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AN ISOMORPHISM THEOREM FOR UNICYCLIC GRAPHS

1. Introduction

In the paper we follow the notation of Harary [1]. By a unicyclic graph we mean any connected graph with exactly one cycle. The graph isomorphism problem can be stated as follows:

For given graphs G_1 and G_2 determine whether or not they are isomorphic and, if they are, derive any isomorphism of G_1 onto G_2 . Two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ are isomorphic ($G_1 \cong G_2$) if there exists a one-to-one mapping ϕ of V_1 onto V_2 such that

$$(u_1, v_1) \in E_1 \quad \text{whenever} \quad (\phi(u_1), \phi(v_1)) \in E_2,$$

for every pair (u_1, v_1) of vertices in V_1 .

In this paper instead of testing isomorphism between two unicyclic graphs U_1 and U_2 we test isomorphism between some matrices M_{U_1} and M_{U_2} corresponding to U_1 and U_2 , respectively. The main theorem is true for unicyclic graphs with at least three so-called offshoots only. (By an offshoot we mean every component of the graph obtained from a unicyclic graph by deleting all the edges of the cycle.) In the last section there are some examples showing that the theorem is not true for graphs with less than three offshoots. In that sense the number "three" is best possible.

Since the exact definition of the matrix M_U for a given unicyclic graph U is given in the next section let us only mention here that many questions concerning the structural properties of U (e.g. the length of the cycle, the number of offshoots or the cardinality of the set of leaves in the particular offshoot) can easily be answered by the use of the matrix M_U . Moreover such a matrix is usually small and it is rather surprising that it provides enough information to define a unicyclic graph U , up to isomorphism.

2. Definitions and lemmas

In order to state the main theorem we shall introduce some definitions

first. We denote by $J(G)$ the set of all vertices of degree one in the graph G . In case G is either a tree or a unicyclic graph we call any vertex belonging to $J(G)$ a leaf. We use \mathcal{U} and \mathcal{U}_p ($p \in \mathcal{N}$, $p \geq 3$) to denote the set of all unicyclic graphs and the set of all unicyclic graphs with a cycle of length p , respectively. By \mathcal{M}_n ($n \in \mathcal{N}$) we mean the set of all matrices $n \times n$ of non-negative elements. Finally, the notation $(i = \overline{k, n})$ means “for every natural i from k to n ”.

DEFINITION 1. Let $A, B \in \mathcal{M}_n$. We say that A is isomorphic to B ($A \cong B$) if there exists a permutation σ of the set $\{1, \dots, n\}$ such that $A[i, j] = B[\sigma(i), \sigma(j)]$ ($i, j = \overline{1, n}$). The matrix A is denoted by $\sigma(B)$.

DEFINITION 2. Let T be a tree with n leaves and let $J(T) = \{u_1, \dots, u_n\}$. Define

$$M_T[i, j] = \begin{cases} \rho_T(u_i, u_j) & \text{if } i \neq j, \\ 0 & \text{if } i = j, \end{cases}$$

where $\rho_T(u_k, u_l)$ ($k, l = \overline{1, n}$) is the distance between the leaves u_k and u_l in T . The matrix M_T is called the matrix of distances between leaves in T .

By Definition 1, it is obvious that for any tree T the matrix M_T is symmetric and has zeros on the main diagonal.

In 1965 Zarecky [3] using results of Smolensky [2] have proved the following:

LEMMA 1 (Zarecky). *Let S_ν ($\nu \geq 2$) be a system of $\nu(\nu - 1)$ natural numbers $\rho_{ij} = \rho_{ji}$ ($i, j = \overline{1, \nu}, i \neq j$). There exists a tree T with the set of leaves $J(T) = \{y_1, \dots, y_\nu\}$ satisfying the conditions $\rho_T(y_i, y_j) = \rho_{ij}$ ($i, j = \overline{1, \nu}, i \neq j$) if and only if the system S_ν has the following properties:*

(1) *for any pairwise different indices $i, j, k \in \{1, \dots, \nu\}$ the numbers $\rho_{ij} + \rho_{ik} - \rho_{jk}$ are even and positive*

and

for any pairwise different indices $i, j, k, l \in \{1, \dots, \nu\}$

(2) *two of the numbers $\rho_{ij} + \rho_{kl}$, $\rho_{ik} + \rho_{jl}$ and $\rho_{il} + \rho_{jk}$ are equal to each other and the third one is not greater than them.*

