondence between the irreducible characters χ of S_n and the (nonincreasing, integer) partitions of n. (Thus, Ferrers-Sylvester diagrams, such as those in Figure 2, play a prominent role in the character theory of S_n.) Those characters χ_r corresponding to partitions of the form $(r, 1^{n-r})$, short for

$$n = r + 1 + \cdots + 1,$$

are called *single-hook characters*. For example, $\chi_1 = \varepsilon$ and $\chi_n = 1$. [In general, $\chi_r(e) = C(n-1, r-1)$, the binomial coefficient $(n-1)$-choose-$(r-1)$.] We will denote by d_r the immanant corresponding to χ_r, so $d_1 = \det$, and $d_n = \text{per}$. [The context should permit the reader to distinguish between the immanant $d_r(L(G))$, the determinantal divisor $d_r(G)$, and the vertex degree d_r.] It turns out that these single-hook immanants can be used to count $h(G)$, the number of *Hamiltonian circuits* in G [91]. (Also, see [53].)

THEOREM 6.4. *Let G be a connected graph on $n \geqslant 3$ vertices. Then the number of Hamiltonian circuits in G is*

$$h(G) = \frac{1}{2n} \sum_{r=2}^{n} (-1)^r d_r(L(G)).$$

If A is an n-by-n positive semidefinite Hermitian matrix, then $(n-1)^r \text{per}\, A \geqslant d_{n-1}(A)$ [99]. Once again, it would seem surprising if a general result like this could not be improved when restricted to a much smaller class of matrices.

CONJECTURE 6.5. If T is a tree on n vertices, then $(n-2)\,\text{per}\, L(T) \geqslant d_{n-1}(L(T))$.

There is a natural affinity between immanants and Laplacians. Recall that $L(G)$ is a Gram matrix based, e.g., on the row vectors $Q_1, Q_2, \ldots, Q_m$ of

$Q(G)$. It turns out that $d_\chi(L(G))$ is $n!/\chi(e)$ times the length of the "decomposable symmetrized tensor" $Q_1 * Q_2 * \cdots * Q_m$. [If G is connected, then $d_\chi(L(G)) > 0$ for all $\chi \neq \varepsilon$.]

Let $M_\chi = \{U : d_\chi(U^{-1}AU) = d_\chi(A) \text{ for all } A\}$. If $\chi = \varepsilon$, then M_χ is the full linear group. Otherwise, it is the monomial group consisting of all nonzero scalar multiples of permutation matrices [48]. Thus, each of the *immanantal polynomials* $d_\chi(xI - L(G))$, as χ ranges over the characters of S_n (irreducible or not), is a graph-theoretic invariant.

At present, only a little is known about general *immanantal roots*. While they need not all be real, those that are lie in the interval $[0, \lambda_1(G)]$ [89]. After determinant and permanent, the most widely studied immanantal polynomial is $d_2(xI - L(G))$. It is known that the d_2-roots lie in the Geršgorin circles [72]. The coefficient of x in the d_2-polynomial is related to *moment sums* in graphs, leading to an extension of the notion of *centroid point* [92].

It turns out that immanantal polynomials, even when they are all taken together, are not much better than the characteristic polynomial when it comes to distinguishing nonisomorphic graphs. J. Turner [135] found a pair of nonisomorphic trees T and T' on 12 vertices such that $d_\chi(xI - A(T)) = d_\chi(xI - A(T'))$ for all 77 irreducible characters χ of S_{12}. Such examples also exist for the Laplacian. Indeed, as we now see, they are *typical* (in the sense of Schwenk and McKay).

THEOREM 6.6 [12]. *Let t_n be the number of nonisomorphic trees on n vertices. Let r_n be the number of such trees T for which there is a nonisomorphic tree T' such that, simultaneously, for every character χ of S_n, both*

(iv) $d_\chi(xI - A(T)) = d_\chi(xI - A(T'))$ *and*
(v) $d_\chi(xI - L(T)) = d_\chi(xI - L(T'))$.

Then $\lim_{n\to\infty} r_n/t_n = 1$.

We have used (iv) and (v) in the statement of Theorem 6.6 because it may be viewed as a continuation of Theorem 5.2.

REFERENCES

1 J. Aihara, Why aromatic compounds are stable, *Sci. Amer.* 266, Mar. 1992, pp. 62–68.
2 N. Alon, Eigenvalues and expanders, *Combinatorica* 6:83–96 (1986).
3 N. Alon, Z. Galil, and V. D. Milman, Better expanders and superconcentrators, *J. Algorithms* 8:337–347 (1987).

