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Graph Isomorphism and Theorems of Birkhoff Type

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Dedicated to Professor W. Knödel on the occasion of his 60th birthday

Abstract — Zusammenfassung

Graph Isomorphism and Theorems of Birkhoff Type. Two graphs G and G' having adjacency matrices A and B are called ds-isomorphic iff there is a doubly stochastic matrix X satisfying $XA = BX$. *Ds*-isomorphism is a relaxation of the classical isomorphism relation. In section 2 a complete set of invariants with respect to *ds*-isomorphism is given. In the case where $A = B$ (*ds*-automorphism) the main question is: For which graphs G the polytope of *ds*-automorphisms of G equals the convex hull of the automorphisms of G? In section 3 a positive answer to this question is given for the cases where G is a tree or where G is a cycle. The corresponding theorems are analoga to the well known theorem of Birkhoff on doubly stochastic matrices.

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Isomorphie von Graphen und Theoreme vom Birkhoff-Typ. Zwei Graphen G und G' werden *ds*-isomorph genannt, wenn eine doppelt stochastische Matrix X existiert mit $XA = BX$, wobei A und B die Adjazenzmatrizen von G und G' sind. *Ds*-Isomorphie ist eine Vergröberung der klassischen Isomorphierelation. In Abschnitt 2 wird ein vollständiges Invariantensystem bezüglich *ds*-Isomorphie vorgestellt. Für den Fall $A = B$ (*ds*-Automorphismus) lautet die Hauptfrage: Für welche Graphen G ist das Polytop der *ds*-Automorphismen gleich der konvexen Hülle der klassischen Automorphismen? In Abschnitt 3 wird diese Frage für Kreise und Bäume positiv beantwortet. Die entsprechenden Theoreme sind Analoga zu dem bekannten Satz von Birkhoff über doppelt stochastische Matrizen.

1. Introduction

We consider undirected graphs $G = (V_n, E)$ with vertex set $V_n = \{1, 2, \ldots, n\}$ and edge set E. The adjacency matrix $A = A(G)$ of such a graph is a symmetric square matrix of order n whose entry A_{ij} at the position (i, j) equals 1 or 0 depending on whether the edge $\langle i, j \rangle$ is in E or not.

Let $G_A = (V_n, E_A)$ and $G_B = (V_n, E_B)$ be two graphs having adjacency matrices A and B, respectively. G_A and G_B are called *isomorphic* iff there exists a permutation matrix P of order n such that

$$PA = BP. \tag{1}$$

The isomorphism problem for graphs is the problem of deciding whether two graphs G_A and G_B are isomorphic or not. The relative complexity of this problem is unresolved. No polynomial time algorithm is known, nor is the problem known to be NP-complete. Many generalizations and restrictions of the isomorphism problem are known to be polynomial time equivalent (see e.g. [2]). Among these there are the restrictions of the problem to particular graph classes such as connected undirected graphs, regular graphs, bipartite graphs, chordal graphs, lattices and many others. These problems are called isomorphism complete. Another isomorphism complete problem is the problem of finding the automorphism partition of a graph. The automorphism partition or G_A is the partition of the vertex set V_n induced by the automorphism group $AUT(A)$ of G_A. Two vertices i and j belong to the same class iff there is an automorphism in $AUT(A)$ which sends i to j.

In this paper we consider a relaxation of the condition (1). Let Σ_n be the set of all doubly stochastic matrices X of order n. An equivalence relation on the set of all undirected graphs $G=(V_n, E)$ on n vertices which is weaker than (1) is given by

$$G_A \simeq_{ds} G_B \tag{2}$$

iff there is an $X \in \Sigma_n$ such that

$$XA = BX. \tag{3}$$

In the case of (2) we shall call G_A and G_B *doubly stochastically isomorphic* (*ds*-isomorphic). Any $X \in \Sigma_n$ satisfying (3) will be called a *doubly stochastic isomorphism* (*ds*-isomorphism) of G_A and G_B.

Analogously, for $A=B$, any $X \in \Sigma_n$ satisfying

$$XA = AX \tag{4}$$

is called a *doubly stochastic automorphism* of G_A (*ds*-automorphism).

Using an n-vector e of 1's and an $n \times n$-matrix 0 of 0's the condition (3) reads

$$\begin{aligned} &XA = BX \\ &Xe = X^T e = e \qquad (DSI) \\ &X \geq 0. \end{aligned}$$

(DSI) is equivalent to a linear programming problem in continuous variables x_{ij}, $1 \leq i, j \leq n$. Hence, given G_A and G_B the problem of deciding whether $G_A \simeq_{ds} G_B$ is true or not is polynomial. This follows from the fact that any linear programming problem can be solved in polynomial time using the ellipsoid method (see [7]) or the algorithm of Karmakar [8]. But in section 2 we shall see that there is a much less complicated method solving the "doubly stochastic isomorphism problem" for (undirected) graphs. The restriction on undirected graphs is not an essential loss of generality in this context.

The solution set of (DSI) is a convex subpolytope of the well studied assignment polytope Σ_n (see [1, 3, 4]). This subpolytope is denoted by $P(A, B)$, or simply by $P(A)$, when $A=B$. Let $IS(A, B)$ denote the set of all classical isomorphisms of G_A and

G_B. By $PIS(A,B)$ we shall denote the convex hull of $IS(A,B)$. $PIS(A,B)$ is another (possibly empty) subpolytope of Σ_n satisfying

$$PIS(A,B) \subset P(A,B) \subset \Sigma_n. \tag{5}$$

When $PIS(A,B) = P(A,B)$, then any linear programming algorithm which finds a basic solution (an extreme point of the solution set) of (DSI) would solve the standard isomorphism problem for G_A and G_B. Hence, an interesting question touched in this paper is the question for which pairs of graphs G_A and G_B equality holds at the first inclusion of (5). In section 3 we present first results in this direction.