If conditions (1) and (2) are satisfied and there exists a tree T' with the set of leaves $J(T') = \{y'_1, \dots, y'_\nu\}$ such that $\rho_{T'}(y'_i, y'_j) = \rho_{ij}$ ($i, j = \overline{1, \nu}, i \neq j$) then the trees T and T' are isomorphic and the isomorphism of T onto T' is defined by the correspondence between leaves with equal indices. The condition (2) for $\nu \leq 3$ and the condition (1) for $\nu = 2$ set no limitations to the numbers belonging to S_ν . ■

We shall focus on the part of Lemma 1 concerning the isomorphism problem. In the notation just introduced we can state the following obvious:

COROLLARY 1. Let T_1 and T_2 be trees. Then $T_1 \cong T_2$ if and only if $M_{T_1} \cong M_{T_2}$.

Now we introduce some definitions for unicyclic graphs.

DEFINITION 3. For any cycle C , by a direction of C we mean any digraph C^+ obtained from the cycle C by orienting its edges such that for every pair of different edges xy and uv of C , if $xy, uv \in E(C^+)$ then $x \neq u$.

Clearly, for any cycle C there are two different directions of C . In order to simplify the notation we use the same symbol uv to denote both a directed and undirected edge. It will not lead to misunderstandings. The set of all pairs (U, C^+) , where $U \in \mathcal{U}$ and C^+ is a direction of the cycle C in U is denoted by \mathcal{U}^+ . Similarly, \mathcal{U}_p^+ denotes the set of all pairs (U, C^+) , where $U \in \mathcal{U}_p$ and C^+ is a direction of the cycle C in U . In both above cases we shall denote a pair (U, C^+) by U^+ and write $U^+ \in \mathcal{U}^+$ (resp. $U^+ \in \mathcal{U}_p^+$) instead of $(U, C^+) \in \mathcal{U}^+$ (resp. $(U, C^+) \in \mathcal{U}_p^+$). We shall also write “a direction in U ” instead of “a direction of the cycle C in U ”.

DEFINITION 4. Let $U^+ \in \mathcal{U}^+$. We define a path between vertices $u, v \in V(U)$ to be a sequence of vertices $\{v_0, \dots, v_n\}$, $v_i \in V(U)$ ($i = \overline{0, n}$), such that

$$(3) \quad v_0 = u, v_n = v,$$

$$(4) \quad v_{i-1}v_i \neq v_{j-1}v_j \quad (i, j = \overline{1, n}, i \neq j),$$

$$(5) \quad \text{if } v_{i-1}v_i \in E(C) \text{ then } v_{i-1}v_i \in E(C^+) \quad (i = \overline{1, n}).$$

The length of a path in $U^+ \in \mathcal{U}^+$ is equal to the number of edges of this path. A path from u to v will be denoted by $[u, v]$.

DEFINITION 5. Let $U^+ \in \mathcal{U}^+$. The pseudodistance between vertices $u, v \in V(U)$ in U^+ , denoted by $\rho_{U^+}(u, v)$, is the length of the shortest path from u to v in U^+ .

Notice that the pseudodistance is not a metric in a graph $U^+ \in \mathcal{U}^+$.

DEFINITION 6. Let $U^+ \in \mathcal{U}^+$ and let $J(U) = \{u_1, \dots, u_n\}$. The matrix $M_{U^+} \in \mathcal{M}_n$ such that $M_{U^+}[i, j]$ is equal to the pseudodistance between vertices u_i and u_j ($i, j = \overline{1, n}$) in U^+ is called the matrix of pseudodistances in U^+ .

Clearly, for any graph $U \in \mathcal{U}$ there exist exactly two, up to isomorphism, matrices of pseudodistances. These matrices correspond to the two different directions in U .

DEFINITION 7. Let $U^+ \in \mathcal{U}_p^+$ for some $p \in \mathcal{N}$. Let us denote vertices of the cycle by c_1, \dots, c_p . For every vertex c_i ($1 \leq i \leq p$) we define the set O_i of all leaves $u \in J(U)$ such that there exists a path $[u, c_i]$ not including

any edge of the cycle. If, for any i ($1 \leq i \leq p$), the set O_i is not empty then it is called the offshoot of U . The vertex c_i is called the base vertex of the offshoot O_i .

