Pebble Games and Linear Equations

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Abstract

We give a new, simplified and detailed account of the correspondence between levels of the Sherali–Adams relaxation of graph isomorphism and levels of pebble-game equivalence with counting (higher-dimensional Weisfeiler–Lehman colour refinement). The correspondence between basic colour refinement and fractional isomorphism, due to Tinhofer [22, 23] and Ramana, Scheinerman and Ullman [17], is re-interpreted as the base level of Sherali–Adams and generalised to higher levels in this sense by Atserias and Maneva [1] and Malkin [14], who prove that the two resulting hierarchies interleave. In carrying this analysis further, we here give (a) a precise characterisation of the level k Sherali–Adams relaxation in terms of a modified counting pebble game; (b) a variant of the Sherali–Adams levels that precisely match the k-pebble counting game; (c) a proof that the interleaving between these two hierarchies is strict. We also investigate the variation based on boolean arithmetic instead of real/rational arithmetic and obtain analogous correspondences and separations for plain k-pebble equivalence (without counting). Our results are driven by considerably simplified accounts of the underlying combinatorics and linear algebra.

Contents

1 Introduction

We study a surprising connection between equivalence in finite variable logics and a linear programming approach to the graph isomorphism problem. This connection has recently been uncovered by Atserias and Maneva [1] and, independently, Malkin [14], building on earlier work of Tinhofer [22, 23] and Ramana, Scheinerman and Ullman [17] that just concerns the 2-variable case.

Finite variable logics play a central role in finite model theory. Most important for this paper are finite variable logics with counting, which have been specifically studied in connection with the question for a logical characterisation of polynomial time and in connection with the graph isomorphism problem (e.g. [6, 8, 9, 12, 13, 16]). Equivalence in finite variable logics can be characterised in terms of simple combinatorial games known as pebble games. Specifically, C^k-equivalence can be characterised by the bijective k-pebble game introduced by Hella [10]. Cai, Fürer and Immerman [6] observed that C^k-equivalence exactly corresponds to indistinguishability by the k-dimensional Weisfeiler-Lehman (WL) algorithm,[1] a combinatorial graph isomorphism algorithm that goes back to work of Weisfeiler and Lehman in the 1970s (for example, [24]; see [6] for an account of the history of the algorithm). The 2-dimensional version of the WL algorithm precisely corresponds to an even simpler isomorphism algorithm known as colour refinement.

The isomorphisms between two graphs can be described by the integral solutions of a system of linear equations and inequalities. If we have two graphs with adjacency matrices A and B, then each isomorphism from the first to the second corresponds to a permutation matrix X such that $X^tAX = B$, or equivalently

$$AX = XB. \tag{1}$$

If we view the entries of X as variables, this equation corresponds to a system of linear equations. We can add inequalities that force X to be a permutation matrix and obtain a system ISO of linear equations and inequalities whose integral solutions correspond to the isomorphisms between the two graphs. In particular, the system ISO has an integral solution if and only if the two graphs are isomorphic.

What happens if we drop the integrality constraints, that is, if we admit arbitrary real solutions of the system ISO? We can ask for doubly stochastic matrices X satisfying equation (1). (A real matrix is *doubly stochastic* if its

[1] The dimensions of the WL algorithm are counted differently in the literature; what we call "k-dimensional" here is sometimes called "$(k-1)$-dimensional".

entries are non-negative and all row sums and column sums are one.) Tinhofer [22, 23] proved a beautiful result that establishes a connection between linear algebra and logic: the system ISO has a real solution if, and only if, the colour refinement algorithm does not distinguish the two graphs with adjacency matrices A and B. Recall that the latter is equivalent to the two graphs being C^2-equivalent.

To bridge the gap between integer linear programs and their LP-relaxations, researchers in combinatorial optimisation often add additional constraints to the linear programs to bring them closer to their integer counterparts. The Sherali–Adams hierarchy [21] of relaxations gives a systematic way of doing this. For every integer linear program IL in n variables and every positive integer k, there is a *rank-k Sherali–Adams relaxation* IL(k) of IL, such that IL(1) is the standard LP-relaxation of IL where all integrality constraints are dropped and IL(n) is equivalent to IL. There is a considerable body of research studying the strength of the various levels of this and related hierarchies (e.g. [4, 5, 7, 15, 20, 19]).

Quite surprisingly, Atserias and Maneva [1] and Malkin [14] were able to lift Tinhofer's result, which we may now restate as an equivalence between ISO(1) and C^2-equivalence, to a close correspondence between the higher levels of the Sherali–Adams hierarchy for ISO and the logics C^k. They proved for every $k \geq 2$:

1. if ISO(k) has a (real) solution, then the two graphs are C^k-equivalent;
2. if the two graphs are C^k-equivalent, then ISO($k-1$) has a solution.

Atserias and Maneva [1] used these results to transfer results about the logics C^k to the world of polyhedral combinatorics and combinatorial optimisation, and conversely, results about the Sherali–Adams hierarchy to logic.

Atserias and Maneva [1] left open the question whether the interleaving between the levels of the Sherali–Adams hierarchy and the finite-variable-logic hierarchy is strict or whether either the correspondence between C^k-equivalence and ISO(k) or the correspondence between C^k-equivalence and ISO($k-1$) is exact. Note that for $k = 2$ the correspondence between C^k-equivalence and ISO($k-1$) is exact by Tinhofer's theorem. We prove that for all $k \geq 3$ the interleaving is strict. However, we can prove an exact correspondence between ISO($k-1$) and a variant of the bijective k-pebble game that characterises C^k-equivalence. This variant, which we call the weak bijective k-pebble game, is actually equivalent to a game called ($k-1$)-sliding game by Atserias and Maneva.

Furthermore, we prove that a natural combination of equalities from ISO(k) and ISO($k-1$) gives a linear program ISO($k-1/2$) that characterises C^k-equivalence exactly. Malkin [14] gives an alternative characterisation of C^k-equivalence in terms of the Sherali-Adams relaxations of a different polytope. Building on our work, yet another algebraic characterisation of C^k-equivalence has recently been given in [3].

To obtain these results, we give simple new, and arguably simpler proofs of the theorems of Tinhofer and of Atserias and Maneva. In fact, the linear algebra we use is so simple that much of it can be carried out not only over the field of real numbers, but over arbitrary semirings. By using similar algebraic arguments over the boolean semiring (with disjunction as addition and conjunction as multiplication), we obtain analogous results to those for C^k-equivalence for the ordinary k-variable logic L^k, characterising L^k-equivalence, i.e., k-pebble game equivalence without counting, by systems of 'linear' equations over the boolean semiring.

2 Finite variable logics and pebble games

We assume the reader to be familiar with the basics of first-order logic FO. We almost exclusively consider first-order logic over finite graphs, which we view as finite relational structures with one binary relation. We assume graphs to be undirected and loop-free. For every positive integer k, we let L^k be the fragment of FO consisting of all formulae that contain at most k distinct variables.

We write $\mathcal{A} \equiv^k_{\mathsf{L}} \mathcal{B}$ to denote that two structures $\mathcal{A}, \mathcal{B}$ are L^k-*equivalent*, that is, satisfy the same L^k-sentences. L^k-equivalence can be characterised in terms of the k-*pebble game*, played by two players on a pair $\mathcal{A}, \mathcal{B}$ of structures. A *play* of the game consists of a (possibly infinite) sequence of *rounds*. In each round, player **I** picks up one of his pebbles and places it on an element of one of the structures $\mathcal{A}, \mathcal{B}$. Player **II** answers by picking up her pebble with the same label and placing it on an element of the other structure.

Note that after each round r there is a subset $p \subseteq \mathcal{A} \times \mathcal{B}$ consisting of the at most k pairs of elements on which the pairs of corresponding pebbles are placed. We call p the *position* after round r. Player **II** wins the play if every position that occurs is a local isomorphism, that is, a local mapping from $\mathcal{A}$ to $\mathcal{B}$ that is injective and preserves membership and non-membership in all relations (adjacency and non-adjacency if $\mathcal{A}$ and $\mathcal{B}$ are graphs).

Theorem 2.1 (Barwise [2], Immerman [11])**.** *$\mathcal{A} \equiv^k_{\mathsf{L}} \mathcal{B}$ if, and only if, player* **II** *has a winning strategy for the k-pebble game on $\mathcal{A}, \mathcal{B}$.*

We extend L^k-equivalence to structures with distinguished elements. For tuples $\mathbf{a}$ and $\mathbf{b}$ of the same length $\ell \leq k$ we let $\mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}$ if $\mathcal{A}, \mathbf{a}$ and $\mathcal{B}, \mathbf{b}$ satisfy the same L^k-formulae $\varphi(\mathbf{x})$ with ℓ free variables $\mathbf{x}$. The pebble game characterisation extends: $\mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}$ if, and only if, player **II** has a winning strategy for the k-pebble game on $\mathcal{A}, \mathcal{B}$ starting with pebbles on $\mathbf{a}$ and the corresponding pebbles on $\mathbf{b}$. The L^k-*type* of a tuple $\mathbf{a}$ in a structure $\mathcal{A}$ is the $\equiv^k_{\mathsf{L}}$-equivalence class of $\mathcal{A}, \mathbf{a}$. More syntactically, we may also view the L^k-type of $\mathbf{a}$ as the set of all L^k-formulae $\varphi(\mathbf{x})$ satisfied by $\mathcal{A}, \mathbf{a}$.

Let us turn to the k-variable counting logics. It is convenient to start with the (syntactical) extension C of FO by *counting quantifiers* $\exists^{\geq n}$. The semantics of these counting quantifiers is the obvious one: $\exists^{\geq n} x\, \varphi$ means that there are at least n elements x such that φ is satisfied. Of course this can be expressed in FO, but only by a formula that uses at least n variables. For all positive integers k, we let C^k denote the k-variable fragment of C. Whereas C and FO have the same expressive power, C^k is strictly more expressive than L^k.

We write $\mathcal{A} \equiv_{\mathsf{C}}^{k} \mathcal{B}$ to indicate that structures $\mathcal{A}$ and $\mathcal{B}$ are C^k-equivalent. C^k-equivalence can be characterised in terms of the *bijective k-pebble game*, which, like the k-pebble game, is played by two players by placing k pairs of pebbles on a pair of structures $\mathcal{A}, \mathcal{B}$. The rounds of the bijective game are as follows. Player **I** picks up one of his pebbles, and player **II** picks up her corresponding pebble. Then player **II** chooses a bijection f between $\mathcal{A}$ and $\mathcal{B}$ (if no such bijection exists, that is, if the structures have different cardinalities, player **II** immediately loses). Then player **I** places his pebble on an element a of $\mathcal{A}$, and player **II** places her pebble on $f(a)$. Again, player **II** wins a play if all positions are local isomorphisms.

Theorem 2.2 (Hella [10]). *$\mathcal{A} \equiv_{\mathsf{C}}^{k} \mathcal{B}$ if, and only if, player **II** has a winning strategy for the bijective k-pebble game on $\mathcal{A}, \mathcal{B}$.*

As with L^k-equivalence, we extend C^k-equivalence to structures with distinguished elements, writing $\mathcal{A}, \mathbf{a} \equiv_{\mathsf{C}}^{k} \mathcal{B}, \mathbf{b}$. Again, the pebble-game characterisation of the equivalence extends. We define C^k-types analogously to L^k-types.

The *colour refinement* algorithm is a simple combinatorial heuristic for testing whether two graphs are isomorphic. Given two graphs $\mathcal{A}$ and $\mathcal{B}$, which we assume to be disjoint, it computes a colouring of their vertices by the following iterative procedure: Initially, all vertices have the same colour. Then in each round, the colouring is refined by assigning different colours to vertices that have a different number of neighbours of at least one colour assigned in the previous round. Thus after the first round, two vertices have the same colour if, and only if, they have the same degree. After the second round, two vertices have the same colour if, and only if, they have the same degree and for each d the same number of neighbours of degree d. The algorithm stops if no further refinement is achieved; this happens after at most $|\mathcal{A}| + |\mathcal{B}|$ rounds. We call the resulting colouring of $\mathcal{A} \cup \mathcal{B}$ the *stable colouring* of $\mathcal{A}, \mathcal{B}$. If the stable colouring differs on the two graphs, that is, for some colour c the graphs have a different number of vertices of colour c, then we say that colour refinement *distinguishes* the graphs.

Theorem 2.3 (Immerman and Lander [12]). *$\mathcal{A} \equiv_{\mathsf{C}}^{2} \mathcal{B}$ if, any only if, colour refinement does not distinguish $\mathcal{A}$ and $\mathcal{B}$.*

The *k-dimensional Weisfeiler-Lehman algorithm* (for short: k-WL) is a generalisation of the colour refinement algorithm, which instead of vertices colours k-tuples of vertices. Given two structures $\mathcal{A}$ and $\mathcal{B}$, which we assume to be disjoint, k-WL iteratively computes a colouring of $\mathcal{A}^k \cup \mathcal{B}^k$. Initially, two tuples $\mathbf{a} = (a_1, \ldots, a_k), \mathbf{b} = (b_1, \ldots, b_k) \in \mathcal{A}^k \cup \mathcal{B}^k$ get the same colour if the mapping defined by $p(a_i) = b_i$ is a local isomorphism. In each round of the algorithm, the colouring is refined by assigning different colours to tuples that for some $j \in [k]$ and some colour c have different numbers of j-neighbours of colour c in their respective graphs. Here we call two k-tuples *j-neighbours* if they differ only in their jth component. The algorithm stops if no further refinement is achieved; this happens after at most $|\mathcal{A}|^k + |\mathcal{B}|^k$ rounds. If after the refinement process the colourings of the two graphs differ, that is, for some colour c the graphs have a different number of k-tuples of colour c, then we say that k-WL *distinguishes* the graphs.

Theorem 2.4 (Cai, Fürer, and Immerman [6]). *$\mathcal{A} \equiv_{\mathsf{C}}^{k} \mathcal{B}$ if, and only if, k-WL does not distinguish $\mathcal{A}$ and $\mathcal{B}$.*

More significantly, Cai, Fürer, and Immerman [6] proved that for all k there are nonisomorphic graphs $\mathcal{A}_k, \mathcal{B}_k$ of size $O(k)$ such that $\mathcal{A} \equiv_{\mathsf{C}}^{k} \mathcal{B}$.

Note that the previous two theorems imply that colour refinement and 2-WL distinguish the same graphs.

There are also 'boolean' versions of the two algorithms characterising L^k-equivalence (see [16]).

3 Basic combinatorics and linear algebra

We consider matrices with entries in $\mathbb{B} = \{0,1\}$, $\mathbb{Q}$ or $\mathbb{R}$. A matrix $X \in \mathbb{R}^{m,n}$ with m rows and n columns has entry X_{ij} in row $i \in [m] = \{1,\dots,m\}$ and column $j \in [n] = \{1,\dots,n\}$. We write E_n for the n-dimensional unit matrix.

We write $X \geqslant 0$ to say that (the real or rational) matrix X has only non-negative entries, and $X > 0$ to say that all entries are strictly positive. We also speak of *non-negative* or *strictly positive matrices* in this sense. For a boolean matrix X, strict positivity $X > 0$ means that all entries are 1.

A square $n \times n$-matrix is *doubly stochastic* if its entries are non-negative and if the sum of entries across every row and column is 1. *Permutation matrices* are doubly stochastic matrices over $\{0,1\}$, with precisely one 1 in every row and in every column. Permutation matrices are orthogonal, i.e., $PP^t = P^tP = E_n$ for every permutation matrix P. The permutation $p \in S_n$ associated with a permutation matrix $P \in \mathbb{R}^{n,n}$ is such that $P\mathbf{e}_j = \mathbf{e}_{p(j)}$, i.e., it describes the permutation of the standard basis vectors $\mathbf{e}_j$ that is effected by P. We also say that P represents p. The permutation matrices form a subgroup of the general linear groups. The doubly stochastic matrices do not form a subgroup, but are closed under transpose and product.