2. A Complete Set of Invariants

In this section we deal with the general case where G_A and G_B are arbitrary undirected graphs. The relation (2) is an equivalence relation. Hence the most natural question to start with is: What are the invariants with respect to ds-isomorphisms? This question will be answered exhaustively in this section. We start with the presentation of two lemma's which are basic also for section 3.

For a graph G_A let d_A be the vector of its vertex degrees, i.e. $d_A = Ae$.

Lemma 1: *For all pairs of graphs G_A and G_B and all $X \in P(A,B)$: If $X_{ij} > 0$, then $d_{A,i} = d_{B,j}$ (i.e. the degree of i in G_A equals the degree of j in G_B).*

Proof: Without loss of generality we may assume that $d_{A,1} \le d_{A,2} \le \dots \le d_{A,n}$ and $d_{B,1} \le d_{B,2} \le \dots \le d_{B,n}$.

$X \in P(A,B)$ implies

$$d_B = Be = BXe = XAe = Xd_A \tag{8}$$

$$d_A = Ae = A^T X^T e = X^T B^T e = X^T d_B. \tag{9}$$

Due to a theorem of Hardy, Littlewood, Polya (see [9]) this is equivalent to $d_A = d_B$. Assume

$$d_A^T = (\underbrace{d_1, \dots, d_1}_{n_1}, \underbrace{d_2, \dots, d_2}_{n_2}, \dots, \underbrace{d_p, \dots, d_p}_{n_p}) \tag{10}$$

$$\sum_{i=1}^{p} n_i = n.$$

Due to (8), for $1 \le i \le n_1$, we find

$$\sum_{j=1}^{n} X_{ij} d_{A,j} = d_1 \sum_{j=1}^{n_1} X_{ij} + \sum_{j>n_1} X_{ij} d_{A,j} = d_1.$$

This implies $X_{ij} = 0$ for $1 \le i \le n_1$ and $j > n_1$. Analoguously, using (9) we find $X_{ij} = 0$ for $1 \le j \le n_1$ and $i > n_1$. The proof of the lemma is completed by induction on p, the number of different degree values $d_1, d_2, \dots, d_p$.

Lemma 2: *Let*

$$\begin{pmatrix} V^1 & V^2 & \dots & V^k \\ W^1 & W^2 & \dots & W^k \end{pmatrix}$$

be a pair of partitions of V_n, *i.e.*

$$\bigcup_{i=1}^{k} V^i = \bigcup_{i=1}^{k} W^i = V_n, \quad V^i \cap V^j = W^i \cap W^j = \phi \quad \text{for } i \neq j$$

and assume $|V^i| = |W^i|$, $1 \leq i \leq k$.

Define

$$A^{i,j} = (A_{st})_{s \in V^i, t \in V^j} \tag{11a}$$

$$B^{i,j} = (B_{st})_{s \in W^i, t \in W^j} \tag{11b}$$

For $U \subset \{1, 2, \dots, k\}^2$ *let* $A(U)$ *be the matrix deduced from* A *by annulling all blocks* $A^{i,j}$, $(i, j) \in U$. *Let* $B(U)$ *be defined analogously. Then if* $X \in P(A, B)$ *satisfies* $X_{st} = 0$ *for all*

$$(s, t) \notin \bigcup_{i=1}^{k} W^i \times V^i,$$

then $X \in P(A(U), B(U))$ *for all* $U \subset \{1, 2, \dots, k\}^2$ (*i.e.* $X \cdot A(U) = B(U) \cdot X$).

Proof: Under the hypothesis of the lemma we have $XA = BX$ if and only if

$$X^{i,i} A^{i,j} = B^{i,j} X^{j,j}, \quad 1 \leq i, j \leq k \tag{12}$$

where

$$X^{i,i} = (X_{st})_{s \in W^i, t \in V^i}, \quad 1 \leq i \leq k. \tag{11c}$$

The conditions (12) are not violated by annulling corresponding blocks $A^{i,j}$ and $B^{i,j}$. This proves the lemma.

Next we want to associate with a graph G_A a certain code matrix $L(A)$. At the end of this section it will be proved that $L(A)$ represents a complete set of invariants with respect to ds-isomorphisms. $L(A)$ is defined by the following rules:

(1) (Initial step): Start with the degree partition of V_n:

$$V^{i,0} := \{v \in V_n \mid d_{A,v} = d_i\}, \quad 1 \leq i \leq p \tag{13}$$

where the d_i's are defined in (10) and where as before $d_1 < \dots < d_p$ is assumed. Define the $n \times 2$-matrix

$$L^0_{kl} := \begin{cases} i & \text{if } l = 0 \text{ and } k \in V^{i,0} \\ d_i & \text{if } l = 1 \text{ and } k \in V^{i,0}. \end{cases} \tag{14}$$

