Fractional isomorphism of graphs

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Abstract

Let the adjacency matrices of graphs G and H be A and B. These graphs are isomorphic provided there is a permutation matrix P with $AP = PB$, or equivalently, $A = PBP^T$. If we relax the requirement that P be a permutation matrix, and, instead, require P only to be doubly stochastic, we arrive at two new equivalence relations on graphs: *linear fractional isomorphism* (when we relax $AP = PB$) and *quadratic fractional isomorphism* (when we relax $A = PBP^T$). Further, if we allow the two instances of P in $A = PBP^T$ to be *different* doubly stochastic matrices, we arrive at the concept of *semi-isomorphism*.

We present necessary and sufficient conditions for graphs to be linearly fractionally isomorphic, we prove that quadratic fractional isomorphism is the same as isomorphism and we relate semi-isomorphism to isomorphism of bipartite graphs.

Key words: Graph isomorphism; Adjacency matrix; Fractional isomorphism

1. Introduction

The most familiar equivalence relation on the set of graphs is certainly the notion of isomorphism. Graphs G and H are said to be *isomorphic* provided that there exists a bijection $f: V(G) \to V(H)$ so that $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$. Isomorphism can be expressed in matrix algebra terms. Suppose the adjacency matrices of the graphs are A and B. The graphs are isomorphic just when there is a permutation matrix P so that any one of the following equivalent conditions holds:

$$A = PBP^{-1} \tag{1}$$

$$AP = PB, \tag{2}$$

$$A = PBP^{\mathsf{T}}. \tag{3}$$

Each of these relations admits a natural relaxation.

For (1) it is natural to simply require that P be any nonsingular matrix. In this case, the graphs G and H are known as *cospectral*. Graph spectra and cospectral graphs have been extensively studied; see, for example, [1, 5, 19, 20].

Equations (2) and (3) can be relaxed in a different way. One can define a permutation matrix as an *integer* matrix of nonnegative numbers whose rows and columns all sum to 1. By omitting the word *integer* one has the notion of a *doubly stochastic matrix*. This gives rise to two notions of *fractional isomorphism* of graphs. These definitions are in the spirit of other combinatorial problems which give rise to 'fractional' parameters. (See, for example, [10] for a discussion of the *fractional chromatic number* of graphs, [6] for the *fractional covering number* of hypergraphs, and [3] for the *fractional dimension* of partially ordered sets.) The unifying idea in all cases is to describe a problem in terms of equations that must be satisfied by 0, 1-variables and then to relax the problem by allowing the variables to take values in [0, 1] instead of {0, 1}.

Definition 1.1 (*Linear Fractional Isomorphism*). Let G and H be graphs with adjacency matrices A and B respectively. We say that G is (*linearly*) *fractionally isomorphic* to H provided there exists a doubly stochastic matrix S so that $AS = SB$. In this case we write $G \cong_f H$.

The adverb *linearly* (which we often omit in the sequel) emphasizes that the system of equations $AS = SB$ is linear in the variables, i.e., the entries in S. This relation is also known as *ds-isomorphism*; see [21] as well as [4, 14, 15].

This notion of fractional isomorphism is discussed in Section 2.

The definition of (linear) fractional isomorphism we have presented arises from relaxing the condition $AP = PB$. An alternative approach is to relax the condition $A = PBP^{\mathsf{T}}$. This leads to several new equivalence relations on graphs.

For $n \times n$ matrices A and B, we writer $A \rightarrow B$ to mean there exists a doubly stochastic matrix S with $B = SAS^{\mathsf{T}}$. The idea is that A is 'mixed' to form B. Further, we write $A \leftrightarrow B$ if $A = SBS^{\mathsf{T}}$ and $B = S^{\mathsf{T}}AS$ for some doubly stochastic matrix S.

Definition 1.2 (*Quadratic Fractional Isomorphism(s)*). Let G and H be graphs with adjacency matrices A and B respectively. We say that G is *weakly quadratically fractionally isomorphic* to H provided $A \rightarrow B$. We say that G is *quadratically fractionally isomorphic* to B provided $A \rightarrow B$ and $B \rightarrow A$. Finally, we say that G is *strongly quadratically fractionally isomorphic* to H provided $A \leftrightarrow B$.

The adjective *quadratic* arises from the fact that the systems of equations $A = SBS^{\mathsf{T}}$ and $B = S^{\mathsf{T}}AS$ are quadratic in the variables (the entries of S). We also use it to distinguish this notion from ordinary (linear) fractional isomorphism.

It is a simple exercise to verify that quadratic fractional isomorphism and strong quadratic isomorphism are equivalence relations. But it is not clear that weak quadratic fractional isomorphism is symmetric. For example, consider the following matrices:

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad \text{and} \quad S = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}.$$

Note that $B = SAS^{\mathsf{T}}$, so $A \to B$. However, there can be no matrices X and Y with $A = XBY$ as A has greater rank than B, thus $B \not\to A$.

The reader may object to this example since the matrices A and B are not adjacency matrices of graphs. The authors have a pretty good excuse — no *graph* example is possible! We show in Section 3 that all three forms of quadratic fractional isomorphism are equivalent to ordinary graph isomorphism.

The various notions of quadratic fractional isomorphism are equivalent to ordinary graph isomorphism. We can relax the condition $A = PBP^{\mathsf{T}}$ not only by allowing P to be doubly stochastic, but also allowing the left and right factors to be different matrices.

Definition 1.3 (*Semi-isomorphism*). Let G and H be graphs with adjacency matrices A and B respectively. We say that G is *semi-isomorphic* to H provided $A = SBR$ where S and R are doubly stochastic.

In Section 4 we relate semi-isomorphism to isomorphism of bipartite graphs.

1.1. Addendum: matrix theory background

We provide here definitions and results from matrix theory which we require in this paper. See also [1, 8, 19].

Every doubly stochastic matrix S can be written as a convex combination of permutation matrices, i.e.,

$$S = \sum_{i=1}^{t} \alpha_i P_i$$

where $\sum \alpha_i = 1$, the α_i's are positive and each P_i is a permutation matrix. This convex combination is known as a *Birkhoff representation of S*.