4 N. Alon and V. D. Milman, λ_1, isoperimetric inequalities for graphs, and superconcentrators, *J. Combin. Theory Ser. B* 38:73–88 (1985).
5 W. N. Anderson and T. D. Morley, Eigenvalues of the Laplacian of a graph, *Linear and Multilinear Algebra* 18:141–145 (1985).
6 A. T. Balaban, Chemical graphs, *Theoret. Chim. Acta (Berl.)* 53:355–375 (1979).
7 R. B. Bapat, A bound for the permanent of the Laplacian matrix, *Linear Algebra Appl.* 74:219–223 (1986).
8 R. B. Bapat and G. Constantine, An enumerating function for spanning forests and color restrictions, *Linear Algebra Appl.* 173:231–237 (1992).
9 K. A. Berman, Bicycles and spanning trees, *SIAM J. Algebraic Discrete Methods* 7:1–12 (1986).
10 F. Bien, Constructions of telephone networks by group representations, *Notices Amer. Math. Soc.* 36:5–22 (1989).
11 N. Biggs, *Algebraic Graph Theory*, Cambridge U.P., 1974.
12 P. Botti and R. Merris, Almost all trees share a complete set of immanantal polynomials, *J. Graph Theory*, to appear.
13 P. Botti, R. Merris, and C. Vega, Laplacian permanents of trees, *SIAM J. Discrete Math.* 5:460–466 (1992).
14 R. A. Brualdi and J. L. Goldwasser, Permanent of the Laplacian matrix of trees and bipartite graphs, *Discrete Math.* 48:1–21 (1984).
15 F. C. Bussemaker and D. M. Cvetković, There are exactly 13 connected, cubic, integral graphs, *Univ. Beograd Publ. Elektrotehn. Fak. Ser. Mat. Fiz.* 544–576:43–48 (1976).
16 S. Chaiken, A combinatorial proof of the all minors matrix tree theorem, *SIAM J. Algebraic Discrete Methods* 3:319–329 (1982).
17 S. Chaiken and D. J. Kleitman, Matrix tree theorems, *J. Combin. Theory Ser. A* 24:377–381 (1978).
18 J. Cheeger, A lower bound for the smallest eigenvalue of the Laplacian, in *Problems in Analysis* (R. C. Gunning, Ed.), Princeton U.P., 1970, pp. 195–199.
19 F. R. K. Chung, Diameters and eigenvalues, *J. Amer. Math. Soc.* 2:187–196 (1989).
20 F. R. K. Chung, V. Faber, and T. Manteuffel, An upper bound on the diameter of a graph from eigenvalues associated with its Laplacian, manuscript.
21 K. L. Collins, On a conjecture of Graham and Lovasz about distance matrices, *Discrete Appl. Math.* 25:27–35 (1989).
22 Factoring distance matrix polynomials, *Discrete Math.*, to appear.
23 Private communication.
24 G. M. Constantine, Schur convex functions on the spectra of graphs, *Discrete Math.* 45:181–188 (1983).
25 *Combinatorial Theory and Statistical Design*, Wiley, New York, 1987.
26 Graph complexity and the Laplacian matrix in blocked experiments, *Linear and Multilinear Algebra* 28:49–56 (1990).
27 D. M. Cvetković, Cubic integral graphs, *Univ. Beograd Publ. Elektrotehn. Fak. Ser. Mat. Fiz.* 498–541:107–113 (1975).
28 D. M. Cvetković and M. Doob, Developments in the theory of graph spectra, *Linear and Multilinear Algebra* 18:153–181.