It will be useful to have the shorthand notation

$$X_{D_1 D_2} = 0$$

for the assertion that $X_{d_1 d_2} = 0$ for all $d_1 \in D_1$, $d_2 \in D_2$. If p and q are permutations in S_n represented by permutation matrices P and Q, then

$$(P^t X Q)_{D_1 D_2} = 0 \quad \text{iff} \quad X_{p(D_1) q(D_2)} = 0.$$

So, if $X_{D_1 D_2} = 0$ and P and Q are chosen such that $p^{-1}(D_1)$ and $q^{-1}(D_2)$ are final and initial segments of $[n]$, respectively, then $P^t X Q$ has a null block of dimensions $|D_1| \times |D_2|$ in the upper right-hand corner.

3.1 Decomposition into irreducible blocks

Definition 3.1. With $X \in \mathbb{R}^{n,n}$ associate the directed graph

$$\mathrm{G}(X) := ([n], \{(i,j) \colon X_{ij} \neq 0\}).$$

The strongly connected components of $\mathrm{G}(X)$ induce a partition of the set $[n] = \{1, \dots, n\}$ of rows/columns of X. X is called *irreducible* if this partition has just the set $[n]$ itself.

Note that X is irreducible iff $P^t X P$ is irreducible for every permutation matrix P.

Observation 3.2. *Let $X \in \mathbb{R}^{n,n} \geqslant 0$ with strictly positive diagonal entries. If X is irreducible, then all powers X^ℓ for $\ell \geqslant n-1$ have non-zero entries throughout. Moreover, if X is irreducible, then so is X^ℓ for all $\ell \geqslant 1$.*

Proof. It is easily proved by induction on $\ell \geqslant 1$ that $(X^\ell)_{ij} \neq 0$ if, and only if there is a directed path of length ℓ from vertex i to vertex j in $G(X)$. For X with positive diagonal entries, $G(X)$ has loops in every vertex, and therefore there is a path of length ℓ from vertex i to vertex j if, and only if, there is path of length M' for every $\ell' \geqslant \ell$ from i to j. If $G(X)$ is also strongly connected, then any two vertices are linked by a path of length up to $n-1$. □

Let us call two matrices $Z, Z' \in \mathbb{R}^{n,n}$ *permutation-similar* or *S_n-similar*, $Z \sim_{S_n} Z'$, if $Z' = P^t Z P$ for some permutation matrix P, i.e., if one is obtained from the other by simultaneously permuting rows and columns with the same permutation.

Lemma 3.3. *Every symmetric $Z \in \mathbb{R}^{n,n} \geqslant 0$ is permutation-similar to some block diagonal matrix $\mathrm{diag}(Z_1, \dots, Z_s)$ with irreducible blocks $Z_i \in \mathbb{R}^{n_i,n_i}$.*

The permutation matrix P corresponding to the row- and column-permutation $p \in S_n$ that puts Z into block diagonal form $P^t Z P = \mathrm{diag}(Z_1, \dots, Z_s)$ with irreducible blocks, is unique up to an outer permutation that re-arranges the block intervals $([k_i+1, k_i+n_i])_{1 \leqslant i \leqslant s}$ where $k_i = \sum_{j<i} n_j$, and a product of inner permutations within each one of these s blocks.

The underlying partition $[n] = \dot{\bigcup}_{1 \leqslant i \leqslant s} D_i$ where $D_i := p([k_i+1, k_i+n_i])$ for $k_i = \sum_{j<i} n_j$, is uniquely determined by Z.[2]

In the following we refer to the *partition induced by a symmetric matrix Z*.

Proof. Obvious, based on the partition of the vertex set $[n]$ of $G(Z)$ into connected components (note that symmetry of Z is preserved under similarity, and strong connectivity is plain connectivity in $G(Z)$ for symmetric Z). □

Observation 3.4. *In the situation of Lemma 3.3, the partition $[n] = \dot{\bigcup}_i D_i$ induced by the symmetric matrix Z is the partition of $[n]$ into the vertex sets*

[2] Here we regard two partitions as identical if they have the same partition sets, i.e., we ignore their indexing/enumeration.

of the connected components of $G(Z)$. Then, for every pair $i \neq j$, $Z_{D_i D_j} = 0$, while all the minors $Z_{D_i D_i}$ are irreducible.[3]

If, moreover, Z has strictly positive diagonal entries, then the partition induced by Z is the same as that induced by Z^ℓ, for any $\ell \geqslant 1$; for $\ell \geqslant n-1$, the diagonal blocks $(Z^\ell)_{D_i D_i}$ have non-zero entries throughout: $(Z^\ell)_{D_i D_i} > 0$.

The last assertion says that for a symmetric $n \times n$ matrix Z with non-negative entries and no zeroes on the diagonal, all powers Z^ℓ for $\ell \geqslant n-1$ are *good symmetric* in the sense of the following definition.

Definition 3.5. Let $Z \geqslant 0$ be symmetric with strictly positive diagonal. Then Z is called *good symmetric* if w.r.t. the partition $[n] = \dot{\bigcup}_i D_i$ induced by Z, all $Z_{D_i D_i} > 0$.

More generally, a not necessarily symmetric matrix $X \geqslant 0$ without null rows or columns is *good* if $Z = XX^t$ and $Z' = X^t X$ are good in the above sense.

The importance of this notion lies in the fact that, as observed above, for an arbitrary symmetric $n \times n$ matrix $Z \geqslant 0$ without zeroes on the diagonal, the partition induced by Z is the same as that induced by the good symmetric matrix $\hat{Z} := Z^{n-1}$; and, as for any good matrix, this partition can simply be read off from $\hat{Z}$: $i, j \in [n]$ are in the same partition set if, and only if, $\hat{Z}_{ij} \neq 0$.

Definition 3.6. Consider partitions $[n] = \dot{\bigcup}_{i \in I} D_i$ and $[m] = \dot{\bigcup}_{i \in I} D'_i$ of the sets $[n]$ and $[m]$ with the same number of partition sets. We say that these two partitions are *X-related* for some matrix $X \in \mathbb{R}^{n,m}$ if

(i) $X \geqslant 0$ has no null rows or columns, and

(ii) $X_{D_i D'_j} = 0$ for every pair of distinct indices $i, j \in I$.

Note that partitions that are X-related are X^t-related in the opposite direction. More importantly, each one of the X/X^t-related partitions can be recovered from the other one through X according to

$$\begin{aligned} D'_i &= \{d' \in [m] \colon X_{dd'} > 0 \text{ for some } d \in D_i\}, \\ D_i &= \{d \in [n] \colon X_{dd'} > 0 \text{ for some } d' \in D'_i\}. \end{aligned}$$

For a more algebraic treatment, we associate with the partition sets D_i of a partition $[n] = \dot{\bigcup}_{i \in I} D_i$ the *characteristic vectors* $\mathbf{d}_i$ with entries 1 and 0 according to whether the corresponding component belongs to D_i:

$$\mathbf{d}_i = \textstyle\sum_{d \in D_i} \mathbf{e}_d,$$

where $\mathbf{e}_d$ is the d-th standard basis vector. In terms of these characteristic vectors $\mathbf{d}_i$ for $[n] = \dot{\bigcup}_{i \in I} D_i$ and $\mathbf{d}'_i$ for $[m] = \dot{\bigcup}_{i \in I} D'_i$, the X/X^t-relatedness of these partitions means that

$$\begin{aligned} D'_i &= \{d' \in [m] \colon (X^t \mathbf{d}_i)_{d'} > 0\}, \\ D_i &= \{d \in [n] \colon (X \mathbf{d}'_i)_d > 0\}. \end{aligned}$$

[3] Note that this does not depend on the enumeration of the partition set D_i, because irreducibility is invariant under permutation-similarity.

Lemma 3.7. *If two partitions $[n] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I} D'_i$ of the same set $[n]$ are X-related for some doubly stochastic matrix $X \in \mathbb{R}^{n,n}$, then $|D_i| = |D'_i|$ for all $i \in I$, and for the characteristic vectors $\mathbf{d}_i$ and $\mathbf{d}'_i$ of the partition sets D_i and D'_i even*

$$\mathbf{d}_i = X\mathbf{d}'_i \quad \text{and} \quad \mathbf{d}'_i = X^t\mathbf{d}_i.$$

Proof. Observe that for all $d \in [n]$ we have $0 \leq (X\mathbf{d}'_i)_d = \sum_{d' \in D'_i} X_{dd'} \leq 1$. It follows immediately from the definition of X-relatedness that $(X\mathbf{d}'_i)_d = 0$ for all $d \notin D_i$. Therefore,

$$|D_i| \geqslant \sum_{d \in D_i} (X\mathbf{d}'_i)_d = \sum_{d \in [n]} (X\mathbf{d}'_i)_d = \sum_{d' \in D'_i} \sum_{d \in [n]} X_{dd'} = |D'_i|.$$

Similarly, $0 \leq (X^t\mathbf{d}_i)_{d'} \leq 1$ for $d' \in [n]$, and $|D'_i| \geq \sum_{d' \in D'_i} (X^t\mathbf{d}_i)_{d'} = |D_i|$. Together, we obtain

$$|D_i| = \sum_{d \in D_i} (X\mathbf{d}'_i)_d = |D'_i| = \sum_{d' \in D'_i} (X^t\mathbf{d}_i)_{d'}.$$

As all summands are bounded by 1, this implies $(X\mathbf{d}'_i)_d = 1$ for all $d \in D_i$ and $(X^t\mathbf{d}_i)_{d'} = 1$ for all $d' \in D_i$. □

Lemma 3.8. *Let $X \geqslant 0$ be an $m \times n$ matrix without null rows or columns. Then the $m \times m$ matrix $Z := XX^t$ and the $n \times n$ matrix $Z' := X^tX$ are symmetric with positive entries on their diagonals. Moreover, the (unique) partitions of $[m]$ and $[n]$ that are induced by Z and Z', respectively, are X/X^t-related.*[4]

Proof. It is obvious that Z and Z' are symmetric with positive diagonal entries. Let partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I'} D'_i$ be obtained from decompositions of Z and Z' into irreducible blocks. We need to show that the non-zero entries in X give rise to a bijection between the index sets I and I' of the two partitions, in the sense that partition sets D_i and D'_j are related if, and only if, some pair of members $d \in D_i$ and $d' \in D'_j$ have a positive entry $X_{dd'}$. Then a re-numbering of one of these partitions will make them X-related in the sense of Definition 3.6. Recall from Observation 3.4 that the D_i are the vertex sets of the connected components of $G(XX^t)$ on $[m]$, while the D'_i the are the vertex sets of the connected components of $G(X^tX)$ on $[n]$.

Consider the uniformly directed bipartite graph $G(X)$ on $[m] \dot{\cup} [n]$ with an edge from $i \in [m]$ to $j \in [n]$ if $X_{ij} > 0$. In light of the symmetry of the whole situation w.r.t. X and X^t, it just remains to argue for instance that no $i \in [m]$ can have edges into two distinct sets of the partition $[n] = \dot{\bigcup}_{i \in I'} D'_i$. But any two target nodes of edges from one and the same $i \in [n]$ are in the same connected component of $G(X^tX)$, hence in the same partition set. □

In the situation of Lemma 3.8, powers of Z induce the same partitions as Z, and the partitions induced by $(Z^\ell X)(Z^\ell X)^t = Z^{2\ell+1}$ are X/X^t-related as well as $Z^\ell X/X^tZ^\ell$-related, for all $\ell \geqslant 1$.

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[4] As X/X^t-relatedness refers to partitions presented with an indexing of the partition sets, we need to allow a suitable re-indexing for at least one of them, so as to match the other one.

For $\ell \geqslant n/2-1$, the matrix $Z^\ell X$ has no null rows or columns: else $Z^\ell X(Z^\ell X)^t = Z^{2\ell+1}$ would have to have a zero entry on the diagonal, contradicting the fact that this symmetric matrix is good symmetric in the sense of Definition 3.5. The same reasoning shows that $Z^\ell X$ is itself good in the sense of Definition 3.5.

Corollary 3.9. *Let $X \geqslant 0$ be an $m \times n$ matrix without null rows or columns, $Z = XX^t$, $Z' = X^tX$ the associated symmetric matrices with non-zero entries on the diagonal. Then for $\ell \geqslant m-1, n-1$, the matrix $\hat{X} := Z^\ell X = X(Z')^\ell$ and its transpose $\hat{X}^t = X^t Z^\ell = (Z')^\ell X^t$ are good and relate the partitions $[m] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$ induced by Z and Z', respectively.*[4] *Moreover,*

(i) $\hat{X}_{D_i D'_i} > 0$ *for all i, and*

(ii) $\hat{X}_{D_i D'_j} = 0$ *for all $i \neq j$.*

Proof. $Z^\ell X$ is good symmetric by the above reasoning. So $(Z^\ell)_{D_i D_i} > 0$ for all i, while $(Z^m)_{D_i D_j} = 0$ for all $j \neq i$. It follows that $(Z^\ell X)_{D_i D'_i} = (Z^\ell)_{D_i D_i} X_{D_i D'_i}$ has only non-zero entries because $X_{D_i D'_i}$ does not have null columns. This proves (i). Assertion (ii) is clear as, for $i \neq j$, $(Z^\ell X)_{D_i D'_j} = (Z^\ell)_{D_i D_j} X_{D_j D'_j} = 0\, X_{D_j D'_j} = 0$. □

Aside: boolean vs. real arithmetic

Looking at matrices with $\{0,1\}$-entries, we may not only treat them as matrices over $\mathbb{R}$ as we have done so far, but also over other fields, or as matrices over the boolean semiring $\mathbb{B} = \{0,1\}$ with the logical operations of $\vee$ for addition and $\wedge$ for multiplication. Though not even forming a ring, boolean arithmetic yields a very natural interpretation in the context where we associate non-negative entries with edges, as we did in passage from X to $G(X)$ (cf. Definition 3.1 and Observation 3.2). The 'normalisation map' $\chi\colon \mathbb{R}_{\geqslant 0} \to \{0,1\}$, $x \mapsto 1$ iff $x > 0$, relates the arithmetic of reals $x, y \geqslant 0$ to boolean arithmetic in

$$\chi(x+y) = \chi(x) \vee \chi(y) \quad \text{and} \quad \chi(xy) = \chi(x) \wedge \chi(y).$$

This is the 'logical' arithmetic that supports, for instance, arguments used in Observation 3.2: for any real $n \times n$ matrix $X \geqslant 0$, $(XX)_{ij} = \sum_k X_{ik} X_{kj} \neq 0$ iff there is at least one $k \in [n]$ for which $X_{ik} \neq 0$ and $X_{kj} \neq 0$ iff $\bigvee_{k \in [n]} (\chi(X_{ik}) \wedge \chi(X_{kj})) = 1$. It is no surprise, therefore, that several of the considerations apparently presented for real non-negative matrices above, have immediate analogues for boolean arithmetic – in fact, one could argue, that the boolean interpretation is closer to the combinatorial essence. We briefly sum up these analogues with a view to their use in the analysis of L^k-equivalence, while the real versions are related to C^k-equivalence. Note also that the boolean analogue of a doubly stochastic matrix with non-negative real entries is a matrix without null rows or columns.

Also note that Definitions 3.1 (irreducibility) and 3.6 (X-relatedness) are applicable to boolean matrices without any changes. Observations 3.2 and 3.4 go through (as just indicated), and so does Lemma 3.3. For Lemma 3.7, one may look at X-related partitions of sets $[m]$ and $[n]$, where not necessarily $n = m$, by any boolean matrix X without null rows or columns and obtains the relationship between the characteristic vectors as stated there, now in terms of boolean arithmetic – but of course we do not get any numerical equalities between the sizes of the partition sets. Lemma 3.8, finally, applies to boolean arithmetic, exactly as stated, and also Corollary 3.9 translates accordingly.

