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On the Terminal Distance Matrix of Graphs

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Abstract. Let G be a simple connected graph. The terminal distance matrix of G is the distance matrix between all pendant vertices of G. In this paper, we study the terminal distance matrix and compute the characteristic polynomial of this matrix for some rooted trees. Also we obtain lower bounds for the spectral radius of the terminal distance matrix of graphs and characterize those graphs for which the bounds are best possible.

Keywords: Terminal distance matrix, Terminal distance spectral radius, Terminal Wiener index.

2000 Mathematics subject classification: 05C12, 05C50.

1. Introduction

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The distance matrix $D = D(G)$ of G is defined so that its (i, j)-entry, d_{ij}, is equal to $d_G(v_i, v_j)$, the distance (= length of any shortest path) between the vertices v_i and v_j of G [1]. Recently, the so-called terminal distance matrix [2]-[4] or reduced distance matrix of graphs was considered. If G has p pendant vertices (= vertices of degree one), labelled by $V^*(G) = \{v_1, v_2, \ldots, v_p\}$, then its terminal distance matrix $D^*(G)$, is the square matrix of order k whose (i, j)-entry is the distance between the vertices v_i and v_j in $V^*(G)$. Concepts based on the distance matrix are intensively employed in the mathematical chemistry. In particular, one of the oldest topological molecular indices, the Wiener index

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, is defined as one half of the sum of all elements of the distance matrix of a graph. Also, the terminal Wiener index of graph G is defined by analogy as the one half of a sum of elements of $D^*(G)$. The terminal Wiener index $TW(G)$ of a connected graph as the sum of the distances between all pairs of pendant vertices. More formally,

$$TW(G) = \sum_{1 \leq i < j \leq p} d_G(v_i, v_j).$$

Terminal distance matrices of trees are of special interest, since a tree can be reconstructed by its terminal distance matrix [6]. Since the distance matrix and related matrices, based on graph-theoretical distances, are rich sources of many graph invariants (topological indices) that found use in the structure- property-activity modelling [6]-[9], it is of interest to study spectra and polynomials of these matrices [10]-[12].

This paper is organized as follows. In the first section we report some properties of graphs with respect to the terminal distance matrix and compute the characteristic polynomial of this matrix for some rooted tree. In the second section we obtain some bounds for the distance spectral radius of graphs and characterize those graphs for which the bounds are best possible.

2. Terminal distance regular graphs

In this section we introduce some definitions and obtain some basic results related to the terminal distance matrix of connected graphs, in particular rooted trees.

Definition 2.1. Let G be a connected graph. Then G is called constant terminal distance if all pendant vertices in G have same distance from each other.

A starlike tree is a tree with exactly one vertex having degree greater two. We denote by $S(k_1, k_2, \ldots, k_n)$, the starlike tree which has a vertex v of degree $n \geq 3$ and has the property that $S(k_1, k_2, \ldots, k_n) - v = P_{k_1} \cup P_{k_2} \cup \ldots \cup P_{k_n}$, where P_{k_i} is a path on k_i vertices for $1 \leq i \leq n$. The starlike tree $S(k_1, k_2, \ldots, k_n)$ is said to be regular, if $k_1 = k_2 = \ldots = k_n$ (see Fig.1).

Theorem 2.2. *Let T be a tree. Then T is constant terminal distance if and only if T is a path or regular starlike tree.*

Proof. If T is a path or regular starlike tree, then T obviously is constant terminal distance.

Conversely let T be a constant terminal distance tree. Suppose that x and y are two vertices in T having degree greater than two. So there exist two pendant

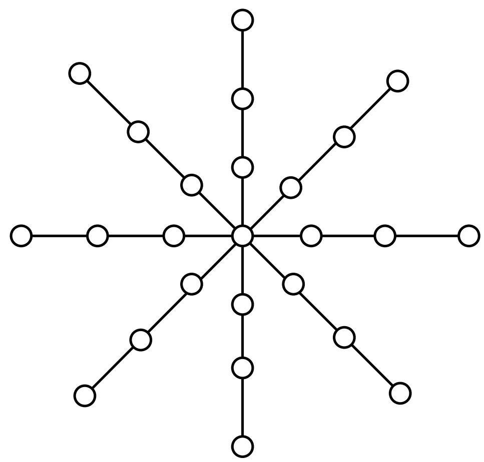

FIGURE 1. A regular starlike tree.