29 D. M. Cvetković, M. Doob, I. Gutman, and A. Torĝasev, *Recent Results in the Theory of Graph Spectra*, North-Holland, Amsterdam, 1988.
30 D. M. Cvetković, M. Doob, and H. Sachs, *Spectra of Graphs*, Academic, New York, 1979.
31 E. A. Dinic, A. K. Kelmans, and M. A. Zaitsev, Nonisomorphic trees with the same T-polynomial, *Inform. Process. Lett.* 6:73–76 (1977).
32 M. Edelberg, M. R. Garey, and R. L. Graham, On the distance matrix of a tree, *Discrete Math.* 14:23–31 (1976).
33 B. E. Eichinger, Elasticity theory. I. Distribution functions for perfect phantom networks, *Macromolecules* 5:496–505 (1972).
34 Configuration statistics of Gaussian molecules, *Macromolecules*, 13:1–11 (1980).
35 Random elastic networks. I. Computer simulation of linked stars, *J. Chem. Phys.* 75:1964–1979 (1981).
36 I. Faria, Permanental roots and the star degree of a graph, *Linear Algebra Appl.* 64:255–265 (1985).
37 M. Fiedler, Algebraic connectivity of graphs, *Czechoslovak Math. J.* 23:298–305 (1973).
38 Eigenvectors of acyclic matrices, *Czechoslovak Math. J.* 25:607–618 (1975).
39 A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory, *Czechoslovak Math. J.* 25:619–633 (1975).
40 Algebraische Zusammenhangszahl der Graphen und ihre Numerische Bedeutung, *Internat. Ser. Numer. Math.* 29, Birkhäuser, Basel, 1975, pp. 69–85.
41 An algebraic approach to connectivity of graphs, in *Recent Advances in Graph Theory*, Academia, Prague, 1975, pp. 193–196.
42 Laplacian of graphs and algebraic connectivity, in *Combinatorics and Graph Theory*, Banach Center Publ. 25, PWN, Warsaw, 1989, pp. 57–70.
43 Absolute algebraic connectivity of trees, *Linear and Multilinear Algebra* 26:85–106 (1990).
44 A geometric approach to the Laplacian matrix of a graph, presented at Algebraic Graph Theory Workshop, Inst. for Math. Appl., Minneapolis, 12 November 1991.
45 M. Fiedler and J. Sedláček, O *W*-basich orientovaných grafů (in Czech), *Čas. Pěst Mat.* 83:214–225 (1958).
46 M. E. Fischer, On hearing the shape of a drum, *J. Combin. Theory* 1:105–125 (1966).
47 W. C. Forsman, Graph theory and the statistics and dynamics of polymer chains, *J. Chem. Phys.* 65:4111–4115 (1976).
48 S. Friedland, Maximality of the monomial group, *Linear and Multilinear Algebra* 18:1–7 (1985).
49 Quadratic forms and the graph isomorphism problem, *Linear Algebra Appl.* 150:423–442 (1991).
50 Lower bounds for the first eigenvalue of certain *M*-matrices associated with graphs, *Linear Algebra Appl.* 172:71–84 (1992).
51 C. Godsil, Real graph polynomials, in *Progress in Graph Theory* (J. A. Bondy and U. S. R. Murty, Eds.), Academic, New York, 1984, pp. 281–293.
52 J. L. Goldwasser, Permanent of the Laplacian matrix of trees with a given matching, *Discrete Math.* 61:197–212 (1986).

53 I. P. Goulden and D. M. Jackson, The enumeration of directed closed Euler trails and directed Hamiltonian circuits by Lagrangian methods, *European J. Combin.* 2:131–135 (1981).

54 R. L. Graham and L. Lovász, Distance matrix polynomials of trees, in *Theory and Applications of Graphs* (Y. Alavi and D. R. Lick, Eds.), Lecture Notes in Math. 642, Springer-Verlag, Berlin, 1978, pp. 186–190.

55 Distance matrix polynomials of trees, *Adv. in Math.* 29:60–88 (1978).

56 R. L. Graham and H. O. Pollak, On the addressing problem for loop switching, *Bell System Tech. J.* 50:2495–2519 (1971).

57 M. Gromov and V. D. Milman, A topological application of the isoperimetric inequality, *Amer. J. Math.* 105:843–854 (1983).

58 R. Grone and R. Merris, Algebraic connectivity of trees, *Czechoslovak Math. J.* 37:660–670 (1987).

59 Cutpoints, lobes and the spectra of graphs, *Portugal. Math.* 45:181–188 (1988).

60 Ordering trees by algebraic connectivity, *Graphs Combin.* 6:229–237 (1990).

61 Coalescence, majorization, edge valuations and the Laplacian spectra of graphs, *Linear and Multilinear Algebra* 27:139–146 (1990).

62 The Laplacian spectrum of a graph II, *SIAM J. Discrete Math.*, to appear.

63 R. Grone, R. Merris, and V. S. Sunder, The Laplacian spectrum of a graph, *SIAM J. Matrix Anal. Appl.* 11:218–238 (1990).

64 R. Grone, R. Merris, and W. Watkins, Laplacian unimodular equivalence of graphs, in *Combinatorial and Graph-Theoretic Problems in Linear Algebra* (R. Brualdi, S. Friedland, and V. Klee, Eds.), *IMA Vol. Math. Appl.* 50, Springer-Verlag, New York, to appear.