Lemma 3.10. *In the sense of boolean arithmetic for matrices with entries in* $\mathbb{B} = \{0, 1\}$*:*

(a) *Any symmetric* $Z \in \mathbb{B}^{n,n}$ *induces a unique partition of* $[n]$ *for which the diagonal minors induced by the partition sets are irreducible and the remaining blocks null;* $d, d' \in [n]$ *are in the same partition set if, and only if,* $(Z^\ell)_{dd'} = 1$ *for any/all* $\ell \geqslant n - 1$*.*

(b) *If two partitions (not necessarily of the same set) with the same number of partition sets are related by some boolean matrix* $X \in \mathbb{B}^{m,n}$*, then the characteristic vectors* $(\mathbf{d}_i)_{i\in I}$ *and* $(\mathbf{d}'_i)_{i\in I}$ *of the partitions are related by* $\mathbf{d}_i = X\mathbf{d}'_i$ *and* $\mathbf{d}'_i = X^t\mathbf{d}_i$*.*

(c) *For any matrix* $X \in \mathbb{B}^{m,n}$ *without null rows or columns, the symmetric boolean matrices* $Z = XX^t$ *and* $Z' = X^tX$ *have diagonal entries* 1 *and induce partitions that are* X/X^t*-related, and agree with the partitions induced by higher powers of* Z *and* Z' *or on the basis of* $Z^\ell X$ *and* $X(Z')^\ell$ *for any* $\ell \in \mathbb{N}$*. For* $\ell \geqslant m-1, n-1$*, the partition blocks in* Z *and* Z' *have entries* 1 *throughout, and* $Z^\ell X$ *and* $X(Z')^\ell$ *have entries* 1 *in all positions relating elements from matching partition sets.*

Observation 3.11. *For a symmetric boolean matrix* $Z \in \mathbb{B}^{n,n}$ *with* $Z_{dd} = 1$ *for all* $d \in [n]$*, the characteristic vectors* $\mathbf{d}_i$ *of the partition* $[n] = \dot{\bigcup}_{i\in I} D_i$ *induced by* Z *satisfy the following 'eigenvector' equation in terms of boolean arithmetic:*

$$Z\mathbf{d}_i = \mathbf{d}_i \quad \text{(boolean)}, \quad \text{for all } i \in I.$$

3.2 Eigenvalues and -vectors

Lemma 3.12. *If* $Z \in \mathbb{R}^{n,n}$ *is doubly stochastic, then it has eigenvalue* 1*. If* Z *is doubly stochastic and irreducible with strictly positive diagonal entries, then the eigenspace for eigenvalue* 1 *has dimension* 1 *and is spanned by the vector* $\mathbf{d} := (1, \ldots, 1)^t$*.*

Proof. Clearly $Z\mathbf{d} = \mathbf{d}$ for any stochastic matrix Z.

If Z is moreover irreducible with positive diagonal entries, then by Observation 3.2, $\hat{Z} := Z^{n-1}$ has strictly positive entries and, being doubly stochastic, therefore entries strictly between 0 and 1.

If $\mathbf{v}$ is an eigenvector for eigenvalue 1 of Z, then it also is an eigenvector for eigenvalue 1 of $\hat{Z}$.If $\mathbf{v} = (v_1, \ldots, v_n)$, this is equivalent to

$$v_i = \textstyle\sum_j \hat{Z}_{ij} v_j \quad \text{for all } i \in [n].$$

Looking at an index i for which $v_j \leqslant v_i$ for all j, we see that the maximal v_i is a convex combination of the v_j to which every v_j contributes. This implies that all $v_j = v_i$, so that $\mathbf{v}$ is a scalar multiple of $\mathbf{d}$ as claimed. □

Corollary 3.13. (a) *Let $Z \in \mathbb{R}^{n,n}$ be doubly stochastic with positive diagonal, and $[n] = \dot{\bigcup}_i D_i$ a partition with $Z_{D_i D_j} = 0$ for $i \neq j$ and such that the minors $Z_{D_i D_i}$ are irreducible for all i. Then the eigenspace for eigenvalue 1 of Z is the direct sum of the 1-dimensional subspaces spanned by the characteristic vectors $\mathbf{d}_i$ of the partition sets D_i.*

(b) *If $Z = X^t X \in \mathbb{R}^{n,n}$ for some doubly stochastic matrix X, then the eigenspace for eigenvalue 1 is the direct sum of the spans of the characteristic vectors $\mathbf{d}_i$ from the unique partition $[n] = \dot{\bigcup}_i D_i$ of $[n]$ induced by Z according to Lemma 3.3.*

Proof. Towards (a), it is clear that $Z\mathbf{d}_i = \mathbf{d}_i$, so that each $\mathbf{d}_i$ is an eigenvector with eigenvalue 1. Let $V_i := \text{span}(\mathbf{e}_d \colon d \in D_i)$; then $\mathbb{R}^n = \bigoplus_i V_i$ is a direct sum decomposition, and $Z_{D_j D_i} = 0$ for $j \neq i$ implies that Z maps V_i to itself. Therefore any eigenvector $\mathbf{v}$ with eigenvalue 1 decomposes as $\mathbf{v} = \sum_i \mathbf{v}_i$, where $\mathbf{v}_i \in V_i$, in such manner that $Z\mathbf{v}_i = \mathbf{v}_i$. Since the restriction of Z to V_i is irreducible with positive diagonal, $\mathbf{v}_i \in \text{span}(\mathbf{d}_i)$ by Lemma 3.12, as claimed.

Statement (b) is s direct consequence, since Z is symmetric with positive diagonal. □

3.3 Stable partitions

Definition 3.14. Let $A \in \mathbb{R}^{n,n}$, $[n] = \dot{\bigcup}_{i \in I} D_i$ be a partition. We call this partition a *stable partition for A* if there are numbers $(s_{ij})_{i,j \in I}$ and $(t_{ij})_{i,j \in I}$ such that for all $i, j \in I$:

$$d \in D_i \quad \Rightarrow \quad \sum_{d' \in D_j} A_{dd'} = s_{ij} \quad \text{and} \quad \sum_{d' \in D_j} A_{d'd} = t_{ij}.$$

If there are s_{ij} such that $\sum_{d' \in D_j} A_{dd'} = s_{ij}$ for all $d \in D_i$, we call the partition *row-stable*; similarly, for t_{ij} such that $\sum_{d' \in D_j} A_{d'd} = t_{ij}$ for all $d \in D_i$, *column-stable.*

For symmetric A, column- and row-stability are equivalent (with $t_{ij} = s_{ij}$).

Note that the row and column sums in the definition are the D_i-components of $A\mathbf{d}_j$ and of $\mathbf{d}_j^t A = (A^t \mathbf{d}_j)^t$, respectively. So, for instance, row stability precisely says that

$$A\mathbf{d}_j = \sum_i s_{ij} \mathbf{d}_i \in \bigoplus_i \text{span}(\mathbf{d}_i).$$

Lemma 3.15. *Let $A \in \mathbb{R}^{n,n}$ commute with some symmetric matrix of the form $Z = XX^t \in \mathbb{R}^{n,n}$ for some doubly stochastic $X \in \mathbb{R}^{n,n}$. Then the partition $[n] = \dot{\bigcup}_i D_i$ of $[n]$ induced by Z according to Lemma 3.3 is stable for A.*

Proof. We use the characteristic vectors $\mathbf{d}_i$ of the partition sets. By Corollary 3.13, the eigenspace for eigenvalue 1 of Z is the direct sum of the spans of the vectors $\mathbf{d}_i$.

Now $ZA\mathbf{d}_i = AZ\mathbf{d}_i = A\mathbf{d}_i$ shows that $A\mathbf{d}_i$ is an eigenvector of Z with eigenvalue 1, whence

$$A\mathbf{d}_i \in \bigoplus_i \text{span}(\mathbf{d}_i).$$

It follows that the partition $[n] = \dot{\bigcup}_i D_i$ is row-stable.

Note again that $(A\mathbf{d}_j)_d = \sum_{d' \in D_j} A_{dd'}$ and $A\mathbf{d}_j \in \bigoplus_i \mathrm{span}(\mathbf{d}_i)$ precisely means that this value $(A\mathbf{d}_j)_d$ only depends on the partition set D_i to which d belongs. I.e., $\sum_{d' \in D_j} A_{dd'} = s_{ij}$ for all $d \in D_i$.

As $Z = XX^t = Z^t$, A^t commutes with Z if A does: $A^t Z = A^t Z^t = (ZA)^t = (AZ)^t = Z^t A^t = ZA^t$. The above reasoning therefore shows that the partition into the D_i is row-stable for A^t as well, hence column stable for A. Hence it is stable for A. □

NB: symmetry of A is not required here. It is essential for deriving commutation of A (and A^t) with $Z = XX^t$ from an equation of the form $AX = XB$, as we shall see below. But first a corollary from the argument just given.

Corollary 3.16. *Let A commute with $Z = XX^t$ and B commute with $Z' = X^t X$, where X is doubly stochastic (cf. Lemma 3.15). Then the partitions induced by Z and Z', which are X-related by Lemma 3.8, are stable for A and B, respectively.*

Aside: boolean arithmetic

We give a separate elementary proof of the analogue of Lemma 3.15 for boolean arithmetic. Here the definition of a *boolean* stable partition is this natural analogue of Definition 3.14.

Definition 3.17. A partition $[n] = \dot{\bigcup}_{i \in I} D_i$ is *boolean stable* for $A \in \mathbb{B}^{n,n}$ if, in the sense of boolean arithmetic, $\sum_{d' \in D_j} A_{dd'}$ and $\sum_{d' \in D_j} A_{d'd}$ only depend on the partition set i for which $d \in D_i$.

Note that boolean stability implies that, for the characteristic vectors $\mathbf{d}_i$ of the partition, $(A\mathbf{d}_j)_d = \sum_{d' \in D_j} A_{dd'}$ is the same for all $d \in D_i$, so that also here $A\mathbf{d}_j$ is a boolean linear combination of the characteristic vectors $\mathbf{d}_i$.

Lemma 3.18. *Let $A \in \mathbb{B}^{n,n}$ commute, in the sense of boolean arithmetic, with some symmetric matrix of the form $Z = XX^t \in \mathbb{B}^{n,n}$ with entries $Z_{dd} = 1$ for all $d \in [n]$. Then the partition $[n] = \dot{\bigcup}_i D_i$ induced by Z according to Lemma 3.10 is boolean stable for A.*

Proof. Recall from Observation 3.11 that the characteristic vectors $\mathbf{d}_i$ of the induced partition behave like eigenvectors with eigenvalue 1 for boolean arithmetic: $Z\mathbf{d}_i = \mathbf{d}_i$. Moreover, we may assume that $Z_{dd'} = 1$ iff d and d' are in the same partition set (after passage to Z^{n-1} if necessary). Let us write $[\![\ell \in D_j]\!]$ for the boolean truth value of the assertion $\ell \in D_j$. Then, for $d \in D_i$,

$$\begin{aligned} \textstyle\sum_{d' \in D_j} A_{dd'} &= (A\mathbf{d}_j)_d = (AZ\mathbf{d}_j)_d \\ &= (ZA\mathbf{d}_j)_d = \textstyle\sum_{k,\ell} Z_{dk} A_{k\ell} \, [\![\ell \in D_j]\!] = \sum_{k \in D_i, \ell \in D_j} A_{k\ell} \end{aligned}$$

does indeed not depend on $d \in D_i$, whence the partition is boolean row-stable. Column-stability again follows from similar considerations based on commutation of $Z = Z^t$ with A^t. □

4 Fractional isomorphism

4.1 C^2-equivalence and linear equations

The *adjacency matrix* of graph $\mathcal{A}$ is the square matrix A with rows and columns indexed by vertices of $\mathcal{A}$ and entries $A_{aa'} = 1$ if aa' is an edge of $\mathcal{A}$ and $A_{aa'} = 0$ otherwise. By our assumption that graphs are undirected and simple, A is a symmetric square matrix with null diagonal. It will be convenient to assume that our graphs always have an initial segment $[n]$ of the positive integers as their vertex set. Then the adjacency matrices are in $\mathbb{B}^{n,n} \subseteq \mathbb{R}^{n,n}$. Throughout this subsection, we assume that $\mathcal{A}$ and $\mathcal{B}$ are graphs with vertex set $[n]$ and with adjacency matrices A, B, respectively. It will be notationally suggestive to denote typical indices of matrices $a, a', \ldots \in [n]$ when they are to be interpreted as vertices of $\mathcal{A}$, and $b, b', \ldots \in [n]$ when they are to be interpreted as vertices of $\mathcal{B}$.

Recall (from the discussion in the introduction) that two graphs $\mathcal{A}, \mathcal{B}$ are isomorphic if, and only if, there is a permutation matrix X such that $AX = XB$. We can rewrite this as the following integer linear program in the variables X_{ab} for $a, b \in [n]$.

ISO

$$\begin{aligned} \sum_{b' \in [n]} X_{ab'} = \sum_{a' \in [n]} X_{a'b} &= 1, \\ \sum_{a' \in [n]} A_{aa'} X_{a'b} &= \sum_{b' \in [n]} X_{ab'} B_{b'b}, \\ X_{ab} &\geq 0 \qquad \text{for all } a, b \in [n]. \end{aligned}$$

Then $\mathcal{A}$ and $\mathcal{B}$ are isomorphic if, and only if, ISO has an integer solution.

Definition 4.1. *Two graphs $\mathcal{A}, \mathcal{B}$ are* fractionally isomorphic*, $\mathcal{A} \approx \mathcal{B}$, if, and only if, the system* ISO *has a real solution.*

Observe that graphs are fractionally isomorphic if, and only if, there is a doubly stochastic matrix X such that $AX = XA$.

Note that fractionally isomorphic graphs necessarily have the same number of vertices (this will be different for the boolean analogue, which cannot count).

The established theorem on fractional isomorphism, by Tinhofer [22, 23] and Ramana, Scheinerman and Ullman from [17, 18], relates fractional isomorphis to the colour refinement algorithm (‘iterated degree sequences’ in [18]) introduced in Section 2 and stable partitions (‘equitable partitions’ in [18]).

A *stable partition* of the vertex set of an undirected graph is a stable partition $[n] = \dot{\bigcup}_{i \in I} D_i$ for its adjacency matrix in the sense of Definition 3.14. Reading that definition for the (symmetric) adjacency matrix A of a graph on $[n]$, and thinking of the partition sets D_i as vertex colours, stability means that the colour of any vertex determines the number of its neighbours in every one of the colours. This is stability in the sense of colour refinement; it means that the colour refinement algorithm produces the coarsest stable partition.

The characteristic parameters for a stable partition $[n] = \dot{\bigcup}_{i\in I} D_i$ for A are the numbers $s_{ij} = s^A_{ij}$ such that $s_{ij} = \sum_{d'\in D_j} A_{dd'}$ for all $d \in D_i$. (As A is symmetric, the parameters t_{ij} of Definition 3.14 are equal to the s_{ij}.) We call two stable partitions $\dot{\bigcup}_{i\in I} D_i$ for a matrix A and $\dot{\bigcup}_{i\in J} D'_i$ for a matrix B *equivalent* if $I = J$ and $|D_i| = |D'_i|$ for all $i \in I$ and $s^A_{ij} = s^B_{ij}$ and for all $i, j \in I$.