Let A be an $a_1 \times a_2$ matrix and B be a $b_1 \times b_2$ matrix. The *direct sum* of A and B, denoted $A \oplus B$ is the $(a_1 + b_1) \times (a_2 + b_2)$ matrix

$$A \oplus B = \begin{bmatrix} A & 0_{a_1, b_2} \\ 0_{b_1, a_2} & B \end{bmatrix}$$

where $0_{m,n}$ denotes an $m \times n$ matrix of 0's. If $M = A \oplus B$ then M is *decomposable*; moreover, we will also say that M is *decomposable* if we can write $PMQ = A \oplus B$ where P and Q are permutation matrices. (In other words, after applying row and/or column

permutations, M can be decomposed as a direct sum.) Otherwise (i.e., if no such permutations exist) we say M is *indecomposable*. Note that a 0, 1 matrix A is indecomposable if and only if the bipartite graph with adjacency matrix

$$\begin{bmatrix} 0 & A \\ A^{\mathsf{T}} & 0 \end{bmatrix}$$

is connected.

A matrix A is *irreducible* if the nonzero entries in A correspond to the nonzero entries in the adjacency matrix of a strongly connected diagraph. Irreducibility implies indecomposability.

The Perron–Frobenius theorem asserts that the eigenvalue of maximum modulus of an irreducible, nonnegative matrix is real, positive and unique (multiplicity one). Furthermore, its associated eigenvector can be taken to be positive.

2. Linear fractional isomorphism

As mentioned in the introduction, (linear) fractional isomorphism has been investigated previously. A 'complete set of invariants' for fractional isomorphism is known.

Let G and H be graphs with adjacency matrices A and B respectively. If $G \cong_f H$ there is not necessarily a bijection per se between the vertices of G and H. Instead, we have a triple, (A, S, B), where S is doubly stochastic and $AS = SB$. We may view S as a weighted bipartite graph linking graphs G and H. Assume that $V(G) = \{v_1, \ldots, v_n\}$ and $V(H) = \{w_1, \ldots, w_n\}$ are disjoint sets. Associate to S a weighted bipartite graph on $V(G) \cup V(H)$ with an edge from v_i to w_j if and only if $s_{ij} \neq 0$; take the weight of this edge to be s_{ij}. So as not to confuse them with the edges of G and H, we refer to the edges of S as *links*. That S is a *fractional isomorphism* implies that (1) for each vertex x of G or of H, the total weight of all links at x is 1 and (2) for every $v \in V(G)$ and $w \in V(H)$, the total weight of edge-link[3] paths from v to w equals the total weight of link-edge paths from v to w. Note that condition (1) is equivalent to S being doubly stochastic and condition (2) is equivalent to the condition that $AS = SB$.

To illustrate this viewpoint, in Fig. 1 we show fractionally isomorphic graphs G and H. In this example, the links all have weight $\frac{1}{2}$.

2.1. Equitable partitions

The main result on fractional isomorphism is that two graphs are fractionally isomorphic if and only if they have a 'common' *equitable* partition (defined below). This gives rise to a complete set of invariants for fractional isomorphism.

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[3] By an *edge-link* path we mean a path of length two, which starts at v, follows an edge of G and then transverses a link of S to w. The weight of such an edge-link path is simply the weight of the link. A *link-edge* path is defined analogously.
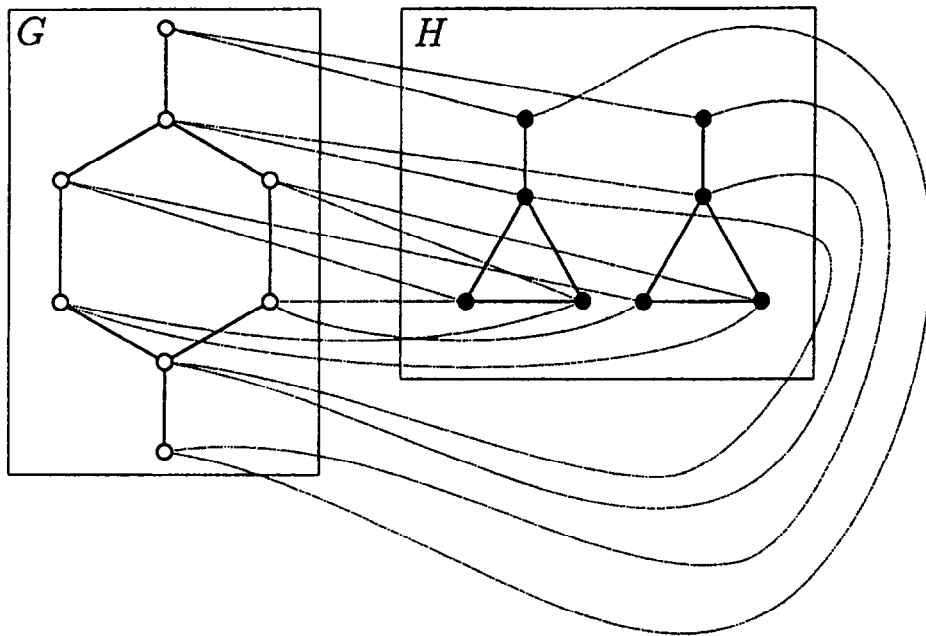
Fig. 1. Two fractionally isomorphic graphs. All links have weight $\frac{1}{2}$.

Let G be a graph. For $v \in V(G)$, we write $N(v)$ for the (open) neighborhood of v. A partition $\{C_1, C_2, \ldots, C_s\}$ of $V(G)$ is called *equitable* provided that for all i and j and for all $v, w \in C_i$, we have $|N(v) \cap C_j| = |N(w) \cap C_j|$

In other words, we have the following two conditions on the parts C_i. First, for each i, the induced subgraph $G[C_i]$ is regular. Second, for each $i \neq j$, the bipartite graph $G[C_i, C_j]$ (which has vertices $C_i \cup C_j$ and edges vw exactly when $v \in C_i$, $w \in C_j$ and $vw \in E(G)$) is *biregular*, i.e., all vertices in C_i have a common degree and all vertices in C_j have a (possibly different) common degree.

The notion of an *equitable partition* of a graph has been previously studied; see, e.g., [14, 16, 19]. See also [5] where they are called *feasible colorations*.

Every graph has an equitable partition: put each vertex in a class by itself. If G is regular, then the singleton $\{V(G)\}$ is an equitable partition. Equitable partitions of a graph are partially ordered under the usual 'is finer than' relation for partitions. The equitable partitions of a graph form a lattice (see [14, 15]). We refer to the maximum element of the equitable partition lattice as the *coarsest equitable* partition of G. (The coarsest equitable partition of a graph is called the *total degree partition* in [21] and simply the *degree partition* in [11].)

The main theorem is that fractionally isomorphic graphs G and H have a 'common' coarset equitable partition. Since G and H are different graphs, we need to make this a bit more precise.

