The Mathematics Student
Vol. 65, Nos. 1–4 (1996), 214–223

THE LAPLACIAN MATRIX OF A GRAPH*

R.B. BAPAT

1. INTRODUCTION

We consider graphs which have no loops or parallel edges, unless stated otherwise. Thus a *graph* $G = (V(G), E(G))$ consists of a finite set of *vertices*, $V(G)$, and a set of *edges*, $E(G)$, each of whose elements is a pair of distinct vertices. We will assume familiarity with basic graph-theoretic notions; see, for example, Bondy and Murty [5].

Given a graph, one associates a variety of matrices with the graph. Some of the important ones will be defined now. Let G be a graph with $V(G) = \{1, \ldots, n\}$, $E(G) = \{e_1, \ldots, e_m\}$.

The *adjacency matrix* $A(G)$ of G is an $n \times n$ matrix with its rows and columns indexed by $V(G)$ and with the (i, j)-entry equal to 1 if vertices i, j are adjacent (i.e., joined by an edge) and 0 otherwise. Thus $A(G)$ is a symmetric matrix with its i-th row (or column) sum equal to $d_i(G)$, which by definition is the degree of the vertex i, $i = 1, 2, \ldots n$. Let $D(G)$ denote the $n \times n$ diagonal matrix, whose i-th diagonal entry is $d_i(G)$, $i = 1, 2, \ldots, n$.

The *Laplacian matrix* of G, denoted by $L(G)$, is simply the matrix $D(G) - A(G)$.

There is another way to view the Laplacian matrix. First we introduce yet another important matrix associated with G. Suppose each edge of G is assigned an orientation, which is arbitrary but fixed. The (vertex-edge) *incidence matrix* of G, denoted by $Q(G)$, is the $n \times m$ matrix defined as follows. The rows and the columns of $Q(G)$ are indexed by $V(G)$, $E(G)$ respectively. The (i, j)-entry of $Q(G)$ is 0 if vertex i and edge e_j are not incident and otherwise it is 1 or -1 according as e_j originates or terminates at i respectively.

*Text of S.S. Pillai Memorial Lecture delivered on 14th April, 1996 at the Physics Lecture Theatre, University of Delhi as a part of the IMS-sponsored programme of Memorial Lectures.

A simple verification reveals that the Laplacian matrix $L(G)$ equals $Q(G)$ $Q(G)^T$, where the superscript T denotes transpose. Observe that although we introduced an orientation for each edge while defining $Q(G)$, the matrix $L(G)$ does not depend upon the particular orientation.

EXAMPLE. Let G be the graph with vertex set $\{1, 2, 3, 4, 5\}$ and edge set $(12, 23, 13, 24, 34, 45)$. Then

$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \quad Q(G = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 1 & 0 & 0 \\ 0 & -1 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

and

$$L(G) = Q(G)Q(G)^T = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}.$$

Let G be a graph with $V(G) = \{1, \ldots, n\}$, $E(G) = \{e_1, \ldots, e_m\}$. Some basic properties of the Laplacian matrix are summarized below.

(i) $L(G)$ is a symmetrix, positive semidefinite matrix.

(ii) The off-diagonal entries of $L(G)$ are nonpositive (in fact, they are either or -1). A positive semidefinite matrix with nonpositive off-diagonal entries is called a *Stieltjes matrix* and thus $L(G)$ is a Stieltjes matrix. Such matrices form an interesting class and possess several nice properties. For example, the square root of a Stieltjes matrix is again a Stieltjes matrix, a fact which is not at all obvious.

(iii) The diagonal entries of $L(G)$ are the vertex degrees and the row sums and the column sums are all zero.

(iv) The quadratic form afforded by $L(G)$ has a rather simple description:

$$\langle L(G)x, x\rangle = \sum_{(i,j) \in E(G)} (x_i - x_j)^2.$$

(v) The rank of $L(G)$ is $n-k$, where k is the number of connected components of G. In particular, if G is connected, then the rank of $L(G)$ is $n-1$.