DEFINITION 8. Let us define a relation $\# \subseteq \mathcal{M}_n \times \mathcal{M}_n$ as the smallest transitive relation (the transitive closure) such that

$$(6) \quad (\forall A, B \in \mathcal{M}_n) (A \# B \text{ if } A \cong B \text{ or } A \cong B^T).$$

3. The unicyclic graph theorem

In this section we state and prove the main theorem of this paper.

THEOREM. Let $U_1, U_2 \in \mathcal{U}$ be graphs with at least three offshoots each. Then $U_1 \cong U_2$ if and only if $M_{U_1^+} \# M_{U_2^+}$, where U_i^+ ($i = \overline{1, 2}$) is the graph U_i with a fixed direction.

Proof. Necessity. Since the proof of necessity is trivial we only mention here that if σ is the isomorphism of U_1 onto U_2 and c_1, \dots, c_p are vertices of the cycle C_1 in U_1 , and for example (without loss of generality) $c_1 c_2 \in E(C_1^+)$, where C_1^+ is the fixed direction in U_1 then either $M_{U_1^+} \# M_{U_2^+}$ (for $\sigma(c_1)\sigma(c_2) \in E(C_2^+)$) or $M_{U_1^+} \# M_{U_2^+}^T$ (for $\sigma(c_2)\sigma(c_1) \in E(C_2^+)$), where C_2^+ is the fixed direction in U_2 .

Sufficiency. By the definition of the relation $\#$, $M_{U_1^+} \# M_{U_2^+}$ implies that either $M_{U_1^+} \cong M_{U_2^+}$ or $M_{U_1^+} \cong (M_{U_2^+})^T$. In fact, since the relation $\#$ is the transitive closure, for every $A, B \in \mathcal{M}_n$ if $A \# B$ then there exist $A_1, \dots, A_l \in \mathcal{M}_n$ such that

$$A = A_1, B = A_l \quad \text{and} \quad A_i \cong A_{i+1} \quad \text{or} \quad A_i^T \cong A_{i+1} \quad (i = \overline{1, l-1}).$$

Furthermore, because isomorphisms and transposes of matrices commute, we obtain $A \cong B$ or $A \cong B^T$. Let us consider two cases.

Case 1). $M_{U_1^+} \cong M_{U_2^+}$.

Let σ be the isomorphism of $M_{U_1^+}$ onto $M_{U_2^+}$. It means (see Definition 1) that $M_{U_1^+} = \sigma(M_{U_2^+}) \stackrel{\text{def}}{=} M$. Let us renumber leaves in U_2^+ according to the permutation σ and denote the obtained graph by U_2^+ again. Now we have got two graphs U_1^+ and U_2^+ , each with a fixed direction such that M is the matrix of pseudodistances corresponding to both of them.

Let $U^+ \in \mathcal{U}^+$ be any graph such that M is its matrix of pseudodistances. We shall prove some properties of U^+ . Let $M \in \mathcal{M}_n$. Let us divide the set $\{1, \dots, n\}$ of indices of the matrix M into classes by the equivalence relation $\mathcal{R} \subseteq \{1, \dots, n\} \times \{1, \dots, n\}$ defined as follows:

$(\forall i, j \in \{1, \dots, n\})$,

$$(i \mathcal{R} j) \iff \underbrace{((\forall k \in \{1, \dots, n\})(M[i, k] - M[k, i] = M[j, k] - M[k, j]))}_{(7)}.$$

First we will show that \mathcal{R} is in fact an equivalence relation on the set $\{1, \dots, n\}$. It is obvious that \mathcal{R} is reflexive and symmetric. In order to prove transitivity of \mathcal{R} we will first show that:

$$(8) \quad \left\{ \begin{array}{l} (\text{a pair } (i, j) \text{ satisfies the condition (7)} \iff \\ (u_i \text{ and } u_j \text{ belong to the same offshoot in the graph } U^+) \end{array} \right.$$

Proof of (8). Necessity. Assume on the contrary that u_i and u_j belong to different offshoots. Since U^+ has at least three offshoots, there exists $k \in \{1, \dots, n\}$ such that u_i, u_j, u_k belong to pairwise different offshoots. Let c_{s1}, c_{s2}, c_{s3} denote the base vertices of these offshoots, respectively. There are two cases up to the orientation of the cycle in U^+ (see Fig. 1).