65 R. Grone and G. Zimmermann, Large eigenvalues of the Laplacian, *Linear and Multilinear Algebra* 28:45–47 (1990).

66 I. Gutman, Graph-theoretical formulation of Forsman's equations, *J. Chem. Phys.* 68:1321–1322 (1978).

67 I. Gutman and D. H. Rouvray, A new theorem for the Wiener molecular branching index of trees with perfect matchings, *Comput. and Chem.*, to appear.

68 F. Harary and A. J. Schwenk, Which graphs have integral spectra?, in *Graphs and Combinatorics* (R. A. Bari and F. Harary, Eds.), Lecture Notes in Math. 406, Springer-Verlag, Berlin, 1974, pp. 45–51.

69 Y. Hattori, Nonisomorphic graphs with the same T-polynomial, *Inform. Process. Lett.* 22:133–134 (1986).

70 H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Japan* 44:2332–2339 (1971).

71 H. Hosoya, M. Murakami, and M. Gotoh, Distance polynomial and characterization of a graph, *Nat. Sci. Rep. Ochanomizu Univ.* 24:27–34 (1973).

72 C. R. Johnson, R. Merris, and S. Pierce, Inequalities involving immanants and diagonal products for H-matrices, *Portugal. Math.* 43:43–54 (1985–1986).

73 F. Juhasz, The asymptotic behavior of Fiedler's algebraic connectivity of graphs, *Discrete Math.* 96:59–63 (1991).

74 M. Kac, Can one hear the shape of a drum, *Amer. Math. Monthly* 73:1–23 (1966).

75 A. K. Kel'mans, Properties of the characteristic polynomial of a graph, (in Russian) *Kibernet. na Službu Kommunizmu* 4:27–41 (1967).

76 A. K. Kelmans and V. M. Chelnokov, A certain polynomial of a graph and graphs with an extremal number of trees, *J. Combin. Theory Ser. B* 16:197–214 (1974).

77 G. Kirchhoff, Über die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Verteilung galvanischer Ströme geführt wird, *Ann. Phys. Chem.* 72:497–508 (1847).

78 M. Lewin, A generalization of the matrix-tree theorem, *Math. Z.* 181:55–70 (1982).

79 D. J. Lorenzini, Arithmetical graphs, *Math. Ann.* 285:481–501 (1989).

80 A finite group attached to the laplacian of a graph, *Discrete Math.* 91:277–282 (1991).

81 L. Lovász, On the Shannon capacity of a graph, *IEEE Trans. Inform. Theory* 25:1–7 (1979).

82 C. Maas, Transportation in graphs and the admittance spectrum, *Discrete Appl. Math.* 16:31–49 (1987).

83 M. Malek, Conversion of the permanent into the determinant, manuscript.

84 A. W. Marshall and I. Olkin, *Inequalities: Theory of Majorization and Its Applications*, Academic, New York, 1979.

85 S. B. Maurer, Matrix generalizations of some theorems on trees, cycles and cocycles in graphs, *SIAM J. Appl. Math.* 30:143–148 (1976).

86 B. D. McKay, On the spectral characterisation of trees, *Ars Combin.* 3:219–232 (1977).

87 The expected eigenvalue distribution of a large regular graph, *Linear Algebra Appl.* 40:203–216 (1981).

88 Private communication.

89 R. Merris, Two problems involving Schur functions, *Linear Algebra Appl.* 10:155–162 (1975).

90 The Laplacian permanental polynomial for trees, *Czechoslovak Math. J.* 32:397–403 (1982).

91 Single-hook characters and Hamiltonian circuits, *Linear and Multilinear Algebra* 4:21–35 (1983).

92 The second immanantal polynomial and the centroid of a graph, *SIAM J. Algebraic Discrete Methods* 7:484–503 (1986).

93 Characteristic vertices of trees, *Linear and Multilinear Algebra* 22:115–131 (1987).

94 An edge version of the matrix-tree theorem and the Wiener index, *Linear and Multilinear Algebra* 25:291–296 (1989).

95 The distance spectrum of a tree, *J. Graph Theory* 14:365–369 (1990).

96 The number of eigenvalues greater than two in the Laplacian spectrum of a graph, *Portugal. Math.* 48:345–349 (1991).

97 Unimodular equivalence of graphs, *Linear Algebra Appl.* 173:181–189 (1992).

98 R. Merris, K. R. Rebman, and W. Watkins, Permanental polynomials of graphs, *Linear Algebra Appl.* 38:273–288 (1981).

99 R. Merris and W. Watkins, Inequalities and identities for generalized matrices, *Linear Algebra Appl.* 64:223–242 (1985).

