A representation of chemical transformations by labeled graphs

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Dedicated to Professor Frank Harary on the occasion of his 70th birthday

A transitional labeling of a graph G is an assignment of one of the elements of the set $\{1, -1, 0\}$ to each vertex and edge of G so that each edge labeled 0 is incident only with vertices labeled 0, and no edge labeled 1 (respectively, -1) is incident with a vertex labeled -1 (respectively, 1). Chemical transformations can be represented by graphs possessing a transitional labeling. The positive (negative) graph of a transitional labeling t of a graph G is the subgraph of G consisting of the nonnegative (nonpositive) elements of G. The linking graph of t is the subgraph consisting of the zero elements of G. A maximum common subgraph of two given graphs G_1 and G_2 is a graph F isomorphic to a common subgraph of G_1 and G_2 such that the sum of the number of vertices and number of edges of F is maximum. A transitional labeling t of a graph G is a transform if there exists an extension t' of t to a supergraph G' of G such that the linking graph of t' is a maximum common subgraph of the positive and negative graphs of t'. Transforms are used to model chemical reaction pathways. Transforms and related concepts are studied in this paper. A characterization of transforms is also given.

1. Introduction

Graph-theoretic models of transformation pathways were introduced in ref. [1], and chemical examples of these models were developed in ref. [2]. It is the goal of this paper to develop these models from another, purely graph-theoretic point of view and to present some theoretical results which are inherited by all chemical interpretations of these general models.

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These formal models require a rigorously defined concept of a transformation that distinguishes those structural features that are changed in the transformation from those that are not. Here, this concept is called a transitional labeling. The type of transitional labeling in which we will be most interested is the transform. A major goal is to present a characterization of transforms, which we will do in section 5. A concept that is comparable to the transitional labeling can be found in Kvasnička and Pospíchal's graph-theoretic formulation of the Dugundji–Ugi theory of organic reactions (ref. [3] and references cited therein). Whereas our definition associates the labels $-1, 0, 1$ with the vertices and the edges of a graph, theirs associates the labels $0, \pm 1, \pm 2, \ldots$ with solely the edges of a graph. Because of their interest in stoichiometric reactions, they require that the edge labels sum to zero. We currently place no stoichiometric constraints on our labels. As a consequence, our formalism extends to non-stoichiometric representations of reactions as are found in metabolic studies, as well as to representations of structural transformations in which the edges of a graph need not correspond to chemical bonds.

2. Transitional labelings of graphs

A *labeling* of a graph G is an assignment of an element of a given set to each vertex and edge of G. A labeling t of G with elements of the set $\{1, -1, 0\}$ is called a *transitional labeling* if

(1) each edge labeled 0 is incident only with vertices labeled 0,

(2) no edge labeled 1 is incident with a vertex labeled -1, and

(3) no edge labeled -1 is incident with a vertex labeled 1.

An edge or vertex is called *positive*, *negative*, or *zero*, according to whether it is labeled $1, -1$, or 0, respectively. The subgraph P of G consisting of the positive and zero elements of G is called the *positive graph* of t, while the subgraph N consisting of the negative and zero elements is the *negative graph* of t. The subgraph L of G consisting of its zero elements is called the *linking graph* of t. Not all of these subgraphs may exist for a transitional labeling of a graph. Figure 1 shows a transitional labeling of a graph H, together with its positive, negative, and linking graphs. The positive edges of a graph are represented by solid lines, the negative edges by dashed lines, and the zero edges by dotted lines. For graph theory terminology not defined here, we follow Chartrand and Lesniak [4].

For a connected graph G and a transitional labeling t of G, a vertex v of G is called a *pole* (with respect to t) is v is not labeled 0. If v is labeled 1, it is a *positive pole*, while if v is labeled -1, it is a *negative pole*. For example, the vertex g of the graph H of fig. 1 is a positive pole, and d is a negative pole.

If G has both positive and negative poles, then t is a *polarization*; otherwise, t is a *quasipolarization*. The transitional labeling t of the graph H of fig. 1 is therefore a polarization. Since a positive pole cannot be adjacent to a negative pole, every transitional labeling of a nontrivial complete graph is a quasipolarization.

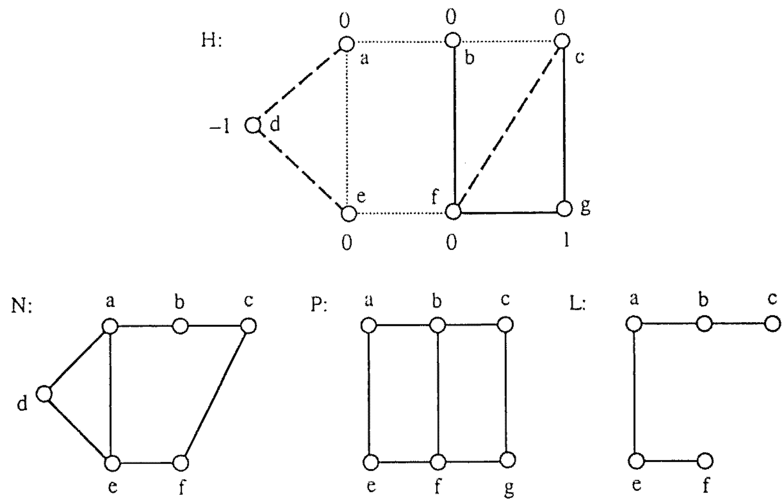

Fig. 1. A transitional labeling of a graph H and its resulting positive, negative, and linking graphs.

Transitional labelings were introduced by Johnson [1] for the purpose of representing chemical transformations. For example, common salt (NaCl) may be formed by reacting metallic sodium directly with hydrochloric acid. This reaction has the chemical equation

$$2\mathrm{Na} + 2\mathrm{HCl} \rightarrow 2\mathrm{NaCl} + \mathrm{H}_2. \tag{1}$$

The (labeled) chemical graph N that represents the two sodium atoms and two molecules of hydrochloric acid is shown in fig. 2, as is the chemical graph P that represents two molecules of sodium chloride and one molecule of H_2. We may think of N as representing chemical compounds prior to the transformation (1), and P the resulting compounds following this transformation.

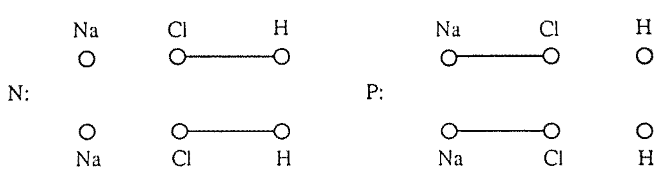

Fig. 2. A graphical representation of the compounds in the chemical transformation (1).

The chemical transformations given by (1) may be interpreted as a process of deletion and addition of certain vertices and edges in the graph N to produce the graph P. Consider the common supergraph G of N and P shown in fig. 3. We now label the vertices and edges

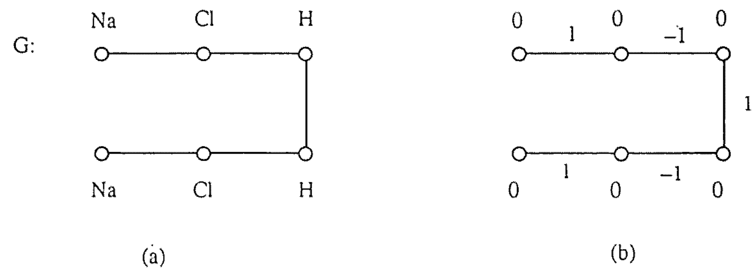

Fig. 3. A graphical representation of the chemical transformation (1).

