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SOME TREES CHARACTERIZED BY EIGENVALUES AND ANGLES

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Abstract. A vertex of a simple graph is called large if its degree is at least 3. It was shown recently that in the class of starlike trees, which have one large vertex, there are no pairs of cospectral trees. However, already in the classes of trees with two or three large vertices there exist pairs of cospectral trees. Thus, one needs to employ additional graph invariant in order to characterize such trees. Here we show that trees with two or three large vertices are characterized by their eigenvalues and angles.

1. Introduction

Let $G = (V, E)$ be a connected simple graph with $n = |V| \geqslant 2$ vertices and $E \subseteq \binom{V}{2}$. Let A be an adjacency matrix of G and let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of A. Let d_i, $i \in V$, denote the degree of a vertex i. Vertex $i \in V$ is called a *large vertex* if $d_i \geqslant 3$. A tree having one, two or three large vertices is called *starlike*, *double starlike* or *triple starlike* tree, respectively. For other undefined notions, we refer the reader to [**1, 4**].

The question 'Which graphs are characterized by eigenvalues?' goes back for about half a century, and originates from chemistry, where the theory of graph spectra is related to Hückel's theory (see an excellent recent survey [**5**]). Concerning trees, Schwenk [**7**] showed that almost every tree has a nonisomorphic cospectral mate. It was shown by Gutman and Lepović [**6**] that in the class of starlike trees there are no pairs of cospectral trees. However, already in the classes of double starlike and triple starlike trees there exist pairs of cospectral trees: by a computer search among trees with up to 18 vertices, we have found a pair of cospectral double starlike trees, shown in Fig. 1, and a pair of cospectral triple starlike trees, shown in Fig. 2.

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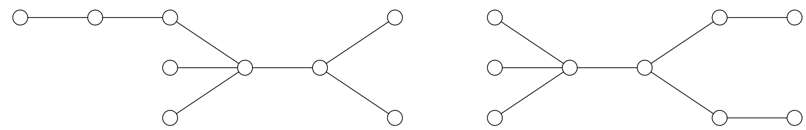

FIGURE 1. A pair of cospectral double starlike trees.

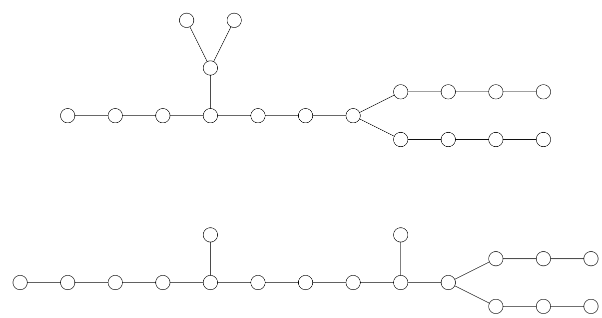

FIGURE 2. A pair of cospectral triple starlike trees.

Thus, in order to characterize double starlike and triple starlike trees we need to employ additional (spectral) invariant. One possible choice is to use graph angles, defined in the following way.

Let $\mu_1 > \mu_2 > \cdots > \mu_m$ be all distinct values among the eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ of A. Further, let $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$ constitute the standard orthonormal basis for R^n. The adjacency matrix A has the spectral decomposition $A = \mu_1 P_1 + \mu_2 P_2 + \cdots + \mu_m P_m$, where P_i represents the orthogonal projection of R^n onto the eigenspace $\mathbf{E}(\mu_i)$ associated with the eigenvalue μ_i (moreover $P_i^2 = P_i = P_i^T$, $i = 1, \dots, m$; and $P_i P_j = 0$, $i \neq j$). The nonnegative quantities $\alpha_{ij} = \cos\beta_{ij}$, where β_{ij} is the angle between $\mathbf{E}(\mu_i)$ and $\mathbf{e}_j$, are called *angles* of G. Since P_i represents orthogonal projection of R^n onto $\mathbf{E}(\mu_i)$ we have $\alpha_{ij} = \|P_i \mathbf{e}_j\|$. The sequence α_{ij}, $j = 1, 2, \dots, n$, is the ith *eigenvalue angle sequence*, while α_{ij}, $i = 1, 2, \dots, m$, is the jth *vertex angle sequence*. The *angle matrix* $\mathbf{A}$ of G is defined to be the matrix $\mathbf{A} = \|\alpha_{ij}\|_{m,n}$ provided its columns (i.e., the vertex angles sequences) are ordered lexicographically. The angle matrix is a graph invariant. For further properties of angles see [**4**, Chapters 4, 5].