Lemma 4.2. *$\mathcal{A}$ and $\mathcal{B}$ are C^2-equivalent if, and only if, there are equivalent stable partitions $\dot{\bigcup}_{i\in I} D_i$ for A and $\dot{\bigcup}_{i\in I} D'_i$ for B.*

Proof. The forward direction follows from Theorem 2.3, because the colour refinement algorithm computes equivalent stable partitions of $\mathcal{A}$ and $\mathcal{B}$.

To establish the converse implication, we use the bijective 2-pebble game, which characterises C^2-equivalence by Theorem 2.2. Suppose we have equivalent stable partitions $\dot{\bigcup}_{i\in I} D_i$ of A and $\dot{\bigcup}_{i\in J} D'_i$ of B. Then it is a winning strategy for player **II** to maintain the following invariant for every position p of the game: p is a local isomorphism (that is, if $\mathrm{dom}(p) = \{a, a'\}$ then $a = a'$ if, and only if, $p(a) = p(a')$, and a and a' are adjacent in $\mathcal{A}$ if, and only if, $p(a)$ and $p(a')$ are adjacent in $\mathcal{B}$), and if $a \in \mathrm{dom}(p) \cap D_i$ then $p(a) \in D'_i$. It follows easily from the definition of stable partitions that player **II** can indeed maintain this invariant. □

Theorem 4.3 (Tinhofer)**.** *Two graphs are C^2-equivalent if, and only if, they are fractionally isomorphic.*

Proof. In view of Lemma 4.2, it suffices to prove that $\mathcal{A}$ and $\mathcal{B}$ have equivalent stable partitions if, and only if, they are fractionally isomorphic.

For the forward direction, suppose that we have equivalent stable partitions $\dot{\bigcup}_{i\in I} D_i$ for A and $\dot{\bigcup}_{i\in J} D'_i$ for B. For all $a \in D_i, b \in D'_j$ we let

$$X_{ab} := \delta(i, j)/n_i,$$

where $n_i := |D_i| = |D'_i|$. (Here and elsewhere we use Kronecker's δ function defined by $\delta(i, j) = 1$ if $i = j$ and $\delta(i, j) = 0$ otherwise.) An easy calculation shows that this defines a doubly stochastic matrix X with $AX = XB$, that is, a solution for ISO.

For the converse direction, suppose that X is a doubly stochastic matrix such that $AX = XB$. Since A and B are symmetric, also $X^tA = BX^t$, and

$$AXX^t = XBX^t = XX^tA \quad \text{and} \quad BX^tX = X^tAX = X^tXB,$$

show that A commutes with $Z := XX^t$ and B with $Z' := X^tX$.

From Lemma 3.15 and Corollary 3.16, the partitions $[n] = \dot{\bigcup}_{i\in I} D_i$ and $[n] = \dot{\bigcup}_{i\in I} D'_i$ that are induced by the symmetric matrices Z and Z' are X-related and stable for A and for B, respectively. We need to show that $|D_i| = |D'_i|$ and that the partitions also agree w.r.t. the parameters s_{ij}.

By Lemma 3.7 we have $|D_i| = |D'_i|$ and

$$\mathbf{d}_i = X\mathbf{d}'_i \quad \text{and} \quad \mathbf{d}'_i = X^t\mathbf{d}_i, \tag{2}$$

where $\mathbf{d}_i$ and $\mathbf{d}'_i$ for $i \in I$ are the characteristic vectors of the two partitions. Thus for all $i, j \in I$,

$$(\mathbf{d}'_i)^t B \mathbf{d}'_j = (X^t \mathbf{d}_i)^t B X^t \mathbf{d}_j = \mathbf{d}_i^t X B X^t \mathbf{d}_j = \mathbf{d}_i^t A X X^t \mathbf{d}_j = \mathbf{d}_i^t A Z \mathbf{d}_j = \mathbf{d}_i^t A \mathbf{d}_j,$$

where the last equality follows from the fact that $\mathbf{d}_j$ is an eigenvector of Z with eigenvalue 1 by Corollary 3.13.

Note that $\mathbf{d}_i^t A \mathbf{d}_j$ is the number of edges of $\mathcal{A}$ from D_i to D_j. By stability of the partition, we have $s_{ij}^A = \mathbf{d}_i^t A \mathbf{d}_j / |D_i|$ and similarly $s_{ij}^B = (\mathbf{d}'_i)^t B \mathbf{d}'_j / |D'_i|$, so that $s_{ij}^A = s_{ij}^B$. □

4.2 L^2-equivalence and boolean linear equations

W.r.t. an adjacency matrix $A \in \mathbb{B}^{n,n}$, a boolean stable partition $[n] = \dot{\bigcup}_{i \in I} D_i$ has as parameters just the boolean values

$$\iota_{ij}^A = \begin{cases} 0 & \text{if } A_{D_i D_j} = 0, \\ 1 & \text{else.} \end{cases}$$

Boolean (row-)stability of the partition for A implies that $\iota_{ij}^A = 1$ if, and only if, for each individual $d \in D_i$ there is at least one $d' \in D_j$ such that $A_{dd'} = 1$, and similarly for column stability.

To capture the situation of 2-pebble game equivalence, though, we now need to work with similar partitions that are stable both w.r.t. A and w.r.t. to the adjacency matrix A^c of the complement of the graph with adjacency matrix A. Here the complement of a graph $\mathcal{A}$ is the graph $\mathcal{A}^c$ with the same vertex set as $\mathcal{A}$ obtained by replacing edges by non-edges and vice versa. Hence $A^c_{aa'} = 1$ if $A_{aa'} = 0$ and $a \neq a'$, and $A^c_{aa'} = 0$ otherwise. While a partition in the sense of real arithmetic is stable for A if, and only if, it is stable for A^c, this is no longer the case for boolean arithmetic. Let us call a partition that is boolean stable for both A and A^c, *boolean bi-stable* for A.

Then the following captures the situation of two graphs that are 2-pebble game equivalent. We note that 2-pebble equivalence is a very coarse notion of equivalence, if we look at just simple undirected graphs – but the concepts explored here form the basis for the analysis of k-pebble equivalence, which is non-trivial even for simple undirected graphs.

L^2-equivalence of two graphs does not imply that the graphs have the same size. In the following, we always assume that $\mathcal{A}, \mathcal{B}$ are graphs with vertex sets $[m], [n]$ respectively and that $A \in \mathbb{B}^{m,m}$ and $b \in \mathbb{B}^{n,n}$ are their adjacency matrices. We call two bi-stable partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ for A (and A^c) and $[n] = \dot{\bigcup}_{i \in J} D'_i$ for B (and B^c) *b-equivalent* if $I = J$ and $\iota_{ij}^A = \iota_{ij}^B$ and $\iota_{ij}^{A^c} = \iota_{ij}^{B^c}$ for all $i, j \in I$. Note that b-equivalence does not imply that $|D_i| = |D'_i|$.

Lemma 4.4. *$\mathcal{A}$ and $\mathcal{B}$ are L^2-equivalent if, and only if, there are b-equivalent bi-stable partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ for A and $[n] = \dot{\bigcup}_{i \in J} D'_i$ for B.*

Proof. The proof is analogous to the proof of Lemma 4.4. For the backward direction, we need bi-stability to guarantee that player **II** can maintain positions p that preserve adjacency, non-adjacency, and (in)equality. Stability alone would only enable her to maintain adjacency and equality. □

Definition 4.5. $\mathcal{A}$ and $\mathcal{B}$ are *boolean isomorphic*, $\mathcal{A} \approx_{\text{bool}} \mathcal{B}$, if there is some boolean matrix X without null rows or columns such that $AX = XB$ and $A^c X = XB^c$.

That is, $\mathcal{A}$ and $\mathcal{B}$ are boolean isomorphic if they satisfy the following system of linear equation over the boolean semiring.

B-ISO

$$\begin{aligned} \sum_{b' \in [n]} X_{ab'} &= \sum_{a' \in [n]} X_{a'b} = 1, \\ \sum_{a' \in [n]} A_{aa'} X_{a'b} &= \sum_{b' \in [n]} X_{ab'} B_{b'b}, \\ \sum_{a' \in [n]} A^c_{aa'} X_{a'b} &= \sum_{b' \in [n]} X_{ab'} B^c_{b'b} \qquad \text{for all } a, b \in [n]. \end{aligned}$$

Theorem 4.6. *Two graphs are L^2-equivalent if, and only if, they are boolean isomorphic.*

Proof. For the forward direction, suppose that $A \equiv^2_{\mathsf{L}} B$, and let $[m] = \dot{\bigcup}_{1 \leqslant i \leqslant s} D_i$ and $[n] = \dot{\bigcup}_{1 \leqslant i \leqslant s} D'_i$ be the similar boolean bi-stable partitions. For all $a \in D_i, b \in D'_j$ we let $X_{ab} := \delta(i,j)$. This defines a boolean matrix $X \in \mathbb{B}^{m,n}$ without null rows or columns. One checks that $AX = XB$, in boolean arithmetic: for $a \in D_i$ and $b \in D'_j$, and for the characteristic vectors $\mathbf{d}_i$ and $\mathbf{d}'_j$ for the partitions,

$$\begin{aligned} (AX)_{ab} = \sum_k A_{ak} X_{kb} &= (A\mathbf{d}_j)_a = \iota^A_{ij} \\ &= \iota^B_{ij} = ((\mathbf{d}'_i)^t B)_b = \sum_k X_{ak} B_{kb} = (XB)_{ab}. \end{aligned}$$

The argument for $A^c X = XB^c$ is completely analogous.

For the converse, suppose that $A \approx_{\text{bool}} B$, and let X be a boolean matrix without null rows or columns such that $AX = XB$ and $A^c X = XB^c$. Since A and B are symmetric, also $X^t A = BX^t$ $X^t A^c = B^c X^t$, and

$$AXX^t = XBX^t = XX^t A \quad \text{and} \quad BX^t X = X^t AX = X^t XB,$$

together with the analogues for the complements, show that both A and A^c commute with $Z := XX^t$ and both B and B^c commute with $Z' := X^t X$. Moreover, the matrices Z and Z' have entries 1 on the diagonal.

From Lemma 3.18 and the straightforward analogue of Corollary 3.16, the partitions $[m] = \dot{\bigcup}_{i \in I} D_i$ and $[n] = \dot{\bigcup}_{i \in I} D'_i$ induced by the symmetric matrices Z and Z' are X-related and boolean bi-stable for A and for B, respectively. We need to show that these partitions also agree w.r.t. the characteristic ι_{ij}. By Lemma 3.10, the characteristic vectors $\mathbf{d}'_i$ and $\mathbf{d}'_i$ of the partitions are related by $\mathbf{d}_i = X\mathbf{d}'_i$ and $\mathbf{d}'_i = X^t \mathbf{d}_i$ in the sense of boolean arithmetic.

Since $AX = XB$ and as the $\mathbf{d}_j$ are boolean eigenvectors of $Z = XX^t$ with eigenvalue 1 by Observation 3.11,

$$\begin{aligned}\iota_{ij}^B &= (\mathbf{d}'_i)^t B \mathbf{d}'_j = (X^t \mathbf{d}_i)^t B X^t \mathbf{d}_j = \mathbf{d}_i^t X B X^t \mathbf{d}_j \\ &= \mathbf{d}_i^t A X X^t \mathbf{d}_j = \mathbf{d}_i^t A Z \mathbf{d}_j = \mathbf{d}_i^t A \mathbf{d}_j \;=\; \iota_{ij}^A.\end{aligned}$$

The argument for $\iota_{ij}^{B^c} = \iota_{ij}^{A^c}$ is strictly analogous. □

4.3 Good solutions for fractional isomorphism

We conclude the analysis of fractional isomorphism with an account that will be useful towards generalisations in higher dimensions. Fractional isomorphism as well as its boolean analogue are based on solutions of linear matrix equations

$$\textsc{Comp}[A, B]: \quad AX = XB,$$

which express a *compatibility* condition. These equations may be read in the sense of real arithmetic or in the sense of boolean arithmetic. For fractional isomorphism between graphs with adjacency matrices A and B we are interested in doubly stochastic real solutions of this single equation; while the boolean analogue involves simultaneous boolean solutions without null rows or columns of the pair of equations $\textsc{Comp}[A, B]$ and $\textsc{Comp}[A^c, B^c]$. We isolate the properties of *good solutions* of equations of this type as follows; compare Definition 3.5 for *good matrices*.

Definition 4.7. For symmetric matrices $A \in \mathbb{B}^{m,m}$ and $B \in \mathbb{B}^{n,n}$, a solution X to the linear matrix equation $\textsc{Comp}[A, B]$ in the sense of real arithmetic (boolean arithmetic) is a *good solution* if X is a doubly stochastic real matrix (a boolean matrix without null rows or columns) and the matrices $Z = XX^t$ and $Z' = X^t X$ induce X-related partitions $[m] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$ such that

- (i) these partitions are equivalent (boolean equivalent) and stable (boolean stable) w.r.t. A and B, respectively;
- (ii) $X_{D_i D'_i} > 0$ for all i;
- (iii) $X_{D_i D'_j} = 0$ for $i \neq j$.

Recall from Corollary 3.9, and from Lemma 3.10 for the boolean case, that good solutions are always obtained from given solutions X through passage to $X' := Z^\ell X$ for sufficiently large ℓ and $Z := XX^t$, which is a symmetric matrix with strictly positive diagonal. Clearly this transformation of solutions into good solutions works for simultaneous solutions to several equations of type $\textsc{Comp}[\cdot, \cdot]$. For simultaneous (boolean) solutions w.r.t. A/B and A^c/B^c we obtain simultaneous good solutions w.r.t. A/B and A^c/B^c, which are therefore (boolean) bi-stable w.r.t. A and B. We thus find the following summary account for the results presented in Sections 4.1 and 4.2 above.

Lemma 4.8. *For graphs $\mathcal{A}$ and $\mathcal{B}$ with adjacency matrices $A \in \mathbb{B}^{m,m}$, $B \in \mathbb{B}^{n,n}$, let X be a good real solution to $\textsc{Comp}[A, B]$ (i.e., a real solution to* ISO*) with induced partitions $[m] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$. Then player* **II** *has a strategy* *in the corresponding bijective* 2*-pebble game to maintain pebble configurations* $p\colon a_1a_2 \mapsto b_1b_2$ *for which*

(i) p *is a local isomorphism:* $a_1 = a_2$ *iff* $b_1 = b_2$ *and* $A_{a_1a_2} = 1$ *iff* $B_{b_1b_2} = 1$*;*

(ii) p *respects the induced partitions: corresponding pebbles are from matching partition sets, i.e.,* $X_{a_1b_1}, X_{a_2b_2} > 0$.

