

Locally constrained graph homomorphisms and equitable partitions ^{*}

Jiří Fiala ^a, Daniël Paulusma ^b, and Jan Arne Telle ^c

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^a Charles University, Faculty of Mathematics and Physics,
DIMATIA and Institute for Theoretical Computer Science (ITI)
Malostranské nám. 2/25, 118 00, Prague, Czech Republic. ¹
fiala@kam.mff.cuni.cz

^b Department of Computer Science, Durham University,
Science Laboratories, South Road,
Durham DH1 3EY, England.
daniel.paulusma@durham.ac.uk

^c Department of Informatics, University of Bergen,
N-5020 Bergen, Norway
telle@ii.uib.no

Abstract

We explore the connection between locally constrained graph homomorphisms and degree matrices arising from an equitable partition of a graph. We provide several equivalent characterizations of degree matrices. As a consequence we can efficiently check whether a given matrix M is a degree matrix of some graph and also compute the size of a smallest graph for which it is a degree matrix in polynomial time. We extend the well-known connection between degree *refinement* matrices of graphs and locally bijective graph homomorphisms to locally injective and locally surjective homomorphisms by showing that also these latter types of homomorphisms impose a quasiorder on degree matrices and a partial order on degree refinement matrices. Computing the degree refinement matrix of a graph is easy, and an algorithm deciding comparability of two matrices in one of these partial orders could be used as a heuristic for deciding whether a graph G allows a homomorphism of the given type to H . For local surjectivity and injectivity we show that the problem of matrix comparability belongs to the complexity class NP.

Keywords: locally constrained graph homomorphism, partial order, degree matrix, computational complexity.

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1 Introduction

Graph homomorphisms have a great deal of applications in graph theory, computer science and other fields. Beyond these computational aspects they give rise to interesting structural properties on graphs, e.g. existence of homomorphism imposes a quasiorder on the class of all graphs, which can be factorized into a partial order on the cores, see the recent monograph [18]. In this paper

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we study similar structural properties derived from *locally constrained* graph homomorphisms [10], where for any vertex u the mapping $f : V_G \rightarrow V_H$ induces a function from the neighborhood of u to the neighborhood of $f(u)$ which is required to be either *bijective* [1, 20], *injective* [11, 12], or *surjective* [15, 21]. We then write $G \xrightarrow{B} H$, $G \xrightarrow{I} H$ and $G \xrightarrow{S} H$, respectively.

The locally bijective homomorphisms, also called graph coverings, originally arose in topological graph theory [4, 23], and have applications in distributed computing [6], in recognizing graphs by networks of processors [2, 3], and in constructing highly transitive regular graphs [5]. The locally injective homomorphisms, also called partial graph coverings, have been studied due to their applications in models of telecommunication [12], in distance constrained labelings of graphs [13] with applications to frequency assignment, and as indicators of the existence of homomorphisms of derivate graphs (line graphs) [24]. The locally surjective homomorphisms, also called role assignments, have applications both in distributed computing [8] and social science [9, 25, 26].

A main computational issue is the one of dichotomy (cf. [17]), i.e., for every graph H classifying the decision problem whether an input graph G has a homomorphism of given type to the fixed graph H as either NP-complete or polynomially solvable. For the locally surjective homomorphisms this classification is known [15], with the problem for every connected H on at least three vertices being NP-complete. For the locally bijective and injective cases there are many partial results, see e.g. [12, 20], but even conjecturing a classification for these two cases is problematic.

An equitable partition of a connected graph G is a partition B_1, \dots, B_k of its vertex set such that any vertex in B_i has the same number $m_{i,j}$ of neighbors in B_j , and we call the matrix $M = \{m_{i,j}\}$ a degree matrix ($1 \leq i, j \leq k$). The degree refinement matrix of a graph G , which can be computed efficiently, is the degree matrix corresponding to the coarsest equitable partition of G . See Figure 1 for a Venn diagram depicting the relation between degree matrices, adjacency matrices and degree refinement matrices. The existence of a locally bijective homomorphism between two graphs implies equality of their degree refinement matrices, and this check for equality forms a well-known heuristic to the question if $G \xrightarrow{B} H$, in particular for the special case of graph isomorphism. In this paper we extend this connection to degree matrices, and we show a connection also between degree refinement matrices and both locally injective and surjective graph homomorphisms.

Our paper is organised as follows. In Section 2 we show that, on the set of connected graphs \mathcal{C} , the three relations $(\mathcal{C}, \xrightarrow{B})$, $(\mathcal{C}, \xrightarrow{I})$ and $(\mathcal{C}, \xrightarrow{S})$ imposed by the existence of a locally constrained graph homomorphism of given type between two graphs are partial orders. In Section 3 we introduce the class \mathcal{M} of degree matrices of connected graphs and present three equivalent characterizations of these matrices. As a consequence we can efficiently check whether a given matrix M is a degree matrix and also compute the size of a smallest graph having degree matrix M . In subsection 3.2 we define three relations $(\mathcal{M}, \xrightarrow{\exists B})$, $(\mathcal{M}, \xrightarrow{\exists I})$ and $(\mathcal{M}, \xrightarrow{\exists S})$ imposed on degree matrices by the existence of graph homomorphisms of given local constraint, e.g. $M \xrightarrow{\exists B} N$ if and only if $\exists G, H \in \mathcal{C} : G \xrightarrow{B} H$ with G and H having degree matrix M and N , respectively. In Section 4 we introduce the class of degree refinement matrices $\mathcal{M}' \subset \mathcal{M}$. We show that the induced relations $(\mathcal{M}', \xrightarrow{\exists B})$, $(\mathcal{M}', \xrightarrow{\exists I})$ and $(\mathcal{M}', \xrightarrow{\exists S})$ are partial orders. These results generalize the use of degree refinement matrices to locally injective and locally surjective homomorphisms.

In Section 5 we give a polynomial-time algorithm that takes as input two degree matrices M and N and decides if $M \xrightarrow{\exists B} N$. In Sections 6 and 7 we prove that the analogous decision problems for $M \xrightarrow{\exists I} N$ and $M \xrightarrow{\exists S} N$ both belong to the complexity class NP. As the size of matrices M and N with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ for some given graphs G and H could be independent of the size of G and H , even these NP algorithms might be plausible as a heuristic for the questions if $G \xrightarrow{I} H$ or $G \xrightarrow{S} H$. Moreover, we consider the universal cover of a graph, defined in subsection 2.2, also known as the infinite unfolding of a graph. As mentioned earlier, $G \xrightarrow{B} H$ is conditioned

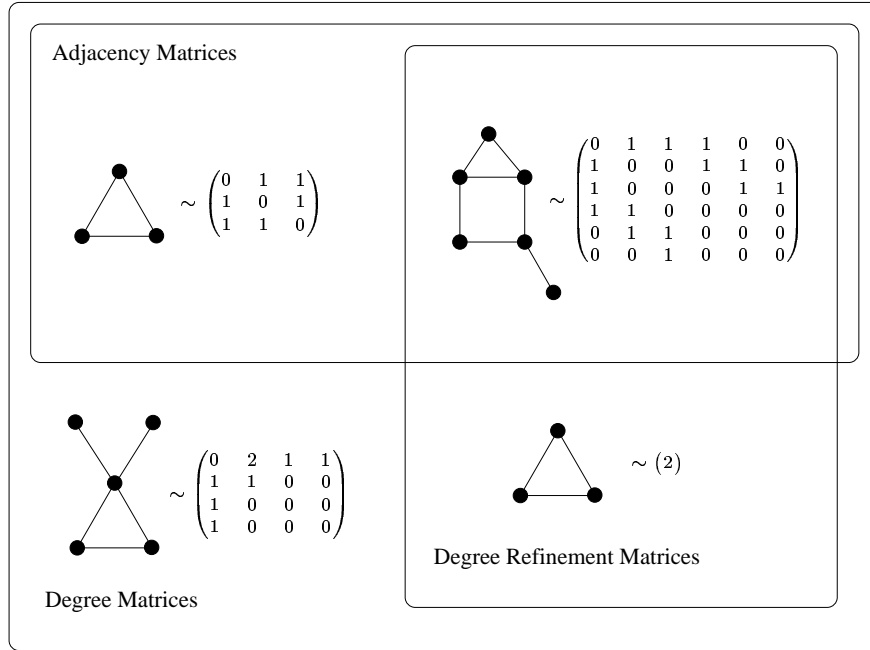


Figure 1: Examples of degree matrices, adjacency matrices and degree refinement matrices.

by the equivalence of the degree refinement matrices of G and H , and this can also be expressed as an isomorphism between the universal covers of G and H [22]. In subsection 6.2 we use the proof technique established in subsection 6.1 to disprove a conjecture that would have established a similarly strong connection between locally injective graph homomorphisms and universal cover inclusion.

2 Graphs

If not stated otherwise graphs considered in this paper are finite and *simple*, i.e. without loops and multiple edges. For graph terminology not defined below we refer to [7].

A graph H is a *subgraph* of a graph G denoted by $H \subseteq G$ if $V_G \subseteq V_H$ and $E_G \subseteq E_H$.

For a mapping $f : V_G \rightarrow V_H$ and a set $S \subseteq V_G$ we use the shorthand notation $f(S)$ to denote the image set of S under f , i.e., $f(S) = \{f(u) \mid u \in S\}$. For any $x \in V_H$, the set $f^{-1}(x)$ is equal to $\{u \in V_G \mid f(u) = x\}$.

For a vertex $u \in V_G$, we denote its *neighborhood* by $N_G(u) = \{v \mid (u, v) \in E_G\}$. A *k-regular* graph is a graph, where all vertices have k neighbors (i.e. are of *degree k*). A *(k, l)-regular bipartite* graph is a bipartite graph where vertices of one class of the bipartition are of degree k and all others are of degree l .

A *complete* graph is a graph with an edge between every pair of vertices. The complete graph on n vertices is denoted by K_n .

A *graph homomorphism* from $G = (V_G, E_G)$ to $H = (V_H, E_H)$ is a vertex mapping $f : V_G \rightarrow V_H$ satisfying the property that for any edge (u, v) in E_G , we have $(f(u), f(v))$ in E_H as well, i.e., $f(N_G(u)) \subseteq N_H(f(u))$ for all $u \in V_G$. Two graphs G and G' are called *isomorphic*, denoted by $G \simeq G'$, if there exists a one-to-one mapping $f : V_G \rightarrow V_{G'}$, where both f and f^{-1} are homomorphisms.

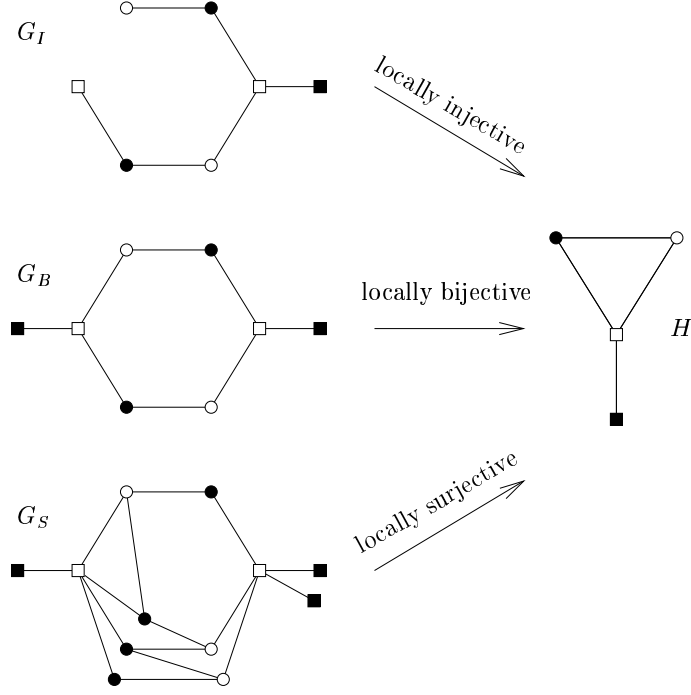


Figure 2: Examples of locally constrained homomorphisms.

Definition 1 For graphs G and H we denote:

- $G \xrightarrow{B} H$ if there exists a so-called locally bijective homomorphism $f : V_G \rightarrow V_H$ satisfying:

$$\text{for all } u \in V_G : f(N_G(u)) = N_H(f(u)) \text{ and } |f(N_G(u))| = |N_G(u)|.$$

- $G \xrightarrow{I} H$ if there exists a so-called locally injective homomorphism $f : V_G \rightarrow V_H$ satisfying:

$$\text{for all } u \in V_G : |f(N_G(u))| = |N_G(u)|.$$

- $G \xrightarrow{S} H$ if there exists a so-called locally surjective homomorphism $f : V_G \rightarrow V_H$ satisfying:

$$\text{for all } u \in V_G : f(N_G(u)) = N_H(f(u)).$$

See Figure 2 for an example. Note that a locally bijective homomorphism is both locally injective and surjective. Hence, any result valid for locally injective or for locally surjective homomorphisms is also valid for locally bijective homomorphisms. We provide an alternative definition of these three kinds of mappings via subgraphs induced by preimages of edges. As far as we know this quite natural definition has not previously appeared in the literature.

Observation 2 Let $f : G \rightarrow H$ be a graph homomorphism. For every edge (x, y) of H , the bipartite subgraph of G induced by the set $f^{-1}(x) \cup f^{-1}(y)$ is

- a perfect matching *if and only if* f is locally bijective,
- of maximum degree one (*i.e.* a matching) *if and only if* f is locally injective,
- of minimum degree one *if and only if* f is locally surjective.