Let $\mathcal{P} = \{C_1, \ldots, C_s\}$ be an equitable partition of a graph G. The *parameters* of $\mathcal{P}$ are a triple (s, n, D) where s is a scalar, n is a vector, and D is a matrix

satisfying:

- s is the number of parts in $\mathscr{P}$,
- $n=(n_1, n_2, \ldots, n_s)^{\mathrm{T}} \in R^s$ is a vector of positive integers whose ith entry, n_i, is the cardinality of C_i, and
- $D \in R^{s \times s}$ is matrix whose (i, j) entry is $d_{ij} = |N(x) \cap C_j|$ where x is any vertex in C_i. Note that $u^{\mathrm{T}} n = \sum n_i = |V(G)|$.

We say that two equitable partitions have the *same parameters* if we can order the parts of the partitions to give identical triples (s, n, D).

Note that if G has an equitable partition with parameters (s, n, D) then we can order the vertices of G so that its adjacency matrix has the following form:

$$A(G) = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1s} \\ A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ A_{s1} & A_{s2} & \cdots & A_{ss} \end{bmatrix}$$

where A_{ij} is an $n_i \times n_j$ matrix with row sums equal to d_{ij}. Note that $A_{ij}^{\mathrm{T}} = A_{ji}$, thus the column sums of A_{ij} equal d_{ji}. Considering the sum of all entries in A_{ij} we observe that

$$n_i d_{ij} = n_j d_{ji} .$$

2.2. Iterated degree sequences

The degree of a vertex v, denoted $d(v)$, is the number of edges incident at v. The *degree sequence* of G, which we denote $d(G)$, is the multiset[4] $\{d(v): v \in V(G)\}$. We generalize these definitions.

For a positive integer k, we define the kth *iterated degree* of a vertex $d_k(v)$ and the kth *iterated degree sequence* of a graph $d_k(G)$ as follows. For $k = 1$, we put $d_1(v) = d(v)$ and $d_1(G) = d(G)$, i.e., the first iterated degree of a vertex is simply its degree and the first iterated degree sequence of a graph is simply its degree sequence. For $k > 1$ we make the following assignments.

- Let $d_k(v)$ be the multiset $\{d_{k-1}(w): wv \in E(G)\}$, i.e., the multiset of $(k-1)$st iterated degrees of v's neighbors, and
- let $d_k(G)$ be the multiset $\{d_k(v): v \in V(G)\}$.

Finally, let $D(G)$ be the vector $[d_1(G), d_2(G), d_3(G), \ldots]$.

The iterated degree sequences are closely allied to equitable partitions as the following result explains.

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[4] Typically, the degree sequence is a sequence (as opposed to a multiset) giving a graph's degrees in, say, nondecreasing order. For our purposes, it is more natural to think of the degree sequence as a multiset. We maintain the word *sequence* as our subsequent definition is a generalization of the traditional degree sequence.

Theorem 2.1. *Let G and H be graphs on n vertices. The following statements are equivalent.*

(1) *G and H have a common coarsest equitable partition.*

(2) *$D(G) = D(H)$.*

(3) *$d_n(G) = d_n(H)$.*

This can be readily shown using the procedure of [11, p. 234].

2.3. Equivalent conditions for fractional isomorphism

The principal result on fractional isomorphism is that two graphs are fractionally isomorphic exactly when they share a common coarsest equitable partition.

Theorem 2.2. *Let G and H be graphs. The following are equivalent.*

(1) *G and H are fractionally isomorphic $(G \cong_f H)$.*

(2) *G and H have some common equitable partition.*

(3) *G and H have a common* coarsest *equitable partition.*

(4) *G and H have the same iterated degree sequences $(D(G) = D(H))$.*

Tinhofer [21] showed the equivalence of (1) and (3). Condition (2) is new in this paper. The equivalence of (3) and (4) is in Theorem 2.1 (see also [11]). For the sake of completeness we present a full proof of the equivalence of (1), (2) and (3).

Before we present the proof, we introduce the following lemma which is important in Section 3 as well. (See [7], [13, Chapter 1 and 2], and [9, Section 3.2]).

Lemma 2.3. *Let R and S be doubly stochastic matrices with Birkhoff representations $R = \sum_i \alpha_i P_i$ and $S = \sum_j \beta_j Q_j$.*

(1) *If there are vectors x and y with $x = Ry$ and $y = Sx$ then $x = P_i y$ and $y = Q_j x$ for all i and j.*

(2) *Let x and y be as in (1). If, in addition, either R or S is indecomposable, then there exists a scalar m with $x = y = mu$, where u is the vector of all 1's.*

(3) *If x and y are 0, 1-vectors, i.e., $x, y \in \{0, 1\}^n$, and $x = P_i y$ for all i.*

The key concept in the proof of this lemma is the following polyhedron (see [18]). Let $z \in R^n$. Let $\Pi(z)$ denote the convex hull of all vectors formed by permuting the entries in z. Note that the extreme points of $\Pi(z)$ are exactly z and all its permutations.

Proof of Lemma 2.3. Let R and S be given as in the statement of lemma. The condition $x = Ry = \sum \alpha_i P_i y$, implies that $x \in \Pi(y)$. Moreover, for any permutation matrix L, $Lx = \sum \alpha_i L P_i y$, so all permutations of x are also in $\Pi(y)$. Therefore $\Pi(x) \subseteq \Pi(y)$. Likewise, the condition $y = Sx$ implies $\Pi(y) \subseteq \Pi(x)$.

To prove (1), observe that we have $\Pi(x) = \Pi(y)$ and each of x and y are extreme points of this polyhedron. Therefore, since $x = \sum \alpha_i P_i y$ we must have each $P_i y = x$. Likewise, $y = Q_j x$ for every j.

For (2), suppose in addition that, say, S is indecomposable. If either x or y is 0, both are 0 and the conclusion is obvious (take $m=0$). So suppose x and y are both nonzero. From (1) we know $x=Py$ for a permutation matrix P. Thus $x=PSx$. Since S is indecomposable, so is PS; in particular, PS is nonnegative and irreducible. Thus by the Perron–Frobenius theorem, PS has a *unique* positive eignevector, which clearly is u, with associated eigenvalue $\lambda=1$. Now x is also an eigenvector of PS with eigenvalue 1, so by the uniqueness of λ, we must have $x=mu$ for some scalar m. Finally $y=Sx=Smu=mu=x$ as required.