Similarly, if X *is a simultaneous good boolean solution to* $\textsc{Comp}[A, B]$ *and* $\textsc{Comp}[A^c, B^c]$*, then the above condition can be maintained in the plain* 2*-pebble game (without counting).*

Proof. We discuss the real version in relation to the bijective 2-pebble game. Consider a position $p\colon a_1a_2 \mapsto b_1b_2$ as described by conditions (i) and (ii), and assume that player **I** starts a round involving relocation of the second pebble pair, so that just $ab := a_1b_1$ of the current position needs to be respected. By the rules of the game, player **II** needs to propose a bijection $\rho\colon [n] \to [n]$ between the vertex sets of $\mathcal{A}$ and $\mathcal{B}$ (recall that $n = m$ as X is doubly stochastic) with $\rho(a) = b$ and such that $A_{aa'} = 1$ iff $B_{b\rho(a')} = 1$ for all a'; in order to maintain conditions (i) and (ii) we additionally want $X_{a'\rho(a')} > 0$ for all a'. The existence of such a bijection follows from the X-equivalence of the partitions $[n] = \dot{\bigcup}_i D_i$ and $[n] = \dot{\bigcup}_i D'_i$. By pre-condition (ii), $a = a_1 \in D_i$ and $b = b_1 \in D'_i$ for the same index i, whence the numbers of A/B-adjacent vertices in D_j in $\mathcal{A}$/in D'_j in $\mathcal{B}$ agree for each index j, and the desired bijection can be pieced together from bijections between D_j and D'_j that respect adjacency with a and b. □

Corollary 4.9. (a) *The following are equivalent for graphs* $\mathcal{A}$ *and* $\mathcal{B}$ *with adjacency matrices* $A \in \mathbb{B}^{m,m}$*,* $B \in \mathbb{B}^{n,n}$*:*

(i) $\mathcal{A}$ *and* $\mathcal{B}$ *are fractionally isomorphic, i.e. the system* ISO *has a real solution;*

(ii) *the matrix equation* $\textsc{Comp}[A, B]$ *admits a good solution* X*;*

(iii) **II** *has a winning strategy in the bijective* 2*-pebble on* $\mathcal{A}$ *and* $\mathcal{B}$*.*

(b) *Similarly the following are equivalent:*

(i) $\mathcal{A}$ *and* $\mathcal{B}$ *are boolean fractionally isomorphic; i.e. the system* B-ISO *has a solution in the sense of boolean arithmetic;*

(ii) *the matrix equations* $\textsc{Comp}[A, B]$ *and* $\textsc{Comp}[A^c, B^c]$ *possess a simultaneous good boolean solution* X*;*

(iii) **II** *has a winning strategy in the plain* 2*-pebble on* $\mathcal{A}$ *and* $\mathcal{B}$*.*

5 Relaxations in the style of Sherali–Adams

In this section we refine the connection between the Sherali–Adams hierarchy of LP relaxations of the integer linear program ISO to equivalence in the finite variable counting logics or the higher-dimensional Lehman–Weisfeiler equivalence.

NB: our parameter $k \geqslant 2$ is the number of pebbles, or the variables available in the k-variable logics C^k or L^k.

As before, $\mathcal{A}$ and $\mathcal{B}$ are graphs with vertex sets $[m]$ and $[n]$, respectively, and A and B are their adjacency matrices. We denote typical elements and tuples of elements from $\mathcal{A}$ and $\mathcal{B}$ as $\mathbf{a} = (a_1, \dots, a_r)$ or $\mathbf{b} = (b_1, \dots, b_r)$, for $0 \leqslant r \leqslant k$; correspondingly, we typically denote entries of the adjacency matrices as, e.g., $A_{aa'}$. This device will help in an intuitive consistency check also in matrix compositions like AX with entries $(AX)_{ab}$ if A is an $m \times m$ matrix over $[m]$ and X, as an $m \times n$ matrix, relates $[m]$ and $[n]$ through entries X_{ab}: $(AX)_{ab} = \sum_{a'} A_{aa'} X_{a'b}$ (which rightly suggests paths of length two in a suitable composition of graphs $\mathcal{A}$ and $G(X)$).

Types. Let $\mathrm{etp}(\mathbf{a})$ denote the equality type of tuple $\mathbf{a}$ in $\mathcal{A}$, $\mathrm{atp}(\mathbf{a})$ its quantifier-free type, and $\mathrm{tp}(\mathbf{a})$ its complete type in the logic C^k, that is, the set of all C^k-formulae $\varphi(\mathbf{x})$ such that $\mathcal{A}$ satisfies $\varphi(\mathbf{a})$. Note that $\mathbf{a} \mapsto \mathbf{b}$ constitutes a local bijection if, and only if, $\mathrm{etp}(\mathbf{a}) = \mathrm{etp}(\mathbf{b})$, and a local isomorphism if, and only if, $\mathrm{atp}(\mathbf{a}) = \mathrm{atp}(\mathbf{b})$.

It will sometimes be useful to view some of the elements whose type we consider as "parameters" and only the remaining as "variables". Formally, we define the *type of a w.r.t. to the parameters* $\mathbf{a}$ simply to be the type of $\mathbf{a}a$, that is, $\mathrm{tp}_{\mathbf{a}}(a) := \mathrm{tp}(\mathbf{a}a)$. The distinction between plain types and types with parameters is one of semantic intention rather than syntactic. It is suggestive when it comes to counting realisations. For example, we let

$$\#^{\mathcal{A}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a}))$$

denote the number of tuples $\mathbf{a}'$ in $\mathcal{A}$ that realise the type of $\mathbf{a}$, i.e., those $\mathbf{a}'$ for which $\mathcal{A}, \mathbf{a}' \equiv^k_{\mathsf{C}} \mathcal{A}, \mathbf{a}$. If the structure in which realisations are counted is obvious or does not matter because of C^k-equivalence, we drop the superscript and write e.g. just $\#_{\mathbf{x}}$ instead of $\#^{\mathcal{A}}_{\mathbf{x}}$ or $\#^{\mathcal{B}}_{\mathbf{x}}$.

The number of realisations of the 1-type of a over parameters $\mathbf{a}$ (in $\mathcal{A}$) is denoted by

$$\#_x(\mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a)) \quad \big(= \#_x(\mathrm{tp}(\mathbf{a}x) = \mathrm{tp}(\mathbf{a}a))\big).$$

Regarding the counting of realisations we note that generally

$$\#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{a}a)) \quad = \quad \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \cdot \#_x(\mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a)). \qquad (3)$$

The equations. In the following we use variables X_p indexed by subsets $p \subseteq [m] \times [n]$ of size up to $k-1$; we may think of such p as being specified by two tuples $\mathbf{a}$ and $\mathbf{b}$ of length $|p|$ that enumerate the first and second components of the pairs in p in any coherent order. In this sense we write $p = \mathbf{ab}$. As remarked before, p is a local bijection between $\mathcal{A}$ and $\mathcal{B}$ iff $\mathrm{etp}(\mathbf{a}) = \mathrm{etp}(\mathbf{b})$, and a local isomorphism iff $\mathrm{atp}(\mathbf{a}) = \mathrm{atp}(\mathbf{b})$ (and neither of these conditions depends on the chosen enumeration of tuples in p, which gives rise to the order of components in both $\mathbf{a}$ and $\mathbf{b}$).

The augmentation of $p \subseteq [m] \times [n]$ by some pair $ab \in [m] \times [n]$ is simply denoted $p^\frown ab$. It is crucial that the notation $p^\frown ab$ does *not* refer to a *tuple* of pairs but to a *set* of pairs, in which the pair (a, b) is not distinguished. In particular, if the pair ab is in p, then $p^\frown ab = p$. Correspondingly, $p \setminus ab$ stands for the set of pairs $a'b' \in p$ that are distinct from ab.

For further reference we isolate and name equation types as follows. For given $n, m \geqslant 1$ and matrices $A \in \mathbb{B}^{n,n}$ and $B \in \mathbb{B}^{m,m}$:

$$X_\emptyset = 1 \qquad \textsc{Cont}(0)$$

$$\left.\begin{array}{l} X_p = \sum_{b'} X_{p^\frown ab'} = \sum_{a'} X_{p^\frown a'b} \\ \text{for } |p| = \ell - 1, a \in [m], b \in [n] \end{array}\right\} \qquad \textsc{Cont}(\ell)$$

$$\left.\begin{array}{l} \sum_{a'} A_{aa'} X_{p^\frown a'b} = \sum_{b'} X_{p^\frown ab'} B_{b'b} \\ \text{for } |p| = \ell - 1, a \in [m], b \in [n] \end{array}\right\} \qquad \textsc{Comp}(\ell)$$

Here *level* ℓ refers to ℓ as the size of the pairings $\mathbf{ab}$ in the typical variables $X_{\mathbf{ab}}$ involved; note that the size of p mentioned in $X_{p^\frown ab}$ therefore remains one below this ℓ. In the generic formats for $\textsc{Cont}(\ell)$ and $\textsc{Comp}(\ell)$ above, we assume $\ell \geqslant 1$. Note that the combination of $\textsc{Cont}(0)$, $\textsc{Cont}(1)$ and $\textsc{Comp}(1)$ precisely corresponds to the equations for fractional isomorphism; in particular the level 1 equation $\textsc{Comp}(1)$ is the same equation that was denoted $\textsc{Comp}[A, B]$ with specific reference to the constituents A/B in Section 4.3.

If we think of the matrix entries $(X_{\mathbf{ab}^\frown ab})_{a \in [n], b \in [m]}$ as specifying extensions of $\mathbf{a} \mapsto \mathbf{b}$ in the form of a distribution on possible pairings $a \mapsto b$, then equations $\textsc{Cont}(\ell)$ may be seen as *continuity conditions*, while equations $\textsc{Comp}(\ell)$ specify *compatibility conditions* with the edge relations encoded in A and B. Variants of the compatibility conditions can be expressed for matrices other than the adjacency matrices A and B that we primarily think of. We saw one such variation in the discussion on boolean isomorphisms above, where $\textsc{Comp}(1)$ was postulated for both A, B and A^c, B^c. Further variants will play a role in Section 5.1.2.

5.1 Sherali–Adams of level $k - 1$

For $k \geqslant 2$, the *level* $k-1$ *Sherali–Adams relaxation* of the integer linear program ISO consists of the collection of the equations $\textsc{Cont}(\ell)$ and $\textsc{Comp}(\ell)$ for $\ell < k$. Note that ISO(1) (i.e., level 1 or ISO$(k-1)$ for $k = 2$) is fractional isomorphism.

ISO$(k-1)$

$$\left.\begin{array}{l} X_\emptyset = 1 \quad \text{and} \\ X_p = \sum_{b'} X_{p^\frown ab'} = \sum_{a'} X_{p^\frown a'b} \\ \text{for } |p| < k - 1, a \in [m], b \in [n] \end{array}\right\} \qquad \textsc{Cont}(\ell) \text{ for } \ell < k$$

$$\left.\begin{array}{l} \sum_{a'} A_{aa'} X_{p^\frown a'b} = \sum_{b'} X_{p^\frown ab'} B_{b'b} \\ \text{for } |p| < k - 1, a \in [m], b \in [n] \end{array}\right\} \qquad \textsc{Comp}(\ell) \text{ for } \ell < k$$

$$X_p \geq 0 \text{ for } |p| \leq k - 1$$

5.1.1 From C^k-equivalence to solutions

Assume that $\mathcal{A} \equiv^k_{\mathsf{C}} \mathcal{B}$. This implies that $\mathcal{A}$ and $\mathcal{B}$ realise exactly the same types of r-tuples for $r \leqslant k$, and with the same number of realisations:

$$\#^{\mathcal{A}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) = \#^{\mathcal{B}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \tag{4}$$

and similarly for all types $\mathrm{tp}(\mathbf{b})$ of r-tuples in $\mathcal{B}$ for $r \leqslant k$. In particular $m = |\mathcal{A}| = |\mathcal{B}| = n$ so that both structures have domain $[n]$.

If $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$, where $\mathbf{a}$ and $\mathbf{b}$ are r-tuples for $r \leqslant k-1$, then, for any $a \in [n]$, there is a $\hat{b} \in [n]$ such that $\mathrm{tp}(\mathbf{b}\hat{b}) = \mathrm{tp}(\mathbf{a}a)$; and for any such choice of $\hat{b}$ we find (cf. equation (3)):

$$\begin{aligned} \#^{\mathcal{A}}_{x}(\mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a)) &= \#^{\mathcal{A}}_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{a}a)) \;/\; \#^{\mathcal{A}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \\ &= \#^{\mathcal{B}}_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{a}a)) \;/\; \#^{\mathcal{B}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \\ &= \#^{\mathcal{B}}_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}\hat{b})) \;/\; \#^{\mathcal{B}}_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b})) \\ &= \#^{\mathcal{B}}_{x}(\mathrm{tp}_{\mathbf{b}}(x) = \mathrm{tp}_{\mathbf{b}}(\hat{b})). \end{aligned} \tag{5}$$

Similarly, for r-tuples $\mathbf{a}$ and $\mathbf{b}$ such that $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$, where $r \leqslant k-2$ (!), and for any a and b, there are $\hat{a}$ and $\hat{b}$ such that $\mathrm{tp}(\mathbf{b}\hat{b}b) = \mathrm{tp}(\mathbf{a}a\hat{a})$ and

$$\#^{\mathcal{A}}_{xy}(\mathrm{tp}_{\mathbf{a}}(xy) = \mathrm{tp}_{\mathbf{a}}(a\hat{a})) = \#^{\mathcal{B}}_{xy}(\mathrm{tp}_{\mathbf{b}}(xy) = \mathrm{tp}_{\mathbf{b}}(\hat{b}b)). \tag{6}$$

For the desired solution put

$$\begin{aligned} &X_{\emptyset} := 1, \\ &X_p := \delta(\mathrm{tp}(\mathbf{a}), \mathrm{tp}(\mathbf{b})) \;/\; \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})), \\ &\qquad\qquad\qquad\qquad \text{for } p = \mathbf{ab},\ 0 < |p| < k. \end{aligned} \tag{7}$$

For the denominator note that $\#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) = \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b}))$ whenever $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$. Clearly $X_p \geqslant 0$. Note that $X_p \neq 0$ implies $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$, which implies that $\mathrm{atp}(\mathbf{a}) = \mathrm{atp}(\mathbf{b})$ whereby $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism.

We check that the given assignment to the variables X_p satisfies all instances of the equations $\textsc{Cont}(\ell)$ and $\textsc{Comp}(\ell)$ in Sherali–Adams of level $k-1$. In fact, we shall prove that the X_p as specified by (7), satisfy all instances of the continuity equations $\textsc{Cont}(\ell)$ of levels $\ell \leqslant k$ (!) and all instances of the compatibility equations $\textsc{Comp}(\ell)$ of levels $\ell < k$, while level $k-1$ Sherali–Adams, i.e. $\mathrm{ISO}(k-1)$, just requires both equation types for levels $\ell < k$. This combination of equations, which seem to be of 'mixed' or intermediate levels in relation to the established Sherali–Adams hierarchy, will be important in our analysis. We denote it as $\mathrm{ISO}(k-1/2)$:

ISO($k-1/2$)

$$\left.\begin{array}{l} X_\emptyset = 1 \quad \text{and} \\ X_p = \sum_{b'} X_{p\frown ab'} = \sum_{a'} X_{p\frown a'b} \\ \text{for } |p| < k, a \in [n], b \in [m] \end{array}\right\} \quad \textsc{Cont}(\ell) \text{ for } \ell \leqslant k$$

$$\left.\begin{array}{l} \sum_{a'} A_{aa'} X_{p\frown a'b} = \sum_{b'} X_{p\frown ab'} B_{b'b} \\ \text{for } |p| < k-1, a \in [n], b \in [m] \end{array}\right\} \quad \textsc{Comp}(\ell) \text{ for } \ell < k$$

$$X_p \geq 0 \text{ for } |p| \leq k$$

Lemma 5.1. *If $\mathcal{A} \equiv^k_{\mathsf{C}} \mathcal{B}$, then* ISO($k-1/2$) *admits a solution.*

Proof. We show that the solution (X_p) proposed as 7 satisfies all relevant instances of $\textsc{Cont}(\ell)$ and $\textsc{Comp}(\ell)$.

Consider an instance of $\textsc{Cont}(\ell)$ for the solution proposed in of level $\ell \leqslant k$, i.e., for $|p| < k$, with $p = \mathbf{ab}$, $a \in [n]$. If $\mathrm{tp}(\mathbf{a}) \neq \mathrm{tp}(\mathbf{b})$, then both sides of the equation are zero. In case $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$, let $\hat{b} \in [n]$ be such that $\mathrm{tp}(\mathbf{b}\hat{b}) = \mathrm{tp}(\mathbf{a}a)$ (such $\hat{b}$ exist as $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$ and since $|p| < k$). Then

$$\begin{aligned} \textstyle\sum_{b'} X_{p\frown ab'} &= \textstyle\sum_{b'} \ \delta(\mathrm{tp}(\mathbf{a}a), \mathrm{tp}(\mathbf{b}b')) \ / \ \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{a}a)) \\ &= \#_x(\mathrm{tp}_{\mathbf{b}}(x) = \mathrm{tp}_{\mathbf{a}}(a)) \ / \ \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{a}a)) \\ &= \#_x(\mathrm{tp}_{\mathbf{b}}(x) = \mathrm{tp}_{\mathbf{b}}(\hat{b})) \ / \ \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}\hat{b})) \\ &= \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b}))^{-1} = X_p, \end{aligned}$$

where the crucial equality leading to the last line is from equation (3).