(i) of G that are common elements of N and P by 0,
(ii) of N that are deleted from N to produce P by -1, and
(iii) of P that are added to N to produce P by 1.

The labeled graph G so obtained is a graph-theoretic representation of the chemical transformation given by (1), which is also shown in fig. 3.

As a second exmple, the hydrocarbon ethylene C_2H_4 is a product of the breakdown of larger hydrocarbon molecules during petroleum refining. For example, ethylene and water react under suitable chemical conditions, producing (diethyl)ether ($C_2H_5OC_2H_5$). This reaction can be represented by the chemical equation

$$2C_2H_4 + H_2O \rightarrow C_2H_5OC_2H_5. \qquad (2)$$

Depending on the amount of water that reacts with the ethylene, ethanol (C_2H_5OH) may be formed, rather than ether. The reaction with water can take place in two stages, namely, (2) and

$$C_2H_5OC_2H_5 + H_2O \rightarrow 2C_2H_5OH. \qquad (3)$$

These two consecutive chemical transformations can be represented by a "transformation digraph" in which the vertices represent chemical compounds and the arcs represent chemical transformations involving these compounds. The first transformation digraphs were proposed by Balaban et al. [5] in 1966. For example, if $C_1 \rightarrow C_2$ and $C_2 \rightarrow C_3$ symbolize the chemical equations (2) and (3), then the transformation digraph of fig. 4 represents the chemical process that takes place when ethylene and water

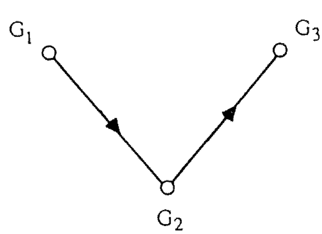

Fig. 4. A chemical transformation digraph.

react to produce ethanol. In fig. 4, G_1, G_2, and G_3 represent the chemical graphs of the compounds C_1, C_2, and C_3, respectively. Systems of chemical compounds and transformations such as the one described by (2) and (3) are called *chemical reaction pathways*. To simplify the modeling of chemical reaction pathways, we may assume that chemical compounds are represented by unlabeled graphs. Thus, the vertices of the corresponding transformation digraph can be labeled by unlabeled graphs.

We return to the chemical transformation described by (2). Figure 5 shows a (labeled) chemical graph N that represents two molecules of ethylene and one molecule of water, and the chemical graph P that represents one molecule of ether. Although the bonds between carbon atoms are different in ethylene and ether, we represent them in the same way for simplification.

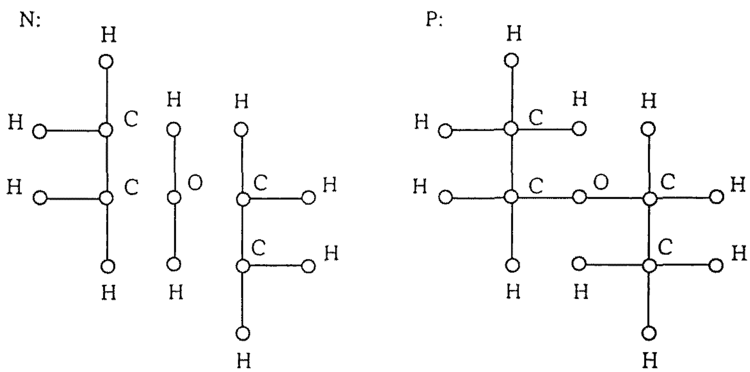

Fig. 5. A graphical representation of the compounds in the chemical transformation (2).

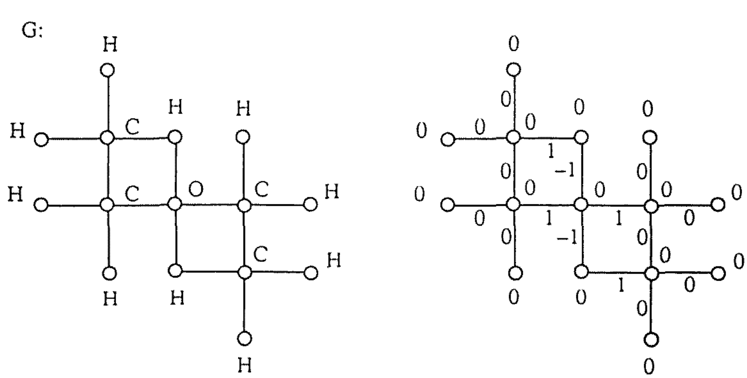

Fig. 6. A graphical representation of the chemical transformation (2).

In order to represent the chemical transformation (2), we consider the common (labeled) supergraph G of N and P shown in fig. 6. Proceeding as before, we obtain the labeling of G (also shown in fig. 6), which is then a representation of the chemical transformation (2).

In certain representations of a chemical transformation (called *nonstoichiometric transformations*), some atoms on one side of the transformation may not be explicitly represented on the other side of the equation. Consequently, under the assumption that atoms from molecules of water do not participate in the atomic balance of the corresponding chemical equation, we obtain a different model for this chemical reaction between ethylene and water. In this case, we have

$$2C_2H_4 \rightarrow C_2H_5OC_2H_5. \quad (4)$$

Here, we obtain the chemical graphs N' and P' of fig. 7. With the aid of the common supergraph G' of N' and P', we obtain the labeling of G' shown in fig. 6. This labeling may be considered as a representation of the chemical reaction (4).

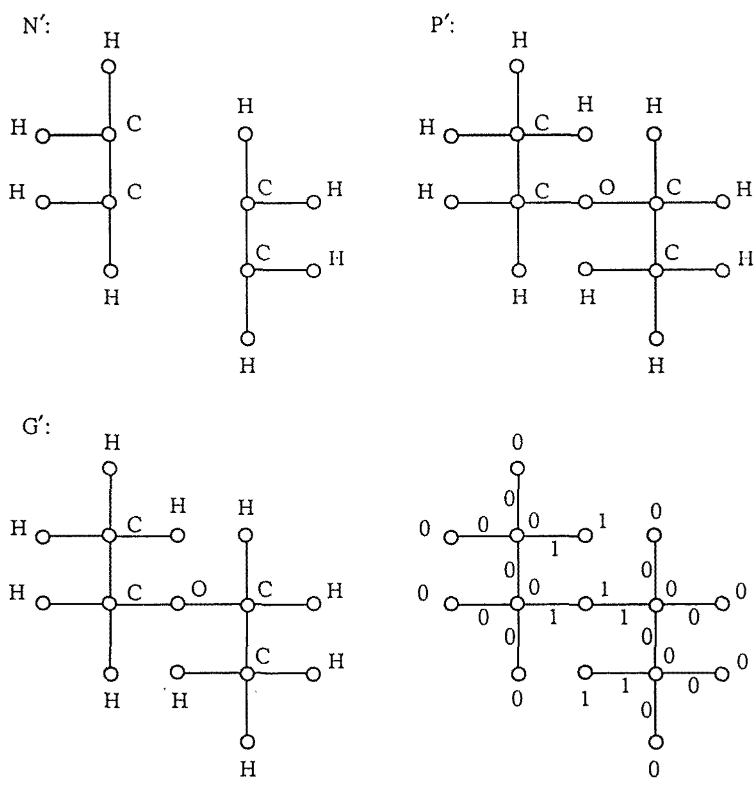

Fig. 7. A common supergraph of two chemical graphs.