For (3), we only assume $x=Ry$, but we also assume that x and y are 0, 1-vectors. Now $x=Ry$ implies $x \in \Pi(y)$. Moreover, $u^T x=u^T Ry=u^T y$, thus x and y have the same number of 1's. This implies that x is permutation of y and therefore an extreme point of $\Pi(y)$. Finally, $x=\sum \alpha_i P_i y$ therefore implies $P_i y=x$ for all i. $\square$

Proof of Theorem 2.2. We show $(1)\Rightarrow(2)$, $(2)\Rightarrow(1)$, and $(1,2)\Rightarrow(3)$. The implication $(3)\Rightarrow(2)$ is trivial. The equivalence $(3)\Leftrightarrow(4)$ is from Theorem 2.1.

$(1)\Rightarrow(2)$: Consider fractionally isomorphic graphs G and H. Let A and B be the adjacency matrices of G and H, and let S be doubly stochastic with $AS=SB$.

Notice that S induces a partition in each $V(G)$ and $V(H)$. We put two vertices u and v of G [resp. H] in a common block exactly when there is a path of *links* (i.e., edges of the weighted bipartite graph S) from u to v. Call these two partitions $\mathscr{P}_G$ and $\mathscr{P}_H$. Note that the parts in $\mathscr{P}_G$ [resp. $\mathscr{P}_H$] are in one-to-one correspondence with the indecomposable blocks of the matrix S. We may assume the vertices are suitably ordered so that S has a block form $S=S_1 \oplus \ldots \oplus S_s$ where S_i is an indecomposable $n_i \times n_i$ doubly stochastic matrix. It follows at once that $\mathscr{P}_G$ and $\mathscr{P}_H$ are partitions of $V(G)$ and $V(H)$, respectively, with s parts of sizes $n_1, n_2, \ldots, n_s$. Let $\mathscr{P}_G=\{V_1, \ldots, V_s\}$ and $\mathscr{P}_H=\{W_1, \ldots, W_s\}$ where V_i and W_i are linked.

We can partition matrices A and B according to the partitions $\mathscr{P}_G$ and $\mathscr{P}_H$. Since $AS=SB$ we have

$$A_{ij}S_j = S_i B_{ij} \tag{$*$}$$

for $1 \leqslant i, j \leqslant s$. Now we can also write $A_{ji}S_i=S_j B_{ji}$ and take transposes to give

$$S_i^T A_{ij} = B_{ij} S_j^T. \tag{$**$}$$

Let $d_{ij}^A=A_{ij}u$ and $d_{ij}^B=B_{ij}u$. Note that each coordinate of d_{ij}^A [resp. d_{ij}^B] gives the number of edges from the corresponding vertex in V_i [resp. W_i] to all vertices in V_j [resp. W_j]. Thus, our aim is to prove that $d_{ij}^A=d_{ij}^B=cu$ for some scalar c.

Multiplying equations $(*)$ and $(**)$ on the right by u we get

$$A_{ij}S_j u = S_i B_{ij} u \quad \Rightarrow \quad d_{ij}^A = S_i d_{ij}^B$$

$$S_i^T A_{ij} u = B_{ij} S_j^T u \quad \Rightarrow \quad S_i^T d_{ij}^A = d_{ij}^B.$$

Now, simply apply Lemma 2.3 to conclude $d_{ij}^A=d_{ij}^B=cu$ for some scalar c. (We can conveniently let the scalar c be called d_{ij}.) Thus the partitions $\mathscr{P}_G$ and $\mathscr{P}_H$ are equitable with parameters (s, n, D), thereby proving (2).

$(2) \Rightarrow (1)$: Suppose G and H have equitable partitions $\mathscr{P}$ and $\mathscr{P}'$ [respectively] with parameters $(s, \boldsymbol{n}, D)$. Thus G and H have the same number of vertices.

Let $V(G) = \{v_1, \ldots, v_n\}$ and $V(H) = \{w_1, \ldots, w_n\}$. We may assume the vertices are labelled so that the first n_1 vertices constitute the first part of $\mathscr{P}$ [resp. $\mathscr{P}'$], the second n_2 vertices constitute the second part, etc.

Let A and B be the adjacency matrices of G and H respectively. They have blocks A_{ij} [resp. B_{ij}] as described above. Note that A_{ij} and B_{ij} have the same size, the same row sums and the same column sums.

Write J_m to denote the $m \times m$ matrix of all 1's. Let $S_i = (1/n_i)J_{n_i}$. Let S be the block diagonal matrix $S_1 \oplus S_2 \oplus \cdots \oplus S_s$. Note that S is doubly stochastic.

Now AS can be written as

$$AS = \begin{bmatrix} A_{11}S_1 & A_{12}S_2 & \cdots & A_{1s}S_s \\ A_{21}S_1 & A_{22}S_2 & \cdots & A_{2s}S_s \\ \vdots & \vdots & \ddots & \vdots \\ A_{s1}S_1 & A_{s2}S_2 & \cdots & A_{ss}S_s \end{bmatrix},$$

and SB is given by

$$SB = \begin{bmatrix} S_1 B_{11} & S_1 B_{12} & \cdots & S_1 B_{1s} \\ S_2 B_{21} & S_2 B_{22} & \cdots & S_2 B_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ S_s B_{s1} & S_s B_{s2} & \cdots & S_s B_{ss} \end{bmatrix}.$$

Now because $n_i d_{ij} = n_j d_{ji}$ we have

$$A_{ij}S_j = \frac{d_{ij}}{n_j} J_{n_i \times n_j} = \frac{d_{ji}}{n_i} J_{n_i \times n_j} = S_i B_{ij}.$$

Thus $AS = SB$ and we conclude that G and H are fractionally isomorphic.

$(1, 2) \Rightarrow (3)$: Suppose G and H are fractionally isomorphic $(AS = SB)$ and have a common equitable partition. We want to show that not only do G and H have some equitable partitions with the same parameters, but that the *coarsest* equitable partitions of G and H have the same parameters as well.

Consider the coarsest equitable partition of G and let $(s, \boldsymbol{n}, D)$ be its parameters. We order the vertices of G as in the $(1) \Rightarrow (2)$ section of this proof and let R be a matrix built up from blocks $R_1 \oplus \cdots \oplus R_s$ where $R_i = (1/n_i)J_{n_i}$. Thus $AR = RA$, hence $ARS = RAS = RSB$.

Now one checks that $RS = R$. This follows for the following reasons: The indecomposable blocks of S correspond, as in the proof of $(1) \Rightarrow (2)$, to an equitable partition of G. Thus the blocks of S refine the blocks of R. Each block of R is a multiple of J (a matrix of all 1's) which, when multiplied by a (doubly stochastic) block of S, remains unchanged.