(2) (Iteration step): Assume that in step j, $j \geq 0$, one has found the partition

$$V^{i,j} \mid 1 \leq i \leq p_j, \quad (p_0 = p) \tag{15}$$

the $n \times (p_{j-1} + 1)$-matrix L^j and a permutation π_j of V_n which assigns a unique row of L^j to each $v \in V_n$. (Let π_0 be the identity and define $p_{-1} := 1$.) For $v \in V_n$ let $N_{ij}(v)$ be the number of neighbours of v which belong to the class $V^{i,j}$, $1 \leq i \leq p_j$. To each $v \in V_n$ assign the list

$$N_j(v) := \left(L^j_{\pi_j(v), 0} \mid N_{1j}(v) | \dots | N_{p_j, j}(v) |\right) \tag{16}$$

and sort the set of lists $\{N_j(v) \mid v \in V_n\}$ lexicographically. Let p_{j+1} be the number of different lists and select vertices $v_1, v_2, \ldots, v_{p_{j+1}} \in V_n$ such that

$$N_j(v_1) \prec N_j(v_2) \prec \ldots \prec N_j(v_{p_{j+1}}).$$

Define the new partition

$$V^{i,j+1} := \{v \in V_n \mid N_j(v) = N_j(v_i)\}, \quad 1 \le i \le p_{j+1}. \tag{17}$$

Let

$$n_{ij} := \sum_{l=1}^{i-1} |V^{l,j+1}|, \qquad 1 \le i \le p_{j+1} \tag{18}$$

and label the vertices of $V^{i,j+1}$ arbitrarily but using the numbers $n_{ij}+1$, $n_{ij}+2, \ldots, n_{i+1,j}$, $1 \le i \le p_{j+1}$. This labelling defines a permutation π_{j+1} of V_n. Now define

$$L_{kl}^{j+1} := \begin{cases} i & \text{if } l=0 \text{ and } N_j(\pi_{j+1}^{-1}(k)) = N_j(v_i) \\ N_{lj}(\pi_{j+1}^{-1}(k)) & \text{otherwise.} \end{cases}$$

Repeat this step as long as $L^{j+1} \neq L^j$. After at most J steps, $0 \le J \le n-1$, we will find $L^J = L^{J+1}$. At this point define

$$\begin{aligned} L(A) &:= L^J, & \pi_A &:= \pi_J, \\ V^i(A) &:= V^{i,J}, & 1 &\le i \le p_J. \end{aligned} \tag{20}$$

The matrix $L(A)$ is uniquely defined. The permutation π_A is not necessarily unique. The partition $(V^i(A) \mid 1 \le i \le p_J)$ is determined by π_A and the blocks of equal rows of $L(A)$. This final partition will be called the *total degree partition* of V_n with respect to G_A. It is a well known tool used in graph isomorphism algorithms in order to reduce drastically the number of permutations which are candidates for an isomorphism of two graphs G_A and G_B (see e.g. [5] or the annotated bibliographies [10], [6]). Furthermore, it is well known that $L(A) = L(B)$ is necessary but not sufficient for the existence of an isomorphism of G_A and G_B.

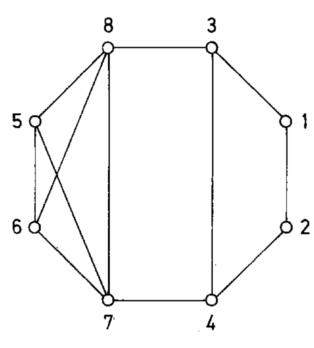

Fig. 1

To have an example consider the graph in Fig. 1. Its vertices are labeled according to non-decreasing degree values. We have

$$V^{1,0}=\{1,2\},\quad V^{2,0}=\{3,4,5,6\},\quad V^{3,0}=\{7,8\}$$

$$L^0=\begin{pmatrix}1&1&2&2&2&2&3&3\\2&2&3&3&3&3&4&4\end{pmatrix}^T.$$

Hence

$$\begin{aligned}
N_0(1)&=(1,\ 1,\ 1,\ 0)\\
N_0(2)&=(1,\ 1,\ 1,\ 0)\\
N_0(3)&=(2,\ 1,\ 1,\ 1)\\
N_0(4)&=(2,\ 1,\ 1,\ 1)\\
N_0(5)&=(2,\ 0,\ 1,\ 2)\\
N_0(6)&=(2,\ 0,\ 1,\ 2)\\
N_0(7)&=(3,\ 0,\ 3,\ 1)\\
N_0(8)&=(3,\ 0,\ 3,\ 1).
\end{aligned}$$

$$\begin{aligned}
&p_1=4\\
&N_0(1)\prec N_0(5)\prec N_0(3)\prec N_0(7)\\
&\pi_1(1)=1,\ \pi_1(2)=2,\ \pi_1(3)=5,\ \pi_1(4)=6,\\
&\pi_1(5)=3,\ \pi_1(6)=4,\ \pi_1(7)=7,\ \pi_1(8)=8.
\end{aligned}$$

This gives

$$L^1=\begin{pmatrix}1&1&1&0\\1&1&1&0\\2&0&1&2\\2&0&1&2\\3&1&1&1\\3&1&1&1\\4&0&3&1\\4&0&3&1\end{pmatrix}\qquad \begin{aligned}V^{1,1}&=\{1,2\}\\ V^{2,1}&=\{5,6\}\\ V^{3,1}&=\{3,4\}\\ V^{4,1}&=\{7,8\}\end{aligned}$$