Consider now an instance of equation $\textsc{Comp}(\ell)$ of level $\ell < k$, i.e., with $|p| < k-1$, with $p = \mathbf{ab}$, $a \in [n]$, $b \in [n]$. Again, the case of $\mathrm{tp}(\mathbf{a}) \neq \mathrm{tp}(\mathbf{b})$ is trivial. So we are left with the case of $p = \mathbf{ab}$ with $\mathrm{tp}(\mathbf{a}) = \mathrm{tp}(\mathbf{b})$ and $|p| \leqslant k-2$. These imply that there are $\hat{a}$ and $\hat{b}$ such that $\mathrm{tp}(\mathbf{a}a\hat{a}) = \mathrm{tp}(\mathbf{b}\hat{b}b)$. Then

$$\begin{aligned} & \textstyle\sum_{a'} A_{aa'} X_{p\frown a'b} \\ = \quad & \textstyle\sum_{a'} A_{aa'} \ \delta(\mathrm{tp}(\mathbf{a}a'), \mathrm{tp}(\mathbf{b}b)) \ / \ \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}b)) \\ = \quad & \frac{\#_y\big(\mathrm{edge}(ay) \wedge \mathrm{tp}_{\mathbf{a}}(y) = \mathrm{tp}_{\mathbf{a}}(\hat{a})\big)}{\#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}b))} \\ = \quad & \frac{\#_{xy}\big(\mathrm{edge}(xy) \wedge \mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a) \wedge \mathrm{tp}_{\mathbf{a}}(y) = \mathrm{tp}_{\mathbf{a}}(\hat{a})\big)}{\#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}b)) \cdot \#_x(\mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a))} \\ = \quad & \frac{\#_{xy}\big(\mathrm{edge}(xy) \wedge \mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a) \wedge \mathrm{tp}_{\mathbf{a}}(y) = \mathrm{tp}_{\mathbf{a}}(\hat{a})\big)}{\#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b})) \cdot \#_x(\mathrm{tp}_{\mathbf{b}}(x) = \mathrm{tp}_{\mathbf{b}}(b)) \cdot \#_x(\mathrm{tp}_{\mathbf{a}}(x) = \mathrm{tp}_{\mathbf{a}}(a))}, \end{aligned} \tag{8}$$

where we use instances of equation (3), and, in the passage from the third to the fourth line, artificially count over all realisations of $\mathrm{tp}_{\mathbf{a}}(a)$ instead of just the fixed parameter a, and compensate for that in the denominator.

The counting term in the enumerator of this expression,

$$\#_{xy}\big(\text{edge}(xy) \wedge \text{tp}_{\mathbf{a}}(x){=}\text{tp}_{\mathbf{a}}(a) \wedge \text{tp}_{\mathbf{a}}(y){=}\text{tp}_{\mathbf{a}}(\hat{a})\big),$$

is the sum of the number of realisations of all those types ($\text{tp}_{\mathbf{a}}(a'', a')$) that simultaneously extend $\text{tp}_{\mathbf{a}}(a)$, $\text{tp}_{\mathbf{a}}(\hat{a})$ and contain the formula edge(xy). Each one of these types has exactly the same number of realisations in $\mathcal{A}$ as the corresponding type that simultaneously extends $\text{tp}_{\mathbf{b}}(\hat{b})$, $\text{tp}_{\mathbf{b}}(b)$ and contains the formula edge(xy). By symmetry of the graphs under consideration, edge(xy) is equivalent with edge(yx) and what we obtained in (8) coincides with the corresponding evaluation of the right-hand side of this instance of equation $\text{COMP}(\ell)$ as desired:

$$\begin{aligned}
&\textstyle\sum_{b'} B_{b'b} X_{p^\frown ab'} \\
= \;& \textstyle\sum_{b'} B_{b'b}\, \delta(\text{tp}(\mathbf{a}a), \text{tp}(\mathbf{b}b')) \;\big/\; \#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x){=}\text{tp}(\mathbf{a}a)) \\
= \;& \frac{\#_{xy}\big(\text{edge}(yx) \wedge \text{tp}_{\mathbf{b}}(x){=}\text{tp}_{\mathbf{b}}(b) \wedge \text{tp}_{\mathbf{a}}(y){=}\text{tp}_{\mathbf{a}}(a)\big)}{\#_{\mathbf{x}x}(\text{tp}(\mathbf{x}x){=}\text{tp}(\mathbf{a}a)) \cdot \#_x(\text{tp}_{\mathbf{b}}(x){=}\text{tp}_{\mathbf{b}}(b))} \\
= \;& \frac{\#_{xy}\big(\text{edge}(yx) \wedge \text{tp}_{\mathbf{b}}(x){=}\text{tp}_{\mathbf{b}}(b) \wedge \text{tp}_{\mathbf{b}}(y){=}\text{tp}_{\mathbf{b}}(\hat{b})\big)}{\#_{\mathbf{x}}(\text{tp}(\mathbf{x}){=}\text{tp}(\mathbf{a})) \cdot \#_x(\text{tp}_{\mathbf{a}}(x){=}\text{tp}_{\mathbf{a}}(a)) \cdot \#_x(\text{tp}_{\mathbf{b}}(x){=}\text{tp}_{\mathbf{b}}(b))}\,.
\end{aligned} \tag{9}$$

□

We shall see in Theorem 5.9 that $\equiv^k_{\mathsf{C}}$ precisely corresponds to $\text{ISO}(k-1/2)$.

5.1.2 From solutions to pebble game equivalence

In the following we discuss what it means that some admissible real or rational non-negative assignment to the variables X_p for all $|p| < k$ satisfies the equations $\text{CONT}(\ell)$ and $\text{COMP}(\ell)$ for $\ell < k$, i.e., $\text{ISO}(k-1)$.

Definition 5.2. A matrix $X = (X_p)_{|p| \leqslant k}$, with non-negative entries indexed by *sets* $p \subseteq [m] \times [n]$ of size up to k is *supported by local bijections* if $X_p > 0$ only for p that are the graphs of local bijections between $[n]$ and $[m]$.We say that X is *supported by local isomorphisms* (w.r.t. to edge relations A and B of graphs $\mathcal{A}$ and $\mathcal{B}$ on $[n]$ and $[m]$, respectively) if $X_p > 0$ moreover implies that the partial bijection p is a local isomorphism.

Lemma 5.3. (a) *If* $(X_p)_{|p|<k}$ *is a solution to* $\text{CONT}(\ell)$ *for* $\ell < k$*, then it is supported by local bijections.*

(b) *For* $k \geqslant 3$*, if* $(X_p)_{|p|<k}$ *is a solution to* $\text{CONT}(\ell)$ *for* $\ell < k$ *and of* $\text{COMP}(\ell)$ *for* $\ell = 2$*, then it is supported by local isomorphisms.*

It follows that any solution to $\text{ISO}(k-1)$ *is supported by local isomorphisms.*

Proof. Suppose that $p = \mathbf{ab}$ is not a local bijection, w.l.o.g. (by symmetry) assume that there are a and $b_1 \neq b_2$ such that $(a, b_1), (a, b_2) \in p$. For $p_0 := p \setminus (a, b_2)$ we clearly have $\ell := |p_0| < k-1$, and looking at the instance of $\text{CONT}(\ell)$ for this p_0 and a, we find that the two summands for $b' = b_i$, $i = 1, 2$, both contribute to the left-hand side. So the equation and non-negativity of all X-assignments imply that $X_{p_0} + X_p \leqslant X_{p_0}$, whence $X_p = 0$.

For (b) we use (a) and instances of the equations $\textsc{Comp}(2)$. Note that for $p = \emptyset$ as well as for $|p| = 1$, $p = ab$, cannot fail to be a local isomorphism (in undirected, loop-free graphs). Note that p is a local isomorphism if all restrictions $p' \subseteq p$ of p of size $|p'| = 2$ are local isomorphisms, and that $X_p > 0$ implies $X_{p'} > 0$ for all $p' \subseteq p$ by instances of $\textsc{Cont}(\ell)$. So it remains to argue that $\textsc{Comp}(2)$ enforces that $X_{a_1a_2b_1b_2} > 0$ only for local isomorphisms $a_1a_2 \mapsto b_1b_2$. As $a_1a_2 \mapsto b_1b_2$ must be a local bijection by (a), it remains to check that

(i) $A_{a_1a_2} = 1 \;\Rightarrow\; B_{b_1b_2} \neq 0$, and

(ii) $B_{b_1b_2} = 1 \;\Rightarrow\; A_{a_1a_2} \neq 0$.

For (i) we use the instance $\sum_{a'} A_{a_1a'} X_{a_1b_1{}^\frown a'b_2} = \sum_{b'} X_{a_1b_1{}^\frown a_1b'} B_{b'b_2}$ of equation $\textsc{Comp}(2)$, whose right-hand side reduces to the single term $X_{a_1b_1} B_{b_1b_2}$ because X is supported by local bijections. As the left-hand side is positive if $A_{a_1a_2} = 1$ and $X_{a_1b_2{}^\frown a_2b_2} > 0$, (i) follows. The case for (ii) is strictly analogous. $\square$

From solutions to good solutions

Recall Definition 4.7 for good solutions to individual equations

$$\textsc{Comp}[A, B]\colon\; AX = XB,$$

which is motivated by the useful properties these solutions have for the analysis of fractional isomorphism in relation to 2-pebble equivalence.

We now want to analyse the solution spaces of $\mathrm{ISO}(k-1)$ and $\mathrm{ISO}(k-1/2)$, and very specifically of the relevant continuity equations with a view to strengthening the analogy with fractional isomorphism. Solutions to the continuity equations up to arity level ℓ can in fact be understood as fractional isomorphisms between graphs of ℓ-tuples that govern the combinatorics of the plain ℓ-pebble game and, by extension, of the k-pebble game with counting. This will in particular also allow us to resort to *good solutions* with similar benefits as in the analysis of plain fractional isomorphism (at level 1).

To this end we switch to a modified view of a solution $(X_p)_{|p|\leqslant \ell}$ that labels entries not by local isomorphisms p as *sets of pairs* $p \subseteq [m] \times [n]$ of size $|p|$, but instead, for $|p| > 0$, by pairs of *full ℓ-tuples* $(\mathbf{a}, \mathbf{b}) \in [m]^\ell \times [n]^\ell$ such that $p(\mathbf{a}) = \mathbf{b}$, where $\mathbf{a}$ is any enumeration of $\mathrm{dom}(p)$ and $\mathbf{b}$ the matching tuple enumerating $\mathrm{image}(p)$. With a solution $X = (X_p)_{|p|\leqslant \ell}$ we want to associate the single matrix

$$\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})_{\mathbf{a}\in[m]^\ell, \mathbf{b}\in[n]^\ell}\colon \qquad \check{X}_{\mathbf{a},\mathbf{b}} := X_p \text{ for } p = \{(a_i, b_i)\colon i \in [\ell]\}.$$

It is easy to see that the continuity equations $\textsc{Cont}(\ell')$ for all $\ell' \leqslant \ell$ for (X_p) imply that the associated matrix $\check{X}$ is doubly stochastic. But the continuity equations for (X_p) also manifest themselves in the fact that $\check{X}$ is a fractional isomorphism w.r.t. a graph representation of the combinatorial layout of the plain k-pebble game over $[m]^\ell, [n]^\ell$, as follows. For $i \in [\ell]$, the matrix $\mathbb{I}^{(i)} = \mathbb{I}^{(i)}_{m,\ell}$ with entries

$$\mathbb{I}^{(i)}_{\mathbf{a},\mathbf{a}'} := \prod_{j \neq i} \delta(a_j, a'_j) \quad \text{for } \mathbf{a}, \mathbf{a}' \in [m]^\ell$$

may be regarded as the adjacency matrix of the reflexive graph

$$\mathcal{I}^{(i)}(m, \ell) := ([m]^\ell, \mathbb{I}^{(i)})$$

associated with legal moves of the i-th pebble in the plain ℓ-pebble game over universe $[m]$. Its reflexive and symmetric edge relation links two tuples in $[m]^\ell$ if they disagree at most in the i-th component. If X solves $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$, then $\check{X}$ describes a fractional isomorphism between $\mathcal{I}^{(i)}(m, \ell)$ and $\mathcal{I}^{(i)}(n, \ell)$, for each $i \in [\ell]$: $\check{X}$ is doubly stochastic and a solution to the matrix equations

$$\textsc{Comp}[\mathbb{I}^{(i)}_{m,\ell}, \mathbb{I}^{(i)}_{n,\ell}]: \quad \mathbb{I}^{(i)}_{m,\ell}\check{X} = \check{X}\mathbb{I}^{(i)}_{n,\ell} \qquad \text{for each } i \in [\ell],$$

as is shown in Lemma 5.6 below. We may modify this solution $\check{X}$ to obtain a *good solution* in the sense of Definition 4.7, as in Corollary 3.9; and this good solution $(\check{X}'_{\mathbf{a},\mathbf{b}})$ then translates back into a solution (X'_p) of the continuity equations up to $\textsc{Cont}(\ell)$ with similar homogeneity benefits.

Definition 5.4. (a) Let $X = (X_p)_{|p| \leqslant \ell}$ be non-negative, labelled by *sets* $p \subseteq [m] \times [n]$ of sizes up to ℓ. Define its *lifting* to tuple co-ordinates to be the array $\check{X} := (\check{X}_{\mathbf{a},\mathbf{b}})_{\mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell}$ where $\check{X}_{\mathbf{a},\mathbf{b}} := X_p$ for $p := \{(a_i, b_i) : i \in [\ell]\}$.

(b) A matrix $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ labelled by *pairs of tuples* $(\mathbf{a}, \mathbf{b}) \in [m]^\ell \times [n]^\ell$ is said to be *consistent* if $\check{X}_{\mathbf{a},\mathbf{b}} = \check{X}_{\mathbf{a}',\mathbf{b}'}$ whenever $\{(a_i, b_i) : i \in [\ell]\} = \{(a'_i, b'_i) : i \in [\ell]\}$.

(c) For any consistent matrix $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ labelled by $(\mathbf{a}, \mathbf{b}) \in [m]^\ell \times [n]^\ell$, define its *projection* to set co-ordinates to be the array $X := (X_p)_{|p| \leqslant \ell}$ with $X_\emptyset := 1$ and $X_p = \check{X}_{\mathbf{a},\mathbf{b}}$ for any $\mathbf{a}, \mathbf{b}$ such that $p = \{(a_i, b_i) : i \in [\ell]\}$.

Note that the natural notions of being supported by local bijections, or by local isomorphisms, in the sense of Definition 5.2, are preserved in the passage from X to $\check{X}$ according to (a), and in the passage from consistent $\check{X}$ to X according to (b). Note also that consistency of a matrix $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ implies that its co-ordinatisation is *permutation invariant* in the sense that $\check{X}_{\mathbf{a},\mathbf{b}} = \check{X}_{\pi(\mathbf{a}),\pi(\mathbf{b})}$ for all permutations $\pi \in S_\ell$. Permutation invariance guarantees in particular that the fractional isomorphism conditions $\mathbb{I}^{(i)}\check{X} = \check{X}\mathbb{I}^{(i)}$ are equivalent for any two choices of $i \in [\ell]$.