It should now be clear that if G is a labeled graph representing a certain chemical transformation as described above, then edges labeled 0 are incident only with vertices labeled 0. Moreover, since additional edges cannot be incident with deleted edges, and deleted edges cannot be incident with added vertices, we see that no edge labeled -1 is incident with a vertex labeled 1, and no edge labeled 1 is incdent with a vertex labeled -1. Therefore, the labeling of G is, in fact, a transitional labeling. Denote this labeling by t.

We note that the subgraph of G consisting of the elements labeled -1 or 0 and the subgraph consisting of the elements labeled 1 or 0 are well defined. These subgraphs are, respectively, the chemical graphs of the involved compounds prior to and following the chemical transformation under consideration. Furthermore, these are, respectively, the negative graph N and the positive graph P of t.

Hevia [6,7] has studied theoretical properties of transitional labelings. In particular, he has investigated transitional labelings of complete graphs and trees. Unless stated otherwise, we shall assume that all transitional labelings under discussion are nonconstant. There is no loss of generality with this assumption since transitional labelings were introduced to model chemical transformations, and a constant transitional labeling indicates that no chemical change has occurred.

Let G_1 and G_2 be two graphs with transitional labelings t_1 and t_2, respectively. We say that t_1 is *isomorphic* to t_2, written $t_1 \equiv t_2$, if there exists a graph isomorphism ϕ from $V(G_1)$ to $V(G_2)$ such that the diagram of fig. 8 is commutative, that is,

$$t_1 = t_2 \circ \overline{\phi},$$

where $\overline{\phi}: V(G_1) \cup E(G_1) \to V(G_2) \cup E(G_2)$ is an extension of ϕ for which $\overline{\phi}(uv) = \phi u\, \phi v$, for each edge uv of G_1. Since ϕ is an isomorphism, it follows that $\phi u\, \phi v$ is an edge of G_2 whenever uv is an edge of G_1. This shows that the extension $\overline{\phi}$ of ϕ always exists.

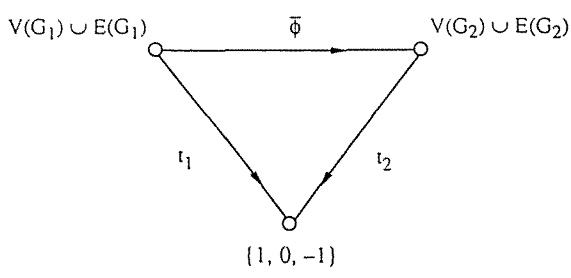

Fig. 8. The commutative diagram for isomorphic transitional labelings.

Figure 9 shows two graphs G_1 and G_2, with corresponding transitional labelings t_1 and t_2. If ϕ: $V(G_1) \to V(G_2)$ is the isomorphism defined by $\phi(u_i) = v_i$ ($i = 1, 2, 3, 4$), then $t_1 = t_2 \circ \overline{\phi}$ and, hence, $t_1 \equiv t_2$. It can be shown that the relation "is isomorphic to" is an equivalence relation of any set of transitional labelings.

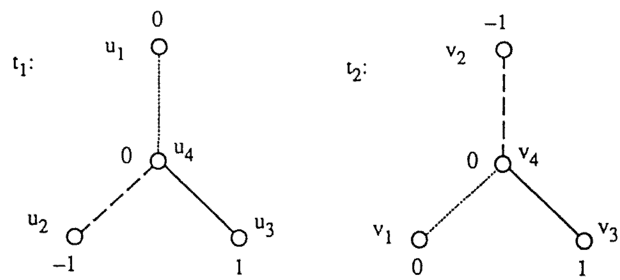

Fig. 9. Isomorphic transitional labelings.

Let t be a nontrivial transitional labeling of a graph G. The *core* t_c of t is the restriction of t to the subgraph obtained from G by deleting all zero edges together with all zero vertices that are incident only with zero edges. Equivalently, the core t_c of G is the restriction of t to the subgraph H of G induced by the nonzero edges of G and the isolated vertices of G that are poles. Figure 10 shows a transitional labeling t of a graph together with its core t_c.

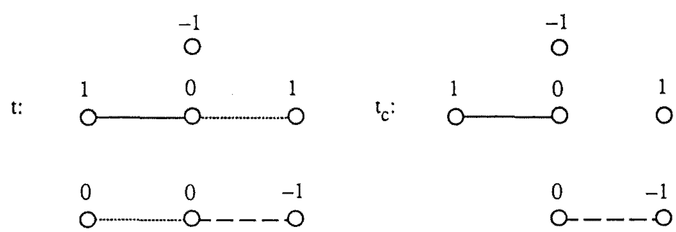

Fig. 10. The core of a transitional labeling.

At this point, we interrupt our discussion briefly to recall a few ideas from the mathematical theory of relations. A *relation* $\sim$ on a set S is a collection of elements (ordered pairs) of the product set $S \times S$. For any $x, y \in S$, it is customary to write $x \sim y$ if and only if (x, y) belongs to the relation $\sim$ and we say *x is related to y by* $\sim$. The relation is called (1) *reflexive* if $x \sim x$ for all $x \in S$, (2) *symmetric* if whenever $x \sim y$, then $y \sim x$, (3) *antisymmetric* if whenever $x \sim y$ and $y \sim x$, then $x = y$, and (4) *transitive* if whenever $x \sim y$ and $y \sim z$, then $x \sim z$. A relation that satisfies the reflexive, symmetric, and transitive properties is referred to as an *equivalence relation.*

If a relation $\sim$ on a set S is reflexive, antisymmetric, and transitive, then it is called a *partial ordering* on S, and we say that $\sim$ *partially orders* S. It is customary to denote a partial ordering by $\leq$. A set S together with a partial ordering on S is called a *partially ordered set* or, more commonly, a *poset.* With each poset, there is associated a diagram called a *Hasse diagram.* For each element of the poset, we associate a point. If x and y belong to the poset and $x \leq y$, then we draw the point