In step 2 we find

$$\begin{aligned}
N_1(1)&=(1,\ 1,\ 0,\ 1,\ 0) & N_1(5)&=(2,\ 0,\ 1,\ 0,\ 2)\\
N_1(2)&=(1,\ 1,\ 0,\ 1,\ 0) & N_1(6)&=(2,\ 0,\ 1,\ 0,\ 2)\\
N_1(3)&=(3,\ 1,\ 0,\ 1,\ 1) & N_1(7)&=(4,\ 0,\ 2,\ 1,\ 1)\\
N_1(4)&=(3,\ 1,\ 0,\ 1,\ 1) & N_1(8)&=(4,\ 0,\ 2,\ 1,\ 1)
\end{aligned}$$

Again

$$\begin{aligned}
&p_2=4\\
&N_1(1)\prec N_1(5)\prec N_1(3)\prec N_1(7),\\
&\pi_2(v)=\pi_1(v),\qquad 1\le v\le 8.
\end{aligned}$$

This gives

$$L^2 = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 2 & 0 & 1 & 0 & 2 \\ 2 & 0 & 1 & 0 & 2 \\ 3 & 1 & 0 & 1 & 1 \\ 3 & 1 & 0 & 1 & 1 \\ 4 & 0 & 2 & 1 & 1 \\ 4 & 0 & 2 & 1 & 1 \end{pmatrix} \qquad \begin{aligned} V^{1,2} &= \{1,2\} \\ V^{2,2} &= \{5,6\} \\ V^{3,2} &= \{3,4\} \\ V^{4,2} &= \{7,8\}. \end{aligned}$$

Since in this step the partition $V^{i,1}$, $1 \leq i \leq 4$ is not refined, in step 3 we would find $L^3 = L^2$. Thus $\{1,2\}$, $\{5,6\}$, $\{3,4\}$, $\{7,8\}$ is the (ordered) total degree partition, and $L(A) = L^2$.

The following theorem shows that $L(A)$ completely characterizes the *ds*-isomorphism class of G_A.

Theorem 1: *Two graphs G_A and G_B are ds-isomorphic iff $L(A) = L(B)$.*

Proof: The proof of the sufficiency part is constructive. Given $L(A) = L(B)$ we will find a "trivial" *ds*-isomorphism. The proof of the necessity part is based on the lemma's above.

First, assume $P(A,B) \neq \emptyset$. Let

$$\begin{aligned} &L^j(A), \quad 0 \leq j \leq J_A \\ &L^j(B), \quad 0 \leq j \leq J_B \end{aligned}$$

be the sequences of matrices L^j leading to $L(A)$ and $L(B)$, respectively. Let

$$\begin{aligned} &V^{i,j}(A), \quad 1 \leq i \leq p_j(A) \\ &V^{i,j}(B), \quad 1 \leq i \leq p_j(B) \end{aligned}$$

be the corresponding partitions found in step j. We will show $J_A = J_B$ and $L^j(A) = L^j(B)$ for $0 \leq j \leq J_A$. The proof is by induction on j.

Due to Lemma 1 we have $L^0(A) = L^0(B)$ and $X_{st} = 0$ for all $X \in P(A,B)$ and all

$$(s,t) \notin \bigcup_{i=1}^{p_0} V^{i,0}(B) \times V^{i,0}(A).$$

Assume $L^j(A) = L^j(B)$ for some $j \geq 0$. Let

$$V^i := V^{i,j}(A), \qquad W^i := V^{i,j}(B), \qquad 1 \leq i \leq p_j$$

and assume $X_{st} = 0$ for all $X \in P(A,B)$ and all

$$(s,t) \notin \bigcup_{i=1}^{p_j} W^i \times V^i.$$

$L^j(A)=L^j(B)$ implies $|V^i|=|W^i|$, $1\le i\le p_j$. Hence, the pair of partitions (V^i), (W^i) satisfies the hypothesis of Lemma 2. For $1\le k, l\le p_j$ define

$$U_{kl}:=\{1,2,\ldots,p_j\}^2-\{(k,l),(l,k)\}.$$

Due to Lemma 2 we have

$$X\in P(A,B)\Rightarrow X\in P\big(A(U_{kl}),B(U_{kl})\big),\qquad 1\le k,l\le p_j. \tag{21}$$

Now, in step $j+1$, for $v\in V^k$ the numbers $N_{lj}(v)$ equal the degrees of v with respect to $G_{A(U_{kl})}$, $1\le l\le p_j$. The same is true for $u\in W^k$, the numbers $N_{lj}(u)$ and the degrees of u in $G_{B(U_{kl})}$, $1\le l\le p_j$. Hence, if $X_{uv}>0$, then $(u,v)\in W^k\times V^k$ for some k (by assumption) and, by (21) and Lemma 1, the lists

$$\big(N_{lj}(u)\big),\ \big(N_{lj}(v)\big),\qquad 1\le l\le p_j$$

are identical. The matrix $X^{k,k}$ as defined in (11 c) is a doubly stochastic square matrix (apart from the different index sets of its rows and columns). Hence, by the well known theorem of Birkhoff (see e.g. [9]) $X^{k,k}$ is a convex sum of permutation matrices. Each permutation matrix used in a representation of $X^{k,k}$ defines a bijection B: $W^k\to V^k$ satisfying

$$B(u)=v\Rightarrow X_{uv}>0.$$

But $X_{uv}>0$ implies $N_j(u)=N_j(v)$ where $N_j(u)$ is used in the computation of $L^{j+1}(B)$ whereas $N_j(v)$ is used in the computation of $L^{j+1}(A)$. This proves that $L^{j+1}(B)$ and $L^{j+1}(A)$ have the same multiset of rows. Thus $L^{j+1}(A)=L^{j+1}(B)$ and by Lemma 1 $X_{st}=0$ for all $X\in P(A,B)$ and all

$$(s,t)\notin\bigcup_{i=1}^{p_{j+1}} V^{i,j+1}(B)\times V^{i,j+1}(A).$$

Hence, we see that $P(A,B)\neq\emptyset$ implies $J_A=J_B$ and $L(A)=L(B)$.