Note that for locally bijective homomorphisms from a graph G to a connected graph H the preimage classes all have the same size and for locally surjective homomorphisms all the preimage classes have size at least one. This yields the following observation:

Observation 3 *Let G be a graph and H be a connected graph. If $G \xrightarrow{S} H$, then either $|V_G| > |V_H|$ or else $G \simeq H$.*

In our paper we frequently involve the following two useful statements:

Proposition 4 ([20]) *For two graphs G, H holds that $G \xrightarrow{I} H$ if and only if G is a subgraph of a graph H' with $H' \xrightarrow{B} H$.*

Theorem 5 ([14]) *Let G be a, possibly infinite, graph and let H be a connected graph. If G allows both a locally injective and a locally surjective homomorphism to H , then both these homomorphisms are locally bijective.*

2.1 Partial orders on graphs

It is well-known that graph homomorphisms define a quasiorder on the class of all graphs, which can be factorized into a partial order on the so-called cores, see e.g. the recent monograph [18]. In contrast, we consider all isomorphism classes of *connected* graphs. We assume that each of these classes is represented by one of its elements, and these representatives form the set \mathcal{C} , called the *set of connected graphs*. We view \xrightarrow{B} , \xrightarrow{I} and \xrightarrow{S} as binary relations on \mathcal{C} , denoted by $(\mathcal{C}, \xrightarrow{*})$, where $*$ indicates the appropriate local constraint, and now show that $(\mathcal{C}, \xrightarrow{*})$ is a partial order for any local constraint $* \in \{B, I, S\}$.

Observe first that for any $G \in \mathcal{C}$ the identity mapping $\text{id} : V_G \rightarrow V_G$ clarifies that all three relations $\xrightarrow{*}$ are *reflexive*.

The composition of two graph homomorphisms of the same kind of local constraint (B, I, S) is again a graph homomorphism of the same kind. Hence each $\xrightarrow{*}$ is also *transitive*.

For antisymmetry, suppose for $G, H \in \mathcal{C}$ that $f : G \xrightarrow{*} H$, $g : H \xrightarrow{*} G$, where f, g are of the same local constraint. For $* \in \{B, S\}$ we can invoke Observation 3 to conclude that $G \simeq H$.

For $* = I$ we have $g \circ f : G \xrightarrow{I} G$ and $\text{id} : G \xrightarrow{S} G$ by the identity mapping id . Then, by Theorem 5, the mapping $g \circ f$ is locally bijective. Since G is in \mathcal{C} , we deduce that $(g \circ f)(V_G) = V_G$. This implies that f is (globally) injective. By the same argument we find that $f \circ g : H \xrightarrow{I} H$ is locally bijective. Since H is in \mathcal{C} , we deduce that $(f \circ g)(V_H) = V_H$. This implies that f is (globally) surjective. Hence, f is a graph isomorphism from G to H . So, all three relations are *antisymmetric*. We would like to mention that the antisymmetry of \xrightarrow{I} also follows from an iterative argument of [24].

Combining the results above with Theorem 5 yields the following.

Theorem 6 $(\mathcal{C}, \xrightarrow{B})$, $(\mathcal{C}, \xrightarrow{I})$ and $(\mathcal{C}, \xrightarrow{S})$ are partial orders with $(\mathcal{C}, \xrightarrow{B}) = (\mathcal{C}, \xrightarrow{I}) \cap (\mathcal{C}, \xrightarrow{S})$.

2.2 Universal covers of graphs

For a connected graph G , the *universal cover* T_G is defined in [2] as follows. The vertices of T_G can be represented as walks in G starting in a fixed vertex u that do not traverse the same edge in two consecutive steps. Edges in T_G connect those walks that differ in the presence of the last edge. The universal cover T_G will be infinite whenever G is not a tree. The mapping $T_G \xrightarrow{B} G$ sending a vertex representing a walk in G to the last vertex of that walk is a locally bijective homomorphism.

Proposition 7 ([2]) *For any graph $G \in \mathcal{C}$ the universal cover is the unique tree (up to isomorphism) that allows $T_G \xrightarrow{B} G$.*

Trivially, a homomorphism from a graph G to a graph H translates into a homomorphism from T_G to T_H , and the following lemma will be useful.

Lemma 8 ([14]) *Let G and H be graphs in \mathcal{C} . If $G \xrightarrow{*} H$, then $T_G \xrightarrow{*} T_H$ for $*$ $\in \{B, I, S\}$.*

The following result follows from Lemma 8 and a simple inductive argument on the two trees T_G and T_H .

Corollary 9 *Let G and H be graphs in \mathcal{C} . If $G \xrightarrow{I} H$ then $T_G \subseteq T_H$, and if $G \xrightarrow{S} H$ then $T_H \subseteq T_G$.*

3 Degree matrices

Any locally bijective graph homomorphism preserves not only vertex degrees but also degrees of neighbors and degrees of neighbors of these neighbors and so on. To capture this property the following notion will be useful. For a matrix M we denote $M_{i,j} = m_{i,j}$ throughout the rest of the paper.

Definition 10 *We call a square matrix M of order k a degree matrix of a connected graph G and write $G \xrightarrow{B} M$ if there is a so-called equitable partition of V_G into blocks $\mathcal{B} = B_1, \dots, B_k$ that, for every i and $u \in B_i$, satisfies:*

$$\forall j : |N_G(u) \cap B_j| = m_{i,j}. \quad (1)$$

Equitable partitions are well-known, see e.g. [16, 27], and although the associated matrices have also been considered we did not find an established terminology for them. Note that degree matrices of disconnected graphs can be defined in the same way, and a graph G can allow several degree matrices, with an adjacency matrix itself being the largest one, and the smallest one being its *degree refinement matrix*, as defined in Section 4 (this latter connection explains our choice of terminology). We let \mathcal{M} be the *set of degree matrices of connected graphs*, i.e., a matrix M is in \mathcal{M} if and only if there exists a nonempty graph $G \in \mathcal{C}$ such that $G \xrightarrow{B} M$. Note that, by definition, whenever we write $G \xrightarrow{B} M$, the graph G is a connected graph (which implies M is in \mathcal{M}). The relation $G \xrightarrow{B} M$ can be viewed as an extension of the locally bijective graph homomorphisms to the codomain \mathcal{M} , by the following observation.

Observation 11 *Let $\text{adj}(H)$ be an adjacency matrix of a connected graph H . Then $G \xrightarrow{B} H$ if and only if $G \xrightarrow{B} \text{adj}(H)$.*

Proof: Assume $V_H = \{v_1, \dots, v_k\}$. Any partition $\{B_1, \dots, B_k\}$ of V_G satisfying equation (1) for $M = \text{adj}(H)$ is in one-to-one correspondence to a locally bijective homomorphism $f : G \xrightarrow{B} H$ such that $f(B_i) = v_i$. \square

We also extend the locally injective and surjective graph homomorphisms to the codomain of degree matrices.

Definition 12 Let G be a connected graph and let $M \in \mathcal{M}$ be a degree matrix of order k . We write $G \xrightarrow{I} M$ if there is a partition of V_G into blocks B_1, \dots, B_k that, for every i and $u \in B_i$, satisfies:

$$\forall j : |N_G(u) \cap B_j| \leq m_{i,j}. \quad (2)$$

Definition 13 Let G be a connected graph and let $M \in \mathcal{M}$ be a degree matrix of order k . We write $G \xrightarrow{S} M$ if there is a partition of V_G into blocks B_1, \dots, B_k that, for every i and $u \in B_i$, satisfies:

$$\forall j : |N_G(u) \cap B_j| \begin{cases} = 0 & \text{if } m_{i,j} = 0 \\ \geq m_{i,j} & \text{if } m_{i,j} > 0. \end{cases} \quad (3)$$

Observation 14 Let $\text{adj}(H)$ be an adjacency matrix of a connected graph H . Then $G \xrightarrow{S} H$ if and only if $G \xrightarrow{S} \text{adj}(H)$ and $G \xrightarrow{I} H$ if and only if $G \xrightarrow{I} \text{adj}(H)$.

3.1 A characterization of degree matrices

As a first step we make the following observation, which is easy to see.

Observation 15 For a graph G and degree matrix M of order k , let $G \xrightarrow{B} M$ by equitable partition $\mathcal{B} = B_1, \dots, B_k$ as in Definition 10. Then $m_{i,j}|B_i| = m_{j,i}|B_j|$ for all $1 \leq i < j \leq k$.

This immediately implies that for any degree matrix $M \in \mathcal{M}$ of order k ,

$$m_{i,j} > 0 \text{ if and only if } m_{j,i} > 0 \text{ for all } 1 \leq i < j \leq k.$$

We call integer matrices that have the above property *zero-symmetric*. There exist zero-symmetric matrices that are *not* in \mathcal{M} . Take for example

$$M = \begin{pmatrix} 0 & 2 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

It is easy to see that M is not in \mathcal{M} : due to equation (1) the vertex set V_G of any graph G with $G \xrightarrow{B} M$ can be partitioned into blocks B_1, B_2, B_3 with $2|B_1| = |B_2| = |B_3| = |B_1|$, which would result in G being empty. Note that M is not a degree matrix of a disconnected graph either. The fact that \mathcal{M} is not trivially characterized makes the following decision problem interesting.

DEGREE MATRIX DETERMINATION

Instance: A matrix M .

Question: Is $M \in \mathcal{M}$?

To determine the complexity of the above problem we will characterize degree matrices and therefore introduce the following definitions. A directed graph $D = (V_D, E_D)$ with possibly loops is called *symmetric* if there exists an arc $(j, i) \in E_D$ whenever there exists an arc $(i, j) \in E_D$.

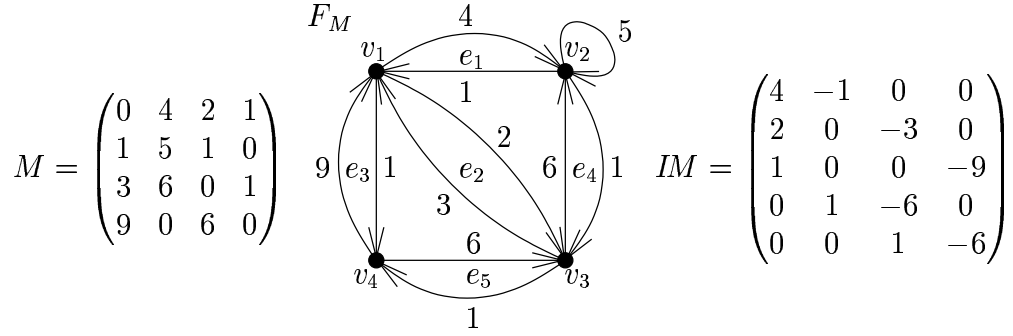


Figure 3: A degree matrix, its quotient graph, and its weighted incidence matrix.

Let $w : E_D \rightarrow \mathbb{N}$ be a positive weight function defined on the arc set of D . We say that a cycle $v_0, v_1, \dots, v_c, v_0$ in D has the *cycle product identity* if

$$1 = \prod_{i=0}^{c-1} \frac{w(v_i, v_{i+1})}{w(v_{i+1}, v_i)},$$

where the subscript of v_{i+1} is computed modulo $c + 1$. In other words, a cycle has the cycle product identity if the product of arc weights going clockwise around the cycle is the same as the product counter-clockwise. We say that D has the *cycle product identity* if every cycle of D has the cycle product identity.

Observation 16 *A symmetric directed graph D has the cycle product identity if and only if every induced cycle of D has the cycle product identity.*

Proof: We prove this by induction on the length of a cycle $C = v_0, v_1, \dots, v_c, v_0$ in D . The base case is when $c = 1$, in which case the cycle is induced by definition of D . For $c \geq 2$, if the cycle is not induced then we have an arc (v_i, v_j) (and an arc (v_j, v_i) by symmetry) for some $0 \leq i < j - 1 \leq c - 1$ splitting the cycle C into two smaller cycles $C_1 = v_0, v_1, \dots, v_i, v_j, v_{j+1}, \dots, v_c, v_0$ and $C_2 = v_i, v_{i+1}, \dots, v_j, v_i$. Note that the product of edge weights clockwise around the cycle C is equal to the the product of edge weights clockwise around the cycles C_1 and C_2 divided by $w(v_i, v_j)w(v_j, v_i)$. Likewise the product of edge weights counter-clockwise around C is equal to the product of counter-clockwise products around cycles C_1 and C_2 divided by $w(v_i, v_j)w(v_j, v_i)$. By induction we conclude that the cycle C has the cycle product identity. \square

For a $k \times k$ matrix M we define the *quotient graph* F_M as follows. Its vertex set V_{F_M} consists of vertices $\{1, \dots, k\}$. For $1 \leq i, j \leq k$, there is an arc or loop from i to j with weight $m_{i,j}$ if and only if $m_{i,j} \geq 1$. See Figure 3 for an example. Note that F_M is a symmetric directed graph if and only if M is zero-symmetric. We say that the matrix M is *connected* if the associated graph F_M is connected. Note that, by definition of \mathcal{M} , any degree matrix in \mathcal{M} is connected.

Let F'_M be the underlying simple graph of F_M , i.e., $V_{F'_M} = V_{F_M} = \{1, \dots, k\}$ and (i, j) is an undirected edge of F'_M , whenever both (i, j) and (j, i) with $i \neq j$ are directed arcs of F_M . We define the *weighted incidence matrix* IM to be the $|E_{F'_M}| \times k$ matrix whose rows are indexed by edges $e = (i, j) \in E_{F'_M}$, $i < j$ and its only nonzero entries in the e -th row are $IM_{e,i} = m_{i,j}$ and $IM_{e,j} = -m_{j,i}$. See Figure 3 for an example.