vertices u_x and v_x in T closer to x than y and there exist two pendant vertices u_y and v_y in T closer to y than x. Without loss generality, let $d_T(u_x, x) + d_T(v_x, x) \leq d_T(u_y, y) + d_T(v_y, y)$ and $d_T(u_y, y) \leq d_T(v_y, y)$, then $d_T(u_x, v_x) < d_T(u_x, v_y)$ which is a contradiction to the fact that T is a constant terminal distance tree. So at most one vertex in T has degree greater than two. If degree of all vertices in T is less than three T is a path. At last if T is a tree with exactly one vertex having degree greater two, then T is a regular distance tree. Therefore the theorem is proved. □

Definition 2.3. Let G be a graph with $V^*(G) = \{v_1, v_2, \ldots, v_p\}$ and the terminal distance matrix D^*. Then the terminal distance degree of v_i, denoted by D_i^* is given by $D_i^* = \sum_{j=1}^{k} d_{ij}$ for $1 \leq i \leq p$. Then G is called terminal distance regular if all pendant vertices of G have same terminal distance degree.

Recall in a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. Let T be a rooted tree with k levels. Denote by T_i, a induced subtree of T rooted at a vertex on the $(k+1-i)$-th level of T for $1 \leq i \leq k$. Obviously T_i is a rooted tree with i levels. Denote by N_i, the number of pendant vertices of T which are belong to $V^*(T_i)$ (hence $N_1 = 1$). Finally, a sequence of induced subtrees of T as $T_1, T_2, \ldots, T_{k-1}$ is called a increasing sequence of subtrees of T if T_i is a induced subtree of T_{i+1} for $1 \leq i \leq k-2$ (see Fig.2). In the following theorem we obtain a description for the terminal distance regular trees.

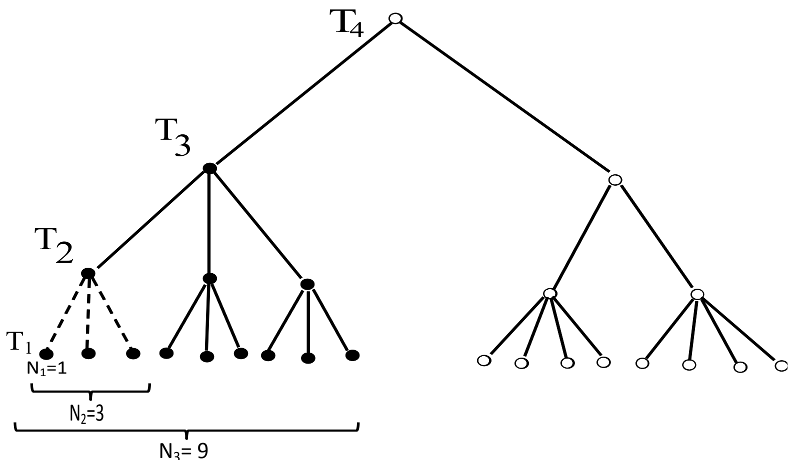

FIGURE 2. A increasing sequence of induced subtrees of a rooted tree.

Lemma 2.4. *A rooted tree is terminal distance regular if and only if sum of the numbers of pendant vertices of subtrees in all increasing sequence of subtrees are same.*

Proof. Let v_1 be an arbitrary pendant vertex of T and $T_1, T_2, \ldots, T_{k-1}$ denote the increasing sequence of subtrees of T contain v_1. If $N_i = |V^*(T_i)|$, then

$$\begin{aligned}\sum_{v \in V^*(T)} d_T(v, v_1) &= 2(N_2 - N_1) + 4(N_3 - N_2) + \ldots + 2(k-1)(N_k - N_{k-1}) \\ &= -2(N_1 + N_2 + \ldots + N_{k-1}) + 2(k-1)N_k.\end{aligned}$$

Since $N_k = |V^*(T)|$ and $N_1 + N_2 + \ldots + N_{k-1}$ denotes sum of the numbers of pendant vertices of the subtrees in a increasing sequence of subtrees of T, hence the lemma is proved. $\square$

For example the graph which is shown in Fig.2 is a terminal distance regular tree. Since sum of the numbers of pendant vertices in all increasing sequence of its subtrees is $N_1 + N_2 + N_3 = 13$. Also for rooted tree which is shown in Fig.3, we have $N_1 + N_2 + N_3 + N_4 = 28$, hence this tree is terminal distance regular.