Now, assume $L(A)=L(B)=L$ for some matrix L. Let $p\ (=L_{n,0})$ be the number of different rows of L. Define

$$V^i:=V^i(A),\qquad W^i:=V^i(B),\qquad 1\le i\le p,$$

$$\lambda:=\pi_A,\qquad \mu:=\pi_B.$$

We have $|V^i|=|W^i|$, $1\le i\le p$. Associated with these two total degree partitions there are block decompositions

$$A^{i,j},\ B^{i,j},\qquad 1\le i,j\le p$$

as defined by (11 a), (11 b) in Lemma 2. Since $L=L(A)$ is not changed by applying an additional iteration step (2), for any fixed pair (i,j) the column sums

$$\sum_{s\in V^i} A_{st}^{i,j}=L_{\lambda(t),i},\qquad t\in V^j$$

are independent of $t\in V^j$. Analogously, the row sums

$$\sum_{t\in V^j} A_{st}^{i,j}=L_{\lambda(s),j},\qquad s\in V^i$$

are independent of $s \in V^i$. Hence, the blocks $A^{i,j}$ have constant row sums and constant column sums. By the same argument the numbers

$$L_{\mu(t),i} = \sum_{s \in W^i} B^{i,j}_{st}, \qquad t \in W^j$$

$$L_{\mu(s),j} = \sum_{t \in W^j} B^{i,j}_{st}, \qquad s \in W^i$$

are independent of $t \in W^j$ and $s \in W^i$. Furthermore, summing up all entries of $A^{i,j}$ gives for any $(s,t) \in V^i \times V^j$:

$$|V^j|\, L_{\lambda(t),i} = |V^i|\, L_{\lambda(s),j}. \tag{22a}$$

Analogously, for any $(s,t) \in W^i \times W^j$:

$$|W^j|\, L_{\mu(t),i} = |W^i|\, L_{\mu(s),j}. \tag{22b}$$

Now, define

$$E(A,B)_{st} := \begin{cases} |V^i|^{-1} & \text{if } (s,t) \in W^i \times V^i \text{ for some } i \\ 0 & \text{otherwise.} \end{cases} \tag{23}$$

Let $E^{i,i}$, $1 \le i \le p$, be the blocks of $E(A,B)$ as defined in (11c). We find for $(s,t) \in W^i \times V^j$:

$$(E^{i,i} A^{i,j})_{st} = |V^i|^{-1} L_{\lambda(t),i},$$
$$(B^{i,j} E^{j,j})_{st} = |V^j|^{-1} L_{\mu(s),j} = |W^i|^{-1} L_{\mu(u),i}$$

where $u \in W^j$ is arbitrary. But $L_{\lambda(t),i} = L_{\mu(u),i}$ for all $t \in V^j$, $u \in W^j$. This implies

$$E^{i,i} A^{i,j} = B^{i,j} E^{j,j}, \qquad 1 \le i,j \le p.$$

Hence, $E(A,B) \in P(A,B)$.

This proves the theorem. □

Let us say that a matrix Y *covers* a matrix X if there is a real number $t > 0$ such that $t \cdot X \le Y$. The proof of Theorem 1 shows that $E(A,B)$ covers any $X \in P(A,B)$. We also see that deciding whether $G_A \simeq_{ds} G_B$ or not is equivalent to deciding whether $L(A) = L(B)$. The latter problem is, of course, polynomial.

It is a well known fact in graph theory that for almost all graphs the total degree partition is of the form $(\{v_i\} \mid 1 \le i \le n)$, i.e. each partition class contains exactly one vertex. This implies that the automorphism group of almost all graphs is trivial. In all these cases $L(A)$ has no equal rows and $L(A) = L(B)$ implies $P(A,B) = PIS(A,B) = \{P\}$ where the permutation matrix P represents the unique isomorphism of G_A and G_B which is related to π_A and π_B by $P_{ij} = 1$ iff $\pi_A(i) = \pi_B(j)$, $1 \le i,j \le n$.

Theorem 1 provides us with a simple polynomial algorithm for deciding whether G_A and G_B are ds-isomorphic or not. But if the answer is "Yes", then the computed ds-isomorphism $E(A,B)$ in (23) is a "trivial" one (having constant positive entries only). This is in general not an extreme point of $P(A,B)$. To see this assume $A = B$ and let G_A be a regular graph of degree r. For such a graph $L(A) = L^0(A)$ and V_n is not partitioned at all. Furthermore,

$$E(A,A) = n^{-1} \cdot E$$

where E is the matrix of order n all of whose entries are equal to 1. $n^{-1} \cdot E$ is the center of Σ_n and, hence, is an interior point of Σ_n while any extreme point of $P(A)$ lies on the boundary of Σ_n.