The Laplacian matrix is also known by several other names in the literature such as the Kirchhoff matrix or the Information matrix. The term Laplacian matrix is justified as follows.

Consider the partial differential equation

$$\frac{\partial^2 z}{\partial x^2}+\frac{\partial^2 z}{\partial y^2}+\lambda z=0,$$

or

$$\nabla z+\lambda z=0,$$

where ∇ is the Laplacian operator and $z=z(x, y)$ is subject to the boundary condition $z(x, y)=0$ on a simple closed curve Γ in the xy-plane.

It is well-known that this problem has a solution only for an infinite sequence of *eigenvalues* $\lambda_1 \leq \lambda_2 \leq \ldots$

An approximate solution to the problem may be found by covering the region enclosed by Γ by a grid and then solving the corresponding finite eigenvalue problem. The coefficient matrix of the finite problem is seen to tbe precisely the *Laplacian matrix* of the graph associated with the grid.

The Laplacian matrix arises in a variety of application areas such as graph isomorphism problems, electrical networks, computational techniques for differential equations, physical chemistry, biochemistry, computer science and design of statistical experiments. We refer to Cvetkovic, Doob and Sachs [9] and Merris [15] for further references concerning these applications.

In this paper we survey some interesting results involving the Laplacian matrix. The emphasis is on giving a glimpse into results with different flavours. We do not aim at completeness and hence this is not a comprehensive survey. For an excellent survey, from which we have borrowed extensively, see Merris [15].

2. Kirchhoff's Matrix-Tree Theorem

Recall that a *tree* is a connected, acyclic graph. A *spanning tree* of the graph $G=(V(G), E(G))$ is a subgraph of G with vertex set $V(G)$, which is a tree. Clearly,

G has a spanning tree if and only if G is connected. The next result gives a formula for the number of spanning trees in a graph in terms of its Laplacian matrix.

THEOREM 1 (Kirchhoff's Matrix-Tree Theorem). *If G is a connected graph, then the cofactors of the Laplacian matrix are all equal and the common value is the number of spanning trees in G.*

As an application of Theorem 1, consider K_n, the complete graph on n vertices. The Laplacian $L(K_n)$ is the $n \times n$ matrix with $n-1$ on the diagonal and -1 elsewhere. It is easily verfied that any cofactor of $L(K_n)$ equals n^{n-2}, which by Theorem 1 is the number of spanning trees in K_n. This result is known as Cayley's Theorem which can be proved in many different ways, see Moon [16].

A proof of Theorem 1 can be given using Cauchy-Binet formula for the determinant applied to the expression $L(G) = Q(G)Q(G)^T$. The technique has been used to get various extensions and generalizations of the theorem, see for example [1, 3, 7, 8].

3. PERRON-FROBENIUS THEOREM

The concept of the Laplacian matrix extends naturally to a directed graph with weights on the edges. Thus consider the complete directed graph on three vertices, 1, 2, 3, where the edge from i to j is assigned weight $w_{ij} \geq 0$. Then the Laplacian matrix is given by

$$\begin{bmatrix} w_{12}+w_{13} & -w_{12} & -w_{13} \\ -w_{21} & w_{21}+w_{23} & -w_{23} \\ -w_{31} & -w_{32} & w_{31}+w_{32} \end{bmatrix}.$$

The Matrix-Tree Theorem has a natural extension to this case and cofactors in the above matrix have interpretation in terms of spanning trees. Thus the cofactor of the (1, 3)-entry is

$$w_{21}w_{32} + w_{21}w_{31} + w_{23}w_{31},$$

which is the sum of the weights of all spanning trees directed towards vertex 1. (The weight of a spanning tree is the product of the edge weights.)