The kernel and rank of a matrix M are denoted by $\ker(M)$ and $\text{rank}(M)$ respectively.

We now present our characterization of degree matrices, which will also be useful in later proofs.

Theorem 17 For a square matrix M over nonnegative integers the following statements are equivalent:

- (i) M is a connected degree matrix, i.e., $M \in \mathcal{M}$.
- (ii) The quotient graph F_M is a connected symmetric directed graph satisfying the cycle product identity.
- (iii) M is zero-symmetric and $\dim(\ker(IM)) = 1$.

Proof: (i) \Rightarrow (ii) Since M is a connected degree matrix, M is zero-symmetric. Hence, F_M is a connected symmetric directed graph. Let $C = i_0, \dots, i_c, i_0$ be a cycle in F_M , where vertex v_i corresponds to row i of M . Use Observation 15 for pairs $(i_0, i_1), \dots, (i_c, i_0)$ to show that C satisfies the cycle product identity.

(ii) \Rightarrow (iii) Since F_M is symmetric, M is zero-symmetric. Consider a path P_{1i} in F_M from the vertex 1 corresponding to the first row of M to any vertex i corresponding to the i -th row of M . We apply Observation 15 for consecutive pairs on P_{1i} . Combining these equalities yields a rational $b_i > 0$ such that $|B_i| = b_i|B_1|$ for the blocks B_i and B_1 of any possible graph G with degree matrix M . Because F_M satisfies the cycle product identity, taking another path P'_{1i} between vertices 1 and i would lead to exactly the same equality $|B_i| = b_i|B_1|$. Define $b_1 = 1$. Then any solution of $\ker(IM)$ is a multiple of the vector $\mathbf{b} = (b_1, \dots, b_k)$. Hence, we conclude that $\dim(\ker(IM)) = 1$.

(iii) \Rightarrow (i) We first determine the block sizes of a candidate graph G with $G \xrightarrow{B} M$. We do this with respect to the following two facts.

- (1) For any $p \geq 1$, there exists a p -regular graph on n vertices if and only if $n \geq p + 1$ and np is even.
- (2) For any $p, q \geq 1$, there exists a (p, q) -regular bipartite graph with the degree- p side having m vertices and the degree- q side having n vertices if and only if $m \geq q, n \geq p$ and $mp = nq$.

We now choose an integer solution \mathbf{s} of $\ker(IM)$ such that

- $s_i \geq m_{i,i} + 1$ for all i .
- $s_i m_{i,i}$ is even for all i . (*)
- $s_i \geq m_{j,i}$ for all i and all $j \neq i$.

Then the following graph G_M has M as one of its degree matrices. Its vertex set V_{G_M} can be partitioned into blocks $B_1 \cup \dots \cup B_k$ with $|B_i| = s_i$ for all $1 \leq i \leq k$. Its edge set E_{G_M} can be chosen such that:

- The subgraph induced by B_i is $m_{i,i}$ -regular for $1 \leq i \leq k$.
- The induced bipartite subgraph between vertices of blocks B_i and B_j is $(m_{i,j}, m_{j,i})$ -regular for all $1 \leq i < j \leq k$.

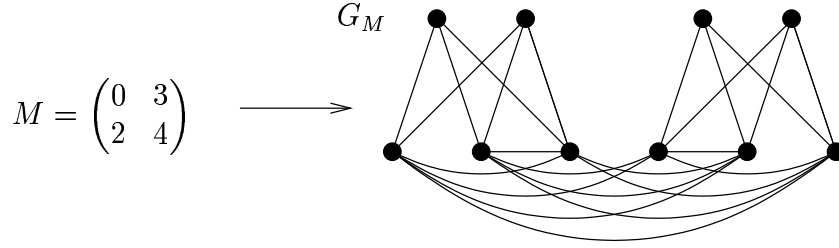


Figure 4: Construction of a smallest graph from the degree matrix.

See Figure 4 for an example of the construction. \square

We note here that for the transposed matrix IM^T the dimension of its kernel could be well expressed since it is equal to the dimension of the cycle space $\mathcal{S}_{F'_M}$ of F'_M : $\dim(\ker(IM)) = 1$ if and only if $\text{rank}(IM^T) = \text{rank}(IM) = k - 1$ if and only if $\dim(\ker(IM^T)) = |E_{F'_M}| - \text{rank}(IM^T) = |E_{F'_M}| - k + 1 = \dim(\mathcal{S}_{F'_M})$.

Theorem 17 has many consequences for the computational complexity of problems related to degree matrices.

Corollary 18 *The DEGREE MATRIX DETERMINATION problem can be solved in polynomial time.*

Proof: First we check whether the matrix M is zero-symmetric. If it is, then we construct its quotient graph F_M in order to find out whether the matrix M is connected. We further check whether $\dim(\ker(IM)) = 1$ and use Theorem 17. \square

Theorem 17 and Corollary 18 immediately imply that for examining whether a graph has the cycle product identity we do not have to check all (induced) cycles, of which there could be an exponential number, explicitly.

Corollary 19 *The problem whether a symmetric directed graph with positive edge weights has the cycle product identity can be solved in polynomial time.*

Note that for many matrices M the smallest graph G having M as a degree matrix could have size exponential in the size of M (assuming the entries of M are encoded in binary). For an example take the 1×1 matrix M with the (only) entry $m_{1,1}$. Then $G = K_{m_{1,1}+1}$ is the smallest $m_{1,1}$ -regular graph, but its size is exponential in $O(\log m_{1,1})$. Thus, in some way the following result is the best we can hope for.

Corollary 20 *For any degree matrix $M \in \mathcal{M}$, the block sizes of a smallest graph G with $G \xrightarrow{B} M$ can be computed in polynomial time.*

Proof: Let $M \in \mathcal{M}$ be a $k \times k$ degree matrix. Let $m = \max\{m_{i,j} \mid 1 \leq i, j \leq k\}$. Let $\langle m \rangle$ be the number of bits required to encode m . Then the size of a $k \times k$ matrix M can be defined as $k^2 \langle m \rangle$. If we compute coefficients b_i as in the proof of Theorem 17, then we find that both nominator and denominator of each b_i have size at most $k \langle m \rangle$. Let α be the product of all denominators of elements b_i . Let b' be a solution of $\ker(IM)$ with entries $b'_i = \alpha b_i$ for all $1 \leq i \leq k$. We divide each b'_i by the greatest common divisor of b'_1, \dots, b'_k . This way we have obtained the smallest integer solution \mathbf{b}^* of $\ker(IM)$ in polynomial time. Now we choose the smallest integer γ such that $\gamma \geq \max_{1 \leq i, j \leq k} \left\{ \frac{m_{i,i+1}}{b_i^*}, \frac{m_{j,i}}{b_i^*} \right\}$, where γ is required to be even if for some i the product $b_i^* m_{i,i}$ is odd.

Then $\mathbf{b} = \gamma \mathbf{b}^*$ satisfies all three conditions (*) in the proof of Theorem 17, i.e., it yields the block sizes of a smallest graph G in the same way as in the proof of Theorem 17. \square

We have shown that verification whether or not a given matrix is a degree matrix can be done in polynomial time. What about the complexity of the problem of deciding whether a given matrix M is a degree matrix of a given graph G ?

DEGREE MATRIX RECOGNITION

Instance: A graph G and a matrix M .

Question: Does $G \xrightarrow{B} M$ hold?

Proposition 21 *The DEGREE MATRIX RECOGNITION problem is NP-complete.*

Proof: A result from [19] is that the H -COVER problem, which takes as input a graph G and asks if $G \xrightarrow{B} H$, is NP-complete already for $H = K_3$. Observation 11 tells us that $G \xrightarrow{B} K_3$ if and only if $G \xrightarrow{B} \text{adj}(K_3)$. \square

The H -PARTIAL COVER problem takes as input a graph G and asks if $G \xrightarrow{I} H$ for some fixed graph H . The H -ROLE ASSIGNMENT problem takes as input a graph G and asks if $G \xrightarrow{S} H$. Both problems are NP-complete for $H = K_3$ [12, 21]. Hence, by a similar argument, using Observation 14 and the NP-completeness of K_3 -ROLE ASSIGNMENT and K_3 -PARTIAL COVER, also the problems of deciding if $G \xrightarrow{S} M$ and $G \xrightarrow{I} M$ are NP-complete.

3.2 Degree matrix comparisons

To study the connection between degree matrices and locally constrained graph homomorphisms we define the following concepts.

Definition 22 *We define three relations $\xrightarrow{\exists B}$, $\xrightarrow{\exists I}$, and $\xrightarrow{\exists S}$ on \mathcal{M} as follows. Let M, N be matrices in \mathcal{M} . We have*

- $M \xrightarrow{\exists B} N$ if there exist graphs G, H with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ such that $G \xrightarrow{B} H$;
- $M \xrightarrow{\exists I} N$ if there exist graphs G, H with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ such that $G \xrightarrow{I} H$;
- $M \xrightarrow{\exists S} N$ if there exist graphs G, H with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ such that $G \xrightarrow{S} H$.

Later we prove that these three relations are quasiorders and that they become partial orders when restricted to degree refinement matrices. We define now the following matrix comparison problems:

MATRIX BIJECTIVITY

Instance: Matrices $M, N \in \mathcal{M}$.

Question: Does $M \xrightarrow{\exists B} N$ hold?

MATRIX INJECTIVITY

Instance: Matrices $M, N \in \mathcal{M}$.

Question: Does $M \xrightarrow{\exists I} N$ hold?

MATRIX SURJECTIVITY

Instance: Matrices $M, N \in \mathcal{M}$.

Question: Does $M \xrightarrow{\exists S} N$ hold?

In Section 5, after our study on degree refinement matrices, we give a polynomial-time algorithm that solves the MATRIX BIJECTIVITY problem based on the well-known algorithm to compute a degree refinement matrix of a given graph. For the other two local constraints considerably more effort is required. In Section 6 we give an NP algorithm for solving the MATRIX INJECTIVITY problem by showing that $M \xrightarrow{\exists I} N$ if and only if there exists a graph G of bounded size with $G \xrightarrow{B} M$ and $G \xrightarrow{I} N$.

In Section 7 we give an NP algorithm for solving the MATRIX SURJECTIVITY problem. Here, we first need to show that $M \xrightarrow{\exists S} N$ holds if and only if there exists a graph G with $G \xrightarrow{B} M$ and $G \xrightarrow{S} N$. Then, in the same way as for the MATRIX INJECTIVITY problem we show that we may assume that this graph G has bounded size.

3.3 Universal covers of degree matrices

For use in later proofs we extend the notion of universal cover to degree matrices. Let M be a degree matrix in \mathcal{M} . We construct its *universal cover* T_M by taking as root of the (possibly infinite) tree T_M a vertex corresponding to row 1 of M , thus of row-type 1, and inductively adding a new level of vertices while maintaining the property that each vertex of row-type i has exactly $m_{i,j}$ neighbors of row-type j . Obviously, $T_M \xrightarrow{B} M$ holds. We make the following observation on universal covers of degree matrices and graphs.

Proposition 23 $T_M = T_G$ for any graph G with $G \xrightarrow{B} M$.

Proof: We have $T_G \xrightarrow{B} G$ and $G \xrightarrow{B} M$. Then we can partition V_{T_G} into (infinite) sets B_1, \dots, B_k such that, for $1 \leq i, j \leq k$, any $u \in B_i$ has $m_{i,j}$ neighbors in B_j . Taking any vertex from B_1 as root, thus of row-type 1, and inductively adding neighbors (children) in T_G on the next level, we maintain precisely the property in the definition of T_M , namely that a vertex of row-type i will have $m_{i,j}$ neighbors of row-type j . Thus $T_M = T_G$. \square

The following result follows from Corollary 9 and Proposition 23.

Corollary 24 Let M and N be matrices in \mathcal{M} . If $M \xrightarrow{\exists I} N$ then $T_M \subseteq T_N$, and if $M \xrightarrow{\exists S} N$ then $T_N \subseteq T_M$.

For the surjective case it is clear that the reverse is not true: for a small counterexample take $M = \text{drm}(P_4)$ and $N = \text{drm}(P_3)$, where P_k denotes a path on k vertices. For the injective case the authors were trying hard to prove the following conjecture (in an attempt to obtain an efficient algorithm for the MATRIX INJECTIVITY problem).

Conjecture 25 For any two matrices $M, N \in \mathcal{M}$: $M \xrightarrow{\exists I} N \iff T_M \subseteq T_N$.

However, the proof technique developed in Section 6 allows the construction of an example disproving Conjecture 25. Due to the relatively large size of this counterexample we cannot easily show its correctness without explaining the technique itself, and therefore postpone its presentation to Section 6.2.

4 Degree refinement matrices

Among all equitable partitions of a graph G , there is a unique one having the fewest number of blocks. This coarsest equitable partition, and a canonical ordering of its blocks, is computed by

the *stepwise refinement* of V_G , which is the following efficient algorithm (cf. [2]). Note that all sequences and vectors defined below are finite.

1. Partition V_G into a sequence of blocks $\mathcal{B}^1 = B_1^1, B_2^1, \dots$ such that two vertices are in the same block B_i^1 if and only if they have the same degree, and such that the blocks are arranged in descending degree value order, i.e., $\deg(u) > \deg(v)$ for $u \in B_i^1, v \in B_j^1$ with $i < j$. Set $t := 1$.
2. Compute for every vertex $u \in V_G$ its *degree vector*

$$\mathbf{d}_t(u) := \left(|N_G(u) \cap B_1^t|, |N_G(u) \cap B_2^t|, \dots \right),$$

consisting of the number of neighbors it has in each block.