In summary, we have a new fractional isomorphism $AR = RB$. The difference is that the partition induced in G is the coarsest equitable partition. Thus, by the equivalence of (1) and (2), the coarsest equitable partition of G shares parameters with some equitable partition in H, and vice versa. Thus it follows that the coarsest equitable partitions of G and H are the same. This completes the proof. □

Given a graph G we can determine, in a mechanical way, all the graphs which are fractionally isomorphic to G. Order the vertices of G according to its coarsest equitable partition. Thus the adjacency matrix of G has the following structure:

$$A(G) = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1s} \\ A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ A_{s1} & A_{s2} & \cdots & A_{ss} \end{bmatrix}$$

where A_{ij} is an $n_i \times n_j$ matrix with row sums d_{ij}. We can from every graph fractionally isomorphic to G by the following substitution procedure.

(1) For each $1 \leqslant i \leqslant s$ select a d_{ii}-regular graph on n_i vertices. Let B_{ii} be its adjacency matrix.

(2) for each $1 \leqslant i < j \leqslant s$ find a bipartite graph $(X \cup Y, E)$ with $|X| = n_i$ and $|Y| = n_j$ in which each X vertex is adjacent to exactly d_{ij} of the Y vertices and each Y vertex is adjacent to d_{ij} of the X's. Let Bd_{ij} be its X, Y incidence matrix and let $B_{ji} = B_{ij}^{T}$.

(3) Finally, replace each A_{ij} block of $A(G)$ by the corresponding B_{ij}.

So created, the graph H with adjacency matrix B is fractionally isomorphic to G. Furthermore, every graph fractionally isomorphic to G has (up to row/column permutation) an adjacency matrix created by the above procedure.

2.4. Cospectrality and trees

We know that fractionally isomorphic graphs have the same degree sequence (and therefore the same number of vertices and edges). Further, it follows from Theorem 2.2 that the graphs must have a common maximum eigenvalue. So it seems natural to ask: If two graphs have the same degree sequence and the same eigenvalues[5], must it be the case that they are fractionally isomorphic? We show by the following example that the answer is 'no'. Let G and H be the trees in Fig. 2. Both trees have degree sequence $(3, 3, 2, 2, 2, 1, 1, 1, 1)$ and routine computations show they both have characteristic polynomial $x^9 - 8x^7 + 19x^5 - 14x^3 + 2x$, and are therefore cospectral. Further, these trees are clearly *not* isomorphic. [Thanks to Allen Schwenk for providing us with this pair of trees.]

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[5] Cospectrality is *not* a necessary condition for fractional isomorphism, but it seems natural to inquire to what extent it is sufficient.
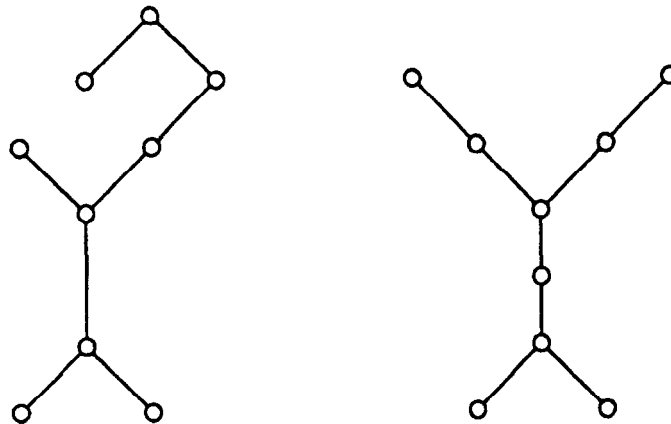
Fig. 2. Trees with equal degree sequences and spectra, but which are *not* fractionally isomorphic.

Below we show that fractionally isomorphic trees must be isomorphic (see Theorem 2.5). Thus the graphs in Fig. 2 have the same degree sequence and are cospectral, yet are not fractionally isomorphic.

In McKay's M.Sc. thesis [14] it is shown that the only equitable partitions of a forest F are those arising as the orbits of some group of automorphisms of F. We will show that *any* graph fractionally isomorphic to a forest F must be isomorphic to F.

We begin by showing that only forests can be fractionally isomorphic to forests.

Lemma 2.4. *Suppose that F and G are fractionally isomorphic graphs and that F is a forest. Then G is a forest.*

Proof. The proof is by induction on the number of edges in F. The result is trivial if F has no edges, so assume F has edges. By Theorem 2.2, F and G have a common coarsest equitable partition. Let L and M be the set of vertices of degree one in F and G, respectively. Note that L and M are nonempty, have the same number of elements, and consist of a union of blocks of the coarsest equitable partition. Let $F' = F \backslash L$ and $G' = G \backslash M$. Then the common coarsest equitable partition of F and G, restricted to the vertex sets of F' and G', form a common equitable partition of F' and G'. By Theorem 2.2, F' and G' are fractionally isomorphic. We infer from the induction hypothesis that G' is a forest. But G is obtained from G' by attaching vertices of degree one. Hence G is a forest. $\square$

We now show that the fractional isomorphism class of a forest is a singleton set, consisting of the forest alone. We require the following definition. A sequence of vertices in a forest is called *successful* if each vertex in the sequence is chosen to be adjacent to a previous vertex in the sequence, if such a choice is available.

Theorem 2.5. *Suppose that F and G are fractionally isomorphic graphs and that F is a forest. Then F is isomorphic to G.*

Proof. By Lemma 2.4, G must be a forest. By Theorem 2.2, F and G have a common coarsest equitable partition. Let $v_1, v_2, \ldots, v_n$ be a successful ordering of the vertices of F. For $v \in V(F)$ and $w \in V(G)$, write $v \sim w$ to mean that v and w are in corresponding blocks of the common coarsest equitable partition. We inductively choose $w_k \in V(G)$ for $1 \leqslant k \leqslant n$ so that the map $\phi: v_j \to w_j$ is an isomorphism from F to G.

Begin by letting w_1 be any vertex in $V(G)$ with $w_1 \sim v_1$. Assuming $w_1, w_2, \ldots, w_{k-1}$ have already been chosen, pick $w_k \in V(G)$ so that

(1) $w_k \neq w_j$ for $1 \leqslant j < k$;

(2) $w_k \sim v_k$;

(3) $\{w_1, w_2, \ldots, w_k\}$ is successful in G; and

(4) for $1 \leqslant j < k$, $v_j v_k \in E(F)$ if and only if $w_j w_k \in E(G)$.