In the following theorem, $P_T(\lambda) = det(D^*(T) - \lambda I)$, the characteristic polynomial of terminal distance matrix of a terminal distance regular tree T is computed. If T is a terminal distance regular, then the terminal distance degree of T will be denoted by D_T.

Theorem 2.5. *Let T be a terminal distance regular tree of levels k, $T_1, T_2, \dots T_r$ denote the induced subtrees obtained by deleting the root of T, $n_i = |V^*(T_i)|$ and $\bar{P}_i = \frac{P_{T_i}(\lambda)}{\lambda - D_{T_i}}$ for $1 \leq i \leq r$. Then the characteristic polynomial of $D^*(T)$ is given as follows:*

$$P_T(\lambda) = (\lambda - D_T)\bar{P}_1 \prod_{i=2}^{r} (\lambda + 2(k-1)n_i - D_{T_i})\bar{P}_i.$$

Proof. Let $M_i = det(D^*(T_i) - \lambda I)$ and $E_{i,j}$ be an $n_i \times n_j$ matrix all of whose entries are $2k$ for $1 \leq i, j \leq r$. Then the characteristic polynomial of $D^*(T)$ is given as

$$P_T(\lambda) = \begin{vmatrix} M_1 & E_{12} & E_{13} & \dots & E_{1r} \\ E_{21} & M_2 & E_{23} & \dots & E_{2r} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ E_{r1} & E_{r2} & E_{r3} & \dots & M_r \end{vmatrix}. \qquad (1)$$

If we replace the first row of (1) with sum of all rows of this determinant and then subtract the first column of the obtained determinant from other columns, then for the obtained matrices $M_i^{'}$ and $E_{ij}^{'}$ for $1 \leq i, j \leq r$, by use of those two linear operations on the entries of (1), we have

$$\begin{aligned} P_T(\lambda) &= (\lambda - D_T)\bar{P}_1 \begin{vmatrix} 1 & E_{12}^{'} & E_{13}^{'} & \dots & E_{1r}^{'} \\ 0 & M_2^{'} & E_{23}^{'} & \dots & E_{2r}^{'} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ 0 & 0 & 0 & \dots & M_r^{'} \end{vmatrix} \\ &= (\lambda - D_T)\bar{P}_1 det(M_2^{'}) det(M_2^{'}) \dots det(M_r^{'}). \qquad (2) \end{aligned}$$

Also with replacing the first row of $det(M_i^{'})$ by sum of all rows and then subtracting the first column of obtained determinant from other columns, for $2 \leq i \leq r$ we have

$$det(M_i^{'}) = (\lambda + 2(k-1)n_i - D_{T_i})\bar{P}_i. \qquad (3)$$

By replacing (3) in (2) we get

$$P_T(\lambda) = (\lambda - D_T)\bar{P}_1 \prod_{i=2}^{r} (\lambda + 2(k-1)n_i - D_{T_i})\bar{P}_i.$$

Therefore the theorem is proved. □

A rooted tree such that its vertices at the same level have equal degrees is called a generalized Bethe tree [12]. By use of Lemma 2.4, a generalized Bethe tree is a terminal distance regular tree. The characteristic polynomial and spectrum of the terminal distance matrix of generalized Bethe trees can be computed by Theorem 2.5 in recursive method.

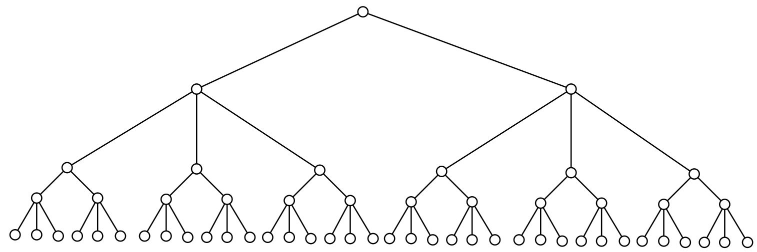

Figure 3. A generalized Bethe tree with 5 levels.