3. Partition the vertices of each block B_i^t into a sequence of new blocks $B_{i_1}^{t+1}, B_{i_2}^{t+1}, \dots$, such that for each distinct degree vector $\mathbf{d} = \mathbf{d}_t(u)$ for some $u \in B_i^t$ there is exactly one block $B_{i_\ell}^{t+1}$ containing the vertices with degree vector \mathbf{d} and such that the new blocks are arranged in lexicographic descending degree vector order. Define the new sequence

$$\mathcal{B}^{t+1} = B_1^{t+1}, B_2^{t+1}, \dots := B_{1_1}^t, B_{1_2}^t, \dots, B_{i_1}^t, B_{i_2}^t, \dots$$

4. If no block was split in step 3, i.e., $\mathcal{B}^{t+1} = \mathcal{B}^t$, then define the *degree partition* $\mathcal{B}^* = B_1^*, B_2^*, \dots := \mathcal{B}^t$ and stop. Otherwise set $t := t + 1$ and go to step 2.

As the degree partition is a special case of an equitable partition we may define:

Definition 26 *The degree refinement matrix $\text{drm}(G)$ of a graph G is the unique degree matrix corresponding to the degree partition \mathcal{B}^* , i.e., its i^{th} row is a degree vector of a vertex in B_i^* .*

Clearly, the stepwise refinement algorithm runs in polynomial time. So the DEGREE MATRIX RECOGNITION problem becomes polynomially solvable when restricted to degree refinement matrices. As an example we consider the graphs G_B and H of Figure 2. We find that

$$\text{drm}(G_B) = \text{drm}(H) = \begin{pmatrix} 0 & 2 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

The graphs G_I and G_S in Figure 2 have degree refinement matrices different from $\text{drm}(H)$, e.g., $\text{drm}(G_I)$ is an adjacency matrix of G_I , and no locally bijective homomorphism from these graphs to H can exist. Indeed, it is clear that any two graphs G and H with $G \xrightarrow{B} H$ must satisfy the condition $\text{drm}(G) = \text{drm}(H)$. For two graphs of the same size the test for this condition constitutes a well-known heuristic for graph isomorphism.

4.1 Partial orders on degree refinement matrices

In a paper from 1982, Leighton showed the following.

Theorem 27 ([22]) *Let G and H be graphs in \mathcal{C} . The following statements are equivalent:*

- (i) $\text{drm}(G) = \text{drm}(H)$.
- (ii) $T_G = T_H$.

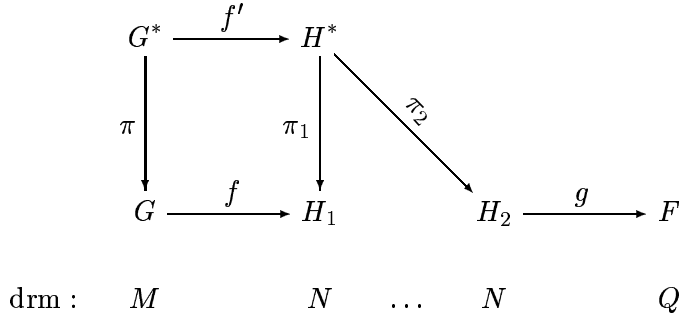


Figure 5: Commutative diagram for transitivity of $\overset{\exists I}{\rightarrow}$ where horizontal mappings are injective and others are bijective.

(iii) There exists a graph $F \in \mathcal{C}$ such that $F \overset{B}{\rightarrow} G$ and $F \overset{B}{\rightarrow} H$.

Theorem 27 implies that the symmetric and transitive closure of the partial order $(\mathcal{C}, \overset{B}{\rightarrow})$ is an equivalence relation whose classes can be naturally represented by degree refinement matrices. It is natural to ask if the other two kinds of locally constrained homomorphisms are also conditioned by the existence of a well-defined relation on the degree refinement matrices. Here, we prove that such relations exist and moreover, that they are partial orders. We let $\mathcal{M}' \subset \mathcal{M}$ denote the *set of connected degree refinement matrices*, i.e., the set of all degree refinement matrices of graphs in \mathcal{C} .

As stated above $(\mathcal{M}', \overset{\exists B}{\rightarrow})$ is a trivial order where no two distinct elements are comparable. For the other two relations $(\mathcal{M}', \overset{\exists I}{\rightarrow})$ and $(\mathcal{M}', \overset{\exists S}{\rightarrow})$, the *reflexivity* of the relation follows directly from the existence of the identity mapping on any underlying graph, where at least one must exist to assert the membership of the matrix in \mathcal{M}' . Antisymmetry and transitivity require more effort.

For proving *antisymmetry* of $(\mathcal{M}', \overset{\exists I}{\rightarrow})$ we involve the notion of universal cover. Assume that $M \overset{\exists I}{\rightarrow} N$ and $N \overset{\exists I}{\rightarrow} M$ for two matrices $N, M \in \mathcal{M}'$. Then there exist graphs G_1, G_2 with $\text{drm}(G_1) = \text{drm}(G_2) = M$ and H_1, H_2 with $\text{drm}(H_1) = \text{drm}(H_2) = N$ such that $G_1 \overset{I}{\rightarrow} H_1$ and $H_2 \overset{I}{\rightarrow} G_2$. By Lemma 8, there exist homomorphisms $f' : T_{G_1} \overset{I}{\rightarrow} T_{H_1}$ and $g' : T_{H_2} \overset{I}{\rightarrow} T_{G_2}$. Due to Proposition 23 we find that $T_{G_1} = T_{G_2} = T_M$ and $T_{H_1} = T_{H_2} = T_N$. Hence we have $f' : T_M \overset{I}{\rightarrow} T_N$ and $g' : T_N \overset{I}{\rightarrow} T_M$. Recall from Section 2 that there exist a homomorphism $f_0 : T_M \overset{B}{\rightarrow} G_1$. We now invoke Theorem 5 to conclude that $f_0 \circ g' \circ f' : T_M \overset{I}{\rightarrow} G_1$ is locally bijective. This implies that f' and g' are locally surjective, and hence locally bijective. Consequently, the universal covers T_M and T_N are isomorphic. Hence, $M = N$ due to Theorem 27. The antisymmetry of $\overset{\exists S}{\rightarrow}$ can be proven according to the same kind of arguments.

For the transitivity property of $\overset{\exists I}{\rightarrow}$ we use the next lemma.

Lemma 28 *Let $G, H_1, H_2, F \in \mathcal{C}$ be such that $G \overset{I}{\rightarrow} H_1$ and $H_2 \overset{I}{\rightarrow} F$, where H_1 and H_2 share the same degree refinement matrix. Then there exists a graph $G^* \in \mathcal{C}$ such that $G^* \overset{I}{\rightarrow} F$ and $G^* \overset{B}{\rightarrow} G$.*

Proof: Using Theorem 27 we first construct a finite graph H^* such that $H^* \overset{B}{\rightarrow} H_1$ via projection π_1 and $H^* \overset{B}{\rightarrow} H_2$ via projection π_2 . The projection $\pi_2 : H^* \overset{B}{\rightarrow} H_2$ composed with a locally injective homomorphism $g : H_2 \overset{I}{\rightarrow} F$ gives that $H^* \overset{I}{\rightarrow} F$. See Figure 5.

By Observation 2, the preimage $\pi_1^{-1}(x)$ has the same size for all vertices $x \in V_{H_1}$, say k . We assume that all vertices of H^* that map onto a vertex x are labeled $\{x_1, x_2, \dots, x_k\}$.

Let $f : G \xrightarrow{I} H_1$. The vertex set of the desired graph G^* is the Cartesian product $V_G \times \{1, \dots, k\}$. Define the edges of G^* as follows:

$$((u, i), (v, j)) \in E_{G^*} \iff (u, v) \in E_G \text{ and } (f(u)_i, f(v)_j) \in E_{H^*}.$$

We define the mappings $f' : (u, i) \rightarrow f(u)_i$ and $\pi : (u, i) \rightarrow u$. Observe that, for any edge $(x_i, y_j) \in E_{H^*}$, the subgraph of G^* induced by the vertex set $f'^{-1}(x_i) \cup f'^{-1}(y_j)$ is isomorphic to the subgraph of G induced by the vertex set $f^{-1}(x) \cup f^{-1}(y)$. Then, according to Observation 2, the mapping f' is a locally injective homomorphism from G^* to H^* . Hence, the mapping $g \circ \pi_2 \circ f'$ is a locally injective homomorphism $G^* \xrightarrow{I} F$. Observe that, for any edge $(u, v) \in E_H$, the subgraph of G^* induced by the vertex set $\pi^{-1}(u) \cup \pi^{-1}(v)$ is isomorphic to the subgraph of H^* induced by the vertex set $\pi_1^{-1}(x) \cup \pi_1^{-1}(y)$, where $f(u) = x$ and $f(v) = y$. Then, according to Observation 2, the mapping π is a locally bijective homomorphism from G^* to G . \square

Indeed, we now find that $M \xrightarrow{\exists I} N$ and $N \xrightarrow{\exists I} Q$ for matrices $M, N, Q \in \mathcal{M}'$ implies $M \xrightarrow{\exists I} Q$: in Lemma 28 we take $M = \text{drm}(G), N = \text{drm}(H_1) = \text{drm}(H_2), Q = \text{drm}(F)$, and obtain $M = \text{drm}(G^*)$ due to $G^* \xrightarrow{B} G$.

A similar lemma as Lemma 28 can be proven for the order $\xrightarrow{\exists S}$ with exactly the same arguments, the only difference is that the preimage in G^* of any edge $(x_i, y_j) \in E_{H^*}$ is a bipartite graph of minimum degree one. We have thus shown:

Theorem 29 *The relations $(\mathcal{M}', \xrightarrow{\exists B})$, $(\mathcal{M}', \xrightarrow{\exists I})$, $(\mathcal{M}', \xrightarrow{\exists S})$ are partial orders. They arise as a factor of the orders $(\mathcal{C}, \xrightarrow{B})$, $(\mathcal{C}, \xrightarrow{I})$, $(\mathcal{C}, \xrightarrow{S})$, respectively, when we unify the graphs that have the same degree refinement matrices.*

Theorem 5 can now be translated to matrices. If $M \xrightarrow{\exists I} N$ and $M \xrightarrow{\exists S} N$ for two degree refinement matrices M and N , then $M \xrightarrow{\exists B} N$, i.e., $M = N$.

Corollary 30 $(\mathcal{M}', \xrightarrow{\exists B}) = (\mathcal{M}', \xrightarrow{\exists I}) \cap (\mathcal{M}', \xrightarrow{\exists S}) = (\mathcal{M}', \{(M, M) : M \in \mathcal{M}'\})$.

Proof: It is clear that $(\mathcal{M}', \xrightarrow{\exists B}) \subseteq (\mathcal{M}', \xrightarrow{\exists I}) \cap (\mathcal{M}', \xrightarrow{\exists S})$. Suppose $G_1 \xrightarrow{I} H_1$ and $G_2 \xrightarrow{S} H_2$ hold with $\text{drm}(G_i) = M$ and $\text{drm}(H_i) = N$ ($i = 1, 2$). By Corollary 24, we have that $T_M \subseteq T_N$ and $T_N \subseteq T_M$. We represent these inclusions by locally injective homomorphisms $f' : T_M \rightarrow T_N$ and $g' : T_N \rightarrow T_M$. Then we may conclude $M = N$ by the same arguments as in the proof of antisymmetry of $\xrightarrow{\exists I}$. \square

5 Degree matrix comparison via local bijectivity

In this section we consider the MATRIX BIJECTIVITY (is $M \xrightarrow{\exists B} N$?) problem. For this purpose we first generalize the stepwise refinement algorithm of Section 4 into an algorithm, called the DRM CONSTRUCTION algorithm and given in the box below, that takes as input a degree matrix M and computes a matrix $\text{drm}(M)$ such that $\text{drm}(M) = \text{drm}(G)$ for any graph G having degree matrix M . Note that this constitutes a definition of $\text{drm}(M)$ for a degree matrix M . For computing the degree refinement matrix of a given graph G , take an adjacency matrix of G as the input of this algorithm. Note that in steps **2** and **3** the canonical order of the blocks is defined.

The time complexity of the DRM CONSTRUCTION algorithm for a $k \times k$ matrix is $O(k^3 \log k)$ (assuming unit time per arithmetic operation). The outer cycle may have at most k rounds, while in each round the major operation is the lexicographic sorting of at most k vectors of length at most k , which can be done in time $O(k^2 \log k)$.

Because of the DRM CONSTRUCTION algorithm we can make the following observation.

Observation 31 *Two graphs G and H have a common degree matrix if and only if G and H have the same degree refinement matrix.*

From Observation 31 we derive that $(\mathcal{M}, \overset{\exists B}{\rightarrow})$ is a quasiorder. Furthermore, together with Lemma 28, it implies that $(\mathcal{M}, \overset{\exists L}{\rightarrow})$ and, for the same reasons, $(\mathcal{M}, \overset{\exists S}{\rightarrow})$ are quasiorders.

By applying the DRM CONSTRUCTION algorithm and Corollary 18 we immediately obtain the following result.

Corollary 32 *Checking whether a given $k \times k$ matrix M is a degree refinement matrix in \mathcal{M}' can be done in polynomial time.*

DRM CONSTRUCTION

Input: A degree matrix M of order k .