3. Theorems of Birkhoff Type

In this section we restrict our considerations to the (technically) more simple case where $A=B$. We want to find a characterization of the subpolytope $P(A)$ of Σ_n, the polytope of all doubly stochastic matrices which commute with A. Of course, this polytope is completely determined by the set $EXTR(P(A))$ of its extremal points. Clearly, we have

$$AUT(A) \subseteq EXTR(P(A)) \tag{24}$$

Now the question is, for which graphs G_A equality holds in (24). Assume that $\mathfrak{A}$ is a class of adjacency matrices for all of which (24) is true with equality. This fact could be formulated in the following way:

For all $A \in \mathfrak{A}$ and all $X \in \Sigma_n$: If X commutes with A, then X is a convex sum of automorphisms of G_A. (25)

We propose to call a theorem of this kind a *theorem of Birkhoff type* because of the following reason. Birkhoffs theorem on doubly stochastic matrices states that any such matrix is a convex sum of permutation matrices. Since the unit matrix I commutes with any matrix of the same order and since any permutation matrix represents an automorphism of G_I Birkhoffs theorem could be stated in the following (more complicated) way:

If $X \in \Sigma_n$ commutes with I, then X is a convex sum of automorphisms of G_I. (25a)

Hence (25) is an analogous statement involving a class of matrices instead of the single element class $\{I\}$.

In this section we shall prove two theorems of Birkhoff type, one for the class $\mathfrak{C}$ of cycles and one for the class $\mathfrak{T}$ of trees. The theorems represent first research results concerning Birkhoff type theorems. One may hope to find more important classes for which (25) is provable.

Theorem 2: *Let A be the adjacency matrix of a cycle. Then any $X \in P(A)$ is a convex sum of automorphisms of G_A.*

Theorem 3: *Let A be the adjacency matrix of a tree. Then any $X \in P(A)$ is a convex sum of automorphisms of G_A.*

Proof of Theorem 2: Without loss of generality we may assume that

$$A_{ij} = \begin{cases} 1 & \text{if } j = i+1 \pmod{n} \text{ or } j = i-1 \pmod{n} \\ 0 & \text{otherwise.} \end{cases}$$

Hence, if we take all indices i and j mod (n), from

$$(XA)_{ij}=(AX)_{ij}$$

it follows

$$X_{i+1,j}+X_{i-1,j}=X_{i,j-1}+X_{i,j+1}$$
$$1\leq i,j\leq n.$$

This implies

$$X_{i+1,j-i}-X_{i,j-i-1}=X_{1,j}-X_{n,j-1} \tag{26}$$
$$X_{i+1,j+i}-X_{i,j+i+1}=X_{1,j}-X_{n,j+1} \tag{27}$$
$$1\leq i,j\leq n.$$

For fixed j the expressions of the right sides of (26) and (27) are constants. Suppose $X\in P(A)$ is such that

$$X_{1,j}-X_{n,j-1}>0.$$

This implies

$$X_{i+1,j-i}>X_{i,j-i-1}\geq 0 \text{ for } 1\leq i\leq n.$$

Hence, X covers the reflection

$$P_{ik}=\begin{cases}1 & \text{for } k=j+1-i \pmod n\\ 0 & \text{otherwise}\end{cases}$$

P is a reflection at the axis through the points $\frac{j+1}{2}$ and $\frac{n+j+1}{2}$ (see Fig. 2). An analoguous result follows when $X_{1,j}-X_{n,j-1}<0$ $\left(\text{reflection at the axis through the points } \frac{j-1}{2} \text{ and } \frac{n+j-1}{2}\right)$.

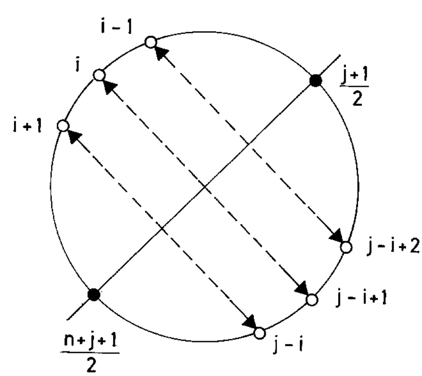

Fig. 2

Now suppose that $X_{1,j}-X_{n,j+1}>0$. This implies

$$X_{i+1,j+i}>X_{i,j+i+1}\geq 0.$$

Hence X covers the rotation (see Fig. 3)

$$P_{ik}=\begin{cases}1 & \text{if } k=j-1+i \pmod n\\ 0 & \text{otherwise.}\end{cases}$$

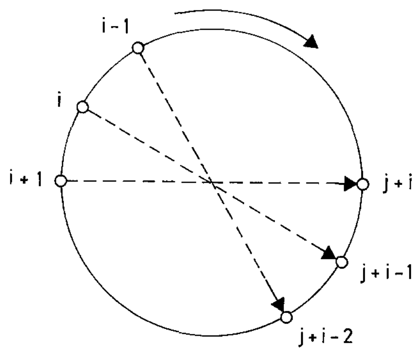

Fig. 3

Again, we find an analoguous result when $X_{1,j}-X_{n,j+1}<0$.

Now in any of the four cases let

$$\lambda=\operatorname{Min}\{X_{ik}\mid P_{ik}=1\}.$$

If $\lambda<1$ define

$$Y=\frac{X-\lambda\cdot P}{(1-\lambda)}.$$

Clearly, $Y\in P(A)$, but the number of non-zero entries of Y is strictly less than the number of such entries in X.