Example 2.6. Let T be the generalized Bethe tree where is shown in Fig. 3. To compute the characteristic polynomial of $D^*(T)$, At first we consider the subtree T^1. In this tree $r = 3$, $D_{T^1} = 4$, $n_1 = n_2 = n_3 = 1$ and $\bar{P}_1 = \bar{P}_2 = \bar{P}_3 = 1$. By use of Theorem 2.5, we have

$$P_{T^1}(\lambda) = (\lambda - 4)(\lambda + 2)^2.$$

For T^2 we have $r = 2$, $D_{T^2} = 16$, $n_1 = n_2 = 3$ and $\bar{P}_1 = \bar{P}_2 = (\lambda + 2)^2$. Therefore

$$P_{T^2} = (\lambda - 16)(\lambda + 8)(\lambda + 2)^4.$$

Now we consider T^3. In this tree $r = 3$, $D_{T^3} = 88$, $n_1 = n_2 = n_3 = 6$, $\bar{P}_1 = \bar{P}_2 = \bar{P}_3 = (\lambda + 8)(\lambda + 2)^4$. Thus

$$P_{T^3}(\lambda) = (\lambda - 88)(\lambda + 20)^2(\lambda + 8)^3(\lambda + 2)^{12}.$$

Finally we consider T. In this tree we have $r = 2$, $D_T = 232$, $n_1 = n_2 = 18$, $\bar{P}_1 = \bar{P}_2 = (\lambda + 20)^2(\lambda + 8)^3(\lambda + 2)^{12}$. Therefore

$$P_T(\lambda) = (\lambda - 232)(\lambda + 56)(\lambda + 20)^4(\lambda + 8)^6(\lambda + 2)^{24}.$$

Therefor the spectrum of T will be computed as roots of $P_T(\lambda)$.

Example 2.7. Let T be the terminal distance regular tree which is shown in Fig. 4. If T^1, T^2 and T^3 denote the induced subtrees obtained by deleting the root of T, then by use of Theorem 2.5,

$$P_{T^1}(\lambda) = (\lambda - 10)(\lambda + 4(2) - 2)(\lambda + 2)(\lambda + 2) = (\lambda - 10)(\lambda + 6)(\lambda + 2)^2,$$

$$P_{T^2}(\lambda) = (\lambda - 16)(\lambda + 4)^4,$$

$$P_{T^3}(\lambda) = (\lambda - 4)(\lambda + 2)^2.$$

Since $D_T = 58$, $2(k-1)n_2 - D_{T_2} = 2(k-1)n_3 - D_{T_3} = 14$, the characteristic polynomial of $D^*(T)$ is computed by use of Theorem 2.5 as follows:

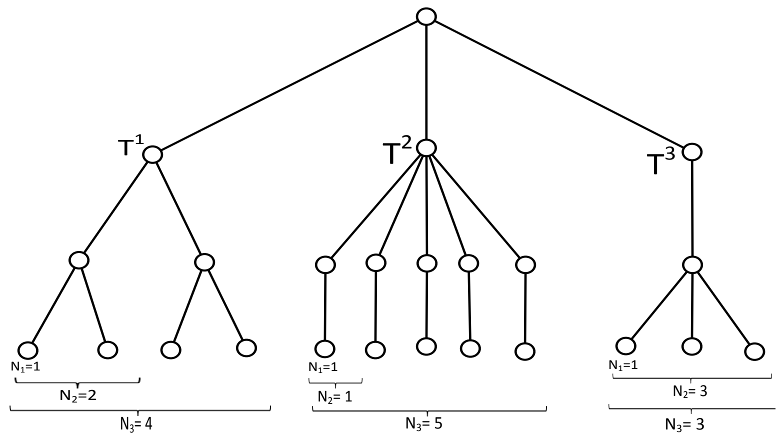

FIGURE 4. A terminal distance regular tree with 4 levels.

