DISTANCE MATRIX POLYNOMIALS OF TREES

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Abstract

For a finite undirected tree T with n vertices, the distance matrix $D(T)$ of T is defined to be the n by n symmetric matrix whose (i, j) entry is d_{ij}, the number of edges in the unique path from i to j. Denote the characteristic polynomial of $D(T)$ by

$$\Delta_T(x) = \det (D(T)-xI) = \sum_{i=0}^{n} \delta_k(T)x^k .$$

In this talk we describe exactly how the coefficients $\delta_k(T)$ depend on the structure of T. In contrast to the corresponding problem for the adjacency matrix of T, the results here are surprisingly difficult, requiring the use of a number of interesting auxiliary results.

1. For a finite undirected tree T with n vertices, the distance matrix $D(T)$ of T is defined to be the n by n symmetric matrix whose (i, j) entry is d_{ij}, the number of edges in the unique path from i to j. Denote the characteristic polynomial of $D(T)$ by

$$(1) \qquad \Delta_T(x) = \det(D(T)-xI) = \sum_{k=0}^{n} \delta_k(T)x^k .$$

In [1], the problem of relating the values of the coefficients $\delta_k(T)$ to the structural properties of T was initiated. In this note, we announce a complete solution to this problem. Proof of the assertions are rather complicated and will be given elsewhere.

For an acyclic graph (i.e., forest) F, let $N_F(T)$ denote the number of subgraphs of T which are isomorphic to F.

Theorem 1. There exist unique coefficients $A_F^{(k)}$ depending only on F and k so that for all trees T with n vertices,

$$(2) \qquad \delta_k(T) = (-2)^n \sum_F A_F^{(k)} N_F(T)$$

where F ranges over all forests having no isolated points and at most $k+1$ edges.

The uniqueness of the $A_F^{(k)}$ follows from a recent result in [4]. This may be compared with the corresponding theorem for the adjacency matrix characteristic polynomial

$$\det(A(T)-xI) = \sum_{k=0}^{n} \alpha_k(T)x^k$$

where $A(T) = (a_{ij})$ with

$$a_{ij} = \begin{cases} 1 & \text{if } d_{ij} = 1, \\ 0 & \text{otherwise.} \end{cases}$$

In this case, it is well known [6] that

$$\alpha_k(T) = \begin{cases} (-1)^t N_{tP_1}(T) & \text{if } k = n-2t, \\ 0 & \text{otherwise.} \end{cases}$$

where tP_1 denotes the forest consisting of t disjoint edges.

The exact values of the $A_F^{(k)}$ are given as follows. For a forest F which is the disjoint union of trees having $n_1, n_2, \ldots,$ and n_r vertices, define $\pi(F)$ to be the integer $n_1 n_2 \ldots n_r$. Let $\mathfrak{F}_n$ denote the set of forests having no isolated vertices and exactly k edges. By convention, $\mathfrak{F}_0$ will consist of only the empty forest F^* having no vertices and $\pi(F^*) = N_{F^*}(T) = 1$ for all T.

<u>Theorem 2</u>. For all trees T with n vertices

$$\delta_k(T) = (-1)^{n-1} 2^{n-k-2} \left\{ \sum_{F \in \mathfrak{F}_{k+1}} a_F \pi(F) N_F(T) + \sum_{F \in \mathfrak{F}_k} b_F \pi(F) N_F(T) \right.$$

$$\left. + \sum_{F \in \mathfrak{F}_{k-1}} c_F \pi(F) N_F(T) \right\}$$

where a_F, b_F, c_F are recursively determined as follows:

(i) $a_{F^*} = b_{F^*} = 0$, $c_{F^*} = -4$

(ii) If F is a <u>tree</u> T' with $n' \geq 1$ vertices and distance matrix (d'_{ij}) then

$$a_{T'} = \frac{1}{n'} \sum_{i<j} d'_{ij}(2-d'_{ij})$$

$$b_{T'} = \frac{4}{n'} \sum_{i<j} (2-d'_{ij})$$

$$c_{T'} = \frac{-4}{n'}$$

(iii) If F is the disjoint union of forests F_1 and F_2 then

$$a_F = a_{F_1} + a_{F_2}$$

$$b_F = b_{F_1} + b_{F_2}$$

$$c_F = c_{F_1} + c_{F_2} + 4$$

As an immediate corollary, taking $k = 0$ we have

$\mathfrak{F}_1 = \{P_1\}$, $a_{P_1} = \frac{1}{2}$, $b_{P_1} = 2$, $c_{P_1} = -2$, $\pi(P_1) = 2$ and

$$(3) \quad \delta_0(T) = (-1)^{n-1}2^{n-2}(\tfrac{1}{2}\cdot 2\cdot N_{P_1}(T) + 0) = (-1)^{n-1}(n-1)2^{n-2}$$

independent of the structure of T (see [2], [3]).

An interesting result used in the proof of Theorem 1 is the following.

Lemma. The inverse $D(T)^{-1} = (d^*_{ij})$ of $D(T)$ is given by

$$d^*_{ij} = \frac{(2-d_i)(2-d_j)}{2(n-1)} + \begin{cases} +\frac{1}{2}a_{ij} & \text{if } i \neq j \\ \\ -\frac{1}{2}d_i & \text{if } i = j \end{cases}$$

where d_i denotes the degree of i^{th} vertex of T.

It is natural to expect that similar results hold for general connected graphs G. It is known [5], for example, that if G has blocks G_j, $j \in J$, then letting cof X denote the sum of the cofactors of a matrix X we have

$$(a) \quad \text{cof } D(G) = \prod_{j \in J} \text{cof } D(G_j)$$

(b) $\det D(G) = \sum_{j \in J} \det D(G_j) \prod_{i \neq j} \operatorname{cof} D(G_i)$

Of course, (3) follows at once from (a) and (b) since all blocks of a tree are isomorphic to P_1 .

It is still not known whether $\Delta_T(x)$ determines T . This is not the case for general graphs G (see [1]) and almost never the case for $\det(A(T)-xI)$ (see [7]) .

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