Assuming for a moment that such choices can be made, it is clear that the resulting ϕ is an isomorphism.

To see that such a w_k exists, we consider two cases. First, suppose there is an index j with $1 \leqslant j < k$ such that $v_j v_k \in E(F)$. Suppose $v_j \in C_1$ and $v_k \in C_2$, where C_1, C_2 are blocks of the coarsest equitable partition. Since the parameter d_{12} is the same for both graphs and since the number of $v_i \in C_2$ with $1 \leqslant i < k$ and with $v_j v_i \in E(F)$ is the same as the number of $w_i \in C_2$ with $1 \leqslant i < k$ and with $w_j w_i \in E(G)$, there must remain at least one $w_k \in C_2$ with $w_j w_k \in E(G)$. Since $\{w_1, w_2, \ldots, w_{k-1}\}$ is successful, $w_i w_k \in E(G)$ for no i with $1 \leqslant i < k$ except for $i = j$. Because the ordering of the vertices of F was chosen to be successful, $v_i v_k \in E(F)$ for no i with $1 \leqslant i < k$ except for $i = j$. Hence w_k has the required properties.

If, on the other hand, there is no index j with $1 \leqslant j < k$ such that $v_j v_k \in E(F)$, then $\{v_1, v_2, \ldots, v_{k-1}\}$ must consist of entire components of the forest F. Let w_k be any vertex satisfying (1) and (2). That such a choice exists follows again from the common coarsest equitable partition. Properties (3) and (4) are automatic in this case. $\square$

3. Quadratic fractional isomorphism

Recall that for matrices A and B we have $A \to B$ provided $B = SAS^T$ for some doubly stochastic matrix S and $A \leftrightarrow B$ provided $B = SAS^T$ and $A = S^T BS$. Let G and H be graphs with adjacency matrices A and B. We say G is (1) *weakly*, (2) *ordinarily*, and (3) *strongly quadratically fractionally isomorphic* to H provided (1) $A \to B$, (2) $A \to B$ and $B \to A$, and (3) $A \leftrightarrow B$, respectively.

Theorem 3.1. *Let G and H be graphs. The following are equivalent.*

(1) *G is weakly quadratically fractionally isomorphic to H.*

(2) *G is quadratically fractionally isomorphic to H.*

(3) *G is strongly quadratically fractionally isomorphic to H.*

(4) *G is isomorphic to H.*

The key notion in our proof is the following operator. Let M_n denote the vector space of all $n \times n$ (real) matrices. For any two matrices $R, S \in M_n$ we define an operator

$f[R, S] : M_n \to M_n$ defined by

$$f[R, S](X) = R X S^\mathrm{T}.$$

It is clear that $f[R, S]$ is linear and can be expressed as an $n^2 \times n^2$ matrix whose ij, kl entry is given by

$$f[R, S]_{ij, kl} = R_{ik} S_{jl}.$$

(In other words, the matrix of $f[R, S]$ with respect to the standard basis for $\mathbf{R}^{n^2}$ is the Kronecker product $R \otimes S$.)

Lemma 3.2. *Let $f[R, S]$ be defined as above.*
  (1) $f[R, S]^\mathrm{T} = f[R^\mathrm{T}, S^\mathrm{T}]$.
  (2) *If R and S are doubly stochastic, then so is $f[R, S]$. Furthermore, if $R = \sum \alpha_i P_i$ and $S = \sum \beta_j P_j$ are Birkhoff representations of R and S, then*

$$\sum_{ij} \alpha_i \beta_j f[P_i, Q_j]$$

is a Birkhoff representation of $f[R, S]$.

Proof of Lemma 3.2. For (1) we simply compute:

$$(f[R, S]^\mathrm{T})_{ij, kl} = f[R, S]_{kl, ij} = R_{ki} S_{lj} = R_{ik}^\mathrm{T} S_{jl}^\mathrm{T} = f[R^\mathrm{T}, S^\mathrm{T}]_{ij, kl}.$$

For (2) suppose R and S are doubly stochastic. Since $f[R, S] \geqslant 0$,

$$f[R, S](J) = R J S^\mathrm{T} = J, \quad \text{and} \quad f[R, S]^\mathrm{T}(J) = R^\mathrm{T} J S = J,$$

it follows that $f[R, S]$ is also doubly stochastic.
  Let

$$R = \sum \alpha_i P_i \quad \text{and} \quad S = \sum \beta_j Q_j$$

for permutation matrices P_i and Q_j. Observe that

$$f[R, S](X) = R X S^\mathrm{T} = \sum_i \sum_j \alpha_i \beta_j P_i X Q_j^\mathrm{T} .$$

Since each $f[P_i, Q_j]$ is an $n^2 \times n^2$ permutation matrix,

$$f[R, S] = \sum_{i, j} \alpha_i \beta_j f[P_i, Q_j]$$

is a Birkhoff representation of $f[R, S]$. $\square$

Proof of Theorem 3.1. Let G and H be graphs with adjacency matrices A and B respectively.
  The implications $(4) \Rightarrow (3) \Rightarrow (2) \Rightarrow (1)$ are trivial. We prove both $(1) \Rightarrow (4)$ and $(2) \Rightarrow (4)$. In our proof of $(2) \Rightarrow (4)$ we make no assumption on the matrices A and B (they can be

arbitrary matrices). For the proof of (1)⇒(4) we need the fact that A and B are 0,1-matrices.

(1)⇒(4): We can write $A \rightarrow B$ as

$$B = f[S, S](A)$$

for some doubly stochastic matrix S. Let the Birkhoff representation of S be $S = \sum \alpha_i P_i$. By (2) of Lemma 3.2, $f[S, S] = \sum_{ij} \alpha_i \alpha_j f[P_i, P_j]$ is a Birkhoff representation. Since A and B are 0,1-matrices, apply (3) of Lemma 2.3 to see that $B = f[P_i, P_j](A)$ for all i and j. Taking $i = j$, we have $B = P_i A P_i^T$ for any i, hence $G \cong H$.