Output: The degree refinement matrix $\text{drm}(M)$ of all graphs with degree matrix M .

1. Set $\mathcal{R}^1 = R_1^1, R_2^1, \dots$ such that

- rows $r, s \in R_i^1$ if and only if $\sum_{i=1}^k m_{r,i} = \sum_{i=1}^k m_{s,i}$.
- row $r \in R_i^1$, row $s \in R_{i'}^1$ with $i < i'$ if and only if $\sum_{i=1}^k m_{r,i} > \sum_{i=1}^k m_{s,i}$.

Set $t := 1$.

2. For each row $r = 1, \dots, k$ compute the row-degree vector

$$\mathbf{d}_t(r) := \left(\sum_{i \in R_1^t} m_{r,i}, \sum_{i \in R_2^t} m_{r,i}, \dots \right).$$

3. Define the new partition \mathcal{R}^{t+1} of $\{1, \dots, k\}$ such that

- rows $r, s \in R_i^{t+1}$ if and only if $\mathbf{d}_t(r) = \mathbf{d}_t(s)$,
- row $r \in R_i^{t+1}$, row $s \in R_{i'}^{t+1}$ with $i < i'$ if and only if
 - * either $r \in R_j^t$, $s \in R_{j'}^t$ with $j < j'$,
 - * or $r, s \in R_j^t$, and $\mathbf{d}_t(r) >_{\text{Lex}} \mathbf{d}_t(s)$.

where $>_{\text{Lex}}$ is the lexicographic order on integer sequences.

4. If $\mathcal{R}^{t+1} = \mathcal{R}^t$ then set $\text{drm}(M) = \begin{pmatrix} \mathbf{d}_t(r) : r \in R_1^t \\ \mathbf{d}_t(r) : r \in R_2^t \\ \vdots \end{pmatrix}$ and stop,

otherwise set $t := t+1$ and go to step 2.

For our algorithm that solves the MATRIX BIJECTIVITY problem we show that it is sufficient to compare degree refinement matrices.

Proposition 33 *Let M and N be matrices in \mathcal{M} . Then $M \overset{\exists B}{\rightarrow} N$ if and only if $\text{drm}(M) = \text{drm}(N)$.*

Proof: Suppose $M \overset{\exists B}{\rightarrow} N$. Then there exist graphs G with $G \overset{B}{\rightarrow} M$ and H with $H \overset{B}{\rightarrow} N$ such that $G \overset{B}{\rightarrow} H$. Hence, we can apply Theorem 27 to conclude that $\text{drm}(M) = \text{drm}(G) = \text{drm}(H) = \text{drm}(N)$.

Suppose $\text{drm}(M) = \text{drm}(N)$. Let G be a graph in \mathcal{C} such that $G \overset{B}{\rightarrow} M$, and let H be a graph in \mathcal{C} such that $H \overset{B}{\rightarrow} N$. We note that $\text{drm}(G) = \text{drm}(M) = \text{drm}(N) = \text{drm}(H)$. Then, by

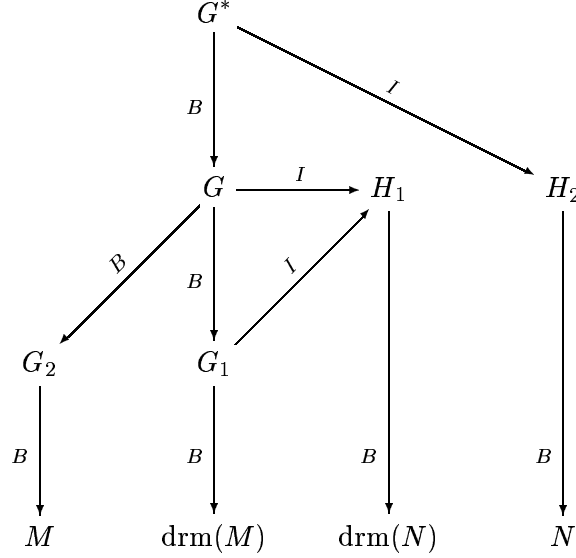


Figure 6: Commutative diagram for the proof of Proposition 35.

Theorem 27, there exists a graph F such that $F \xrightarrow{B} G$ and $F \xrightarrow{B} H$. Since $G \xrightarrow{B} M$, we derive that $F \xrightarrow{B} M$. Recall that $H \xrightarrow{B} N$. Hence, we conclude that $M \xrightarrow{\exists B} N$ via graphs F and H . \square

Corollary 34 *The MATRIX BIJECTIVITY problem is solvable in polynomial time.*

6 Degree matrix comparison via local injectivity

In this section we consider the MATRIX INJECTIVITY problem. We observe that according to the definition of the quasiorder $(\mathcal{M}, \xrightarrow{\exists I})$, there is no obvious bound on the sizes of graphs G and H with M and N as degree refinement matrices that should justify the comparison $M \xrightarrow{\exists I} N$.

Note that it is sufficient to compare degree refinement matrices.

Proposition 35 *Let M and N be matrices in \mathcal{M} . Then $M \xrightarrow{\exists I} N$ if and only if $\text{drm}(M) \xrightarrow{\exists I} \text{drm}(N)$.*

Proof: Suppose $M \xrightarrow{\exists I} N$. Then there exist two graphs $G, H \in \mathcal{C}$ with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ such that $G \xrightarrow{I} H$. Since $G \xrightarrow{B} \text{drm}(M)$ and $H \xrightarrow{B} \text{drm}(N)$ we immediately obtain that $\text{drm}(M) \xrightarrow{\exists I} \text{drm}(N)$.

Suppose $\text{drm}(M) \xrightarrow{\exists I} \text{drm}(N)$. Then there exist two graphs $G_1, H_1 \in \mathcal{C}$ with $G_1 \xrightarrow{B} \text{drm}(M)$ and $H_1 \xrightarrow{B} \text{drm}(N)$ such that $G_1 \xrightarrow{I} H_1$. Let G_2 be a graph with $G_2 \xrightarrow{B} M$. Then G_2 has degree refinement matrix $\text{drm}(G_2) = \text{drm}(M)$. Due to Theorem 27 there exists a graph G with $G \xrightarrow{B} G_2$, which implies $G \xrightarrow{B} M$ and with $G \xrightarrow{B} G_1$, which implies $G \xrightarrow{I} H_1$. Let H_2 be a graph with $H_2 \xrightarrow{B} N$. Then H_2 has degree refinement matrix $\text{drm}(H_2) = \text{drm}(N)$. We use Lemma 28 (with $F = H_2$) to conclude that there exists a graph G^* with $G^* \xrightarrow{B} G$, which implies $G^* \xrightarrow{B} M$ and with $G^* \xrightarrow{I} H_2$. (See Figure 6.) Since $H_2 \xrightarrow{B} N$, we have found G^* and H_2 as witnesses for $M \xrightarrow{\exists I} N$. \square

If we apply Proposition 4 on the universe of connected degree matrices we obtain the following result, which we will use for the construction of our algorithm that solves the MATRIX INJECTIVITY problem. (Since such a result can not be derived for the $\overset{\exists S}{\rightarrow}$ relation, solving the MATRIX SURJECTIVITY problem requires more effort.)

Corollary 36 *Let M, N be matrices in \mathcal{M} . Then $M \overset{\exists I}{\rightarrow} N$ if and only if there exists two graphs G, H with $G \overset{B}{\rightarrow} M$ and $H \overset{B}{\rightarrow} N$ such that G is a subgraph of H .*

6.1 Computational complexity

For computational complexity purposes $\langle X \rangle$ denotes the size of the instance X (graph, matrix, etc.) in usual binary encoding of numbers. Formally we represent vertices of a graph G by numbers $\{1, 2, \dots, |V_G|\}$ and its edges as a list of its vertices. A graph with m edges on n vertices hence requires space $\langle G \rangle = \Theta(m \log n)$. Recall that the size of an integral-valued $k \times l$ matrix A is defined as $kl \langle a^* \rangle = kl \log a^*$, where $a^* = \max(\{2\} \cup \{|A_{i,j}| \mid 1 \leq i \leq k \text{ and } 1 \leq j \leq l\})$.

We will need the following technical lemma for our NP algorithm.

Lemma 37 *Let A be an integral-valued $k \times l$ matrix with $l > k$. If $A\mathbf{x} = \mathbf{0}$ allows a nontrivial nonnegative solution, then it allows a nontrivial nonnegative integer solution \mathbf{x} with at most $k + 1$ nonzero entries and with $\langle x_i \rangle = O(k \log(ka^*))$ for each entry x_i .*

Proof: If a nonnegative solution \mathbf{x} with more than $k + 1$ positive entries exists, then the columns corresponding to $k + 1$ of these variables are linearly dependent. Let the coefficients of such a linear combination together with zeros for the other entries form a vector \mathbf{x}' . Obviously $A\mathbf{x}' = \mathbf{0}$, but the entries of \mathbf{x}' may not be necessarily nonnegative.

Without loss of generality we assume that at least one of the entries in \mathbf{x}' is positive. Then, for $\alpha = -\min\{\frac{x'_i}{x_i} \mid x'_i > 0\}$ the vector $\mathbf{x} + \alpha\mathbf{x}'$ is also a nontrivial nonnegative solution with more zero entries than \mathbf{x} .

Repeating this trimming iteratively we obtain a nontrivial nonnegative solution with at most $k + 1$ nonzero entries. As the other entries are zero, we may restrict the matrix A to columns corresponding to nonzero entries of the solution. It may happen that the rank of the modified matrix decreases. Then we reduce the number of rows until the remaining ones become linearly independent. We repeat the whole process until we finally get a $k' \times (k' + 1)$ matrix B of rank $k' \leq k$, such that $B\mathbf{y} = \mathbf{0}$ allows a nontrivial solution \mathbf{y} with $y_i > 0$ for $i = 1, \dots, k' + 1$. Such a vector \mathbf{y} can be extended to a solution \mathbf{x} of the original system by inserting zero entries.

Without loss of generality we assume that the first k' columns of B are linearly independent, and we arrange them in a regular matrix R . Note that the last column of B is a linear combination of the other columns with unique coefficients $-\frac{y_i}{y_{k'+1}} < 0$ for $i = 1, \dots, k'$. The inverse of R can be expressed as $R^{-1} = \frac{adj(R)}{\det(R)}$, where $adj(R)$ is the adjoint matrix of R . By the determinant expansion we have that $\det(R) \leq k'!(a^*)^{k'} \leq k!(a^*)^k \leq k^k(a^*)^k$. Then we find that $\langle \det(R) \rangle = O(k \log(ka^*))$. Each element of $adj(R)$ is a determinant of a minor of R and hence is smaller than $(k-1)^{k-1}(a^*)^{k-1}$.

Now consider the integral valued matrix $B' = \det(R) \cdot R^{-1}B$. Then

- \mathbf{y} is a solution of $B'\mathbf{y} = \mathbf{0}$ if and only if $B\mathbf{y} = \mathbf{0}$ (recall that $\text{rank}(R) = k'$).
- The first k' columns of B' form the matrix $\det(R) \cdot I_{k'}$.
- In the last column the entries $z_i = \det(R) \frac{y_i}{y_{k'+1}}$ for $i = 1, \dots, k'$ are all negative (if $\det(R) > 0$) or all positive (otherwise).

If $\det(R) > 0$ then $\mathbf{y} = (-z_1, \dots, -z_{k'}, \det(R))$ is a nonnegative nontrivial integral solution to $B\mathbf{y} = \mathbf{0}$. In the other case we swap the sign and choose $\mathbf{y} = (z_1, \dots, z_{k'}, -\det(R))$. As each $z_i \leq ka^* \max_{ij}(\text{adj}(R)_{i,j}) \leq k^k (a^*)^k$, we obtain $\langle z_i \rangle = O(k \log(ka^*))$, which concludes the proof. \square

We now give the main theorem of this section. In the remainder we write $m_{i,j} = M_{i,j}$ and $n_{i,j} = N_{i,j}$ for matrices M and N respectively. For a square matrix M of order k we let $m^* = \max(\{2\} \cup \{m_{i,j} \mid 1 \leq i, j \leq k\})$.

Theorem 38 *For two connected degree matrices M and N of order k and l respectively, $M \xrightarrow{\exists!} N$ holds if and only if there exists a graph G of size $(klm^*)^{O(k^2l^2)}$ such that $G \xrightarrow{B} M$ and $G \xrightarrow{L} N$.*

Proof: Let $M, N \in \mathcal{M}$ be of order k and l respectively. Throughout this proof we assume that indices i, j, r, s used later always belong to feasible intervals $1 \leq i, r \leq k$ and $1 \leq j, s \leq l$. For clarity we often abbreviate pairs of sub-/super-scripts i, j by ij , so in this notation, ij does not mean multiplication.

Suppose $M \xrightarrow{\exists!} N$ holds. Then there exist graphs $G, H \in \mathcal{C}$ with $G \xrightarrow{B} M$ and with $H \xrightarrow{B} N$ such that $G \xrightarrow{L} H$ holds. Hence, we find that $G \xrightarrow{L} N$ holds. Let $\{U_1, \dots, U_k\}$ be a partition of V_G for $G \xrightarrow{B} M$, and $\{V_1, \dots, V_l\}$ be a partition of V_G for $G \xrightarrow{L} N$. For each pair of indices r and s we define the set

$$W_{rs} = \{v \mid v \in U_r \cap V_s\},$$

and for each vertex $u \in W_{rs} \subseteq V_G$ we can write a vector $\mathbf{p}(u) = (|N_G(u) \cap W_{11}|, \dots, |N_G(u) \cap W_{kl}|)$ describing the distribution of neighbors of u in the classes W_{11}, \dots, W_{kl} .