Observation 5.5. *The conditions of being doubly stochastic and of permutation-invariance, as well as of being supported by local bijections or by local isomorphisms, are compatible with transposition and matrix products: e.g., if $\check{X}, \check{Y}$ are consistent then so are $\check{X}^t$ and $\check{X}\check{Y}$. For matrices that are supported by local bijections, consistency is also preserved in transposition and matrix products.*

Proof. The proofs are straightforward and we just sketch the argument for consistency. Symmetry of the condition immediately implies compatibility with transposition. For products consider matrices $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ and $\check{X} = (\check{X}_{\mathbf{b},\mathbf{c}})$ that are both consistent and supported by local bijections. Let $X = (X_p)$ and $Y = (Y_p)$ be their projections to set co-ordinates, which are therefore also supported by local bijections. Let $\check{Z} := \check{X}\check{Y}$ and consider index pairs $(\mathbf{a}, \mathbf{c})$ and $(\mathbf{a}', \mathbf{c}')$ such that $\{(a_i, c_i) \colon i \in [\ell]\} = \{(a'_i, c'_i) \colon i \in [\ell]\}$. Let s be the size of these sets. Then

$$\check{Z}_{\mathbf{a},\mathbf{c}} = \sum_{\mathbf{b}} \check{X}_{\mathbf{a},\mathbf{b}} \check{Y}_{\mathbf{b},\mathbf{c}} = 1/s! \sum_{q \circ p \colon \mathbf{a} \mapsto \mathbf{c}} X_p Y_q = 1/s! \sum_{q \circ p \colon \mathbf{a}' \mapsto \mathbf{c}'} X_p Y_q = \check{Z}_{\mathbf{a}',\mathbf{c}'}.$$

Note that the p, q-sums are over all pairs of local bijections whose compositions are represented by the graph $\{(a_i, c_i) \colon i \in [\ell]\} = \{(a'_i, c'_i) \colon i \in [\ell]\}$. That just local bijections need to be considered, is due to the support of $\check{X}$ and $\check{Y}$ by local bijections: all other terms vanish; the uniform translation of these terms into set co-ordinates relies on consistency of $\check{X}$ and $\check{Y}$. □

Lemma 5.6. (a) *Let $X = (X_p)_{|p| \leqslant \ell}$ be labelled by sets $p \subseteq [m] \times [n]$ of sizes up to ℓ and let $\check{X}$ be its consistent lifting. If X solves the continuity equations up to level ℓ, then $\check{X}$ is doubly stochastic (which implies $n = m$) and commutes with the $\mathbb{I}^{(i)} = \mathbb{I}^{(i)}_{n,\ell}$:*

$$\mathbb{I}^{(i)} \check{X} = \check{X} \mathbb{I}^{(i)} \quad \textit{for } i \in [\ell].$$

In other words, $\check{X}$ is a fractional automorphism of the (reflexive) graph $\mathcal{I}^{(i)}(n, k)$, for each $i \in [\ell]$.

(b) *Conversely, let $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$, labelled by $(\mathbf{a}, \mathbf{b}) \in [m]^\ell \times [n]^\ell$, be consistent and let $X = (X_p)_{|p| \leqslant \ell}$ be its projection to set co-ordinates. If $\check{X}$ is a fractional isomorphism between $\mathcal{I}^{(i)}(m, \ell)$ and $\mathcal{I}^{(i)}(n, \ell)$ for some i (and hence for each i), then $n = m$ and X satisfies the continuity equations up to level ℓ.*

Proof. For part (a), assume first that X solves the continuity equations up to level k. By induction on the number $|[\mathbf{a}]|$ of distinct components in $\mathbf{a} \in [n]^\ell$, we show that the row sum $\sum_{\mathbf{b}} \check{X}_{\mathbf{a},\mathbf{b}} = 1$. For $|[\mathbf{a}]| = 1$, $\mathbf{a} = a^\ell$ and $\sum_{\mathbf{b}} \check{X}_{\mathbf{a},\mathbf{b}} = \sum_b \check{X}_{a^\ell, b^\ell} = \sum_b X_{\emptyset \frown ab} = X_\emptyset = 1$ by the continuity equations for X. The induction step is treated analogously: if $|[\mathbf{a}]|$ is such that, e.g., $a_\ell \notin \{a_1, \ldots, a_{\ell-1}\}$, we associate with any $\mathbf{b} \in [n]^\ell$ such that $\check{X}_{\mathbf{a},\mathbf{b}} > 0$ the local bijection $p = \{(a_i, b_i) \colon i < \ell\}$ and use the identity $\check{X}_{\mathbf{a},\mathbf{b}} = X_{p \frown a_\ell b_\ell}$ to first rewrite

$$\sum_{b_\ell} \check{X}_{\mathbf{a},\mathbf{b}} = \sum_{b_\ell} X_{p \frown a_\ell b_\ell} = X_p = \check{X}_{\mathbf{a}\frac{a_1}{\ell}, \mathbf{b}\frac{b_1}{\ell}}$$

using continuity equations for X. Therefore,

$$\sum_{\mathbf{b}} \check{X}_{\mathbf{a},\mathbf{b}} = \sum_{b_1,\ldots,b_{\ell-1}} \sum_{b_\ell} X_{\mathbf{ab}} = \sum_{b_1,\ldots,b_{\ell-1}} \check{X}_{\mathbf{a}\frac{a_1}{\ell}, \mathbf{b}\frac{b_1}{\ell}} = \sum_{\mathbf{b}} \check{X}_{\mathbf{a}\frac{a_1}{\ell}, \mathbf{b}} = 1$$

by inductive hypothesis. For the commutation condition $\mathbb{I}^{(i)} \check{X} = \check{X} \mathbb{I}^{(i)}$ we check that, for any $\mathbf{a}, \mathbf{b} \in [n]^\ell$, and for $p := \{(a_j, b_j) \colon j \neq i\}$:

$$(\mathbb{I}^{(i)} \check{X})_{\mathbf{a},\mathbf{b}} = \sum_{\mathbf{a}'} \mathbb{I}^{(i)}_{\mathbf{a},\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{a'} \check{X}_{\mathbf{a}\frac{a'}{i}, \mathbf{b}} = \sum_{a'} X_{p \frown a' b_i} = X_p$$

and similarly

$$(\check{X}\mathbb{I}^{(i)})_{\mathbf{a},\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'}\mathbb{I}^{(i)}_{\mathbf{b}',\mathbf{b}} = \sum_{b'} \check{X}_{\mathbf{a},\mathbf{b}\frac{b'}{i}} = \sum_{b'} X_{p^\frown a_i b'} = X_p.$$

Towards the converse, (b), the last two equations also show that the fractional isomorphism conditions for $\check{X}$ w.r.t. $\mathbf{I}^{(i)}$ imply that the sums

$$\sum_{a'} X_{p^\frown a' b_i} = \sum_{b'} X_{p^\frown a_i b'}$$

must be independent of the choice of a_i and b_i. Their value, therefore, must be equal to $\sum_{b'} X_{p^\frown a_1 b'} = X_{p^\frown a_1 b_1} = X_p$, whence the continuity equations at all levels $2 \leqslant \ell' \leqslant \ell$ are established. For level 1, $1 = X_\emptyset = \sum_a X_{ab} = \sum_b X_{ab}$ follows from the doubly stochastic nature of $\check{X}$, which implies, e.g., that $1 = \sum_{\mathbf{b}} \check{X}_{a^\ell \mathbf{b}} = \sum_b \check{X}_{a^\ell b^\ell} = \sum_b X_{ab}$. □

Definition 5.7. A solution $X = (X_p)_{|p| \leqslant \ell}$ to $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$ is *good* if its lifting $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ to tuple co-ordinates is a good solution (in the sense of Definition 4.7) to $\textsc{Comp}[\mathbb{I}^{(i)}(m,\ell), \mathbb{I}^{(i)}(n,\ell)]$ (simultaneously for every $i \in [\ell]$).

Recall from Definition 4.7 that a good solution, $\check{X}$ in tuple co-ordinates, induces $\check{X}$-related partitions of the vertex sets $[m]^\ell = \dot{\bigcup}_s D_s$ and $[n]^\ell = \dot{\bigcup}_s D'_s$ of the $\mathbb{I}^{(i)}$ such that

(i) these partitions are equivalent and stable w.r.t. the edge relations of the $\mathbb{I}^{(i)}$, for every $i \in [\ell]$;
(ii) $\check{X}_{D_s D'_s} > 0$ for all s;
(iii) $\check{X}_{D_s D'_t} = 0$ for $s \neq t$.

Note that, if (X_p) is a good solution that is supported by local isomorphisms, then the $\check{X}$-related partitions (D_s) and $D'_s)$ are such that $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism between $\mathcal{A}$ and $\mathcal{B}$ whenever $\check{X}_{\mathbf{a},\mathbf{b}} > 0$, i.e., whenever $\mathbf{a}$ and $\mathbf{b}$ are from matching partition sets D_s and D'_s.

Suppose that $X = (X_p)_{|p| \leqslant \ell}$ is a solution to $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$ that is supported by local isomorphisms. Note that by Lemma 5.3 this is the case for any solution to ISO$(k-1)$ and for $\ell = k-1$. Then by Lemma 5.6 (a) the lifting $\check{X}$ of X to tuple co-ordinates is a fractional isomorphism between $\mathbb{I}^{(i)}(m,\ell)$ and $\mathbb{I}^{(i)}(n,\ell)$, which is also supported by local isomorphisms between $\mathcal{A}$ and $\mathcal{B}$ in the sense that $\check{X}_{\mathbf{a},\mathbf{b}} > 0$ implies that $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism between $\mathcal{A}$ and $\mathcal{B}$. The associated matrices $\check{Z} := \check{X}^t\check{X}$ and $\check{Z}' := \check{X}\check{X}^t$ are doubly stochastic, symmetric with strictly positive diagonal, and also supported by local isomorphisms between $\mathcal{A}$ and $\mathcal{B}$ in the above sense. As in Corollary 3.9., we thus obtain a good solution $\check{X}'$ for the fractional isomorphism between $\mathbb{I}^{(i)}(m,\ell)$ and $\mathbb{I}^{(i)}(n,\ell)$. This good solution is of the form $\check{X}' = \check{Z}^n\check{X}$. Note that, by Lemma 5.6 (b), the projection of $\check{X}'$ to set co-ordinates, $X' = (X'_p)_{|p| \leqslant \ell}$, is again a solution to $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$, and it is supported by local isomorphisms. Regarding the relationship between (X_p) and (X'_p), also note that $X_p > 0$ implies $X'_p > 0$ as $\check{Z}$ and its powers have strictly positive diagonal.

We summarise these observations regarding solutions to $\textsc{Cont}(\ell)$ that are supported by local isomorphisms in a corollary before turning to the status of the induced solutions w.r.t. levels of $\textsc{Comp}(\ell)$.

Corollary 5.8. *If the equations* $\textsc{Cont}(\ell')$ *for* $\ell' \leqslant \ell$ *for* $\mathcal{A}$ *on* $[m]$ *and* $\mathcal{B}$ *on* $[n]$ *admit any solution* $X = (X_p)_{|p| \leqslant \ell}$ *that is supported by local isomorphisms between* $\mathcal{A}$ *and* $\mathcal{B}$*, then they also admit a solution* $X' = (X'_p)_{|p| \leqslant \ell}$ *that is* good *in the sense of Definition 5.7 and supported by local isomorphisms. Moreover, the natural good solution* X' *associated with a given solution* X *is strictly positive where* X *is.*

We are now ready to prove the converse of Lemma 5.1, thus matching C^k-equivalence to $\mathrm{ISO}(k-1/2)$. Recall $\mathrm{ISO}(k-1/2)$ (cf. the table given for Lemma 5.1 above): these intermediate levels Sherali–Adams levels combine the equations $\textsc{Comp}(\ell)$, concerning compatibility with the edge relations, of level $\ell < k$ with the continuity equations $\textsc{Cont}(\ell)$ of levels $\ell \leqslant k$.

Let $\mathcal{A}$, $\mathcal{B}$ be graphs with vertex sets $[m], [n]$, respectively, A, B be their symmetric adjacency matrices. We know from Lemma 5.1 that C^k-equivalence of $\mathcal{A}$ and $\mathcal{B}$ implies the existence of a solution for exactly this combination of equations. The following theorem says that the converse is also true.

Theorem 5.9. $\mathrm{ISO}(k-1/2)$ *has a solution if, and only if,* $\mathcal{A} \equiv^k_{\mathsf{C}} \mathcal{B}$*.*

Proof. It remains to argue for the implication from solvability of $\mathrm{ISO}(k-1/2)$ to C^k-equivalence. In fact, if $(X_p)_{|p| \leqslant k}$ is any solution to $\mathrm{ISO}(k-1/2)$, then

$$X_{\mathbf{ab}} > 0 \quad \Longrightarrow \quad \mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{C}} \mathcal{B}, \mathbf{b}.$$

We know from Lemma 5.3 that any solution $X = (X_p)$ to $\mathrm{ISO}(k-1/2)$ is supported by local isomorphisms. By Corollary 5.8 we may therefore assume without loss of generality that the given solution is good in the sense of Definition 5.7. So its lifting $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ to tuple co-ordinates induces $\check{X}$-related partitions $[n]^k = \dot{\bigcup}_s D_s$ and $[n]^k = \dot{\bigcup}_s D'_s$ that are equivalent stable partitions w.r.t. $\mathbb{I}^{(j)}(n,k)$ for each $j \in [k]$, and $\check{X}_{\mathbf{a},\mathbf{b}} > 0$ precisely if the tuples $\mathbf{a}$ and $\mathbf{b}$ are from matching partition sets. It suffices to provide strategy a for **II** to maintain this condition. For a round played in component j,

$$\#_a(\mathbf{a}\tfrac{a}{j} \in D_t) = \#_b(\mathbf{b}\tfrac{b}{j} \in D'_t)$$

follows from equivalence and stability of the partitions w.r.t. the edge relation of $\mathbb{I}^{(j)}$. Player **II** can offer a bijection $a \mapsto b$ that matches partition indices for $\mathbf{a}\frac{a}{j}$ and $\mathbf{b}\frac{b}{j}$, and thus maintains strict positivity of $\check{X}$ and X. □

Note that, of the compatibility equations in $\mathrm{ISO}(k-1/2)$, we only had to use the level 2 equation $\textsc{Comp}(2)$, which is sufficient to establish support by local isomorphisms (cf. Lemma 5.3 (b)). The rest of the compatibility levels are actually redundant, and this only changes when the levels of compatibility and continuity equations are properly matched, as they are in the regular Sherali–Adams relaxation levels of the isomorphism problem. To understand the nature of ISO$(k-1)$ we need to take the higher levels of the compatibility equations into account. To this end we turn to the interpretation of the compatibility equations $\textsc{Comp}(\ell)$ in terms of liftings to tuple co-ordinates.