$$\begin{aligned} P_T(\lambda) &= (\lambda-58)(\lambda+6)(\lambda+2)^2\Big((\lambda+14)(\lambda+4)^4(\lambda+14)(\lambda+2)^2\Big) \\ &= (\lambda-58)(\lambda+14)^2(\lambda+6)(\lambda+4)^4(\lambda+2)^4. \end{aligned}$$

3. Bounds on the terminal distance spectral radius

The terminal distance matrix of G is a real symmetric matrix. Thus its eigenvalues are real numbers. We denote by $\varrho(G)$ the largest eigenvalue of $D^*(G)$, and call it the terminal distance spectral radius of G. By the Perron-Frobenius theorem, we know that $\varrho(G) > 0$ and there exists a unique positive vector $X = (x_1, x_2, \ldots, x_p)^T$, called Perron eigenvector such that $D^*(G)X = \varrho(G)X$, where x_i is the coordinate for the pendant vertex v_i of G. In the following lemma the range of variation of $\varrho(G)$ will be determined.

Lemma 3.1. *Let $\varrho(G)$ denote the terminal distance spectral radius of G and D_i^* denote the terminal distance degree corresponding of vertex i in G . Then*

$$\min_{i\in V^*(G)} D_i^* \le \varrho(G) \le \max_{i\in V^*(G)} D_i^*.$$

Proof. Let $X = (x_1, x_2, \ldots, x_p)^T$ be a Perron eigenvector of $D^*(G)$ corresponding to the $\varrho = \varrho(G)$, such that $x_r = \min_{1\le i\le p} x_i$ and $x_s = \max_{1\le i\le p} x_i$.

From the eigenvalue equation $D^*X = \varrho X$, written for the component x_r we have

$$\varrho x_r = \sum_{i=1}^{p} d_{ri}x_i \ge x_r \sum_{i=1}^{p} d_{ir}.$$

Therefore $\varrho(G) \geq \min_{i\in V^*(G)} D_i^*$.

Analogously for the component x_s we have

$$\varrho x_s = \sum_{i=1}^{p} d_{ri}x_i \leq x_s \sum_{i=1}^{p} d_{ir}.$$

Thus $\varrho(G) \leq \max_{i\in V^*(G)} D_i^*$ and the lemma is proved. □

Corollary 3.2. *Let G is a terminal distance regular graph. Then $\varrho(G) = D_G$.*

In order to verifying the terminal reditus we determine the component of a Perron eigenvalue of D^* for the terminal distance regular graphs in the following lemma.

Lemma 3.3. *A connected graph G is terminal distance regular if and only if its Perron eigenvector of terminal distance matrix is constant.*

Proof. Let G be a terminal distance regular graph and $X = (x_1, x_2, \ldots, x_p)^T$ denote a Perron eigenvector of $D^*(G)$ corresponding to the $\varrho = \varrho(G)$, such that

$$x_r = \min_{1\leq i\leq p} x_i$$

Since $\varrho = D_i^*$ for $1 \leq i \leq p$, from the eigenvalue equation $D^*X = \varrho X$, written for the component x_i we have

$$(\sum_{j=1}^{p} d_{ij})x_i = \sum_{j=1}^{p} d_{ij}x_j \Rightarrow \sum_{j\neq i=1}^{p} (x_i - x_j)d_{ij} = 0.$$

Since D^* is a non negative matrix, so $x_i - x_j = 0$ for $1 \leq i \leq p$ and all of the components of X are same.

Conversely let $X = (x_1, x_2, \ldots, x_p)^T$, the Perron eigenvector of $D^*(G)$ be constant. From the eigenvalue equation for $1 \leq i \leq p$, we have

$$\varrho x_i = \sum_{j=1}^{p} d_{ij}x_j \Rightarrow \varrho = \sum_{j=1}^{p} d_{ij}.$$

Thus G is a terminal distance regular graph. □

Now we can obtain an lower bound for terminal distance spectral radius of connected graphs in terms of its terminal Wiener index.

Theorem 3.4. *Let G be a connected graph with $p \geq 2$ pendant vertices. Then*

$$\varrho(G) \geq \frac{2TW(G)}{p}$$

with equality if and only if G is terminal distance regular.