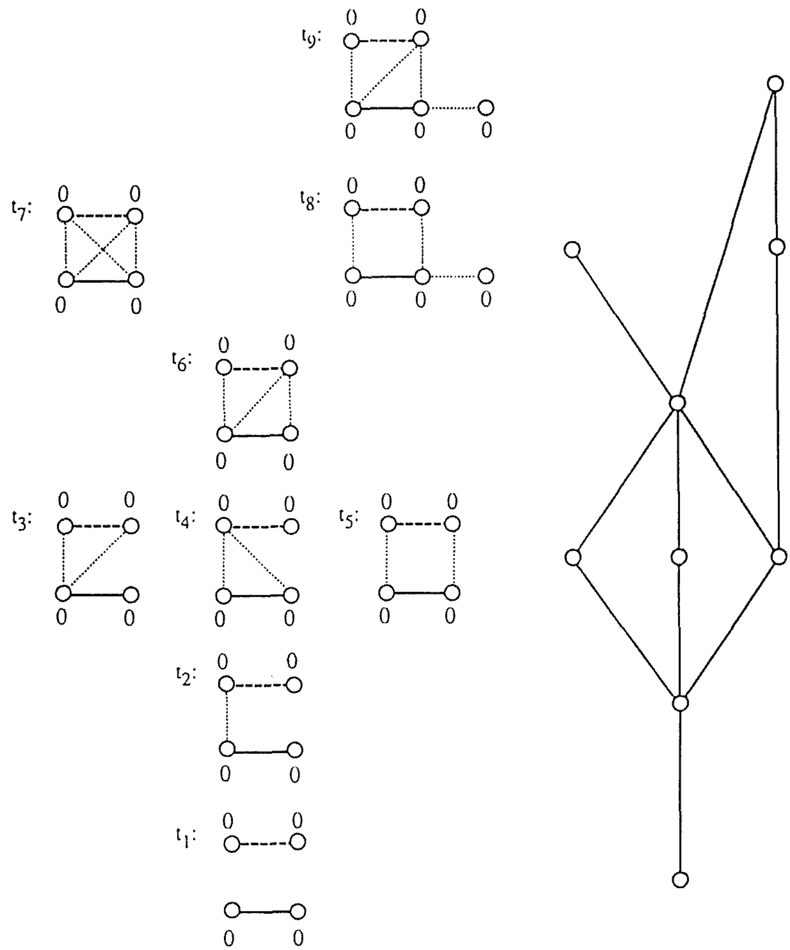

Fig. 11. The Hasse diagram of a set of transitional labelings.

corresponding to x below the point corresponding to y. Furthermore, if $x \leq y$ and there is no element z of the poset distinct from x and y such that $x \leq z \leq y$, then we join x and y by a line segment.

We now return to our primary discussion. Let t and t' be transitional labelings of graphs G and G', respectively. They are said to have the *same core* if $t_c \cong t'_c$. (This relation is an equivalence relation on any set of transitional labelings.) Let t and t' be transitional labelings having the same core. Then we write $t \leq t'$ if t is isomorphic to a restriction of t'. Thus, $t \leq t'$ if and only if a transitional labeling isomorphic to t' can be constructed from t by adding appropriate zero elements to G. Note that, by definition, if $t \leq t'$, then $t_c \cong t'_c$. If $t \leq t'$, then t is called a *restriction* of t', and t' is an *extension* of t. If $t \leq t'$ and $t \not\cong t'$, then t' is a *proper extension* of t.

The relation $\leq$ partially orders any set $\mathcal{T}$ of transitional labelings. Certainly, $\leq$ is reflexive and transitive. To see that $\leq$ is also antisymmetric, suppose that t

and t' are transitional labelings of graphs G and G', respectively, such that $t \leq t'$ and $t' \leq t$. Then t and t' must have an equal number of zero elements and, consequently, $t \equiv t'$.

For example, let $\mathcal{T}$ be the set of transitional labelings $t_1, t_2, \ldots, t_9$ shown in fig. 11. These transitional labelings have isomorphic cores. Thus, $(\mathcal{T}, \leq)$ is a poset and may be represented by the Hasse diagram of fig. 11. The transitional labelings shown in fig. 11 will be referred to often throughout the remainder of this paper.

3. Transforms

In this section, we describe a secial kind of transitional labeling called a transform, in which we will be interested throughout the remainder of the paper. It is necessary to define a few additional terms before introducing this concept.

We define the *cardinality* $|G|$ of a graph G as the sum of its order and size, that is,

$$|G| = |V(G)| + |E(G)|.$$

A graph F is called a *maximum common subgraph* of graphs G_1 and G_2 if F is a graph of maximum cardinality that is isomorphic to a common subgraph of G_1 and G_2. A graph G is a *minimum common supergraph* of G_1 and G_2 if G is a graph of minimum cardinality that is isomorphic to a common supergraph of G_1 and G_2. These two concepts were introduced by Johnson in ref. [8]. For the graphs G_1 and G_2 of fig. 12, $|G_1| = 10$ and $|G_2| = 9$. The graph F is the unique maximum common subgraph of G_1 and G_2, and G is a minimum common supergraph (though not unique) of G_1 and G_2.

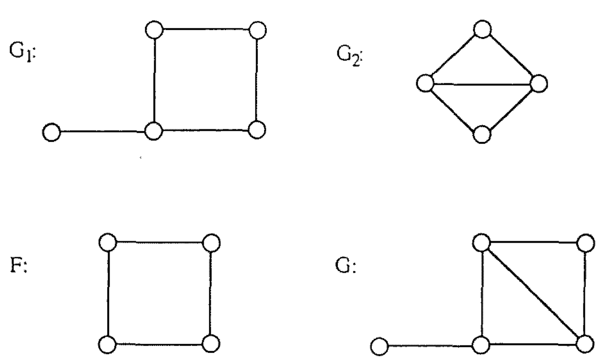

Fig. 12. A maximum common subgraph and minimum common supergraph of two graphs.

For subgraphs H_1 and H_2 of a (labeled) graph G, we define the *union* $H_1 \cup H_2$ as that subgraph of G with vertex set $V(H_1) \cup V(H_2)$ and edge $E(H_1) \cup E(H_2)$. The *intersection* $H_1 \cap H_2$ of H_1 and H_2 is defined analogously.

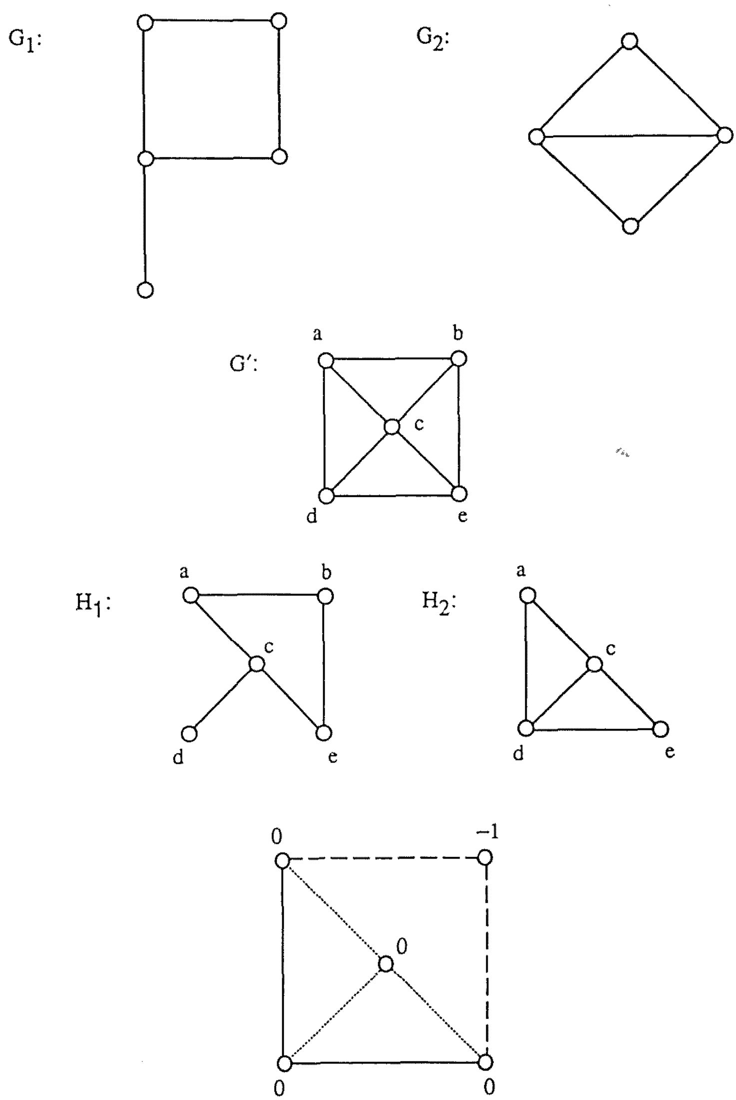

Fig. 13. The construction of a transitional labeling with prescribed negative and positive graphs.