Eigenvalues and angles still cannot characterize all trees: following Schwenk's approach, Cvetković [**2**] showed that for almost every tree there is a nonisomorphic cospectral mate with the same angles. The smallest pair of cospectral trees with the same angles, shown in Fig. 3, has four large vertices.

Thus, the question remains whether double and triple starlike trees are characterized by eigenvalues and angles. We answer this question affirmatively: in

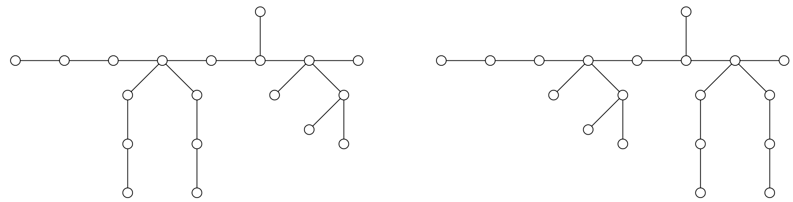

FIGURE 3. A pair of cospectral trees with the same angles and four large vertices.

Section 2 we prove this for double starlike trees, while in Section 3 we consider triple starlike trees. Some other classes of graphs, characterized by eigenvalues and angles, may be found in [**3**].

2. Double starlike trees

Following [**2**], we call a graph or a vertex invariant *EA-reconstructible*, if it can be determined from the eigenvalues and angles of graph. Denote by $w_s(j,G)$ the number of closed walks of length s in graph G starting and terminating at vertex j. The basic property of angles is given in the following lemma.

LEMMA 2.1. [**4**] *For $j \in v(G)$ and $s \in N$, the value $w_s(j,G)$ is EA-reconstructible.*

PROOF. Recall that $w_s(j,G)$ is equal to the (j,j)-entry of A^s. Since $\alpha_{ij}^2 = \|P_i\mathbf{e}_j\|^2 = \mathbf{e}_j^T P_i \mathbf{e}_j$, the numbers $\alpha_{i1}^2, \alpha_{i2}^2, \ldots, \alpha_{in}^2$ appear on the diagonal of P_i. From the spectral decomposition of A we have $A^s = \sum_{i=1}^m \mu_i^s P_i$, whence

$$w_s(j,G) = \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^s. \tag{2.1}$$ □

From Lemma 2.1 the degree d_j of the vertex j is given by

$$d_j = \sum_{i=1}^{m} \alpha_{ij}^2 \mu_i^2$$

and, thus, degree sequence of a graph is EA-reconstructible. In [**2**] it is proven that the knowledge of the characteristic polynomials of vertex deleted subgraphs is equivalent to the knowledge of angles, since we have

$$P_{G-j}(\lambda) = P_G(\lambda) \sum_{i=1}^{m} \frac{\alpha_{ij}^2}{\lambda - \mu_i},$$

where $P_G(\lambda)$, $P_{G-j}(\lambda)$ are the characteristic polynomials of G and $G-j$, respectively. Vertices belonging to components having the same largest eigenvalue as the graph are EA-reconstructible, since by the Perron–Frobenius theory of nonnegative matrices angles belonging to μ_1 are nonzero precisely for these vertices. As a corollary, the property of a graph of being connected is EA-reconstructible. Since the numbers of vertices and edges are clearly EA-reconstructible, the property of a graph of being a tree is also EA-reconstructible. Further, the number of large vertices is known from the degree sequence. Thus, we have the following

LEMMA 2.2. *The property of being a double starlike tree is EA-reconstructible. The property of being a triple starlike tree is EA-reconstructible.*

A *branch* of a tree at the vertex u is a maximal subtree containing u as a leaf. The union of one or more branches of u is called a *limb at* u.