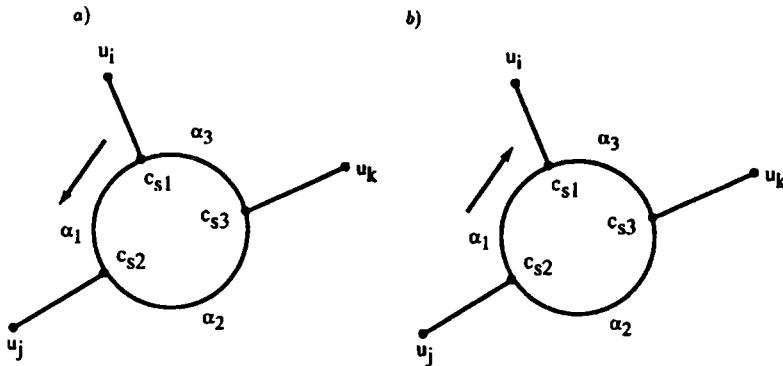


Figure 1.

In the case a), denote $\alpha_1 = \rho(c_{s1}, c_{s2})$, $\alpha_2 = \rho(c_{s2}, c_{s3})$ and $\alpha_3 = \rho(c_{s3}, c_{s1})$. Then

$$M[i, k] - M[k, i] = \alpha_1 + \alpha_2 - \alpha_3 \quad \text{and} \quad M[j, k] - M[k, j] = \alpha_2 - \alpha_3 - \alpha_1.$$

Thus $\alpha_1 + \alpha_2 - \alpha_3 = \alpha_2 - \alpha_3 - \alpha_1$ and therefore $\alpha_1 = 0$. It is a contradiction because, by the assumption, u_i and u_j belong to different offshoots.

In the case b) we proceed analogously.

Sufficiency. Let u_i and u_j belong to the same offshoot, say O_1 . The proof of sufficiency is divided into two cases.

Case a). $u_k \in O_1$. By the definition of the pseudodistance we trivially get: $M[i, k] - M[k, i] = 0 = M[j, k] - M[k, j]$.

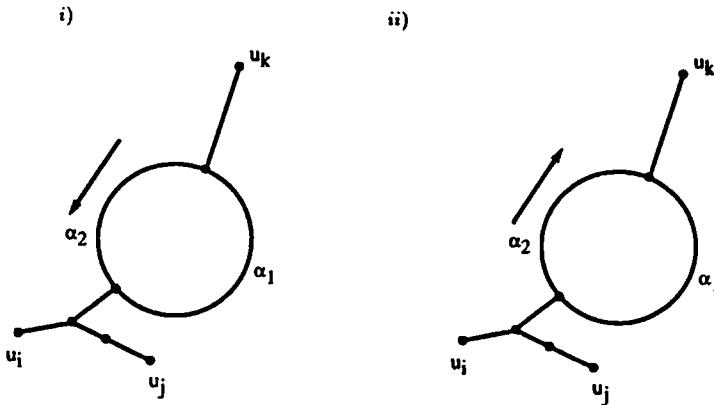


Figure 2.

Case b). $u_k \notin O_1$. Two subcases are possible (see Fig. 2). Since they are analogous, we consider the case *i*) only. Clearly, $M[i, k] - M[k, i] = \alpha_1 - \alpha_2 = M[j, k] - M[k, j]$. The proof of (8) is completed.

Transitivity of the relation \mathcal{R} is now immediate. By (8), if $i \mathcal{R} j$ and $j \mathcal{R} k$ then the vertices u_i and u_j belong to the same offshoot and so do u_j and u_k . Thus u_i and u_k (and clearly u_j as well) belong to the same offshoot, so by (8), $i \mathcal{R} k$.

The relation \mathcal{R} defines a partition of the set $\{1, \dots, n\}$ of indices of the matrix M into t classes F_1, \dots, F_t . This partition corresponds to the partition of the set of leaves in the graph U^+ into offshoots. More precisely, indices i, j belong to the same class if and only if corresponding leaves u_i and u_j belong to the same offshoot in U^+ . Hence, we shall identify a class F_s with a set of leaves belonging to an offshoot O_s ($s = \overline{1, t}$). In order to streamline the notation we use the symbol c_s ($s = \overline{1, t}$) to denote a base vertex of an offshoot O_s and conversely an offshoot corresponding to a base vertex c_s is denoted by O_s ($s = \overline{1, t}$). We have established so far that U^+ has got t offshoots, where $t \geq 3$.