Let G_1 and G_2 be two given graphs. In ref. [1], Johnson shows how to construct a graph G and a transitional labeling t of G such that the negative graph of t is isomorphic to G_1 and the positive graph of t is isomorphic to G_2. We briefly describe this procedure. Let G' be a common supergraph of G_1 and G_2. Let H_1 and H_2 be two subgraphs of G' that are isomorphic to G_1 and G_2, respectively. Define a transitional labeling t of $G = H_1 \cup H_2$ by

$$t(x) = \begin{cases} -1 & \text{if } x \text{ is an element of } H_1 \text{ but not of } H_2, \\ 1 & \text{if } x \text{ is an element of } H_2 \text{ but not of } H_1, \\ 0 & \text{if } x \text{ is a common element of } H_1 \text{ and } H_2. \end{cases} \quad (5)$$

We illustrate this procedure. Let G_1 and G_2 be the two graphs shown in fig. 13. Choose the common supergraph G' of G_1 and G_2 and the subgraphs H_1 and H_2 of G' of fig. 13. We then obtain the transitional leveling t of $G = H_1 \cup H_2$ shown in fig. 13.

For given graphs G_1 and G_2, let G be a minimum common supergraph of G_1 and G_2 and let H_i denote a subgraph of G isomorphic to G_i, $i = 1, 2$. Then

$$|G| = |H_1| + |H_2| - |F|$$

and so

$$|G| = |G_1| + |G_2| - |F|, \quad (6)$$

where $F = H_1 \cap H_2$. Thus, F is a common subgraph of G_1 and G_2. From eq. (6), it follows that F is a maximum common subgraph of G_1 and G_2. Therefore, in constructing the transitional labeling t described in (5), if we choose G' as a minimum common supergraph of G_1 and G_2, then the linking graph of t is a maximum common subgraph of G_1 and G_2. Figure 14 shows a transitional labeling s whose negative and positive graphs are isomorphic to the graphs G_1 and G_2 of fig. 13, respectively, and where the linking graph of s is a maximum common subgraph of G_1 and G_2.

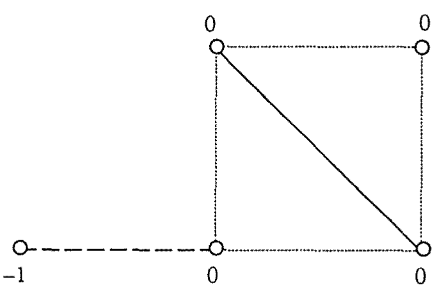

Fig. 14. The construction of a transitional labeling with prescribed negative and positive graphs and whose linking graph is a maximum common subgraph.

A transitional labeling t is said to be of *maximum linkage* if its linking graph is a maximum common subgraph of the positive and negative graphs of t. Thus, the transitional labeling shown in fig. 14 is of maximum linkage.

A characteristic of transitional labelings of maximum linkage is now established.

THEOREM 1

If t is a transitional labeling of maximum linkage of a graph G, then t is a quasipolarization of G.

Proof

Let N and P be the negative and positive graphs of t, respectively. Since t is of maximum linkage, G is a minimum common supergraph of N and P. Suppose, to the contrary, that t is a polarization. Let u and v be poles with distinct signs. Let H be the graph obtained by identifying u and v. Then H is a common supergraph of N and P whose cardinality is less than the cardinality of G, contradicting the minimality of G. □

The converse of theorem 1 is not true in general, as is illustrated by the quasipolarization shown in fig. 15.

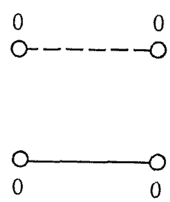

Fig. 15. A quasipolarization that is not a transitional labeling of maximum linkage.

A transitional labeling t is called a *transform* if there exists an extension t' of t that is of maximum linkage, that is, the linking graph t' is a maximum common subgraph of the negative and positive graphs of t'. Thus, every transitional labeling of maximum linkage is a transform. Transforms were introduced by Johnson [1] for the purpose of modeling chemical reaction pathways.

We return to the example given in fig. 11. Figure 16 shows the transitional labelings t_1 and t_3 of fig. 11, together with their corresponding negative and positive graphs. Since the linking graph of t_3 is a maximum common subgraph of the negative graph N_3 and positive graph P_3 of t_3, it follows that t_3 is of maximum linkage. The linking graph of t_1 is *not* a maximum common subgraph of the negative graph N_1 and the positive graph P_1 of t_1, so t_1 is *not* of maximum linkage. However, because t_3 is of maximum linkage and $t_1 \leq t_3$, it follows that t_1 and, of course, t_3 are transforms.

Now consider the transitional labeling t of the graph G shown in fig. 17, with linking graph L, negative graph N, and positive graph P. Observe that $L \cong K_1$ and $N \cong P \cong K_2$. Let s be an extension of t, with linking graph L^*, negative graph N^*, and positive graph P^*. Since s is obtained from t by adding zero edges and/or zero

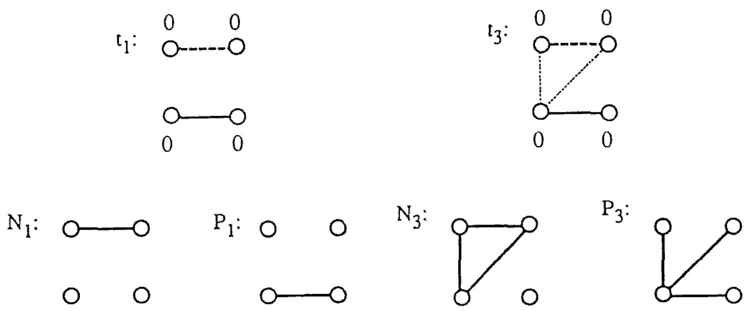

Fig. 16. Transitional labelings that are transforms.

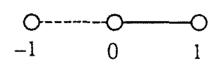

Fig. 17. A transitional labeling that is not a transform.

vertices to t, it follows that $N^* \cong P^*$ and L^* is a proper subgraph of N^* (equivalently P^*). Because $N^* \cong P^*$, the maximum common subgraph of N^* and P^* is also isomorphic to N^*. Hence, L^* is not a maximum common subgraph of N^* and P^*, so t is not a transform.

4. Actions, transform kits, and metadigraphs

Let t be a transform. An ordered pair (G_1, G_2) of (unlabeled) graphs is called an *action* of t if there exists an extension t' of maximum linkage of t such that the negative graph of t' is isomorphic to G_1 and the positive graph of t' is isomorphic to G_2. Equivalently, then, (N, P) is an action of t if t is of maximum linkage with negative graph N and positive graph P. For example, for the graphs N_3 and P_3 of fig. 16, the ordered pair (N_3, P_3) is an action of the transforms t_1 and t_3.

