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LAPLACIAN MATRIX AND DISTANCE IN TREES

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Abstract. We provide a simple proof of an expression for the distance between vertices of a tree T in terms of the Laplacian matrix L of this tree. Let v_i and v_j be distinct vertices of T, at distance $d(v_i, v_j)$. Then $d(v_i, v_j) = \det L[i,j]$, where $L[i,j]$ is the submatrix, obtained by deleting the i-th and the j-th rows and columns from L.

INTRODUCTION

In this paper we are concerned with graphs without multiple and directed edges and without self–loops. Let G be such a graph, let n be the number of its vertices, and let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be its vertex set.

The *distance* between two distinct vertices v_i and v_j of G, denoted by $d(v_i, v_j | G)$ is equal to the length of (number of edges in) the shortest path that connects v_i and v_j. Conventionally, $d(v_i, v_i | G) = 0$.

The *degree* of a vertex v_j, denoted by δ_j, is equal to the number of vertices adjacent to v_j. A vertex of degree one is said to be *pendent*.

The *Laplacian matrix* of the graph G, denoted by $L = L(G) = ||L_{ij}||$, is a square matrix of order n whose elements are defined as

$$L_{ij} = \begin{cases} \delta_i & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and the vertices } v_i\,,\ v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j \text{ and the vertices } v_i\,,\ v_j \text{ are not adjacent}\,. \end{cases}$$

A *forest* is a graph without cycles. A *tree* is a connected graph without cycles. Any tree with $n \geq 2$ vertices has at least two pendent vertices. The n-vertex tree with exactly two pendent vertices is the *path*, denoted by P_n.

If M is a square matrix, then by $M[i_1, i_2, \ldots, i_p]$ we denote the submatrix obtained by deleting from M the i_1-th, i_2-th, $\ldots$, i_p-th rows and the i_1-th, i_2-th, $\ldots$, i_p-th columns.

In this paper we point out a relation between the submatrix $L(G)[i,j]$ of the Laplacian matrix and the distance $d(v_i, v_j|\, G)$ in case when G is a tree. In particular, we prove:

Theorem 1. *Let v_i and v_j be distinct vertices of a tree T, at distance $d(v_i, v_j|\, T)$. If T possesses at least three vertices, then*

$$\det L(T)[i,j] = d(v_i, v_j|\, T) \tag{1}$$

where $L(T)[i,j]$ is the submatrix, obtained by deleting the i-th and the j-th rows and columns from the Laplacian matrix of T.

Numerous results are known, connecting various determinant–related invariants of the Laplacian matrix of a graph with the spanning forests of this graph. Of these the best known is the classical Kirchhoff theorem [2], according to which, for any i, $1 \leq i \leq n$, the determinant of $L[i]$ is equal to the number of spanning trees of G. Another famous result of this kind is the Kel'mans theorem [2] relating the coefficient c_k of the Laplacian characteristic polynomial,

$$\psi(G, \lambda) = \det(\lambda\, I - L) = \sum_{k \geq 0} c_k\, \lambda^{n-k}$$

to the $(n-k)$-component spanning forests of G. Recently Bapat and Kulkarni [1] found expressions in terms of spanning forests for $\det L(G)[i_1, i_2, \ldots, i_p]$ for any p $2 \leq p \leq n-1$. For $p = 2$ their result reads:

Theorem 2. *Let v_i and v_j be distinct vertices of a graph G. Then* $\det L(G)[i,j]$ *is equal to the number of 2-component spanning forests of G in which v_i and v_j belong to different components.*

Theorem 1 can be viewed as a special case of Theorem 2. In what follows we describe an alternative proof of Theorem 1, in which spanning forests are not encountered.

PROOF OF THEOREM 1

We first show that the claim of Theorem 1 holds if T is the n-vertex path P_n, $n \geq 3$, and v_i, v_j are its two pendent vertices. This is the exceptional case, when a tree T has no pendent vertices other than v_i and v_j.

Lemma 3. If v_i and v_j are the terminal vertices of the path P_n, then

$$\det L(P_n)[i,j] = n-1 = d(v_i, v_j |\, P_n) \ .$$

Proof. Without loss of generality the vertices of P_n may be labelled so that v_k is adjacent to v_{k+1}, $k = 1, 2, \ldots n-1$. Then $i = 1$ and $j = n$, and $L(P_n)[1,n]$ assumes the form

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix} .$$

Denote $\det L(P_n)[1,n]$ by D_n. Expanding D_n with regard to its first row we obtain

$$D_n = 2\, D_{n-1} - D_{n-2}$$

which together with the initial conditions $D_3 = 2$ and $D_4 = 3$, yields $D_n = n - 1$. This, in turn, is just the distance between the terminal vertices of P_n. $\square$

In what follows we prove Theorem 1 by induction on the number n of vertices. For trees with three and four vertices the validity of Theorem 1 can be verified by direct checking.