(2)⇒(4): As $A \rightarrow B$ and $B \rightarrow A$ we can write

$$B = f[R, R](A) \quad \text{and} \quad A = f[S, S](B)$$

for doubly stochastic R and S. Let $R = \sum \alpha_i P_i$ and $S = \sum \beta_k Q_k$ be Birkhoff representations of R and S respectively. Then

$$f[R, R] = \sum_{ij} \alpha_i \alpha_j f[P_i, P_j] \quad \text{and} \quad f[S, S] = \sum_{kl} \beta_k \beta_l f[Q_k, Q_l].$$

By (1) of Lemma 2.3,

$$B = f[P_i, P_j](A) \quad \text{and} \quad A = f[Q_k, Q_l](B)$$

for any i, j, k, l. In particular, $B = P_i A P_i^T$ for some i, so $G \cong H$.   □

4. Semi-isomorphism

It is tempting to weaken the condition $A \rightarrow B(B = SAS^T)$ even further and simply require $B = RAS$ for some pair of doubly stochastic matrices R and S, i.e., relax the requirement that $R = S^T$ in the definition of quadratic fractional isomorphism. We say that G is *semi-isomorphic* to H provided $B = RAS$ where A and B are the adjacency matrices of G and H respectively.

Following the arguments of Section 3, we see that since A and B are 0, 1 matrices, we have $B = PAQ$ for some pair of *permutation* matrices P and Q. We can rewrite this as $B = PQQ^TAQ$ and let $C = Q^TAQ$, giving $B = (PQ)C$. In other words, after a suitable renaming of the vertices, we form the adjacency matrix of H by permuting only the rows of G's adjacency matrix; this motivates the term *semi*-isomorphic.

There is another way to describe semi-isomorphism of graphs without mention of adjacency matrices. Recall that $N(v)$ denotes the set of vertices adjacent to v. Note that G and H are *isomorphic* graphs exactly when there is a bijection $\phi: V(G) \rightarrow V(H)$ so that $uv \in E(G)$ iff $\phi(u)\phi(v) \in E(H)$. Let $\phi^*: 2^{V(G)} \rightarrow 2^{V(H)}$ be the set-wise mapping induced by ϕ; that is, for $X \subseteq V(G)$ we put $\phi^*(X) = \{\phi(x) : x \in X\}$. Thus a bijection ϕ is an isomorphism provided $\phi^*[N(v)] = N[\phi(v)]$ for all $v \in V(G)$.

Let $N(G)$ denote the *multiset* of neighborhoods of G, that is $N(G) = \{N(v) : v \in V(G)\}$. If two vertices have the same neighborhood, they are included twice in $N(G)$. Thus

a bijection $\phi: V(G) \to V(W)$ is an isomorphism provided ϕ^* is a bijection from $N(G)$ onto $N(H)$ with one further condition: for every $v \in V(G)$, if $\phi(v) = w$, then $\phi^*[N(v)] = N(w)$.

For *semi-isomorphism* we simply drop the side condition: G is semi-isomorphic to H exactly when there is a bijection $\phi: V(G) \to V(H)$ so that ϕ^* is a bijection between $N(G)$ and $N(H)$.

In other words, two graphs are semi-isomorphic if they can be relabeled so that the neighborhood lists for both graphs are identical. In Fig. 3 graphs C_6 and $2K_3$ are labeled so that $N(C_6) = N(2K_3)$ thereby showing they are semi-isomorphic.

Semi-isomorphism lies 'between' isomorphism and (linear) fractional isomorphism.

Theorem 4.1. *Consider the following statements about graphs G and H:*

(1) *G is isomorphic to H.*

(2) *G is semi-isomorphic to H.*

(3) *G is (linearly) fractionally isomorphic to H.*

Then $(1) \Rightarrow (2) \Rightarrow (3)$, *but neither implication can be reversed.*

Proof. The implication $(1) \Rightarrow (2)$ is trivial. To show $(2) \Rightarrow (3)$ suppose G is semi-isomorphic to H. Then $B = PAQ^T$ for permutation matrices P and Q, hence $BQ = PA$. Taking transposes, we have $B = QAP^T$, hence $BP = QA$. This gives $AS = SB$ where $S = \frac{1}{2}(P + Q)$, hence G is fractionally isomorphic to H.

We show that (2) does not imply (1) by the following example. Let

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Put

$$A = \begin{bmatrix} 0 & I & H \\ I & 0 & I \\ H & I & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & H & I \\ H & 0 & H \\ I & H & 0 \end{bmatrix}, \quad \text{and} \quad P = \begin{bmatrix} H & 0 & 0 \\ 0 & H & 0 \\ 0 & 0 & H \end{bmatrix}.$$

Note that $B = PAI_6$, but A and B are not adjacency matrices of isomorphic graphs; A is the adjacency matrix of C_6, while B is an adjacency matrix of $2K_3$ (see Fig. 3).
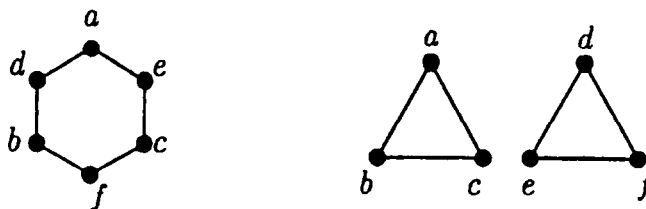

Fig. 3. Semi-isomorphic graphs C_6 and $2K_3$ which have been labeled so that $N(C_6) = N(2K_3) = \{\{a, b\}, \{a, c\}, \{b, c\}, \{d, e\}, \{d, f\}, \{e, f\}\}$.

To show that (3) does not imply (2), let $G = C_7$ and $H = C_4 + C_3$. As both graphs are 2-regular, they are fractionally isomorphic. However, the adjacency matrices of G and H are, respectively, nonsingular and singular. Were G and H semi-isomorphic, their adjacency matrices would have (up to sign) the same determinant. Thus G and H are not semi-isomorphic. $\square$

An alternative way to see that $G = C_7$ is not semi-isomorphic to $H = C_4 + C_3$ is to observe that H has a pair of identical neighborhoods, while no two neighborhoods of G are the same.

The notion of semi-isomorphism can be reduced to isomorphism by the following construction. Given a graph G, with $V(G) = \{v_1, \dots, v_n\}$, define a new bipartite graph, $B(G)$ with vertex set $\{x_1, \dots, x_n, y_1, \dots, y_n\}$ in which $x_i y_j$ is an edge iff $v_i v_j$ is an edge of the original graph G. In matrix terms, if A is the adjacency matrix of G, then the adjacency matrix of $B(G)$ is

$$\begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix}.$$

Theorem 4.2. *Graphs G and H are semi-isomorphic if and only if $B(G)$ and $B(H)$ are isomorphic.*

Proof. Let the adjacency matrices of G and H be A and B respectively.