A *metadigraph* $M = (D, g)$ is a (possibly infinite) digraph D together with a labeling g of the vertices of D with unlabeled graphs such that if $u, v \in V(D)$, $u \neq v$, then $g(u) \not\cong g(v)$. Figure 18 shows a metadigraph M of order 3 whose vertices are labeled with the graphs G_1, G_2, and G_3. Two metadigraphs $M_1 = (D_1, g_1)$ and $M_2 = (D_2, g_2)$ are *isomorphic* if there exists an isomorphism $\phi: V(D_1) \to V(D_2)$ such that $g_1(u) \cong g_2(\phi(u))$ for all $u \in V(D_1)$.

A *transform kit* K is an ordered pair (T_g, T_b) of sets of transforms. The elements of T_g are called the *generating transforms* of K and the elements of T_b are referred to as *blocking transforms* of K. Let $K = (T_g, T_b)$ be a transform kit, and let $t \in T_g$ and $t' \in T_b$. An action (G_1, G_2) of t is said to be *blocked* by t' if

(i) (G_1, G_2) is an action of t', and

(ii) $t \leq t'$, that is, t' is an extension of t.

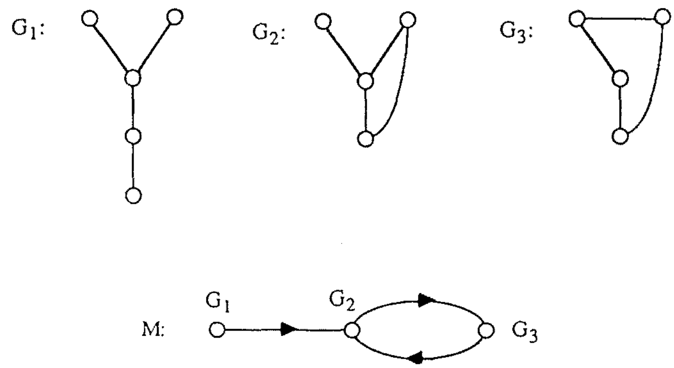

Fig. 18. A metadigraph.

We return to the transitional labelings shown in fig. 11. Consider the transform kit $K = (T_g, T_b)$, where $T_g = \{t_1\}$ and $T_b = \{t_3\}$. We have seen that $a_1 = (N_3, P_3)$ is an action of t_1 and t_3, where N_3 and P_3 are the graphs shown in fig. 16. Since $t_1 \leq t_3$, the action a_1 of t_1 is blocked by t_3. Let N_8 and P_8 denote the negative and positive graphs of the transitional labeling t_8 of fig. 11 (see fig. 19). We claim that $a_2 = (N_8, P_8)$

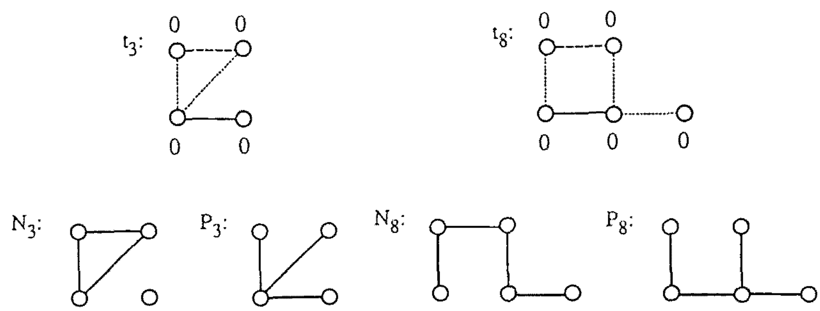

Fig. 19. An action (N_8, P_8) of t_1 is not blocked by t_3.

is an action of t_1 that is not blocked by t_3. In order to see this, we assume, to the contrary, that a_2 is blocked by t_3. Then a_2 is an action of t_3. So, there exists some extension of t_3 whose negative graph N is isomorphic to N_8. Since the negative graph N_3 of t_3 is a subgraph of N, the graph N_8 contains a triangle, which produces a contradiction. Let $T_b' = \{t_2\}$. Then for the transform kit $K' = (T_g, T_b')$, the actions a_1 and a_2 of t_1 are blocked by the transform t_2.

By an *action of a transform kit* K, we mean an action of the generating transforms of K that is not blocked by any blocking transform of K. Thus, for the transform kit $K = (T_g, T_b)$ described above in which $T_g = \{t_1\}$ and $T_b = \{t_3\}$, $a_2 = (N_8, P_8)$ is an action of K.

Let Δ be a nonempty set of unlabeled graphs, and let K be a transform kit. With Δ and K, we can associate a metadigraph $D(\Delta, K)$. Each vertex of $D(\Delta, K)$ corresponds to an element (unlabeled graph) of Δ. Let u and v be distinct vertices of $D(\Delta, K)$ with corresponding graphs G_1 and G_2, respectively. Then (u, v) is an arc of $D(\Delta, K)$ if and only if (G_1, G_2) is an action of K.

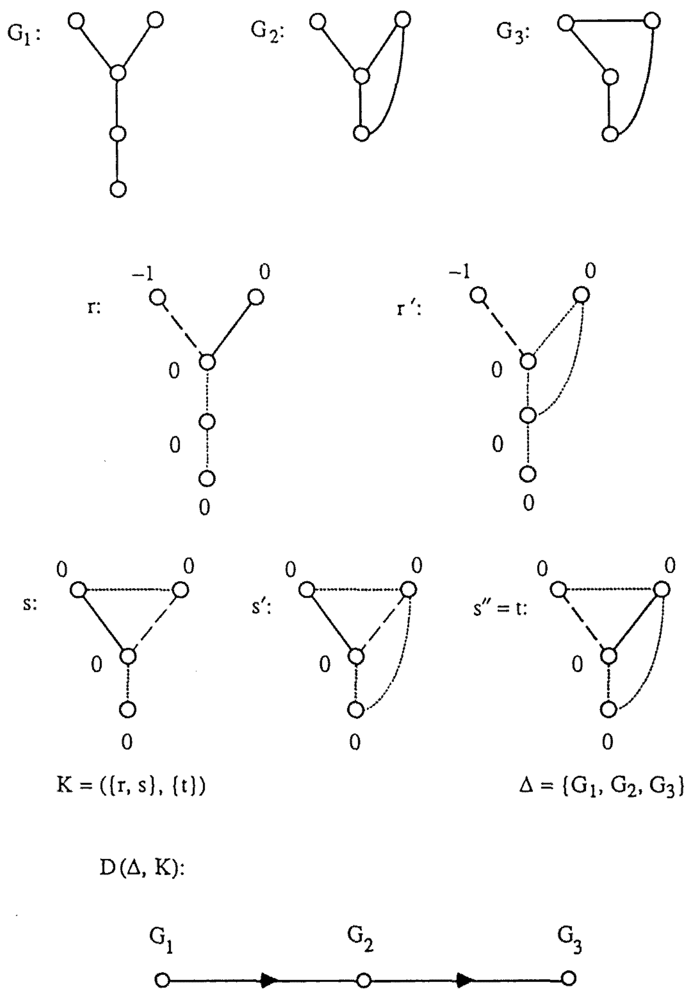

Fig. 20. Actions, a transform kit, and a metadigraph.