RECONSTRUCTION LEMMA. [**2**] *Given a limb R of a tree T at a vertex u which is adjacent to a unique vertex of T not in R, that vertex is among those vertices j such that $P_{T-j}(\lambda) = g_u^R(\lambda)$, where*

$$g_u^R(\lambda) = \frac{P_R(\lambda)}{[P_{R-u}(\lambda)]^2}\big[P_R(\lambda)P_{T-u}(\lambda) - P_{R-u}(\lambda)P_T(\lambda)\big]. \tag{2.2}$$

LEMMA 2.3. *For every leaf of a tree T, its distance from the nearest vertex v with $d_v \neq 2$ and the angles of v are EA-reconstructible.*

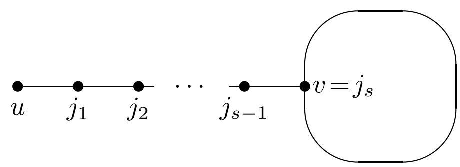

FIGURE 4. Leaf u of a tree with the nearest vertex v with $d_v \neq 2$.

PROOF. Let $u = j_0, j_1, j_2, \dots, j_{s-1}, j_s = v$ be the unique path in T between a leaf u and the nearest vertex v with $d_v \neq 2$ (see Fig. 4). From the Reconstruction Lemma we get:

$$\begin{aligned} P_{T-j_1}(\lambda) &= g_{j_0}^{P_1}(\lambda) = g_u^{P_1}(\lambda), \\ P_{T-j_2}(\lambda) &= g_{j_1}^{P_2}(\lambda), \\ &\dots \\ P_{T-v}(\lambda) = P_{T-j_s}(\lambda) &= g_{j_{s-1}}^{P_s}(\lambda). \end{aligned}$$

Hence, we know the angles of j_k for $k = 0, 1, \dots, s$. The vertex $v = j_s$ is recognized from the condition $d_{j_s} = \sum_{i=1}^m \alpha_{ij_s}^2 \mu_i^2 \neq 2$. □

THEOREM 2.1. *A double starlike tree is characterized by eigenvalues and angles.*

PROOF. Let T' be a double starlike tree and let T be a graph having the same eigenvalues and angles as T'. From Lemma 2.2 we can see that T is also a double starlike tree.

Let c_1 and c_2 be large vertices of T, and let T_m be a subtree of T induced by c_1, c_2, path P connecting c_1 and c_2, and vertices at distance at most m from either

c_1 or c_2. For $i = 1, 2$ let S_i denote the set of vertices of T that do not belong to P and for which c_i is a closer large vertex.

We show by induction that T_m is EA-reconstructible for all $m \geqslant 0$. Let T have e edges and let L be a set of leaves of T. For each leaf $l \in L$ Lemma 2.3 gives its distance f_l from a closer large vertex. Length of path P is then equal to $e - \sum_{l \in L} f_l$, because every edge belongs either to P or to a path connecting a large vertex to a leaf, and it belongs to exactly one such path. Hence, T_0 is EA-reconstructible.

Suppose T_m is constructed for some $m \geqslant 0$. Then T_{m+1} will be determined if we know the number of vertices in S_i at distance $m+1$ from c_i for $i = 1, 2$. All vertices of T at distance at most m from c_i belong to T_m. Tree T_m also contains all vertices not in S_i that are at distance exactly $m+1$ from c_i. Namely, these vertices either belong to P or they are at distance at most m from the other large vertex. Therefore, the only closed walks of length $2m+2$ starting from c_i that are not contained in T_m are those between c_i and the vertices in S_i at distance $m+1$ from c_i. The number of these closed walks is equal to $w_{2m+2}(c_i, T) - w_{2m+2}(c_i, T_m)$, which is also equal to the number of vertices in S_i at distance $m+1$ from c_i. This proves that T_{m+1} is EA-reconstructible.