Assume thus that Theorem 1 holds for all trees with fewer than n vertices.

Let T be an n-vertex tree and let v_i and v_j be its two vertices. In view of Lemma 3 we need to examine only the case when T possesses at least one pendent vertex, different from v_i and v_j. Let this pendent vertex be v_n and its (unique) neighbor v_{n-1}.

Let T' be the $(n-1)$-vertex tree, obtained by deleting v_n from T. Then the Laplacian matrix of T is of the form

$$L(T) = \begin{bmatrix} L^*(T') & \underline{u}^t \\ \underline{u} & 1 \end{bmatrix} \tag{2}$$

where $\underline{u} = (0, 0, \ldots, 0, -1)$, and where $L^*(T')$ is a square matrix of order $n-1$, whose elements are equal to those of $L(T')$, except that $L^*(T')_{n-1,n-1} = L(T')_{n-1,n-1} + 1$.

Without loss of generality we may require that $i < j$. Then two cases need to be distinguished: (1) $j < n-1$ and (2) $j = n-1$.

Case 1: $j < n-1$. Then in view of Eq. (2),

$$L(T)[i,j] = \begin{bmatrix} L^*(T')[i,j] & \underline{u}^t \\ \underline{u} & 1 \end{bmatrix} . \tag{3}$$

The determinant of the right–hand side of (3) is equal to the determinant of the matrix

$$\begin{bmatrix} L(T')[i,j] & \underline{0}^t \\ \underline{u} & 1 \end{bmatrix} \tag{4}$$

obtained by adding the n-th row of $L(T)[i,j]$ to its $(n-1)$-th row. In formula (4) $\underline{0}$ stands for an all-zero $(n-1)$-dimensional vector. Clearly,

$$\det \begin{bmatrix} L(T')[i,j] & \underline{0}^t \\ \underline{u} & 1 \end{bmatrix} = \det L(T')[i,j]$$

which, by the induction hypotheses is equal to $d(v_i, v_j|\, T')$. Because $d(v_i, v_j|\, T') = d(v_i, v_j|\, T)$, we conclude that relation (1) is satisfied.

Case 2: $j = n-1$. Then in view of Eq. (2),

$$L(T)[i,j] = \begin{bmatrix} L(T')[i,j] & \underline{0}^t \\ \underline{0} & 1 \end{bmatrix}$$

from which it immediately follows

$$\det L(T)[i,j] = \det L(T')[i,j] = d(v_i, v_j|\, T') = d(v_i, v_j|\, T)$$

implying the validity of relation (1) also in Case 2.

This completes the proof of Theorem 1. $\square$

DISCUSSION

Earlier studies revealed several other relations between the Laplacian matrix and distances in trees. Of these we mention here the following. The distance matrix $D = D(G)$ of a graph G is the matrix whose (i,j)-entry is equal to $d(v_i, v_j|\, G)$.

Theorem 4a. *Let T be a tree on n vertices, $n \geq 2$, with Laplacian matrix L and with distance matrix D. Then $L\,D\,L = -2\,L$.*

Denote the eigenvalues of L by $\mu_1, \mu_2, \ldots, \mu_n$ and label them so that $\mu_n = 0$ (and therefore, if the underlying graph is connected, $\mu_1, \mu_2, \ldots, \mu_{n-1}$ are positive–valued) [6]. The eigenvector corresponding to μ_k is $\underline{X}_k = (X_{1k}, X_{2k}, \ldots, X_{nk})^t$, i. e.,

$$L\,\underline{X}_k = \mu_k\,\underline{X}_k$$

holds for $k = 1, 2, \ldots, n$. We choose these eigenvectors to be real, normalized and mutually orthogonal (which always is possible).

Theorem 4b. *If T is an n-vertex tree, then*

$$d(v_i, v_j|\, T) = \sum_{k=1}^{n-1} \frac{1}{\mu_k} (X_{ik} - X_{jk})^2 \tag{5}$$

and

$$W(T) = n \sum_{k=1}^{n-1} \frac{1}{\mu_k} \tag{6}$$

where $W(T)$ denotes the Wiener number, i. e., the sum of distances between all pairs of vertices of T.

The result stated in Theorem 4a was obtained by Xiao and one of the present authors [4]. Formula (6) was first reported by Merris [5], but was independently discovered several times; for details see the review [3]. Formula (5) was recently communicated in [7].

Theorem 1 is one more result of the same kind, perhaps the most explicit connection between the Laplacian matrix and graph metrics.

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