As an example, let $\Delta = \{G_1, G_2, G_3\}$ and $K = (\{r, t\}, \{s\})$, where the graphs G_1, G_2, G_3 and transitional labelings r, s, t are shown in fig. 20. The extension r' and r shown in fig. 20 is of maximum linkage, and the negative and positive graphs of r' are isomorphic to G_1 and G_2, respectively. Therefore, (G_1, G_2) is an action of r that cannot be blocked by t since r and t have distinct cores. Then (G_1, G_2) is an action of K. On the other hand, if (G_1, G_2) is an action of a certain transform u of a graph G, then G must have a positive pole. This implies that such a transform u cannot be an extension of r or of s. Therefore, (G_1, G_2) is neither an action of r nor of s and, consequently, is not an action of K. That (G_2, G_3) and (G_3, G_2) are actions of s can be seen by considering the extension s' and s'' (of maximum linkage), respectively. In particular, since $t = s''$ is a blocking transform of K, the action (G_3, G_2) is blocked by t. Thus, (G_3, G_2) is not an action of K. The action (G_2, G_3) of s cannot be blocked by t since the negative graph N of any extension of t contains a 4-cycle and so $G_2 \not\cong N$. Therefore, (G_2, G_3) is an action of K.

The graphs G_1 and G_3 have a unique maximum common subgraph, namely, P_4. So, if t^* is a transitional labeling of maximum linkage whose negative and positive graphs are isomorphic to G_1 and G_3, or to G_3 and G_1, respectively, then t^* has a core distinct from that of r and s. From this, it follows that (G_1, G_3) and (G_3, G_1) are not actions of r and s and, consequently, are not actions of K. The remaining metadigraph is shown in fig. 20.

Let M be a metadigraph. If there exists a set Δ of unlabeled graphs and a transform kit K such that M is isomorphic to the metadigraph $D(\Delta, K)$, then (Δ, K) is said to be a *specification* for M.

Recall that a transitional labeling t of maximum linkage is a transform. Also, if N and P are the negative and positive graphs of t, then (N, P) is an action of t. The next result concerns this situation.

THEOREM 2

Let t be a transitional labeling of maximum linkage in a graph G, and let N and P denote the negative and positive graphs of t. Then there exists no transform t' that is a proper extension of t such that (N, P) is an action of t'.

Proof

Suppose, to the contrary, that there exists a transform t' that is a proper extension of t such that (N, P) is an action of t'. Since (N, P) is an action of t', there exists a transitional labeling of t'' of some graph G'' that is of maximum linkage and whose negative and positive graphs are isomorphic to N and P. Thus, G and G'' are minimum common supergraphs of N and P, and, consequently, $|G| = |G''|$. However, t'' is a proper extension of t so that $|G| < |G''|$, producing a contradiction. □

An immediate consequence now follows.

COROLLARY 3

If $K = (T_g, T_b)$ is a transform kit and $t \in T_g \backslash T_b$ is of maximum linkage, then (N, P) is an action of K, where N and P are the negative and positive graphs of t.

Proof

Since $t \in T_g \backslash T_b$, any extension t' of t in T_b is a proper extension of t. By theorem 2, (N, P) is not an action of t' for any $t' \in T_b$. Therefore, (N, P) is an action of K. □

Let G_1 and G_2 be two given graphs. By $\mathcal{T}(G_1, G_2)$, we mean the set of all transitional labelings of maximum linkage whose negative and positive graphs are isomorphic to G_1 and G_2, respectively. For example, if G_1 and G_2 are the graphs of fig. 20 (also shown in fig. 21), then $\mathcal{T}(G_1, G_2) = \{t_1, t_2\}$, where t_1 and t_2 are the transitional labelings shown in fig. 21.

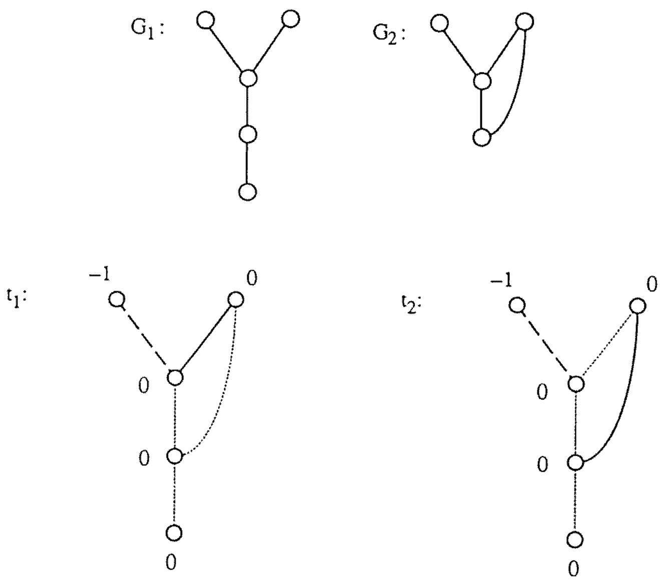

Fig. 21. The transitional labelings of maximum linkage whose negative and positive graphs are isomorphic to G_1 and G_2.

THEOREM 4

Let $K = (T_g, T_b)$ be a transform kit. If G_1 and G_2 are graphs for which $\mathcal{T}(G_1, G_2) \subseteq T_b$, then (G_1, G_2) is not an action of K.

Proof

Suppose that (G_1, G_2) is an action of some transform $t \in T_g$. Then there exists a transitional labeling t' of maximum linkage such that $t \leq t'$ and the negative and positive graphs of t' are isomorphic to G_1 and G_2. Since (G_1, G_2) is an action of t' and $t' \in \mathcal{T}(G_1, G_2) \subseteq T_b$, the action (G_1, G_2) is blocked by t'. Thus, (G_1, G_2) is not an action of K. □

We are now in a position to establish the existence of a specification (Δ, K) for any given metadigraph M. This result is due to Johnson [1], but we include a proof for completeness.

THEOREM 5 (Johnson)

For any metadigraph M, there exists a specification (Δ, K) such that M is isomorphic to $D(\Delta, K)$.

Proof

Let $M = (D, g)$ be a metadigraph. Let $\Delta = \{g(v) \mid v \in V(D)\}$. For each arc $e = (u, v)$ of D, construct a transitional labeling t_e of maximum linkage whose negative and positive graphs are isomorphic to $g(u)$ and $g(v)$, respectively. Let

$$T_g = \{t_e \mid e \in E(D)\}$$

and $T_b = \overline{T}_g$, where $\overline{T}_g$ is the complement of T_g with respect to the set of all transforms. Let $K = (T_g, T_b)$. We show that (Δ, K) is a specification for M.

Suppose that $e = (u, v)$ is an arc of D. Then the transform t_e is an element of $T_g \backslash T_b$. By corollary 3, $(g(u), g(v))$ is an action of K, and so the vertex of $D(\Delta, K)$ labeled $g(u)$ is adjacent to the vertex labeled $g(v)$.

Next, suppose that $e = (u, v)$ is not an arc of D. In this case, $\mathcal{T}(g(u), g(v)) \subseteq T_b$. By theorem 4, $(g(u), g(v))$ is not an action of K, and so the vertex labeled $g(u)$ in $D(\Delta, K)$ is *not* adjacent to the vertex labeled $g(v)$.