Now T is also EA-reconstructible, since $T = T_{m_0}$ for some $m_0 \geqslant 1$. This means that T is a unique graph with the eigenvalues and angles of T', and thus it must hold that $T \cong T'$. $\square$

3. Triple starlike trees

THEOREM 3.1. *A triple starlike tree is characterized by eigenvalues and angles.*

PROOF. Let T' be a triple starlike tree and let T be a graph having the same eigenvalues and angles as T'. From Lemma 2.2 we can see that T is also a triple starlike tree. Let c_1, c_2 and c_3 be large vertices of T, and let P be the shortest path containing all large vertices. We call the large vertices at ends of P the *peripheral* vertices, the large vertex inside P the *central* vertex, while P itself is called the *central path* of T. There are three cases to consider now:

a) Large vertices c_1, c_2 and c_3 all have distinct vertex angle sequences. Then for each leaf u of T we can determine from Lemma 2.3 the nearest large vertex c_i and its distance from c_i. Thus for each large vertex c_i we can determine the maximal limb M_i at c_i not containing other large vertices. Such limb at a peripheral large vertex contains one branch less than its degree, while at the central large vertex it contains two branches less than its degree. Thus, for each large vertex we can also determine whether it is peripheral or central. To determine T completely, it only remains to determine the distances from peripheral vertices to the central vertex, for which we use the following modification of Lemma 2.3.

LEMMA 3.1. *Let R be a limb of a tree T at a vertex u containing $d_u - 1$ branches, and let v be the nearest vertex from u, with $d_v \neq 2$, which does not belong to R. The distance between u and v, as well as the vertex angle sequence of v, are EA-reconstructible.*

PROOF. Let $u = j_0, j_1, j_2, \dots, j_{s-1}, j_s = v$ be the unique path in T between u and v. From the Reconstruction Lemma we get:

$$\begin{aligned} P_{T-j_1}(\lambda) &= g_{j_0}^{R_1}(\lambda) = g_u^R(\lambda), \\ P_{T-j_2}(\lambda) &= g_{j_1}^{R_2}(\lambda), \\ &\dots \\ P_{T-v}(\lambda) = P_{T-j_s}(\lambda) &= g_{j_{s-1}}^{R_s}(\lambda), \end{aligned}$$

where R_i is the limb R with the path P_i attached at u. Hence, we know the angles of j_k for $k = 0, 1, \dots, s$. The vertex $v = j_s$ is recognized from the condition $d_{j_s} = \sum_{i=1}^{m} \alpha_{ij_s}^2 \mu_i^2 \neq 2$. □

Applying Lemma 4 with u being a peripheral and v being the central vertex of T gives us distances between each peripheral and central vertex, and the tree T is now completely determined. This means that T is a unique graph with the eigenvalues and angles of T', and thus it must hold that $T \cong T'$.

b) Two of the large vertices c_1, c_2, c_3 have the same vertex angle sequences, while the third one has a different vertex angle sequence. Without loss of generality, we may suppose that c_1 and c_2 have equal, while c_3 has a distinct vertex angle sequence. By Lemma 3 we can determine all leaves for which c_3 is the nearest large vertex and the distance from c_3. Thus, we can determine the maximal limb M_3 at c_3 not containing other large vertices. If c_3 is a peripheral vertex, then M_3 contains $d_{c_3} - 1$ branches, otherwise, if c_3 is the central vertex, it contains $d_{c_3} - 2$ branches. Thus, we can also determine whether c_3 is a peripheral or the central vertex.

In case c_3 is a peripheral vertex, by Lemma 4 we can determine the distance d from c_3 to the central vertex. Then we can also determine the distance D between c_1 and c_2, as it is equal to the difference between the number of edges in T and the total numbers of edges in limb M_3, path between c_3 and the central vertex and branches from leaves for which either c_1 or c_2 is the nearest large vertex. Now, we have that the following part of T is reconstructed (see Fig. 5).

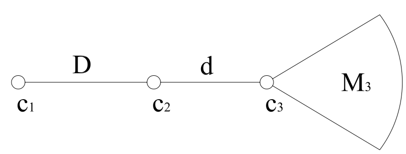

FIGURE 5. Partial reconstruction of T when c_3 is a peripheral vertex.

Denote it by T_0 and let T_m be a supertree of T_0 obtained by adding vertices of T at distance at most m from either c_1 or c_2. Similar as in the proof of Theorem 1, we can inductively prove that T_m is EA-reconstructible for all $m \geqslant 0$. Now T is also EA-reconstructible as $T = T_{m_0}$ for some $m_0 \geqslant 1$, so that T is a unique graph with the eigenvalues and angles of T', and thus it must hold that $T \cong T'$.