We first research the structure of such vectors. Let \mathbf{p}^{rs} be a vector of length kl whose entries are nonnegative integers and are indexed by pairs ij . If the vector \mathbf{p}^{rs} further satisfies

$$\sum_{j=1}^l p_{ij}^{rs} = m_{ri} \quad \text{for all } 1 \leq i \leq k, \quad (4)$$

$$\sum_{i=1}^k p_{ij}^{rs} \leq n_{sj} \quad \text{for all } 1 \leq j \leq l, \quad (5)$$

then we call \mathbf{p}^{rs} an *injective distribution row for indices r and s* . Due to (4), the set

$$T(r, s) = \{\mathbf{p}^{rs(1)}, \dots, \mathbf{p}^{rs(t(r,s))}\}$$

of injective distribution rows is bounded by $t(r, s) \leq \binom{m^*+l-1}{m^*}^k = O((m^*+1)^{kl})$ for every pair of indices r, s . The total number of distribution rows is then

$$t_0 = \sum_{r,s} t(r, s) = O(kl(m^*+1)^{kl}).$$

The vector \mathbf{w} with entries $w^{rs(t)} = |\{u : \mathbf{p}(u) = \mathbf{p}^{rs(t)}\}|$ is a nontrivial solution of the following homogeneous system of k^2l^2 equations in t_0 variables

$$\sum_{t=1}^{t(r,s)} p_{ij}^{rs(t)} w^{rs(t)} = \sum_{t'=1}^{t(i,j)} p_{rs}^{ij(t')} w^{ij(t')} \quad 1 \leq i, r \leq k, \quad 1 \leq j, s \leq l, \quad (6)$$

since in each equation both sides are equal to the number of edges connecting sets W_{rs} and W_{ij} .

So the system (6) has a nontrivial nonnegative solution. Note that all coefficients $p_{ij}^{rs(t)}$ of this system are at most m^* . Then, by Lemma 37, we find a nontrivial nonnegative integer solution $\tilde{\mathbf{w}} = (\tilde{w}^{11(1)}, \dots, \tilde{w}^{kl(t(k,l))})$ whose entry sizes $\tilde{w}^{rs(t)}$ are bounded by $O(k^2 l^2 \log(klm^*))$. We use this solution to construct a graph G' of size $\langle G' \rangle = (klm^*)^{O(k^2 l^2)}$, such that $G' \xrightarrow{B} M$ and $G' \xrightarrow{L} N$.

Since we can multiply $\tilde{\mathbf{w}}$ by two if necessary, we may assume that each entry in $\tilde{\mathbf{w}}$ is even. We first build a multigraph G_0 upon t_0 sets of vertices $\tilde{W}^{11(1)}, \dots, \tilde{W}^{kl(t(k,l))}$, where $|\tilde{W}^{rs(t)}| = \tilde{w}^{rs(t)}$ (some sets may be empty) as follows:

Denote $\tilde{W}^{rs} = \tilde{W}^{rs(1)} \cup \dots \cup \tilde{W}^{rs(t(r,s))}$. Recall fact (1) of the proof of Theorem 17. Our choice of even values $\tilde{w}^{rr(t)}$ allows us to build an arbitrary $p_{rr}^{rr(t)}$ -regular multigraph on each set $\tilde{W}^{rr(t)}$. Recall fact (2) of the proof of Theorem 17. As $\tilde{\mathbf{w}}$ satisfies (6), we can easily build a bipartite multigraph between any pair of different sets \tilde{W}^{rs} and \tilde{W}^{ij} such that the number of edges between them is equal to $\sum_{t=1}^{t(r,s)} p_{ij}^{rs(t)} \tilde{w}^{rs(t)} = \sum_{t'=1}^{t(i,j)} p_{rs}^{ij(t')} \tilde{w}^{ij(t')}$.

For any vertex u in $\tilde{W}^{rs(t)}$ with more than $p_{ij}^{rs(t)}$ neighbors in \tilde{W}^{ij} there exists a vertex u^* in some $\tilde{W}^{ij(t^*)}$ with less than $p_{ij}^{rs(t^*)}$ neighbors, and vice versa. Now we remove an edge between u and some neighbor $v \in \tilde{W}^{ij}$ and add the edge (u^*, v) . We repeat this procedure until all vertices of \tilde{W}^{rs} have the right number of neighbors in \tilde{W}^{ij} . Then we do the same for vertices in \tilde{W}^{ij} .

This way we have constructed a bipartite multigraph between \tilde{W}^{rs} and \tilde{W}^{ij} such that each vertex of each $\tilde{W}^{rs(t)}$ is incident with exactly $p_{ij}^{rs(t)}$ edges, and each vertex of each $\tilde{W}^{ij(t')}$ is incident with exactly $p_{rs}^{ij(t')}$ edges.

It may happen in some instances that multiple edges are unavoidable. In that case let $d \leq m^*$ be the maximal edge multiplicity in G_0 . We obtain the graph G' by taking d copies of the multigraph G_0 and replace each collection of d parallel edges of multiplicity $d' \leq d$ by a simple d' -regular bipartite graph.

Due to the construction, it is straightforward to check that vertices from sets that share the same index r form the r -th block of a partition of $V_{G'}$ satisfying equation (1), and that vertices from sets that share the same index s form the s -th block of a partition of $V_{G'}$ satisfying equation (3). In other words: $G' \xrightarrow{B} M$ and $G' \xrightarrow{L} N$ hold. Since we took at most m^* copies of G_0 to obtain G' , we find that $\langle G' \rangle = (klm)^{O(k^2 l^2)}$.

For the other direction of the proof, suppose there exists a graph G of size $(klm^*)^{O(k^2 l^2)}$ such that $G \xrightarrow{B} M$ and $G \xrightarrow{L} N$. In order to show $M \xrightarrow{\exists!} N$ we construct a graph H with $H \xrightarrow{B} N$ and $G \xrightarrow{L} H$.

Let $\{V'_1, \dots, V'_l\}$ be a partition of V_G for $G \xrightarrow{L} N$. Since N is a degree matrix in \mathcal{M} , the dimension of the solution space of the following homogeneous system whose equations represent the number of edges between two different blocks in N is equal to one by Theorem 17:

$$n_{sj}v_s = n_{js}v_j \quad 1 \leq j, s \leq l \quad (7)$$

This implies that we can form sets V_1, \dots, V_l by further inserting new vertices into V'_1, \dots, V'_l until for each s, j we have that $|V_s|n_{sj} = |V_j|n_{js}$ and $|V_s| > 0$ is even.

Next we build a multigraph H_0 by constructing an (n_{sj}, n_{js}) -regular bipartite multigraph between any two sets V_s and V_j , and an n_{jj} -regular multigraph on each V_j . In case multiple edges cannot be avoided we take sufficient copies of H_0 and make the appropriate reparations. So we perform these steps in the same way as before, however without removing any edges between vertices in (any copy of) G .

Clearly, G is a subgraph of the resulting graph H and H has N as its degree refinement matrix. So we have $G \xrightarrow{L} H$ with $G \xrightarrow{B} M$ and $H \xrightarrow{B} N$ as was required. \square

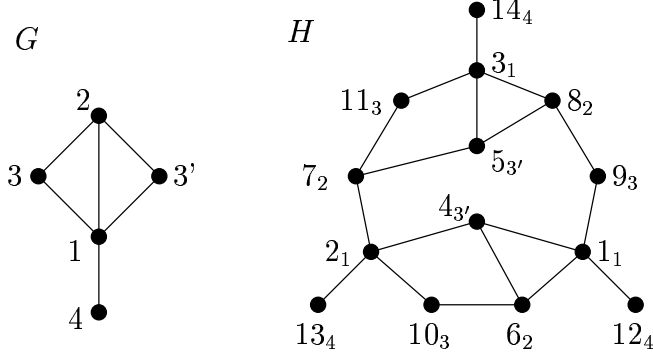


Figure 7: Graphs G and H , vertices of H are labeled by $u_{f(u)}$ for a $f : H \xrightarrow{s} G$.

We can now settle the computational complexity result for the following matrix comparison problem.

Corollary 39 *The MATRIX INJECTIVITY problem belongs to the complexity class NP.*

Proof: The proof of Theorem 38 showed that $M \xrightarrow{\exists!} N$ if and only if system (6) has a nontrivial nonnegative solution. Then by Lemma 37 there exists a nontrivial nonnegative integral solution with at most k^2l^2+1 nonzero entries, which are each bounded in size by $O(k^2l^2 \log(klm^*))$. The certificate for membership in NP consists of the k^2l^2+1 nonzero entries of the vector \mathbf{w} together with the corresponding injective distribution rows. The size of this certificate is $O(k^4l^4 \log(klm^*))$, which is polynomial in the size of both matrices M and N . It can be tested in linear time (with respect to the length of the certificate) whether all injective distribution rows are valid, i.e., satisfy equations (4) and (5). The test whether the vector \mathbf{w} satisfies (6) can also be performed in polynomial time. \square

6.2 An example

We give an example to illustrate the proof technique of Theorem 38 that also serves as a counterexample for disproving Conjecture 25. Let us add that we have not been able to find a smaller counterexample.

Corollary 40 *There exist connected degree matrices M and N of order 4 and 14 respectively, such that $T_M \subseteq T_N$, but $M \not\xrightarrow{\exists!} N$.*

Proof: We first construct graphs G and H such that $H \xrightarrow{s} G$. Denote $M = \text{drm}(G)$ and $N = \text{drm}(H)$. Then according to Corollary 24 we get that $T_M \subseteq T_N$. We will now show that the MATRIX INJECTIVITY problem for matrices M and N has a negative answer.

The graphs G and H together with a mapping $f : H \xrightarrow{s} G$ are depicted in Figure 7.

The graph G has 4 classes in its degree refinement and H has 14 classes. Then N is the adjacency matrix of H and the degree refinement matrix of G is

$$M = \begin{pmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 2 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

In order to obtain a contradiction suppose $M \xrightarrow{\exists I} N$ holds. By Corollary 36 there exist a graph G' with $\text{drm}(G') = M$ and a graph H' with $\text{drm}(H') = N$ such that $G' \subseteq H'$. Let $\{U_1, \dots, U_4\}$ be the degree partition for G' and $\{V_1, \dots, V_{14}\}$ the one for H' . We define the sets W_{rs} as in the proof of Theorem 38.

As we have seen in the proof of Theorem 38 the pair (G', H') corresponds to a nontrivial solution of (6). Below we will show, however, that (6) only allows the trivial solution. For simplicity reasons we will first restrict the length of the injective distribution rows.

A vertex in class U_1 has four neighbors in G' . A vertex in class V_4 has three neighbors in H' . This means that a vertex of U_1 can never be in V_4 , i.e., $W_{1,4}$ is empty. Hence the set $T(1, 4)$ is empty. By the same argument we find that the sets $T(r, s)$ with $(r, s) = (1, 5), \dots, (1, 14), (2, 9), \dots, (2, 14), (3, 12), \dots, (3, 14)$ are empty.

A vertex in U_2 has a neighbor of degree four in G' . A vertex in V_1 does not have a neighbor of degree four in H' . Hence the set $T(2, 1)$ is empty. By the same argument we exclude pairs $(2, 2), (2, 3), (3, 1), (3, 2), (3, 3), (4, 1), (4, 2), (4, 3)$.

Any vertex in U_4 has degree one in G' . Suppose $u \in U_4$ belongs to V_4 . So it does not have degree one in H' . Let $v \in U_1$ be the (only) neighbor of u in G' . Then v has degree four in G' and must belong to $V_1 \cup V_2$. The other three neighbors of v all have degree greater than one in G' . However, one of these three remaining neighbors of v must have degree one in H' . Hence, the set $T(4, 4)$ is empty. In the same way we may exclude pairs $(4, 5), \dots, (4, 11)$.

Every vertex in $W_{2,4}$ needs a neighbor in $W_{3,1}$ or $W_{3,2}$. These sets are empty, since both $T(3, 1)$ and $T(3, 2)$ are empty. Hence $T(2, 4)$ is empty, and consequently, by a similar argument, $T(3, 6)$ is empty. Furthermore, $T(2, 4) = \emptyset$ implies that a vertex in $W_{1,2}$ does not have neighbor in $W_{3,7}$. Since every vertex in $W_{3,7}$ must have a neighbor in $W_{1,2}$, the latter implies $T(3, 7) = \emptyset$, and consequently $T(2, 5) = \emptyset$, which implies $T(3, 8) = \emptyset$.

Only the pairs $(3, 4)$ and $(3, 5)$ allow two injective distribution rows, the other pairs all allow one. So we have reduced the total number of feasible injective distribution rows to $4 \cdot 14 - 20 - 9 - 8 - 5 + 2 = 16$.

The equation (6) for $p, q = 1, 1$ and $i, j = 2, 6$ gives $w^{1,1} = w^{2,6}$. Analogously, $w^{1,1} = w^{3,4(1)}$ while $w^{2,6} = w^{3,4(1)} + w^{3,4(2)}$. Hence $w^{3,4(2)} = 0$. Further $w^{3,4(2)} = w^{1,2} = w^{3,10} = w^{2,6}$, and $w^{1,2} = w^{2,7} = w^{3,11} = w^{1,3}$. Consequently, $w^{1,1} = w^{1,2} = w^{1,3} = 0$.