Now let us consider any triple $s_1, s_2, s_3 \in \{1, \dots, t\}$ such that $s_1 \neq s_2 \neq s_3 \neq s_1$ and let $i, j, k \in \{1, \dots, n\}$ be any indices such that $i \in F_{s_1}, j \in F_{s_2}$ and $k \in F_{s_3}$. We define p as follows:

$$p = |M[i, j] + M[j, k] + M[k, i] - M[j, i] - M[k, j] - M[i, k]|.$$

Now we show that p is a well-defined number equal to the length of the cycle in the graph U^+ . Actually, up to the orientation of the cycle, two cases are possible (see Fig. 3).

Let $\alpha_i \stackrel{\text{def}}{=} \rho_{U^+}(u_i, c_{s_1})$, $\alpha_j \stackrel{\text{def}}{=} \rho_{U^+}(u_j, c_{s_2})$, $\alpha_k \stackrel{\text{def}}{=} \rho_{U^+}(u_k, c_{s_3})$.

Case a). $c_{s_3} \in [c_{s_1}, c_{s_2}]$.

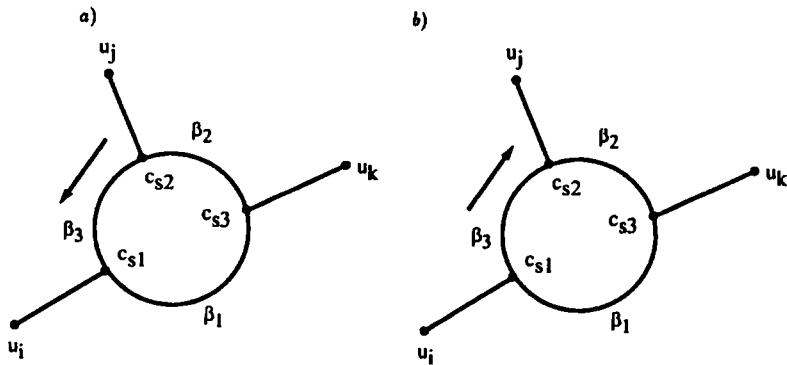


Figure 3.

Define $\beta_1 = \rho_{U^+}(c_{s_1}, c_{s_3})$, $\beta_2 = \rho_{U^+}(c_{s_3}, c_{s_2})$, $\beta_3 = \rho_{U^+}(c_{s_2}, c_{s_1})$. Then

$$p = |\beta_1 + \beta_2 + \beta_3| = \text{the length of the cycle}.$$

Case b). $c_{s_3} \in [c_{s_2}, c_{s_1}]$.

Similarly, define $\beta_1 = \rho_{U^+}(c_{s_3}, c_{s_1})$, $\beta_2 = \rho_{U^+}(c_{s_1}, c_{s_2})$, $\beta_3 = \rho_{U^+}(c_{s_2}, c_{s_3})$. Then

$$p = |-(\beta_1 + \beta_2 + \beta_3)| = \text{the length of the cycle}.$$

Since p does not depend on the indices i, j, k , it is well-defined. We have obtained that $U^+ \in \mathcal{U}_p^+$.

Now consider any $u_i \in O_{s_1}$, $u_j \in O_{s_2}$, $u_k \in O_{s_3}$, where $O_{s_1}, O_{s_2}, O_{s_3}$ are the offshoots of U^+ and $s_1 \neq s_2 \neq s_3 \neq s_1$, and let

$$W(i, j, k) = M[i, j] + M[j, k] + M[k, i] - M[j, i] - M[k, j] - M[i, k].$$

Notice that

$$(9) \quad \begin{cases} (c_{s_3} \in [c_{s_1}, c_{s_2}]) \iff (W(i, j, k) = p), \\ (c_{s_3} \in [c_{s_2}, c_{s_1}]) \iff (W(i, j, k) = -p). \end{cases}$$

Now for every index i of the matrix M ($i \in F_{m_1}, 1 \leq m_1 \leq t$) let us define a number

$$DIST(i) = \begin{cases} 1/2(M[k, i] + M[i, j] - M[k, j]) & \text{if } W(i, j, k) = -p, \\ 1/2(M[j, i] + M[i, k] - M[j, k]) & \text{if } W(i, j, k) = p \end{cases}$$

(see Fig. 4), where $j \in F_{m_2}$ and $k \in F_{m_3}$ are any indices such that $m_1 \neq m_2 \neq m_3 \neq m_1$, $1 \leq m_2, m_3 \leq t$, (which of course implies $i \neq j \neq k \neq i$).