Finally, suppose that for some $X\in P(A)$

$$X_{1,j}=X_{n,j-1}=X_{n,j+1} \quad \text{for } 1\leq j\leq n.$$

In this case

$$X_{i+1,j}=X_{i,j+1}=X_{i-1,j}=X_{i,j-1}$$

for all $1\leq i,j\leq n$. Hence, $X=U+V$ where

$$U_{ij}=\begin{cases}\alpha & \text{for } i-j=0 \pmod 2\\ 0 & \text{otherwise}\end{cases}$$

$$V_{ij}=\begin{cases}\beta & \text{for } i-j=1 \pmod 2\\ 0 & \text{otherwise.}\end{cases}$$

If $\alpha>0$ then U covers a sum of reflections, and so does V, if $\beta>0$. In any case we can proceed like in the previous cases, i.e. we can decompose X into a convex sum

$$X=(1-\lambda)\,Y+\lambda P$$

where P is an automorphism of G_A and $Y\in P(A)$ having at least one less positive entry than X. If $\alpha=\beta=0$, then $X=0$.

Now the theorem follows by induction on the number of positive entries of X. □

The theorem cannot be extended to a disjoint union of cycles. A disjoint union of two cycles of length 3 and 4, respectively, possesses the "trivial" ds-automorphism (23) which, of course, is not a convex sum of automorphisms.

To prove Theorem 3 we first present some lemma's.

For a tree $T=(V_n, E)$ let C be the center of T and define

$$V^{(s)}=\{i\in V_n \mid d(i,C)=s\}, \qquad 1\leq s\leq\delta$$

where $d(i,C)$ is the edge-distance of i from the center C and δ is the excentricity of T, i.e. $\delta=\mathrm{Max}\,\{d(i,C)\mid i\in V_n\}$. Considering T as rooted at its center the sets $V^{(s)}$ are usually called the levels of T. The following lemma tells us that the levels of a tree are invariant under ds-automorphisms.

Lemma 3: *Let A be the adjacency matrix of a tree T.* Then for any $X\in P(A)$

$$X_{ij}>0\Rightarrow\{i,j\}\subset V^{(s)} \text{ for some } s,\ 0\leq s\leq\delta.$$

Proof: Let

$$D_{A,ij}=\begin{cases} d_{A,i} & \text{for } i=j\\ 0 & \text{for } i\neq j.\end{cases}$$

Clearly, $XD_A=D_AX$ for any $X\in P(A)$. Define

$$D^{(t)}_{ij}=\begin{cases} 1 & \text{if the unique path between } i \text{ and } j \text{ has length } t\\ 0 & \text{otherwise.}\end{cases}$$

We have

$$D^{(1)}=A,\quad D^{(2)}=A^2-D_A.$$

Thus $X\in P(A)$ implies

$$XD^{(t)}=D^{(t)}X,\quad t=1,2.$$

Assume $XD^{(t)}=D^{(t)}X$ for all $X\in P(A)$, $1\leq t\leq k$ and some $k\geq 2$. We have

$$D^{(k)}A=D^{(k+1)}+L^{(k)},$$

where

$$L^{(k)}_{ij}=(d_{A,j}-1)\,D^{(k-1)}_{ij}.$$

Due to Lemma 1 we find $XL^{(k)}=L^{(k)}X$ for $X\in P(A)$. Hence, $D^{(k+1)}X=XD^{(k+1)}$, and we have proved that $X\in P(A)$ implies $X\in P(D^{(t)})$ for all $t\geq 1$. Now, let $D=D^{(\delta+1)}$. We have

$$d_{D,i}=\begin{cases} 0 & \text{if } i\in C\\ >0 & \text{if } i\notin C\end{cases}$$

by definition of C. This proves

$$X_{ij}=0 \text{ for } i\in C=V^{(0)},\ j\in V^{(s)},\ s>0.$$

Assume that $X_{ij}=0$ is true for $X\in P(A)$ and

$$i\in U=\bigcup_{s=0}^{k} V^{(s)},\quad j\in W=\bigcup_{s=k+1}^{\delta} V^{(s)} \tag{28}$$

and some $k \geq 0$. Then X is of the form

$$X = \begin{pmatrix} X_U & 0 \\ 0 & X_W \end{pmatrix}$$

and according to Lemma 2 $X_{ij}=0$ for all $i \in V^{(k+1)}$, $j \in V^{(s)}$, $s>k+1$, since i has exactly one neighbour in U whereas j has no neighbour in U. Thus, $X_{ij}=0$ for all i and j satisfying (28) for some k, $0 \leq k < \delta$. This proves the Lemma.

Lemma 4: *Let A be the adjacency matrix of a tree T. For $i \in V^{(s)}$, $s \geq 1$, let $v(i)$ be the unique neighbour of i which belongs to $V^{(s-1)}$). Let $N(i)$ be the set of neighbours of i which belong to $V^{(s+1)}$, $0 \leq s \leq \delta$. For any $X \in P(A)$ the following statements are true:*

(*a*) *For $0 \leq s < \delta$ and all $i, j \in V^{(s)}$ we have*

$$X_{ij} = \begin{matrix} \sum_{l \in N(i)} X_{lk} \text{ for any } k \in N(j) \\ \sum_{k \in N(j)} X_{lk} \text{ for any } l \in N(i). \end{matrix}$$