In case c_3 is the central vertex, we can determine the distance d between c_3 and the closer peripheral vertex using the following

LEMMA 3.2. *Let R be a limb of a tree T at a vertex u containing $d_u - m$ branches, and let v be the nearest vertex to u, with $d_v \neq 2$, which does not belong to R. The distance between u and v is EA-reconstructible.*

PROOF. Let l be the distance between u and v, and let R_k be the limb R with m copies of a path P_{k+1} attached at u, for $0 \leqslant k \leqslant l+1$. Then

$$w_{2k}(u,T) = w_{2k}(u,R_k), \text{ for } 0 \leqslant k \leqslant l,$$

while

$$w_{2l+2}(u,T) \neq w_{2l+2}(u,R_k).$$

Thus, we can determine l from R and the vertex angle sequence of v in T. □

We can also determine the distance D between c_3 and the farther peripheral vertex, as it is equal to the difference between the number of edges in T and the total numbers of edges in limb M_3, path between c_3 and the nearer peripheral vertex and branches from leaves for which either c_1 or c_2 is the nearest large vertex. Thus, we have the following part of T, denote it by T_0, reconstructed (see Fig. 6).

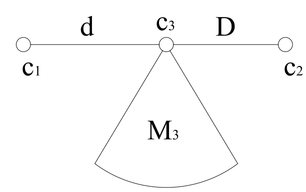

FIGURE 6. Partial reconstruction of T when c_3 is a central vertex.

Peripheral vertices c_1 and c_2 have equal vertex angle sequences, so we may freely choose how to denote the peripheral vertex closer to c_3. Let T_m be a supertree of T_0 obtained by adding vertices of T at distance at most m from either c_1 or c_2. Again, similar as in the proof of Theorem 1, we can inductively prove that T_m is EA-reconstructible for all $m \geqslant 0$. The tree T is also EA-reconstructible, as $T = T_{m_0}$ for some $m_0 \geqslant 1$. Thus, T is a unique graph with the eigenvalues and angles of T' and so it must hold that $T \cong T'$.

c) Large vertices c_1, c_2 and c_3 all have equal vertex angle sequences. Without loss of generality, let c_1 and c_3 be peripheral vertices, c_2 the central vertex, D the distance between c_1 and c_2, d the distance between c_2 and c_3, and let $d \leqslant D$. For nonnegative integer m and a vertex u of T, let $T_m[u]$ be a subgraph of T induced by the vertices at distance at most m from u.

We first prove that $T_m[c_1] \cong T_m[c_2]$ for each $0 \leqslant m \leqslant d$ by induction. For $m = 0$ we have $T_0[c_1] \cong T_0[c_2] \cong K_1$. Suppose that $T_{m_0}[c_1] \cong T_{m_0}[c_2]$ for some $m_0 \leqslant d-1$. Since $m_0 < D$, we have that $T_{m_0+1}[c_1]$ and $T_{m_0+1}[c_2]$ are both starlike trees. It is easy to see that a starlike tree S is characterized by a sequence $(s_n)_{n\geqslant 0}$, where s_n is the number of vertices at distance n from the center of S. Now

$$s_{m_0+1}(c_i) = w_{2m_0+2}(c_i, T) - w_{2m_0+2}(c_i, T_{m_0}[c_i])$$

gives the number of vertices of T at distance $m_0 + 1$ from c_i for $i = 1, 2$. Since $T_{m_0}[c_1] \cong T_{m_0}[c_2]$, we have that $s_{m_0+1}(c_1) = s_{m_0+1}(c_2)$, and thus it follows that $T_{m_0+1}[c_1] \cong T_{m_0+1}[c_2]$. Continuing inductively, we conclude that $T_d[c_1] \cong T_d[c_2]$.

Let $\Delta = d_{c_3} - 1$ and let, as in Fig. 7, m_1 be the number of vertices at distance $d+1$ from c_1 and distance $D+d+1$ from c_2, m'_1 the number of vertices at distance $d+2$ from c_1 and distance $D+d+2$ from c_2, m_2 the number of vertices at distance $d+1$ from c_2, distance $2d+1$ from c_3 and distance $D+d+1$ from c_1, m'_2 the number of vertices at distance 2 from c_3, distance $d+2$ from c_2 and distance $D+d+2$ from c_1, and m''_2 the number of vertices at distance $d+2$ from c_2, distance $2d+2$ from c_3 and distance $D+d+2$ from c_1.