The number $DIST(i)$ ($i = \overline{1, n}$) is well defined and equal to the distance between the leaf u_i and the vertex c_{m_1} , where $u_i \in O_{m_1}$ in the graph U^+ .

Now let l_1 ($1 \leq l_1 \leq n$) be any fixed element of F_1 and l_s ($1 \leq l_s \leq n$) be any element of F_s ($s = \overline{2, t}$). Then

$$\rho_{U^+}(c_1, c_s) = M[l_1, l_s] - DIST(l_1) - DIST(l_s) \quad (s = \overline{2, t}).$$

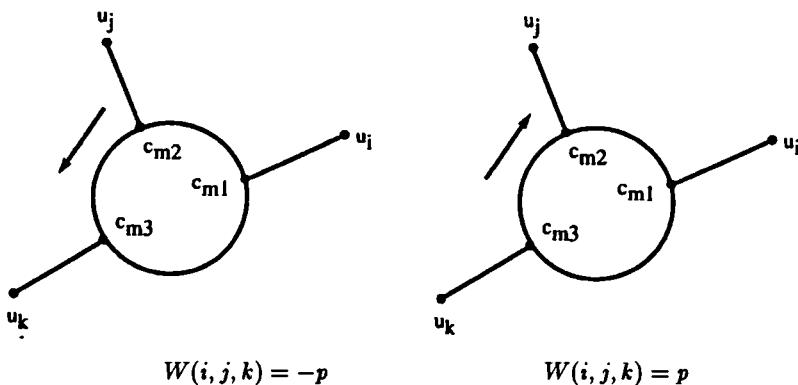


Figure 4.

Therefore, if we fix the vertex c_1 on the cycle of length p then we uniquely determine the positions of the base vertices c_s of the offshoots O_s ($s = \overline{2, t}$).

Let us introduce the ordering relation \prec on the set $\{F_1, \dots, F_t\}$ defined as follows:

$$(10) \quad F_1 \prec F_r \quad (r = \overline{2, t}),$$

$$(11) \quad (F_i \prec F_j) \iff (\rho_{U^+}(c_1, c_i) < \rho_{U^+}(c_1, c_j)) \quad (i, j = \overline{2, t}).$$

Now renumber the classes F_1, \dots, F_t according to the order \prec and reorder the rows and the columns of the matrix M simultaneously in such a way that the successive rows (resp. columns) correspond to indices belonging to the successive classes F_1, \dots, F_t . At the same time let us renumber the leaves in the graph U^+ in the same way as we have renumbered the rows and the columns of the matrix M .

Now the matrix M has the form depicted in Fig. 5.

K_1				
K_2				
•				
•				
•				
K_t				
	K_1	K_2	•	K_t

Figure 5.

Let

$$MAX \stackrel{\text{def}}{=} 1 + \max_{i,j \in \{1, \dots, n\}} M[i, j].$$

Let b_1, \dots, b_p denote the successive vertices of the cycle in U^+ and let $b_1 = c_1$ and $b_1 b_2 \in E(C^+)$, where C^+ is the direction in U^+ .

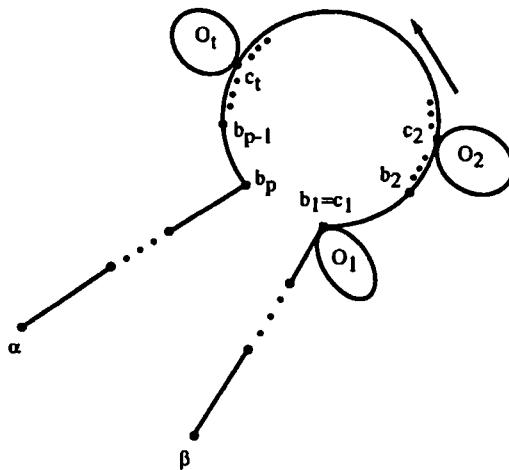


Figure 6.

Remove the edge $b_p b_1$ from the graph U^+ and add paths of length MAX with end-vertices in b_p and b_1 . Let α and β be the other ends of these paths (see Fig. 6), and denote by T the tree obtained this way, i.e.

$$\rho_T(b_p, \alpha) = \rho_T(b_1, \beta) = MAX.$$

According to the above construction applied to U^+ we change the matrix M (and obtain the matrix M') in the following way:

1°). We add the $(n + 1)'th$ and the $(n + 2)'th$ rows and columns corresponding to the vertices α and β , respectively.