(*b*) *If $X_{ij}=0$, then $X_{lk}=0$ for all $l \in N(i)$, $k \in N(j)$.*

(*c*) *If $X_{ij}>0$, then $X_{v(i),v(j)}>0$ (provided $s>0$).*

(*d*) *If $X_{uv}>0$ for some $u \in N(i)$, $v \in N(j)$, then there is a bijection $B: N(i) \to N(j)$ with*

$$B(u) = v$$
$$B(l) = k \Rightarrow X_{lk} > 0, \text{ for all } l \in N(i), k \in N(j).$$

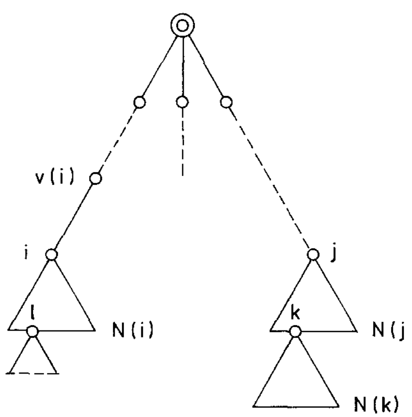

Fig. 4

Proof: (a) $(XA)_{ik} = (AX)_{ik}$, $k \in N(j)$, implies

$$X_{i,v(k)} + \sum_{l \in N(k)} X_{il} = X_{v(i),k} + \sum_{l \in N(i)} X_{lk}.$$

Hence, due to Lemma 3, since $j = v(k)$ (see Fig. 4) we find

$$X_{ij} = \sum_{l \in N(i)} X_{lk}.$$

Analogously, $(XA)_{lj}=(AX)_{lj}$, $l\in N(i)$, implies

$$X_{ij}=\sum_{k\in N(j)} X_{lk}.$$

This proves (a). (b) and (c) are immediate consequences of (a).

In order to prove (d) assume $X_{uv}>0$ for some $u\in N(i)$, $v\in N(j)$. By (c) this implies $X_{ij}>0$, and by Lemma 1, $|N(i)|=|N(j)|$. Thus

$$Y_{lk}=X_{ij}^{-1}\cdot X_{lk}, \qquad l\in N(i),\ k\in N(j)$$

is a doubly stochastic matrix which by Birkhoffs theorem is a convex sum of a set of permutation matrices $P^{(r)}$, $r=1,2,\ldots$. Each $P^{(r)}$ is covered by Y and defines a bijection between $N(i)$ and $N(j)$. Since $X_{uv}>0$ there must be an r such that $P^{(r)}_{uv}=1$. This proves (d).

Proof of Theorem 3: Start with a pair (i,j) such that

$$X_{ij}=\mathrm{Min}\,\{X_{uv}\,|\,X_{uv}>0\}.$$

W.l.o.g. we may assume $X_{ij}<1$. Assume $i,j\in V^{(t)}$ and let

$$W_i=\langle i_t=i,\, i_{t-1},\ldots,i_0\rangle$$
$$W_j=\langle j_t=j,\, j_{t-1},\ldots,j_0\rangle$$

be the unique paths from i and j to the center C of T. Since $X_{ij}>0$, by Lemma 4c we have $X_{i_\alpha j_\alpha}>0$ for $0\le\alpha\le t$. For $w\ge 0$ let

$$U^{(w)}=\bigcup_{s=0}^{w} V^{(s)}.$$

By Lemma 4d there is a bijection $B: N(i_0)\to N(j_0)$ with $B(i_1)=j_1$. Let us extend B to a permutation B^1 of $U^{(1)}$ defining

$$B^1(i_0)=j_0$$
$$B^1(u)=B(u) \text{ for all } u\in N(i_0).$$

Now assume that B^w is a permutation of $U^{(w)}$, $w\ge 1$, satisfying

(a) $B^w(i_\alpha)=j_\alpha$, $0\le\alpha\le\mathrm{Min}\,\{t,w\}$.

(b) $B^w(k)=l \Rightarrow B^w(N(k))=N(l)$ for $k,l\in U^{(w)}-V^{(w)}$.

(c) $B^w(k)=l \Rightarrow X_{kl}>0$ for $k,l\in U^{(w)}$.

We will show how one can extend B^w to a permutation B^{w+1} of $U^{(w+1)}$ preserving the conditions (a)–(c). Let $V^{(w)}=\{r_1,r_2,\ldots,r_\mu\}$. Let $B^w(r_\beta)=s_\beta$, $1\le\beta\le\mu$. If $r_\beta=i_\alpha$ for some β and some $\alpha<t$, then $s_\beta=j_\alpha$, by assumption, and due to Lemma 4d there is a bijection $B_\beta: N(i_\alpha)\to N(j_\alpha)$ satisfying $B_\beta(i_{\alpha+1})=j_{\alpha+1}$. If $r_\beta\notin\{i_0,i_1,\ldots,i_{t-1}\}$, then again by Lemma 4d there is a bijection $B_\beta: N(r_\beta)\to N(s_\beta)$. In both cases $B_\beta(k)=l$ implies $X_{kl}>0$. Thus define

$$B^{w+1}(r)=\begin{cases} B^w(r) & \text{if } r\in U^{(w)}\\ B_\beta(r) & \text{if } r\in N(r_\beta), \quad 1\le\beta\le\mu.\end{cases}$$

B^{w+1} is a permutation of U^{w+1} satisfying (a)–(c). By construction, B^{δ} is an automorphism of the tree T. Hence, any $X \in P(A)$ covers a permutation matrix P which represent an automorphism of T. The proof of the Theorem is completed by induction on the number of positive entries in X.

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