This extension of the Matrix-Tree Theorem is related to the Perron-Frobenius Theorem as we indicate now. Let A be an $n \times n$ *stochastic* matrix, i.e. the entries of A are all nonnegative and the row sums are all 1. Let G be the directed graph associated with A. Thus G has vertices $\{1, 2, \ldots, n\}$ and there is an edge from i to j if and only if $a_{ij} > 0$. We assume that G is strongly connected, that is to say, that A is irreducible. It is well-known that A has a left eigenvector x with positive entries for the eigenvalue 1. This fact is usually proved using the Perron-Frobenius Theorem, in the context of Markov chains, where x is called the *steady state* vector. However we give an alternative proof. Since A is irreducible, $I_n - A$ is singular with rank $n-1$. Thus there exists a nonzero vector x, which is unique up to a scalar multiple, such that $x^T(I_n - A) = 0$. Clearly x is proportional to any column of the cofactor matrix of $I_n - A$. But $I_n - A$ is a weighted version of the Laplacian matrix of G. By the Matrix-Tree Theorem its cofactors represent the sum of the weights of certain spanning trees and hence are all positive. Thus we have shown the existence of a vector x with positive components such that $x^T A = x^T$.

4. Spectral Properties

Let G be a graph and let $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G) = 0$ denote the eigenvalues of the Laplacian $L(G)$. The main problem that is addressed in the area of spectral graph theory is the study of the relation between graph structure and the spectrum of certain matrices associated with the graph. There is considerable work on the spectrum of the adjacency matrix (see [9]) but there are several interesting results concerning the spectrum of a Laplacian as well.

To begin with, note that G is connected if and only if $\lambda_{n-1}(G) > 0$. To describe additional results, let us denote by $d_1(G) \geq d_2(G) \geq \ldots \geq d_n(G)$, the vertex degrees in G.

A simple application of the variational principle for the largest eigenvalue shows that $\lambda_1(G) \geq d_1(G)$. Similarly, by the Gershgorin Discs Theorem we conclude that $\lambda_1(G) \leq 2d_1(G)$. We now show that the first of these two statements can be sharpened.

Theorem 2. *For any graph G, $\lambda_1(G) \geq d_1(G) + 1$.*

Proof. We write d_1 instead of $d_1(G)$. Let

Let

$$L(G) = \begin{bmatrix} d_1 & x^T \\ x & L_{11} \end{bmatrix}$$

$$F = \begin{bmatrix} \sqrt{d_1} & 0 \\ \frac{1}{\sqrt{d_1}} x & (L_{11} - \frac{xx^T}{d_1})^{1/2} \end{bmatrix}$$

Then $L(G) = FF^T$. Now

$$F^T F = \begin{bmatrix} \sqrt{d_1} & \frac{1}{\sqrt{d_1}} x^T \\ * & * \end{bmatrix} \begin{bmatrix} \sqrt{d_1} & * \\ \frac{1}{\sqrt{d_1}} x & * \end{bmatrix}$$

$$= \begin{bmatrix} d_1 + 1 & * \\ * & * \end{bmatrix}.$$

Now observe that $\lambda_1(G)$, which by definition is the maximum engenvalue of FF^T, equals the maximum eigenvalue of $F^T F$ and since $d_1 + 1$ is a main diagonal entry of $F^T F$, we conclude that $\lambda_1(G) \geq d_1 + 1$. ∎

Theorem 2 is due to Merris. A more general result is described in the next section.

5. Majorization

If $x \in R^n$, we donote by $x_{[1]} \geq \ldots \geq x_{[n]}$, the components of x in decreasing order. If $x, y \in R^n$, we say that x is *majorized* by y, if

$$\sum_{i=1}^{k} x_{[i]} \leq \sum_{i=1}^{k} y_{[i]}, \quad k = 1, 2, \ldots, n-1$$

and

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

By a classical result of Schur, if A is an $n \times n$ real, symmetric matrix, then the diagonal elements $a_{11}, \ldots, a_{nn}$ of A are majorized by the eigenvalues of A. Applying this result to the Laplacian matrix we conclude that the degree sequence $d_1(G) \geq \ldots \geq d_n(G)$ is majorized by the eigenvalues $\lambda_1(G) \geq \ldots \geq \lambda_n(G)$ of the Laplacian.