100 M. Michalski, Branching extent and spectra of trees, *Publ. Inst. Math.* 39:35–43 (1986).
101 B. Mohar, Laplacian matrices of graphs, *Preprint Ser. Dept. Math. Univ. E. K. Ljubljana* 26:385–392 (1988).
102 Isoperimetric inequalities, growth, and the spectra of graphs, *Linear Algebra Appl.* 103:119–131 (1988).
103 Isoperimetric numbers of graphs, *J. Combin. Theory Ser. B* 47:274–291 (1989).
104 The Laplacian spectrum of graphs, in *Graph Theory, Combinatorics, and Applications* (Y. Alavi, G. Chartrand, O. R. Ollermann, and A. J. Schwenk, Eds.), Wiley, New York, 1991, pp. 871–898.
105 Eigenvalues, diameter, and mean distance in graphs, *Graphs Combin.* 7:53–64 (1991).
106 B. Mohar and T. Pisanski, How to compute the Wiener index of a graph, *J. Math. Chem.* 2:267–277 (1988).
107 B. Mohar and S. Poljak, Eigenvalues and the max-cut problem, *Czechoslovak Math. J.* 40:343–352 (1990).
108 Eigenvalues in combinatorial optimization, IMA Preprint Ser. 939, Inst. for Math. Appl., Univ. of Minnesota, Minneapolis, 1992.
109 I. Motoc and A. T. Balaban, Topological indices: Intercorrelations, physical meaning, correlational ability, *Rev. Roumaine Chim.* 26:593–600 (1981).
110 N. A. Neuburger and B. E. Eichinger, Computer simulation of the dynamics of trifunctional and tetrafunctional end-linked random elastic networks, *J. Chem. Phys.* 83:884–891 (1985).
111 A. Nilli, On the second eigenvalue of a graph, *Discrete Math.* 91:207–210 (1991).
112 S. Pierce, Permanents of correlation matrices, in *Current Trends in Matrix Theory* (R. Grone et al., Eds.), Elsevier, Amsterdam, 1987, pp. 247–249.
113 O. E. Polansky and D. Bonchev, Theory of the Wiener number of a graph. II. Transfer graphs and some of their metric properties, *Match* 25:3–39 (1990).
114 A. Pothen, H. D. Simon, and K.-P. Liou, Partitioning sparse matrices with eigenvectors of graphs, *SIAM J. Matrix Anal. Appl.* 11:430–452 (1990).
115 M. Protter, Can one hear the shape of a drum? revisited, *SIAM Rev.* 29:185–197 (1987).
116 R. C. Read, An introduction to chromatic polynomials, *J. Combin. Theory* 4:52–71 (1968).
117 D. H. Rouvray, Should we have designs on topological indices, in *Chemical Applications of Topology and Graph Theory* (R. B. King, Ed.), Elsevier, Amsterdam, 1983, pp. 159–177.
118 Predicting chemistry from topology, *Sci. Amer.* 255, Sept. 1986, pp. 40–47.
119 The role of the topological distance matrix in chemistry, in *Mathematics and Computational Concepts in Chemistry* (N. Trinajstić, Ed.), Horwood, Chichester, 1986, pp. 295–306.
120 Characterization of molecular branching using topological indices, in *Applications of Discrete Mathematics* (R. O. Ringesen et al., Eds.), SIAM, Philadelphia, 1988, pp. 176–178.
121 The challenge of characterizing branching in molecular species, *Discrete Appl. Math.* 19:317–338 (1988).