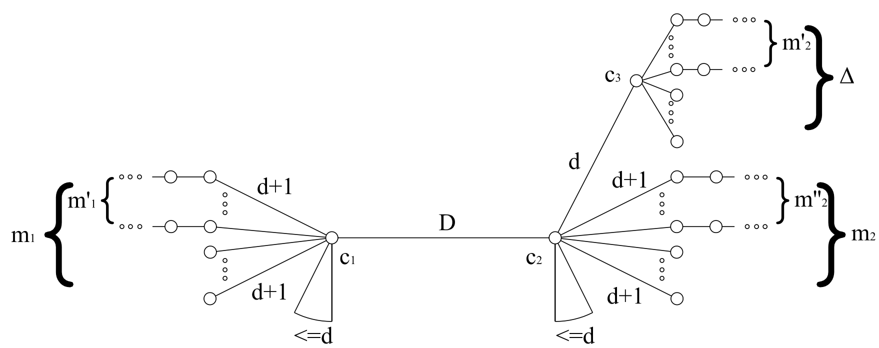

FIGURE 7. Structure of T in case c).

First, consider $(2d + 2)$-closed walks from c_1 and c_2, respectively. At c_2 it is equal to $w_{2d+2}(c_2, T_d[c_2]) + \Delta + m_2$, while at c_1 it is equal to $w_{2d+2}(c_1, T_d[c_1]) + m_1$. Thus, it must hold that $m_1 = \Delta + m_2$.

Now, consider $(2d + 4)$-closed walks at c_1 and c_2, respectively. Their numbers must be equal and they can be divided into the following categories. At c_1:

i) those belonging to $T_d[c_1]$;

ii) those belonging to $T_{d+1}[c_1]$, using a vertex from $T_{d+1}[c_1] \setminus T_d[c_1]$;

iii) those belonging to $T_{d+2}[c_1]$, using a vertex from $T_{d+2}[c_1] \setminus T_{d+1}[c_1]$. There are m'_1 such walks.

At c_2:

i) those belonging to $T_d[c_2]$;

ii) those belonging to $T_{d+1}[c_2]$, using a vertex from $T_{d+1}[c_2] \setminus T_d[c_2]$;

iii) those belonging to $T_{d+2}[c_2]$, using a vertex from $T_{d+2}[c_2] \setminus T_{d+1}[c_2]$. There are $m'_2 + m''_2$ such walks.

iv) those belonging to $T_{d+1}[c_2]$, using more than one neighbor of c_3. There are Δ^2 such walks.

Now, the numbers of type *i*) walks at c_1 and c_2 are equal, since $T_d[c_1] \cong T_d[c_2]$. The number of type *ii*) walks at c_1 and c_2 are also equal, as we may construct a bijection between the closed walks at c_2 reaching one of Δ neighbors of c_3 and the closed walks at c_1 reaching fixed Δ out of m_1 vertices at distance $d+1$ from c_1, and also between the closed walks reaching remaining m_2 vertices at distance $d+1$ from c_2 and the closed walks reaching remaining m_2 vertices at distance $d+1$ from c_1. As a consequence we must have that the number of type *iii*) walks at c_1 and the types *iii*) and *iv*) walks at c_2 must be equal and thus it holds that

$$m_1' = m_2' + m_2'' + \Delta^2.$$

Therefore we have that

$$d_{c_1} \geqslant m_1 + 1 \geqslant m_1' + 1 \geqslant \Delta^2 + 1 > \Delta + 1 = d_{c_3},$$

which is a contradiction to the assumption that c_1 and c_3 have equal vertex angle sequences. Thus, this case is impossible. □

Question. We have just proved that it is impossible that all three large vertices have the same vertex angle sequences. While it is allowed by proof of case b), we did not come across an example of a triple starlike tree having a peripheral and the central vertex with the same vertex angle sequences. Does such a triple starlike tree exist?

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