Proof. Let $X = (1, 1, \ldots, 1)^T$ be a p-vector. Then by Raleigh principle, applied to the terminal distance matrix D^* of G, we get

$$\begin{aligned}\varrho(G) \geq \frac{X^T D^* X}{X^T X} & \\ &= \frac{(D_1^*, D_2^*, \ldots, D_p^*)(1, 1, \ldots, 1)^T}{p} \\ &= \frac{\sum_{i=1}^{p} D_i^*}{p} = \frac{2TW(G)}{p}.\end{aligned}$$

Now suppose G is terminal distance regular. Then by use of the Lemma 3.3, $X = (1, 1, \ldots, 1)^T$ is a Perron eigenvector of $D^*(G)$. Thus

$$\varrho(G) = \frac{X^T D^* X}{X^T X} = \frac{2TW(G)}{p}.$$

Conversely if $\varrho(G) = \frac{2TW(G)}{p}$, then $X = (1, 1, \ldots, 1)^T$ is a Perron eigenvector of $D^*(G)$. By use of the Lemma 3.3, G is terminal distance regular.

Therefore the theorem is proved. □

Theorem 3.5. *Let G be a connected graph with distance degree sequence $\{D_1^*, D_2^*, \ldots, D_p^*\}$. Then*

$$\varrho(G) \geq \sqrt{\frac{{D^*}_1^2 + {D^*}_2^2 + \ldots + {D^*}_p^2}{p}}. \tag{3.1}$$

The equality holds if and only if G is terminal distance regular.

Proof. Let $X = (x_1, x_2, \ldots, x_p)^T$ be a Perron eigenvector of $D^*(G)$ and $Y = (1, 1, \ldots, 1)^T$ be a p-vector. Then

$$\varrho(D^*) = \sqrt{\frac{X^T (D^*)^2 X}{X^T X}} \geq \sqrt{\frac{Y^T (D^*)^2 Y}{Y^T Y}}.$$

Now

$$Y^T (D^*)^2 Y = (D^* Y)^T (D^* Y) = {D^*}_1^2 + {D^*}_2^2 + \ldots + {D^*}_p^2.$$

Thus

$$\varrho = \varrho(D^*) \geq \sqrt{\frac{Y^T (D^*)^2 Y}{Y^T Y}} = \sqrt{\frac{\sum_{i=1}^{p} {D^*}_i^2}{p}}.$$

On the other hand equality in Eq.(3.1) is hold if and only if $X = (1, 1, \ldots, 1)^T$ is a Perron eigenvector of D^*. Hence by use of the Lemma 3.3 equality in Eq.(3.1) if and only if G is terminal distance regular. Therefore the theorem is proved. □

In the following theorem we give another bound for terminal distance spectral radius of connected graphs which cannot be compared with the bounds so far obtained.

Theorem 3.6. *Let G be graph with terminal Wiener index TW and distance degree sequence $\{D_1^*, D_2^*, \dots, D_p^*\}$. Then*

$$\varrho(G) \geq \max_i \frac{1}{p-1}\left((TW - D_i^*) + \sqrt{(TW - D_i^*)^2 + (p-1){D_i^*}^2}\right).$$

Proof. Let x_i be a pendant vertex of G with terminal distance degree D_i^*. Then this vertex gives rise a partition to the terminal distance matrix with following quotient matrix

$$B = \begin{bmatrix} 0 & \frac{D_i^*}{\sqrt{p-1}} \\ \frac{D_i^*}{\sqrt{p-1}} & \frac{2(TW-D_i^*)}{p-1} \end{bmatrix}.$$

Then B has eigenvalues

$$\mu_1 = \frac{(TW - D_i^*) + \sqrt{(TW - D_i^*)^2 + (p-1){D_i^*}^2}}{p-1},$$

$$\mu_2 = \frac{(TW - D_i^*) - \sqrt{(TW - D_i^*)^2 + (p-1){D_i^*}^2}}{p-1}.$$

By the theorem of interlacing, we have eigenvalues of B interlace those of D^*. Thus

$$\varrho(G) \geq \mu_1 = \frac{(TW - D_i^*) + \sqrt{(TW - D_i^*)^2 + (p-1){D_i^*}^2}}{p-1}.$$

Since this is true for all i, the theorem is proved. □

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