2°). We put

$$M[i, n+1] = DIST(i) + \rho_{U+}(c_{s_i}, b_p) + MAX = M[n+1, i] \quad (i = \overline{1, n}),$$

$$M[n+2, i] = MAX + \rho_{U+}(b_1, c_{s_i}) + DIST(i) = M[i, n+2] \quad (i = \overline{1, n}),$$

$$M[n+1, n+1] = M[n+2, n+2] = 0,$$

$$M[n+2, n+1] = p - 1 + 2MAX = M[n+1, n+2],$$

where c_{s_i} is a base vertex of an offshoot O_{s_i} such that $u_i \in O_{s_i}$ ($i = \overline{1, n}$).

3°). We define M' as follows:

$$M'[i, j] = \begin{cases} M[i, j] & \text{if } i \leq j, \\ M[j, i] & \text{if } i > j. \end{cases} \quad (i, j = \overline{1, n+2}),$$

The matrix M' is the matrix of distances between leaves in the tree T (see Fig. 6), i.e. $M' = M_T$ (see Definition 2).

Now let us come back to the graphs U_1^+ and U_2^+ . Since U^+ was any such graph that M was its matrix of pseudodistances we can step by step apply the above construction to the graphs U_1^+ and U_2^+ .

Let T_1 and T_2 be the trees obtained from the graphs U_1^+ and U_2^+ , respectively. Then $M' = M_{T_1}$ and $M' = M_{T_2}$, and by Corollary 1, $T_1 \cong T_2$.

Now, cut out the paths of length MAX from T_1 and T_2 and add one left edge to each of the resulting graphs. The obtained graphs are isomorphic to U_1 and U_2 , respectively. Since $T_1 \cong T_2$, we are done in the case 1).

Case 2). $M_{U_1^+} \cong (M_{U_2^+})^T$.

Let us notice that transposing of the matrix $M_{U_2^+}$ is equivalent to changing the direction on U_2 . Then the proof from case 1) can be applied. Details are left to the reader. ■

Examples

The following examples show that the assumption about existence of three offshoots in the graphs U_1 and U_2 cannot be weakened.

1°). If U_1 and U_2 have no offshoots at all then they are just cycles so clearly $U_1 \not\cong U_2$ for cycles of different length.

2°). If U_1 and U_2 have the exactly one offshoot each then even if the lengths of the cycles in U_1 and U_2 are equal, the graphs may still not be isomorphic, though $M_{U_1^+} \cong M_{U_2^+}$ (see Fig. 7 and Fig. 8).

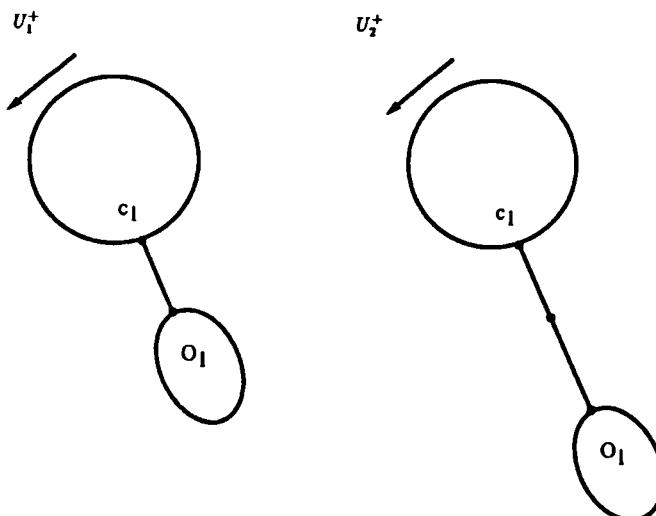


Figure 7.