It can be further shown that (6) allows only trivial solution via values of $w^{r,s}$. However, at this moment we can already claim that no witnesses G, H for $M \xrightarrow{\exists I} N$ exist, since it is impossible to map vertices from the first class of the degree partition of G on any vertex of H . \square

7 Degree matrix comparison via local surjectivity

In this section we consider the MATRIX SURJECTIVITY problem. Let M and N be two degree matrices for which we have to decide whether $M \xrightarrow{\exists S} N$. By the same kind of arguments as in the proof of Proposition 35 we can show it is sufficient to compare degree refinement matrices to each other.

Proposition 41 *Let M and N be matrices in \mathcal{M} . Then $M \xrightarrow{\exists S} N$ if and only if $\text{drm}(M) \xrightarrow{\exists S} \text{drm}(N)$.*

However, for an algorithm we cannot use the same approach as for the MATRIX INJECTIVITY problem immediately. Even if we construct a graph G with $G \xrightarrow{E} M$, there is no evident rule (as given by Corollary 36 for \xrightarrow{I}) how to construct some plausible graph H with $H \xrightarrow{E} N$ such that

| i | 1 | 1 | 1 | 2 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 4 | 4 | 4 |
|--------------|---|---|---|---|---|---|---|---|---|----|----|----|----|----|
| j | 1 | 2 | 3 | 6 | 7 | 8 | 4 | 5 | 9 | 10 | 11 | 12 | 13 | 14 |
| $p^{1,1}$ | | | | 1 | | | 1 | | 1 | | | 1 | | |
| $p^{1,2}$ | | | | | 1 | | 1 | | | 1 | | | 1 | |
| $p^{1,3}$ | | | | | | 1 | | 1 | | | 1 | | | 1 |
| $p^{2,6}$ | 1 | | | | | | 1 | | | 1 | | | | |
| $p^{2,7}$ | | 1 | | | | | | 1 | | | | 1 | | |
| $p^{2,8}$ | | | 1 | | | | | 1 | 1 | | | | | |
| $p^{3,4(1)}$ | 1 | | | 1 | | | | | | | | | | |
| $p^{3,4(2)}$ | | 1 | | 1 | | | | | | | | | | |
| $p^{3,5(1)}$ | | | 1 | | 1 | | | | | | | | | |
| $p^{3,5(2)}$ | | | | 1 | | 1 | | | | | | | | |
| $p^{3,9}$ | 1 | | | | | | | | | | 1 | | | |
| $p^{3,10}$ | | 1 | | 1 | | | | | | | | | | |
| $p^{3,11}$ | | | 1 | | 1 | | | | | | | | | |
| $p^{4,12}$ | 1 | | | | | | | | | | | | | |
| $p^{4,13}$ | | 1 | | | | | | | | | | | | |
| $p^{4,14}$ | | | 1 | | | | | | | | | | | |

Table 1: The injective distribution rows for M (only nonzero entries are shown).

$G \xrightarrow{S} H$ holds. The main theorem of the following section shows how these initial difficulties can be dissolved.

7.1 The graph construction theorem

In the following two lemmas we consider some cases in which the target matrix N is relatively simple. These cases will be the basic cases for the graph construction in our main theorem.

Lemma 42 *Let $N \in \mathcal{M}$ be a degree matrix of order two with zeros on the diagonal. Let G be a graph with $G \xrightarrow{S} N$. Then for any graph H with $H \xrightarrow{B} N$ there exists a connected graph G^* such that $G^* \xrightarrow{B} G$ and $G^* \xrightarrow{S} H$.*

$$\begin{array}{ccccc}
 G^* & \xrightarrow{B} & G & & \\
 & \searrow^S & & \searrow^S & \\
 & & H & \xrightarrow{B} & N
 \end{array}$$

Proof: Since $G \xrightarrow{S} N$, we have a partition $\{V_1, V_2\}$ of V_G satisfying equation (3). Let H be an arbitrary graph with $H \xrightarrow{B} N$ witnessed by a partition $\{W_1, W_2\}$ of V_H satisfying equation (1). We will construct a graph G^* such that $G^* \xrightarrow{B} G$ and $G^* \xrightarrow{S} H$.

Firstly, take an arbitrary mapping $\rho : E_G \rightarrow \{1, \dots, n_{1,2}\}$ that is surjective on edges incident with an arbitrary $u \in V_1$. Analogously take some $\sigma : E_G \rightarrow \{1, \dots, n_{1,2}\}$ that is surjective on edges incident with any $v \in V_2$.

For each vertex $x \in W_1$ we fix a numbering of its neighbors by $\{y_1, \dots, y_{n_{1,2}}\}$. Note that it is possible for a vertex $y \in W_2$ with neighbors x, x' to be $y = y_i$ in the numbering for x and $y = y_j$ in

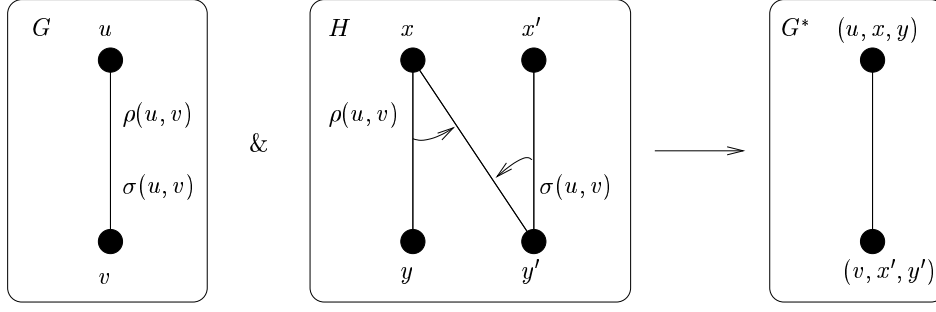


Figure 8: Construction of the graph G^* .

the numbering for x' such that $i \neq j$ holds. Analogously, for each vertex $y \in W_2$ we fix a numbering of its neighbors by $\{x_1, \dots, x_{n_{2,1}}\}$.

Then, for any $x \in W_1$ and $i, j \in \{1, \dots, n_{1,2}\}$ we define the action $y_i \xrightarrow{x, j} y_{(i+j) \bmod n_{1,2}}$. (To be precise, since we do not start from 0, subtract 1 before taking modulo and add 1 after.) Note that both y_i and $y_{(i+j) \bmod n_{1,2}}$ are neighbors of x . Analogously, for every $y \in W_2$ and $i, j \in \{1, \dots, n_{2,1}\}$, we define the action $x_i \xrightarrow{y, j} x_{(i+j) \bmod n_{2,1}}$. Note that both x_i and $x_{(i+j) \bmod n_{2,1}}$ are neighbors of y .

We are now ready to construct the desired graph G^* . We let

$$V_{G^*} = V_G \times E_H = \{(t, x, y) \mid t \in V_G, x \in W_1, y \in W_2, (x, y) \in E_H\}.$$

The edges are defined as follows (See Figure 8):

$$((u, x, y), (v, x', y')) \in E_{G^*} \iff \begin{cases} (u, v) \in E_G & \text{and} \\ y \xrightarrow{x, \rho(u,v)} y' & \text{and} \\ x' \xrightarrow{y, \sigma(u,v)} x \end{cases} \quad (8)$$

To show $G^* \xrightarrow{B} G$ we define the mapping $f : (t, x, y) \rightarrow t$. By the first condition of (8), the mapping f is a graph homomorphism. To argue that it is locally bijective observe that, whenever we take some (u, x, y) with $u \in V_1$ and a neighbor v of u , then there exist a unique $x' \in W_1$ such that $x' \xrightarrow{y, \sigma(u,v)} x$ and a unique $y' \in W_2$ such that $y \xrightarrow{x, \rho(u,v)} y'$, i.e., there is only one neighbor (v, x', y') of (u, x, y) that f maps to v . The local bijectivity on vertices (v, x', y') with $v \in V_2$ can be shown analogously.

It remains to prove that $G^* \xrightarrow{S} H$. We define a mapping $g : V_{G^*} \rightarrow V_H$ as follows: For $u \in V_1$ we let $g(u, x, y) = x$ and for $v \in V_2$ we let $g(v, x', y') = y'$. Consider any edge $((u, x, y), (v, x', y')) \in E_{G^*}$. Since y is a neighbor of x and $y \xrightarrow{x, \rho(u,v)} y'$, vertex y' must be a neighbor of x , which implies that g is a homomorphism. To argue that it is locally surjective, we fix an arbitrary (u, x, y) , where $u \in V_1$, and a neighbor y' of x . Then there exist a unique $q \in \{1, \dots, n_{1,2}\}$ such that $y \xrightarrow{x, q} y'$. Further, by the definition of ρ there is at least one neighbor v of u such that $\rho(u, v) = q$. To fulfill the local surjectivity condition we take the unique vertex x' such that $x' \xrightarrow{y, \sigma(u,v)} x$ to construct a neighbor (v, x', y') of (u, x, y) that is mapped to y' . An analogous argument gives local surjectivity for vertices (v, x', y') with $v \in V_2$. \square

The case of matrices of order one cannot be treated directly as in the above case. The reason is that the construction heavily depends on the bipartition of the graph H , which cannot be assumed in this new setting. We present here a useful trick (motivated by [12]) that allows us to focus on bipartite graphs.

Lemma 43 *Let $N \in \mathcal{M}$ be a degree matrix of order one. Let G be a graph with $G \xrightarrow{S} N$. Then for any graph H with $H \xrightarrow{B} N$ there exists a connected graph G^* such that $G^* \xrightarrow{B} G$ and $G^* \xrightarrow{S} H$.*

Proof: Let us first recall the notion of Kronecker double cover $G \times K_2$ of a graph G . For vertices we take twice the vertex set of G , i.e., $V_{G \times K_2} = V_G \times \{1, 2\}$ and define the edges as $E_{G \times K_2} = \{(u, i), (v, j) \mid (u, v) \in E_G, i \neq j\}$. If the graph G is bipartite then its Kronecker double cover consists of two disjoint copies of G . Otherwise the resulting graph is connected and bipartite. In both cases it allows a locally bijective homomorphism $\pi : G \times K_2 \xrightarrow{B} G$ by the projection to the first coordinate: $\pi(u, i) = u$.

For the proof of the lemma we take $G' = G \times K_2$, and $H' = H \times K_2$. We define the matrix

$$N' = \begin{pmatrix} 0 & n_{1,1} \\ n_{1,1} & 0 \end{pmatrix}.$$

Then $H' \xrightarrow{B} N'$, and we can apply Lemma 42 for N' , G' and H' . Any component G_i^* of the resulting graph G^* satisfies $G_i^* \xrightarrow{B} G' \xrightarrow{B} G$ and $G_i^* \xrightarrow{S} H' \xrightarrow{B} H$, which proves the statement. \square

We now present our graph construction theorem.

Theorem 44 *Let M and N be matrices in \mathcal{M} . The following statements are equivalent.*

- (i) $M \xrightarrow{\exists S} N$.
- (ii) There exists a graph G such that $G \xrightarrow{B} M$ and $G \xrightarrow{S} N$.
- (iii) For any graph H such that $H \xrightarrow{B} N$ there exists a graph G^* such that $G^* \xrightarrow{B} M$ and $G^* \xrightarrow{S} H$.

Proof: (iii) \Rightarrow (i) This is trivially true since $M \xrightarrow{\exists S} N$ requires the existence of only a single pair G and H with $G \xrightarrow{B} M$, $H \xrightarrow{B} N$, and $G \xrightarrow{S} H$.

(i) \Rightarrow (ii) Since $M \xrightarrow{\exists S} N$, there exist a graph G and a graph H such that $G \xrightarrow{B} M$, $H \xrightarrow{B} N$ and $G \xrightarrow{S} H$. The composition of $G \xrightarrow{S} H$ and $H \xrightarrow{B} N$ gives $G \xrightarrow{S} N$.

(ii) \Rightarrow (iii) This is the core implication of the proof. Let M and N have order k and l , respectively. Let G be the graph with $G \xrightarrow{B} M$ and $G \xrightarrow{S} N$. Since $G \xrightarrow{S} N$, we have a partition $\{V_1, \dots, V_l\}$ of V_G satisfying equation (3). Let H be an arbitrary graph with $H \xrightarrow{B} N$ witnessed by a partition $\{W_1, \dots, W_l\}$ of V_H satisfying equation (1). We will construct a graph G^* with $G^* \xrightarrow{B} M$ such that $G^* \xrightarrow{S} H$ via partition $\{V_1^*, \dots, V_l^*\}$.

For $1 \leq i < j \leq l$ with $n_{i,j} > 0$, let $H^{\{i,j\}}$ be the (bipartite) subgraph of H induced by $W_i \cup W_j$, and let $G^{\{i,j\}}$ be the (bipartite) subgraph of G induced by $V_i \cup V_j$. For $1 \leq i \leq l$ with $n_{i,i} > 0$, let $H^{\{i\}}$ be the subgraph of H induced by W_i , and let $G^{\{i\}}$ be the subgraph of G induced by V_i .

For $1 \leq i < j \leq l$ with $n_{i,j} > 0$, we construct a graph $G^{\{i,j\}*}$ as in the proof of Lemma 42. Recall that $V_{G^{\{i,j\}*}}$ consists of all vertices (u, x, y) with $u \in V_{G^{\{i,j\}}}$, $x \in W_i$, $y \in W_j$ such that $(x, y) \in E_{H^{\{i,j\}}}$, and we defined edges in such a way that we have mappings $f^{\{i,j\}} : G^{\{i,j\}*} \xrightarrow{B} G^{\{i,j\}}$, and $g^{\{i,j\}} : G^{\{i,j\}*} \xrightarrow{S} H^{\{i,j\}}$. Let $V_{G^{\{i,j\}*}} = V_i^{\{i,j\}*} \cup V_j^{\{i,j\}*}$, such that $g^{\{i,j\}}$ maps all vertices in $V_i^{\{i,j\}*}$ into vertices of the block W_i and all vertices in $V_j^{\{i,j\}*}$ into vertices of W_j .