One expects that for a Laplacian, which is a special symmetric matrix with more structure, one should be able to strengthen this result. Indeed, it was recently proved by Grone [12] that for a connected graph G, the sequence $d_1(G)+1$, $d_2(G), \ldots, d_{n-1}(G), d_n(G)-1$ is majorized by $\lambda_1(G), \ldots, \lambda_n(G)$. In particular, $\lambda_1(G) \geq d_1(G)+1$, an inequality which was established in the previous section.

6. Automorphism Group of a Graph

Let S_n denote the symmetric group of degree n. If $\sigma \in S_n$, let P^σ denote the permutation matrix corresponding to σ. Thus P^σ has 1 at positions $(i, \sigma(i))$, $i = 1, 2, \ldots, n$ and zeros elsewhere. Let $G = (V(G), E(G))$ be a graph with n vertices. A permutation $\sigma \in S_n$ is called an *automorphism* of G if σ applied to $V(G)$ preserves adjacency. In other words, σ is an automorphism if $A(G) = P^\sigma A(G) P^{\sigma T}$, where $A(G)$ is the adjacency matrix of G. The set of automorphisms of G is clearly a subgroup of S_n and is called the *automorphism group* of G, denoted $\Gamma(G)$.

There are many results in the literature regarding automorphism groups of graphs; see, for example, [9]. We just give one example.

THEOREM 3. *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.*

Here are some consequences of the above result.

COROLLARY 4. *If some permutation in $\Gamma(G)$ has a cycle of length at least 3, then $L(G)$ has a repeated eigenvalue.*

COROLLARY 5. *If the eigenvalues of $L(G)$ are all distinct then each element in $\Gamma(G)$ has order 2 and, in particular, $\Gamma(G)$ is abelian.*

7. Laplacian Spectrum of a Tree

There are a large number of results in the literature concerning the Laplacian spectrum of a tree. We give some sample results here and refer to Merris [15] for further details.

A vertex is called a *pendant vertex* if it has degree 1.

THEOREM 6. *Let T be a tree and let λ be an eigenvalue of the Laplacian $L(T)$. Then the multiplicity of λ is at most $p(T)-1$ where $p(T)$ is the number of pendant vertices in T.*

THEOREM 7. *Let T be a tree with n vertices. If $\lambda > 1$ is an integer eigenvalue of $L(T)$, then λ divides n.*

For any graph G, Fiedler has defined the *algebraic connectivity* of G as the second largest eigenvalue λ_{n-1} of $L(G)$. Note that G is connected if and only if its algebraic connectivity is positive. The next result gives bounds for the algebraic connectivity of a tree.

THEOREM 8. *For any tree T, the algebraic connectivity $a(T)$ satisfies*

$$2(1 - \cos \frac{\pi}{n}) \leq a(T) \leq 1.$$

Equality holds in the first inequality if and only if T is a path, while it holds in the second inequality if and only if T is a star (i.e., a tree in which all vertices except one have degree 1.)

We remark that Fiedler [10] has obtained some interesting and deep results concerning the eigenvector of $L(T)$ corresponding to the algebraic connectivity $a(T)$.

8. DISTANCE MATRIX

Let G be a connected graph with $V(G) = \{1, 2, \ldots, n\}$. The distance $d(i, j)$ between vertices i, j is defined to be the length of the shortest path between i, j. The *distance matrix* $\Delta(G)$ of G is the $n \times n$ matrix $[d(i, j)]$. This matrix turns up in some applications in biochemistry.

For an arbitrary graph the distance matrix is quite intractable, but for a tree, it has nice properties, some of which involve the Laplacian.

The next result due to Graham and Pollak [11] shows that the determinant of the distance matrix of a tree depends only on the number of vertices.

THEOREM 9. *If T is a tree with n vertices, then the determinant of $\Delta(T)$ is* $(-1)^{n-1}(n-1)2^{n-2}$.

The *Wiener index* of a graph G with vertex set $\{1, 2, \ldots, n\}$ is defined to be $\sum_{i<j} d(i, j)$. The Wiener index arises in several applications. For example:

(i) In biochemistry, it represents n^2 times the mean squared radius of gyration of a polymer molecule.