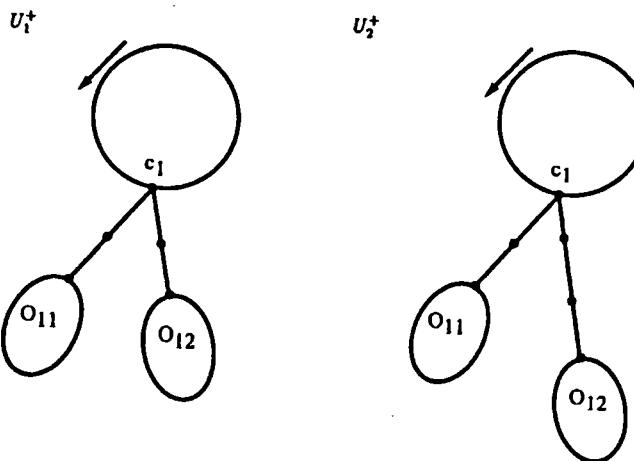
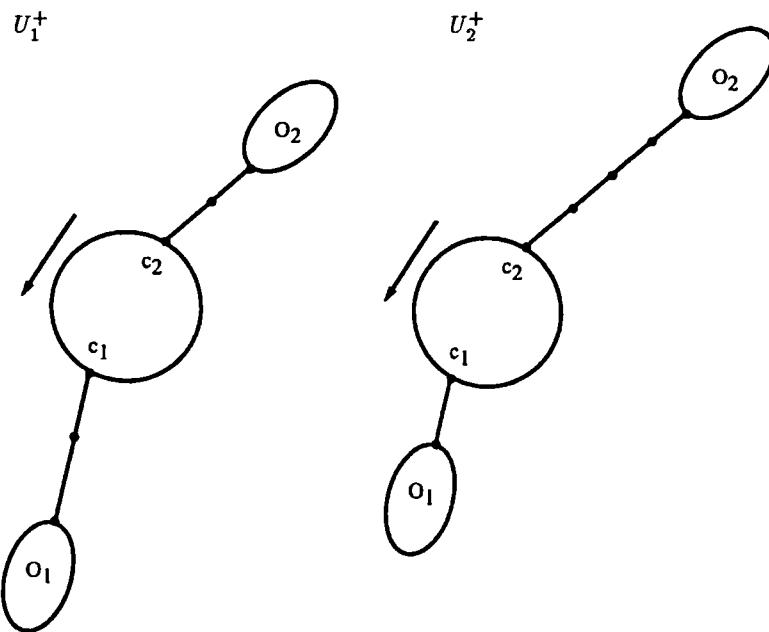


Figure 8.



$$M_{U_1^+} \cong M_{U_2^+}$$

$$\rho_{U_1^+}(c_1, c_2) = \rho_{U_2^+}(c_1, c_2) > 0$$

Figure 9.

3°). Similar example applies for the case of U_1 and U_2 with exactly two offshoots each (see Fig. 9).

4°). Let both U_1 and U_2 have the cycle of length p , where p is the even number. Following the construction of classes F_1, \dots, F_t from the proof of

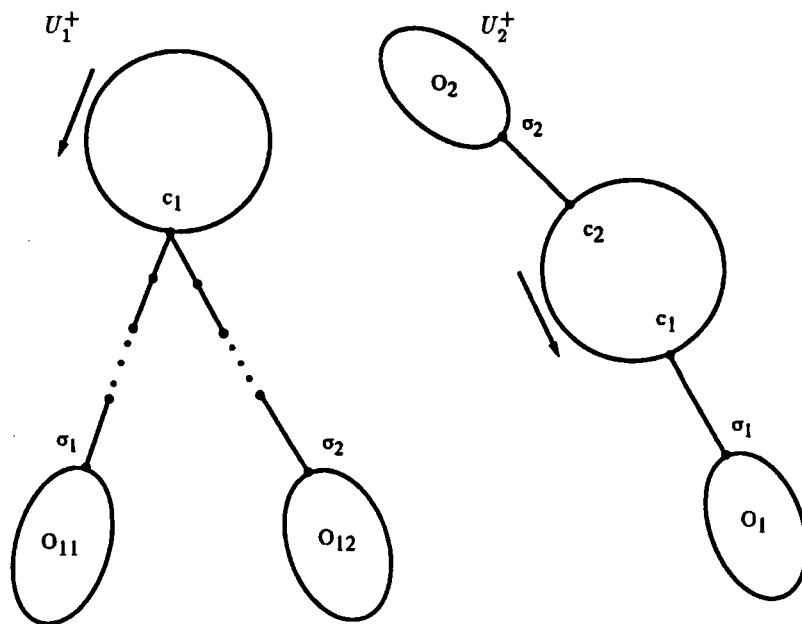


Figure 10.

Theorem we can invent a “mixed” example (see Fig. 10), where $M_{U_1^+} \cong M_{U_2^+}$, whereas U_1 has got one offshoot and U_2 has got two offshoots. Clearly, the above “mixed” example cannot be constructed for graphs with cycles of odd length.

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