Suppose G is semi-isomorphic to H, i.e., $A = PBQ$ for permutation matrices P and Q. Then check that

$$\begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix} = \begin{bmatrix} P & 0 \\ 0 & Q^T \end{bmatrix} \cdot \begin{bmatrix} 0 & B \\ B & 0 \end{bmatrix} \cdot \begin{bmatrix} P^T & 0 \\ 0 & Q \end{bmatrix}$$

proving that $B(G)$ and $B(H)$ are isomorphic.

To prove the opposite assertion we consider first the case that $B(G)$ and $B(H)$ are connected and $B(G) \cong B(H)$. Thus we can write

$$\begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \cdot \begin{bmatrix} 0 & B \\ B & 0 \end{bmatrix} \cdot \begin{bmatrix} P_{11}^T & P_{21}^T \\ P_{12}^T & P_{22}^T \end{bmatrix}.$$

From this we derive that $A = P_{12} B P_{21}^T + P_{11} B P_{22}^T$. Since $B(G)$ and $B(H)$ are isomorphic, connected bipartite graphs, it must be the case that the isomorphism preserves the bipartition. Thus either $P_{11} = P_{22} = 0$ or $P_{12} = P_{21} = 0$. In the first case $P_{12} B P_{21}^T = A$ and in the second case $P_{11} B P_{22}^T = A$.

In case $B(G)$ and $B(H)$ are not connected the above analysis can be applied to their (necessary pairwise isomoprhic) connected components. $\square$

Theorem 4.2 gives necessary and sufficient conditions for graphs to be semi-isomorphic. In case the graphs in question are both bipartite, semi-isomorphism implies isomorphism.

Corollary 4.3. *If G and H are bipartite graphs, then G is semi-isomorphic to H if and only if G is isomorphic to H.*

Proof. Observe that when G is biprartite, $B(G) \cong 2G$. Thus if bipartite graphs G and H are semi-isomorphic we have $2G \cong B(G) \cong B(H) \cong 2H$ and $G \cong H$. The reverse implication is trivial.   □

Note that the requirement that *both* G and H be bipartite cannot, in general, be relaxed to *at least one of* G or H be bipartite, as the example $G = C_6$ and $H = 2K_3$ shows.

4.1. Computational complexity

The problem of determining whether or not two given graphs are isomorphic has a celebrated history in the computer science literature. In particular, it is unknown if this problem can be solved in polynomial time, or is NP-complete, or of some other computational complexity. What can we say about the problems of determining whether two given graphs are fractionally isomorphic or semi-isomorphic?

To be a bit more formal, let us define the SEMI-ISOMORPHISM problem as follows:

Problem: SEMI-ISOMORPHISM
Instance: Two graphs G and H.
Question: Are G and H semi-isomorphic?

The FRACTIONAL ISOMORPHISM problem, ISOMORPHISM problem, etc. are defined similarly.

By linear programming, or by use of Theorem 2.2, we observe that the FRACTIONAL ISOMORPHISM decision problem can be resolved in polynomial time. The QUADRATIC FRACTIONAL ISOMORPHISM problem is identical to the ISOMORPHISM problem, so they are of the same computational complexity. Finally, we can use Corollary 2.3 to show that the SEMI-ISOMORPHISM and the ISOMORPHISM problems have the same computational complexity.

Corollary 4.4. *The SEMI-ISOMORPHISM problem and the ISOMORPHISM problem are polynomially equivalent.*

Proof. By [2] the BIPARTITE ISOMORPHISM problem is polynomially equivalent to the ISOMORPHISM problem. The corollary is now immediate by Corollary 4.3.   □

5. Remarks and problems

Although our main results are stated in terms of graphs, most have a broader interpretation. Theorem 2.2 remains true if G and H have 'adjacency' matrices which

are arbitrary symmetric matrices. If these matrices are populated by nonnegative integer values, our interpretation can be that they are the adjacency matrices of multigraphs. If the matrices have non-negative *real* entries, one might dare say that our results are about 'fuzzy multigraphs' in which having a fractional number of edges between vertices makes sense.

In Theorem 3.1 the equivalence of statements (2), (3) and (4) remains true when the adjacency matrices of G and H are replaced by arbitrary matrices. The equivalence of (1) with the other statements does require that the matrices have 0, 1-entries, but does not require symmetry. Thus this theorem extends to digraphs.

5.1. Algorithmic implications

An interesting aspect of Theorem 3.1 is that it offers a new approach to the graph isomorphism problem. The problem of determining if graphs G and H can be expressed as the feasibility of a system of quadratic and linear equations and linear inequalities:

$$A = SBS^T \qquad Su = u \qquad S^T u = u$$

$$S \geqslant 0$$

Nonlinear programming methods are being developed for the solution of this sort of nonlinear system. It is not clear at this point whether these approaches will lead to a polynomial time algorithm for graph isomorphism.

5.2. Reconstruction

The celebrated graph reconstruction problem asks: Let G and H be graphs with vertex sets $v_1, \ldots, v_n$ and $w_1, \ldots, w_n$ (with $n > 2$) such that $G - v_i \cong H - w_i$ for all i. Such graphs are called *hypomorphic*. Must it be the case that $G \cong H$?

We pose two fractional versions of this problem.

First, must hypomorphic graphs be fractionally isomorphic? Partial evidence in favor of this weaker version of the reconstruction problem is the fact that hypomorphic graphs must share the same degree sequence and the same degree sequence (in the notation of Section 2, $d_1(G) = d_1(H)$ and $d_2(G) = d_2(H)$); see [12] or [17],

Second, are *fractionally* hypomorphic graphs fractionally isomorphic? By this we mean to ask if $G \cong_f H$ whenever $G - v_i \cong_f H - w_i$ for all i.

5.3. Walk generating functions

Let $w_k(v)$ denote the number of walks of length k starting at v. Let

$$f_v(x) = \sum_{k=0}^{\infty} w_k(v) x^k.$$

Finally, let $f_G(x)$ denote the vector of $f_v(x)$'s. It is not hard to show that if $G \cong_f H$, then $f_G(x)$ is simply a permutation of $f_H(x)$. The question is, does the converse hold? In other words, if the walk generating functions of the vertices of G are the same as the walk generating functions of the vertices of H, must G and H be fractionally isomorphic? We can show that the answer is 'yes' in some special cases, namely: (1) if all the vertices have the same degree (hence all entries in $f_G(x)$ are the same), (2) if there are only two distinct entries in $f_G(x)$, and (3) if no two vertices of G [resp. H] have the same walk generating function (i.e., all entries in $f_G(x)$ are distinct).

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