For $1 \leq i \leq l$ with $n_{i,i} > 0$, we define a graph $G^{\{i\}*}$ as in the proof of Lemma 43. Note that this graph is in fact constructed in Lemma 42 for the product graphs $G^{\{i\}} \times K_2$, whose vertices (u, i) we below denote as u_i , and $H^{\{i\}} \times K_2$, whose vertices (x, i) will be denoted as x_i . So the vertex set of $G^{\{i\}*}$ consists of all vertices (u_1, x_1, y_2) and (u_2, y_1, x_2) with $u \in V_{G^{\{i\}}}$, $x, y \in W_i$ such that $(x, y) \in E_{H^{\{i\}}}$, and its edges have been defined in such a way that we have mappings $f^{\{i\}} : G^{\{i\}*} \xrightarrow{\beta} G^{\{i\}}$, and $g^{\{i\}} : G^{\{i\}*} \xrightarrow{\xi} H^{\{i\}}$. We denote the vertex set of $G^{\{i\}*}$ by $V_i^{\{i\}*}$.

Let F_N be the (symmetric directed) quotient graph of N , where $V_{F_N} = \{1, 2, \dots, l\}$, such that vertex i corresponds to the i -th row and column of N . Recall that $(i, j), (j, i)$ with $i < j$ are arcs in F_N if and only if $n_{i,j} > 0$ (and consequently $n_{j,i} > 0$, since N is a degree matrix), and that (i, i) is a loop in F_N if and only if $n_{i,i} > 0$. We define a variable $\alpha^e > 0$ for each $e = \{i, j\}$ that corresponds to arcs $(i, j), (j, i)$ with $i < j$ in F_N and for each $e = \{i\}$ that corresponds to a loop (i, i) in F_N . We show that we can define the block sizes of G^* as

$$|V_i^*| = \alpha^e \cdot |V_i^{e*}| \text{ whenever } i \in e,$$

for some appropriate values for the variables α^e . In order to see this, we first note that, for some arc (i, j) in F_N with $i \neq j$, the sizes of sets V_i^* and V_j^* are uniquely determined if we fix $\alpha^{\{i,j\}} > 0$. Suppose (j, j) is a loop in F_N . Then also $\alpha^{\{j\}}$ is uniquely determined. Suppose (j, h) is an arc in F_N with $j \neq h$. Then also $\alpha^{\{j,h\}}$ is uniquely determined, and so on. Since F_N is connected, this way values of all variables α^e are determined. In order to see that the cycles in F_N do not cause any conflicts, consider the following equation, which expresses the size of $V_i^* \subset V_i^{\{i,j\}*}$, for some arc (i, j) in F_N , in terms of the block sizes of the original graphs G and H .

$$|V_i^*| = \alpha^{\{i,j\}} \cdot |V_i^{\{i,j\}*}| = \alpha^{\{i,j\}} \cdot |V_i| \cdot |E_{H^{\{i,j\}}}| = \alpha^{\{i,j\}} \cdot |V_i| \cdot |W_i| \cdot n_{i,j} \quad (9)$$

Assume without loss of generality that F_N contains a cycle $1, \dots, c, 1$. Then the size of V_c^* can be expressed in two ways as

$$|V_1^*| \cdot \frac{|V_c|}{|V_1|} \cdot \frac{|W_c|}{|W_1|} \cdot \frac{n_{c,1}}{n_{1,c}} = |V_c^*| = |V_1^*| \cdot \frac{|V_c|}{|V_1|} \cdot \frac{|W_c|}{|W_1|} \cdot \prod_{j=1}^{c-1} \frac{n_{j+1,j}}{n_{j,j+1}}.$$

Here in the first case we have considered only the arc $(1, c)$, while in the other we have iterated (9) along the path $1, 2, \dots, c$. As each cycle of F_N satisfies the cycle product identity due to Theorem 17, the two expressions above cause no conflict. Hence, values for all α^e can be derived from a single entry $\alpha^{\{i,j\}} > 0$ regardless which paths were used during the computation. Since all coefficients in the system of linear equations determining the values for the variables α^e are integers, we may assume that the chosen values $\alpha^e > 0$ are integer as well.

We now show how we construct the desired graph G^* on blocks V_i^* with block sizes $|V_i^*| = \alpha^e |V^{e*}|$, where $e = \{i, j\}$ for some arc (i, j) in F_N . For each e that corresponds to an arc in F_N , we take α^e copies of G^{e*} .

Suppose (i, j) is an arc in F_N with $i < j$. Fix a vertex $u \in V_i$ and a vertex $x \in W_i$. Then the total number of vertices (u, x, y) with $y \in W_j$ in the disjoint union of the $\alpha^{\{i,j\}}$ copies $V_i^{\{i,j\}*}$ has size $\alpha^{\{i,j\}} n_{i,j}$. For any other arc (i, h) in F_N with $i \neq h$, the total number of vertices (u, x, z) (or (u, z, x) if $i < h$) with $z \in W_h$ in the disjoint union of the $\alpha^{\{i,h\}}$ copies of $V_i^{\{i,h\}*}$ has size $\alpha^{\{i,h\}} n_{i,h}$. Since $\alpha^{\{i,j\}} |V_i| |W_i| n_{i,j} = \alpha^{\{i,j\}} |V_i^{\{i,j\}*}| = \alpha^{\{i,h\}} |V_i^{\{i,h\}*}| = \alpha^{\{i,h\}} |V_i| |W_i| n_{i,h}$, we find that

$$\alpha^{\{i,j\}} n_{i,j} = \alpha^{\{i,h\}} n_{i,h}.$$

If (i, i) is a loop in F_N , then, in the same way, we find that the total number of vertices (u_1, x_1, x'_2) and (u_2, x'_1, x_2) with $x' \in W_i$ in the disjoint union of the $\alpha^{\{i\}}$ copies of $V^{\{i\}*}$ is equal to $\alpha^{\{i\}}n_{i,i} = \alpha^{\{i,j\}}n_{i,j}$. This means that, for $p = 1, \dots, \alpha^{\{i,j\}}n_{i,j}$, we can take a vertex from each disjoint union of α^e copies of V_i^{e*} with $i \in e$, and merge them into a single vertex $(u, x)_p$. We do this for each pair (u', x') with $u' \in V_i$ and $x' \in W_i$, and this way we obtain the block V_i^* of desired size $|V_i^*| = \alpha^{\{i,j\}}n_{i,j}|V_i| |W_i| = \alpha^{\{i,j\}}|V_i^{\{i,j\}*}|$. After performing such a series of unification for all $i = 1, \dots, l$, we get the desired graph G^* .

The mapping $G^* \xrightarrow{B} G$ is the projection to the original vertices of G , i.e., $(u, x)_p \rightarrow u$. The mapping $G^* \xrightarrow{S} H$ follows from the partial mappings $g^{\{i,j\}}$ and $g^{\{i\}}$, i.e., $(u, x)_p \rightarrow x$. (If G^* is disconnected, we take one of its components.) \square

7.2 Computational complexity

We are now ready to show computational complexity of the MATRIX SURJECTIVITY problem, i.e., deciding if $M \xrightarrow{\exists S} N$ for two degree matrices M and N . Recall that $m^* = \max(\{2\} \cup \{m_{i,j} \mid 1 \leq i, j \leq k\})$ for a matrix M of order k with $M_{i,j} = m_{i,j}$.

Theorem 45 *For two connected degree matrices M and N of order k and l respectively, $M \xrightarrow{\exists S} N$ holds if and only if there exists a graph G of size $(klm^*)^{O(k^2l^2)}$ such that $G \xrightarrow{B} N$ and $G \xrightarrow{S} M$.*

Proof: Let $M, N \in \mathcal{M}$ be two degree matrices of order k and l respectively. Throughout this proof we assume that indices i, j, r, s used later always belong to feasible intervals $1 \leq i, r \leq k$ and $1 \leq j, s \leq l$. Just as in the proof of Theorem 38, we often abbreviate pairs of sub-/super-scripts i, j by ij .

Suppose $M \xrightarrow{\exists S} N$ holds. Due to Theorem 44, we find that there exists a graph G such that $G \xrightarrow{B} M$ and $G \xrightarrow{S} N$. Let $\{U_1, \dots, U_k\}$ be a partition of V_G for $G \xrightarrow{B} M$, and $\{V_1, \dots, V_l\}$ be a partition of V_G for $G \xrightarrow{S} N$. For each pair of indices r and s we define the set $W_{rs} = \{v \mid v \in U_r \cap V_s\}$, and for each vertex $u \in W_{rs} \subseteq V_G$ we can write a vector $\mathbf{p}(u) = (|N_G(u) \cap W_{11}|, \dots, |N_G(u) \cap W_{kl}|)$ describing the distribution of neighbors of u in the classes W_{11}, \dots, W_{kl} .

We first consider the structure of such vectors. Let \mathbf{p}^{rs} be a vector of length kl whose entries are nonnegative integers and are indexed by pairs ij . If the vector \mathbf{p}^{rs} further satisfies

$$\sum_{j=1}^l p_{i,j}^{r,s} = m_{r,i} \quad \text{for all } 1 \leq i \leq k, \quad (10)$$

$$n_{s,j} > 0 \quad \Rightarrow \quad \sum_{i=1}^k p_{i,j}^{r,s} \geq n_{s,j} \quad \text{for all } 1 \leq j \leq l. \quad (11)$$

$$n_{s,j} = 0 \quad \Rightarrow \quad \sum_{i=1}^k p_{i,j}^{r,s} = 0 \quad \text{for all } 1 \leq j \leq l. \quad (12)$$

then we call \mathbf{p}^{rs} a *surjective distribution row for indices r and s* . Due to (10), the set

$$T(r, s) = \{\mathbf{p}^{rs(1)}, \dots, \mathbf{p}^{rs(t(r,s))}\}$$

of surjective distribution rows is bounded by $t(r, s) \leq \binom{m^*+l-1}{m^*}^k = O((m^*+1)^{kl})$ for every pair of indices r, s . The total number of distribution rows is then

$$t_0 = \sum_{r,s} t(r, s) = O(kl(m^*+1)^{kl}).$$

The vector \mathbf{w} with entries $w^{rs(t)} = |\{u : \mathbf{p}(u) = \mathbf{p}^{rs(t)}\}|$ is a nontrivial solution of the following homogeneous system of k^2l^2 equations in t_0 variables

$$\sum_{t=1}^{t(r,s)} p_{ij}^{rs(t)} w^{rs(t)} = \sum_{t'=1}^{t(i,j)} p_{rs}^{ij(t')} w^{ij(t')} \quad 1 \leq i, r \leq k, 1 \leq j, s \leq l, \quad (13)$$

since in each equation both sides are equal to the number of edges connecting sets W_{rs} and W_{ij} .

So the system (6) has a nontrivial nonnegative solution. Note that all coefficients $p_{ij}^{rs(t)}$ of this system are at most m^* . Then, by Lemma 37, we find a nontrivial nonnegative integer solution whose entry sizes are bounded by $O(k^2l^2 \log(klm^*))$. We use this solution to construct a graph G' of size $\langle G' \rangle = (klm^*)^{O(k^2l^2)}$, such that $G' \xrightarrow{B} M$ and $G' \xrightarrow{S} N$, analogously to the construction of the graph for the locally injective homomorphisms in the proof of Theorem 38.

For the other direction of the proof, suppose there exists a graph G of size $(klm^*)^{O(k^2l^2)}$ such that $G \xrightarrow{B} M$ and $G \xrightarrow{S} N$. Then $M \xrightarrow{\exists S} N$ holds due to Theorem 44. \square

We can now settle the computational complexity result for the following matrix comparison problem. The proof is analogous to the proof of Corollary 39.

Corollary 46 *The MATRIX SURJECTIVITY problem belongs to the complexity class NP.*

Another corollary of our proof technique is that for a given connected graph G , if the $\text{drm}(G) \xrightarrow{\exists S} \text{drm}(H)$ heuristic for the $G \xrightarrow{S} H$ question gives an affirmative answer, then this implies the existence of an infinite set of connected graphs G' for which $\text{drm}(G') = \text{drm}(G)$ and $G' \xrightarrow{S} H$ (this follows easily from case (iii) of Theorem 44).

8 Conclusion

We have shown that graph homomorphisms with local constraints impose interesting orders not only on the class of graphs but also on the class of degree (refinement) matrices, and given algorithms for matrix comparability under these orders. We have also shown that these degree matrices arising from equitable partitions can be efficiently recognized.

There are several avenues for future work. On the computational side we may ask if MATRIX INJECTIVITY ($M \xrightarrow{\exists I} N$) and MATRIX SURJECTIVITY ($M \xrightarrow{\exists S} N$) are NP-complete, also for small, fixed degree matrices N . Here we have only partial results. It would also be nice to find combinatorial constraints on pairs of degree refinement matrices equivalent to the existentially defined relations $M \xrightarrow{\exists I} N$ and $M \xrightarrow{\exists S} N$.

Finally, we would like to stress the fact that we have restricted ourselves to connected graphs only for the clarity of presentation. Our methods and results can be straightforwardly generalized to disconnected graphs.

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