122 E. Ruch and I. Gutman, The branching extent of graphs, *J. Combin. Inform. System Sci.* 4:285–295 (1979).
123 S. N. Ruzieh and D. L. Powers, The distance spectrum of the path P_n and the first distance eigenvector of connected graphs, *Linear and Multilinear Algebra* 28:75–81 (1990).
124 E. M. de Sa, Note on graphs and weakly cyclic matrices, *Discrete Math.* 34:275–281 (1981).
125 I. Schur, Über eine Klasse von Mittelbildungen mit Anwendungen die Determinanten, *Sitzungsber. Berlin. Math. Gesellschaft* 22:9–20 (1923).
126 Über endliche Gruppen und Hermitesche Formen, *Math. Z.* 1:184–207 (1918).
127 S. Schuster, Interpolating theorem for the number of end-vertices of spanning trees, *J. Graph Theory* 7:203–208 (1983).
128 A. J. Schwenk, Almost all trees are cospectral, in *New Directions in Graph Theory* (F. Harary, Ed.), Academic, New York, 1973, pp. 275–307.
129 Exactly thirteen connected cubic graphs have integral spectra, in *Theory and Applications of Graphs* (Y. Alavi and D. R. Lick, Eds.), Lecture Notes in Math. 642, Springer-Verlag, Berlin, 1978, pp. 516–553.
130 L. Y. Shy and B. E. Eichinger, Large computer simulations on elastic networks: Small eigenvalues and eigenvalue spectra of the Kirchhoff matrix, *J. Chem. Phys.* 90:5179–5189 (1989).
131 W. So, Rank one perturbation and its application to the Laplacian spectrum of a graph, manuscript.
132 H. M. Trent, A note on the enumeration and listing of all maximal trees of a connected linear graph, *Proc. Nat. Acad. Sci. U.S.A.* 40:1004–1007 (1954).
133 N. Trinajstić, *Chemical Graph Theory*, Vol. I, CRC Press, Boca Raton, Fla., 1983.
134 *Chemical Graph Theory*, Vol. II, CRC Press, Boca Raton, Fla., 1983.
135 J. Turner, Generalized matrix functions and the graph isomorphism problem, *SIAM J. Appl. Math.* 16:520–536 (1968).
136 Y. C. de Verdière, Sur un nouvel invariant des graphes et un critère de planarité, *J. Combin. Theory Ser. B* 50:11–21 (1990).
137 Spectres de variétés Riemanniennes et spectres de graphes, manuscript.
138 A. Vrba, The permanent of the Laplacian matrix of a bipartite graph, *Czechoslovak Math. J.* 36:397–403 (1982).
139 Principal subpermanents of the Laplacian matrix, *Linear and Multilinear Algebra* 19:335–346 (1986).
140 W. Watkins, The Laplacian matrix of a graph: Unimodular congruence, *Linear and Multilinear Algebra* 28:35–43 (1990).
141 Unimodular congruence of the Laplacian matrix of a graph, *Linear Algebra Appl.*, to appear.
142 D. Welsh, Matroids and their applications, in *Selected Topics in Graph Theory 3* (L. W. Beineke, and R. J. Wilson, Eds.), Academic, New York, 1988, pp. 43–70.
143 H. Whitney, A logical expansion in mathematics, *Bull. Amer. Math. Soc.* 38:572–579 (1932).
144 2-isomorphic graphs, *Amer. J. Math.* 55:245–254 (1933).

145 P. J. Cameron, J. M. Goethals, J. J. Seidel, and E. E. Shult, Line graphs, root systems, and elliptic geometry, *J. Algebra* 43:305–327 (1976).

146 B. Cipra, You can't hear the shape of a drum, *Science* 255:1642–1643 (27 Mar. 1992).

147 C. Godsil, D. A. Holton, and B. McKay, The spectrum of a graph, in *Combinatorial Mathematics V*, Lecture Notes in Math. 622, Springer-Verlag, Berlin, 1977, pp. 91–117.

148 C. Gordon, D. L. Webb, and S. Wolpert, One cannot hear the shape of a drum, *Bull. Amer. Math. Soc.* 27:134–138 (1992).

149 I. P. Goulden and D. M. Jackson, Immanants of combinatorial matrices, *J. Algebra* 148:305–324 (1992).

150 M. Fiedler, Aggregation in graphs, Colloq. Math. Soc. János Bolyai 18:315–330 (1976).

151 An estimate for the nonstatistic eigenvalues of doubly stochastic matrices, IMA Preprint Ser. 902, Inst. for Math. Appl., Univ. of Minnesota, 1991.

152 J. J. Seidel, Distance matrices and Lorentz space, in *Workshop Vladimir USSR*, Aug. 1991, pp. 1–2.

153 J. A. Sjogren, Cycles and spanning trees, *Math. Comput. Modelling* 15:87–102 (1991).

154 I. Faria, Multiplicity of integer roots of polynomials of graphs, *Linear Algebra Appl.*, to appear.

155 R. Grone, On the geometry and Laplacian of a graph, *Linear Algebra Appl.* 150:167–178 (1991).

Received 27 July 1992; final manuscript accepted 1 March 1993