Therefore, the restriction $g': V(D) \to \Delta$ of g is an isomorphism of M and $D(\Delta, K)$. □

5. A characterization of transforms

Transforms have played a central role throughout this paper. In this section, we present a characterization of transforms.

Let G_1 and G_2 be graphs with $|V(G_1)| \geq |V(G_2)| = z$, and let $f: V(G_2) \to V(G_1)$ be a one-to-one function. Suppose that $V(G_2) = \{v_1, v_2, \ldots, v_z\}$ and $f(v_i) = u_i$ for $i = 1, 2, \ldots, z$. With f we can associate a quasipolarization for a graph G, as we now describe. We construct a common supergraph G of G_1 and G_2 by identifying u_i and v_i for each i $(1 \leq i \leq z)$. Let H_1 and H_2 denote subgraphs of G isomorphic to G_1 and G_2, respectively. Then $G = H_1 \cup H_2$. Define the transitional labeling t of G as we did in (5), namely,

$$t(x) = \begin{cases} -1 & \text{if } x \text{ is an element of } H_1 \text{ but not of } H_2, \\ 1 & \text{if } x \text{ is an element of } H_2 \text{ but not of } H_1, \\ 0 & \text{if } x \text{ is a common element of } H_1 \text{ and } H_2. \end{cases}$$

Indeed, *every* quasipolarization with negative graph isomorphic to G_1 and positive graph isomorphic to G_2 can be thought of as being associated with a one-to-one function from $V(G_2)$ to $V(G_1)$. We employ these ideas in the proof of the next result.

THEOREM 6

A transitional labeling t of a graph G is a transform if and only if t is a quasipolarization.

Proof

Suppose, first, that t is a transform. Then there exists an extension t' of t that is of maximum linkage. By theorem 1, t' is a quasipolarization. Since $t \leq t'$, the transitional labelings t and t' have the same core, and so t is also a quasipolarization.

Conversely, assume that t is a quasipolarization of G. Suppose, without loss of generality, that G has no positive pole. Let $\{w_1, w_2, \ldots, w_z\}$ be the set of zero vertices of G, which is, consequently, the vertex set of the positive graph of t. We extend t to a quasipolarization t' of a graph G' by adding zero elements to the (labeled) graph G. In particular, for each $i = 1, 2, \ldots, z$, we add b^i new vertices and join each of these to w_i, where b is a fixed integer satisfying the inequality

$$b \geq \max\{2, 2|G| - z\}.$$

Denote the resulting graph by G'. The $\sum_{i=1}^{z} b^i$ newly added vertices and $\sum_{i=1}^{z} b^i$ new edges are labeled 0, resulting in a transitional labeling t' of G' that is an extension of t.

We claim that t' is of maximum linkage. Let G_1 and G_2 be graphs isomorphic to the negative and positive graphs of t'. Then the order of G_2 is

$$z' = z + \sum_{i=1}^{z} b^i.$$

Thus, the order of G_1 is at least z'. Let L be the linking graph of t'. The claim is verified by showing that for each one-to-one function $f: V(G_2) \to V(G_1)$, we have $|F| \leq |L|$, where F is the linking graph of the quasipolarization s of the graph G'' that is associated with f, which then proves that L is a maximum common subgraph of G_1 and G_2.

Let $V(G_2) = \{v_1, v_2, \ldots, v_z, v_{z+1}, \ldots, v_{z'}\}$, where the vertex v_i $(1 \leq i \leq z)$ corresponds to w_i, and where the vertices $v_{z+1}, v_{z+2}, \ldots, v_{z'}$ are those end-vertices that were added to G to obtain G'. Thus, for $i = 1, 2, \ldots, z$,

$$\deg v_i = b^i + \deg_G w_i.$$

Let $f(v_i) = u_i$ for $i = 1, 2, \ldots, z'$. Denote the vertices of G_1 corresponding to $w_1, w_2, \ldots, w_z$ by $x_1, x_2, \ldots, x_z$. The remainder of the proof is divided into two cases.

Case 1. Assume $u_j \neq x_j$ for some j $(1 \leq j \leq z)$. We know that

$$\deg v_j = b^i + \deg_G w_j.$$

There are now two possibilities to consider, namely, $u_j \neq x_i$ for all i $(1 \leq i \leq z)$ and $u_j = x_k$ for some $k \neq j$ $(1 \leq k \leq z)$.

If $u_j \neq x_i$ for all i $(1 \leq i \leq z)$, then

$$\deg u_j \leq |G| - 1,$$

since, in constructing t', we have only modified the degrees of the zero vertices of G. On the other hand, if $u_j = x_k$ for some $k \neq j$ $(1 \leq k \leq z)$, then

$$\deg u_j = \deg x_k = b^k + \deg_G w_k.$$

In either case, it follows that

$$|\deg u_j - \deg v_j| \geq b - |G| + 1.$$

Therefore, at least $b - |G| + 1$ edges of G'' have a nonzero label, so

$$|F| \leq |G''| - (b - |G| + 1).$$

However,

$$|G''| = |G| + 2\sum_{i=1}^{z} b^i,$$

so

$$|F| \leq |G| + 2\sum_{i=1}^{z} b^i - (b - |G| + 1) \leq z + 2\sum_{i=1}^{z} b^i - 1 - (b - 2|G| + z).$$

According to the definition of b,

$$b - 2|G| + z \geq 0,$$

so

$$|F| < z + 2\sum_{i=1}^{z} b^i \leq |L|.$$

Case 2. Assume $u_i = x_i$ for all i $(1 \leq i \leq z)$. Here, it follows in a straightforward manner that $|F| \leq |L|$.

Therefore, L is a maximum common subgraph of G_1 and G_2 and, hence, t' is a transitional labeling of G' of maximum linkage. Since t' is an extension of t, the labeling t is a transform. □

We close by illustrating the construction described in the proof of theorem 6. Figure 22 shows a graph G and a transitional labeling t of G. In this case, there are two zero vertices, so $z = 2$. The integer b satisfies the inequality

$$b \geq \max\{2, 2|G| - z\} = \max\{2, 8\} = 8$$

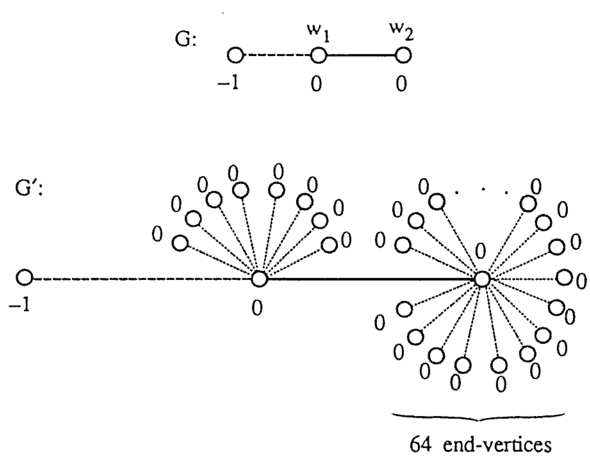

Fig. 22. Construction of an extension of a transitional labeling that is of maximum linkage.

here. Choosing $b = 8$, we construct the graph G' shown in fig. 22, with the resulting transitional labeling t'.

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