(ii) In design of experiments, minimization of the Wiener index is the well-known A-optimality criterion.

THEOREM 10. *Let T be a tree with Laplacian eigenvalues $\lambda_1(T) \geq \ldots \lambda_{n-1}(T) \geq \lambda_n(T) = 0$. Then the Wiener index of T equals $n \sum_{i=1}^{n-1} \frac{1}{\lambda_i(G)}$.*

If A is an $n \times m$ matrix, then an $m \times n$ matrix G is called a *generalized inverse* of A if $AGA = A$. The *Moore-Penrose inverse* of A, denoted by A^+, is an $m \times n$ matrix satisfying the equations $AGA = A$, $GAG = G$, $(AG)^T = AG$ and $(GA)^T = GA$. It is well-known that any complex matrix admits a unique Moore-Penrose inverse; see, for example, [4, 6].

Let T be a tree with n vertices and let A, Δ be the adjacency matrix and the distance matrix of T respectively. Merris [15] has observed that $A^T \Delta A = 2I_n$.

As shown in [2], $AA^+ = I_n - \frac{1}{n} J_n$, where J_n is the matrix of all ones. Thus it follows, using elementary properties of the Moore-Penrose inverse, that if $L^+ = [l_{ij}^+]$ is the Moore-Penrose inverse of the Laplacian matrix of T, then

$$l_{ii}^+ + l_{jj}^+ - 2l_{ij}^+ = d(i,j),$$

for all i, j. We refer to [2] for further details and for combinatorial formulae for A^+ and L^+.

REFERENCES

[1] R.B. Bapat, Mixed discriminants and spanning trees, *Sankhya* (Special volume in memory of Professor R.C. Bose), **54** (1992), 49–55.

[2] ______, Moore-Penrose inverse of the incidence matrix of a tree, *Linear and Multilinear Algebra* (to appear).

[3] R.B. Bapat and G. Constantine, An enumerating function for spanning forests with color restrictions, *Linear Algebra and Its Applications*, **173** (1992), 231–237.

[4] A. Ben-Israel and T.N.E. Greville, *Generalized Inverses: Theory and Applications*, Wiley-Interscience, 1974.

[5] J.A. Bondy and U.S.R. Murty, *Graph Theory with Applications*, Macmillan, 1976.

[6] S.L. Campbell and C.D. Meyer, Jr., *Generalized Inverses of Linear Transformations*, Pitman, 1979.

[7] S. Chaiken, A combinatorial proof of the all minors matrix tree theorem, *SIAM J. Algebraic and Discrete Methods*, **3** (1982). 319–329.

[8] S. Chaiken and D.J. Kleitman, Matrix tree theorems, *Journal of Combinatorial Theory*, Series A, **24** (1978), 377–381.

[9] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs*, Academic Press, New York, 1979.

[10] M. Fiedler, Eigenvectors of acyclic matrices, *Czechoslovak Math. J.*, **23** (1973), 298–305.

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

[12] R. Grone, Eigenvalues and the degree sequences of graphs, *Linear and Multilinear Algebra*, **39** (1995), 133–136.

[13] R. Merris, An edge version of he matrix-tree theorem and the Wiener index, *Linear and Multilinear Algebra*, **25** (1989), 291–296.

[14] ______, The distance spectrum of a tree, *Linear and Multilinear Algebra*, **14** (1990), 365–369.

[15] R. Merris, Laplacian matrices of graphs: a survey, *Linear Algebra Appl.*, **197**, **198** (1994), 143–176.

[16] J.W. Moon, Various proofs of Cayley's formula for counting trees, in F. Harary (ed.), *A seminar on Graph Theory*, Holt, Rinehart and Winston, Inc., New York, 1967.

[17] ______, On the adjoint of a matrix associated with trees, *Linear and Multilinear Algebra*, **39** (1995), 191–194.

Indian Statistical Institute
New Mehrauli Road
New Delhi-110 016