By Lemma 5.3, even the level 2 equations $\textsc{Comp}(2)$ guarantee that solutions are supported by local isomorphisms. But if $X = (X_p)_{|p|\leqslant\ell}$ satisfies $\textsc{Comp}(\ell')$ for all levels $\ell' \leqslant \ell$, then its lifting $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ to tuple co-ordinates also satisfies the following equations for all $\mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell, a \in [m], b \in [n]$ and each $i \in [\ell]$:

$$\sum_{a'} A_{aa'} \check{X}_{\mathbf{a}\frac{a'}{i},\mathbf{b}\frac{b}{i}} = \sum_{b'} \check{X}_{\mathbf{a}\frac{a}{i},\mathbf{b}\frac{b'}{i}} B_{b'b}.$$

For this it suffices to note that the set projection of $(\mathbf{a}\frac{a}{i}, \mathbf{b}\frac{b}{i})$ is $p\widehat{\ }ab$ for $p = \{a_j b_j : j \neq i\}$. In order to view these equations as commutativity conditions in the style of fractional isomorphism, we artificially lift the adjacency matrices A and B to tuple co-ordinates with entries $A_{\mathbf{a},\mathbf{a}'}$ and $B_{\mathbf{b},\mathbf{b}'}$ for pairs of tuples $\mathbf{a}, \mathbf{a}' \in [m]^\ell$ and $\mathbf{b}, \mathbf{b}' \in [n]^\ell$ by putting, for instance in the case of A, for $i \in [\ell]$:

$$A^{(i)}_{\mathbf{a},\mathbf{a}'} := \prod_{j\neq i} \delta(a_j, a'_j) A_{a_i a'_i}.$$

Note that these matrices are symmetric if A is. We obtain an equivalence between $\textsc{Comp}(\ell)$ for X and $\textsc{Comp}[A^{(i)}, B^{(i)}]$ for $\check{X}$.

Lemma 5.10. *For any matrix $X = (X_p)_{|p|\leqslant\ell}$ labelled by sets $p \subseteq [m] \times [n]$ of size up to ℓ and its lifting to tuple co-ordinates $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ labelled by tuples $\mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell$, the following are equivalent:*

(i) *$X = (X_p)$ satisfies the equations $\textsc{Comp}(\ell')$ for $\ell' \leqslant \ell$;*

(ii) *$\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ satisfies $\textsc{Comp}[A^{(i)}, B^{(i)}]$ for some (and hence any) $i \in [\ell]$.*

Proof. The equation $\textsc{Comp}[A^{(i)}, B^{(i)}]$ for $\check{X}$ is

$$\sum_{\mathbf{a}'\in[m]^\ell} A^{(i)}_{\mathbf{a},\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'\in[n]^\ell} \check{X}_{\mathbf{a},\mathbf{b}'} B^{(i)}_{\mathbf{b}',\mathbf{b}},$$

and its equivalence with the equations $\textsc{Comp}(\ell')$ for levels ℓ' up to ℓ is immediate from the definition of $A^{(i)}/B^{(i)}$ in terms of A/B and of $\check{X}$ in terms of X. □

The following summarise the relevant translations of continuity and compatibility equations, which are expressed in terms of set co-ordinates X_p, to their liftings to tuple co-ordinates $\check{X}_{\mathbf{a},\mathbf{b}}$; compare Lemmas 5.6 and 5.10.

$\sum_{\mathbf{a}'} \check{X}_{\mathbf{a}'\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a}\mathbf{b}'} = 1$ $\sum_{\mathbf{a}'} \mathbb{I}^{(i)}_{\mathbf{a}\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'} \mathbb{I}^{(i)}_{\mathbf{b}'\mathbf{b}}$ for all $\mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell$, and all $i \in [\ell]$	lifting of $\textsc{Cont}(\ell'), \ell' \leqslant \ell$
$\sum_{\mathbf{a}'} A^{(i)}_{\mathbf{a},\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'} B^{(i)}_{\mathbf{b}',\mathbf{b}}$ for all $\mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell$, and all $i \in [\ell]$	lifting of $\textsc{Comp}(\ell'), \ell' \leqslant \ell$

As in the analysis of solutions for the fractional isomorphism problem, we see that passage to a good solution $\check{X}'$ of the form $\check{X}' = \check{Z}^n \check{X}$ for $\check{Z} = \check{X}\check{X}^t$ is compatible with this type of commutativity condition.

Starting from a solution X to $\mathrm{ISO}(k-1)$, whose lifting to tuple co-ordinates $\check{X}$ satisfies the above combination of equations for $\ell = k-1$, we obtain a good solution $\check{X}'$, which induces $\check{X}'$-related partitions of $[m]^{k-1}$ and $[n]^{k-1}$ as in Definition 5.7. These partitions are now simultaneously stable w.r.t. the $\mathbb{I}^{(i)}$ and w.r.t. the liftings of the edge relations $A^{(i)}$ and $B^{(i)}$, for each $i \in [\ell]$. In other words, we obtain a simultaneous good solution $\check{X}'$ in the sense of Definition 4.7 for

$$\textsc{Comp}[\mathbb{I}^{(i)}_{m,k-1}, \mathbb{I}^{(i)}_{n,k-1}]\,,\ \textsc{Comp}[A^{(i)}, B^{(i)}] \quad \text{for all } i \in [k-1].$$

We thus obtain the following, by reverse translation of a good solution $\check{X}'$ into set co-ordinates.

Corollary 5.11. *Let $k \geqslant 3$. Any solution $X = (X_p)_{|p|<k}$ to $\mathrm{ISO}(k-1)$ induces a* good *solution $X' = (X'_p)_{|p|<k}$ to $\mathrm{ISO}(k-1)$ with $\check{X}'$-related induced partitions of $[m]^{k-1} = \dot{\bigcup}_s D_s$ and $[n]^{k-1} = \dot{\bigcup}_s D'_s$ such that*

(i) *these partitions are equivalent stable partitions w.r.t. the edge relations of the $\mathbb{I}^{(i)}$ for each $i \in [\ell]$;*

(ii) *these partitions are equivalent stable partitions w.r.t. the liftings of the edge relations $A^{(i)}$ on $[m]^{k-1}$ and $B^{(i)}$ on $[n]^{k-1}$, for each $i \in [\ell]$;*

(iii) $\check{X}'_{D_s D'_s} > 0$ *for all s;*

(iv) $\check{X}'_{D_s D_t} = 0$ *for all $s \neq t$.*

In particular, $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism between $\mathcal{A}$ and $\mathcal{B}$ for $\mathbf{a}$ and $\mathbf{b}$ from matching partition sets. Moreover, X' is strictly positive where the given X is.

Level $k-1$ solutions and $\mathsf{C}^{<k}$-equivalence

As we shall see in Section 5.2, a solution $X = (X_p)_{|p|<k}$ to $\mathrm{ISO}(k-1)$ is in fact not strong enough to guarantee C^k-equivalence between $\mathcal{A}$ and $\mathcal{B}$. Instead it matches to a slightly lesser level of equivalence,

$$\mathcal{A} \equiv^{<k}_{\mathsf{C}} \mathcal{B},$$

which we characterise in terms of a modified game, the *weak bijective k-pebble game* over $\mathcal{A}, \mathcal{B}$. The game is played by two players. If $m \neq n$, player **II** loses immediately. Otherwise, a play of the game proceeds in a sequence of rounds. Positions of the game are sets $p \subseteq [m] \times [n]$ of size $|p| \leq k-1$. Normally, the initial position is $\emptyset$, but we will also consider plays of the game starting from other initial positions. A single round of the game, starting in position p, is played as follows.

1. If $|p| = k-1$, player **I** selects a pair $ab \in p$.
   If $|p| < k-1$, this step is omitted.

2. Player **II** selects a bijection between $[m]$ and $[n]$ (recall that $m = n$).

3. Player **I** chooses a pair $a'b'$ from this bijection.

4. If $p^+ := p^\frown a'b'$ is a local isomorphism then the new position is

$$p' := \begin{cases} (p \backslash ab)^\frown a'b' & \text{if } |p| = k-1, \\ p^\frown a'b' & \text{if } |p| < k-1. \end{cases}$$

   Otherwise, the play ends and player **II** loses.

Player **II** wins a play if it lasts forever, i.e., if $m = n$ and she never loses in step 4 of a round.

By comparison, a round in the ordinary bijective $(k-1)$-pebble game, which characterises $\equiv_{\mathsf{C}}^{k-1}$ according to Theorem 2.2, can be described as follows.

1. If $|p| = k-1$, player **I** selects a pair $ab \in p$.
   If $|p| < k-1$, this step is omitted.

2. Player **II** selects a bijection between $[m]$ and $[n]$.

3. Player **I** chooses a pair $a'b'$ from this bijection.

4. The new position is

$$p' := \begin{cases} (p \backslash ab)^\frown a'b' & \text{if } |p| = k-1, \\ p^\frown a'b' & \text{if } |p| < k-1, \end{cases}$$

   provided it is a local isomorphism. Otherwise, the play ends and player **II** loses.

Note that the weak bijective k-pebble game requires more of the second player than the bijective $(k-1)$-pebble game, because p^+ rather than just p' is required to be a local isomorphism. On the other hand, it requires less than the bijective k-pebble game: the bijective k-pebble game precisely requires the second player to choose the bijection without prior knowledge of the pair ab that will be removed from the position (cf. the alternative presentation of the bijective k-pebble game on page 37). A strategy for player **II** in the weak version is good for the usual version if it is fully symmetric or uniform w.r.t. the pebble pair that is going to be removed.

However, this is only relevant if $k \geq 3$. The weak bijective 2-pebble game and the bijective 2-pebble game are essentially the same.

Definition 5.12. $\mathcal{A}$ and $\mathcal{B}$ are $\mathsf{C}^{<k}$-equivalent, $\mathcal{A} \equiv_{\mathsf{C}}^{<k} \mathcal{B}$, if the second player has a winning strategy in the weak bijective k-pebble game on $\mathcal{A}$, $\mathcal{B}$.

Furthermore, for tuples $\mathbf{a}$ and $\mathbf{b}$ of the same length $\ell < k$ we let $\mathcal{A}, \mathbf{a} \equiv_{\mathsf{C}}^{<k} \mathcal{B}, \mathbf{b}$ if the second player has a winning strategy in the weak bijective k-pebble game on $\mathcal{A}$, $\mathcal{B}$ with initial position $\mathbf{ab}$.

Observation 5.13. *$\mathcal{A} \equiv_{\mathsf{C}}^{2} \mathcal{B} \Leftrightarrow \mathcal{A} \equiv_{\mathsf{C}}^{<2} \mathcal{B}$, and for all $k \geqslant 3$:*

$$\mathcal{A} \equiv_{\mathsf{C}}^{k} \mathcal{B} \quad \Rightarrow \quad \mathcal{A} \equiv_{\mathsf{C}}^{<k} \mathcal{B} \quad \Rightarrow \quad \mathcal{A} \equiv_{\mathsf{C}}^{k-1} \mathcal{B}.$$

Remark 5.14. *The weak bijective k-pebble game is equivalent to a bisimulation-like game with $k-1$ pebbles where in each round the first player may slide a pebble along an edge of one of the graphs and player* **II** *has to answer by sliding the corresponding pebble along an edge of the other graph. In this version, the game coresponds to the $(k-1)$-pebble sliding game introduced by Atserias and Maneva [1]. They prove that equivalence of two graphs with respect to the $(k-1)$-pebble sliding game implies that* $\mathrm{ISO}(k-1)$ *has a solution. In view of the equivalence of the sliding game with our weak bijective k-pebble game, this implies the backward direction of Theorem 5.16 below.*

Let $\wp_r$ be the set of positions of size $k-1$ of the weak bijective k-pebble game over $\mathcal{A}, \mathcal{B}$ in which the second player has a strategy to survive through r rounds. Let $\sim^r$ stand for the equivalence relation induced by $\wp_r$, i.e., the symmetric transitive closure of the relation that puts $\mathbf{a} \sim^r \mathbf{b}$ if $p = \mathbf{ab} \in \wp_r$. Note that $\sim^r$ is compatible with permutations in the sense that, for instance, $\mathbf{a} \sim^r \mathbf{b}$ iff $\pi(\mathbf{a}) \sim^r \pi(\mathbf{b})$ for any $\pi \in S_{k-1}$. We write $\pi(\mathbf{a})$ for the application of the permutation $\pi \in S_{k-1}$ to the components of $\mathbf{a} = (a_1, \dots, a_{k-1})$, which results in $\pi(\mathbf{a}) = (a_{\pi(1)}, \dots, a_{\pi(k-1)})$.

For $r = 0$, the set $\wp_0$ consists of all local isomorphisms of size $k-1$. We characterise $\wp_{r+1}$ and $\sim^{r+1}$ in terms of $\wp_r$ by means of back&forth conditions for a single round: $\mathbf{a} \sim^{r+1} \mathbf{b}$ ($p = \mathbf{ab} \in \wp_{r+1}$) iff position $\mathbf{ab}$ is good in the following sense: for $1 \leqslant j \leqslant k-1$, the second player has a response that guarantees a target position in $\wp_r$ if the first player chooses index j.

I.e., for each $1 \leqslant j \leqslant k-1$, the second player needs to have a bijection ρ_j between $[m]$ and $[n]$ such that for every $ab \in \rho_j$

$$\mathrm{atp}(\mathbf{a}a) = \mathrm{atp}(\mathbf{b}b) \quad \text{ and } \quad \mathbf{a}\tfrac{a}{j}\mathbf{b}\tfrac{b}{j} \in \wp_r.$$

The first condition says that $p\widehat{\ }ab$ is a local isomorphism, the second that the new position is good for r further rounds.

Note that, since $\mathcal{A}$ is a graph, the quantifier-free type $\mathrm{atp}(\mathbf{a}a)$ is fully determined by $\mathrm{atp}(\mathbf{a})$ and the $\mathrm{atp}(a_i a)$ for $1 \leqslant i \leqslant k-1$. The condition that $\mathrm{atp}(\mathbf{a}) = \mathrm{atp}(\mathbf{b})$ is a pre-condition for the round to be played; the condition that $\mathrm{atp}(a_i a) = \mathrm{atp}(b_i b)$ for all $i \neq j$, on the other hand, is part of the post-condition that $p \setminus a_j b_j \widehat{\ } ab$ is a local isomorphism.

Let $(\alpha_i)_{i \in I}$ be an enumeration of the $\sim^r$-classes over $\mathcal{A}$ and $\mathcal{B}$. Then the above conditions on membership of $p = \mathbf{ab}$ in $\wp_{r+1}$ are equivalent to the following:

for each $1 \leqslant j \leqslant k-1$,
for every $\sim^r$-class α, and
for every quantifier-free type $\eta(x, y)$:
$\#_a^{\mathcal{A}}\big(\mathbf{a}\tfrac{a}{j} \in \alpha \wedge \mathrm{atp}(a_j a) = \eta\big) \;=\; \#_b^{\mathcal{B}}\big(\mathbf{b}\tfrac{b}{j} \in \alpha \wedge \mathrm{atp}(b_j b) = \eta\big).$

Note, towards the claimed equivalence, that these numerical equalities allow the second player to piece together a bijection that respects the partition of $[m]$ and $[n]$ according to different combinations of α and η, which in turn guarantees that any pair ab drawn from the bijection respects this partition and hence leads to a position $\mathbf{a}\tfrac{a}{j}\mathbf{b}\tfrac{b}{j} \in \wp_r$ as required.

Conversely, if one of these equalities were violated, then any bijection will have to have at least one pair that does not respect the partition of $[m]$ and $[n]$ w.r.t. the α and η. If the first player picks such a bad pair ab, then the second player loses during this round because $\mathrm{atp}(\mathbf{a}a) \neq \mathrm{atp}(\mathbf{b}b)$, or because the resulting new position $\mathbf{a}\frac{a}{j}\mathbf{b}\frac{b}{j}$ is not in $\wp_r$.

For later use we state the condition on full $\mathsf{C}^{<k}$-equivalence, corresponding to the stable limit of the above refinement step. For $\mathbf{a} \in [m]^{k-1}$ and $\mathbf{b} \in [n]^{k-1}$, $\mathcal{A}, \mathbf{a} \equiv^{<k}_{\mathsf{C}} \mathcal{B}, \mathbf{b}$ iff

$$\begin{array}{l} \text{for each } 1 \leqslant j \leqslant k-1, \\ \text{for all } \mathsf{C}^{<k}\text{-equivalence classes } \alpha, \text{ and} \\ \text{for every quantifier-free type } \eta(x,y)\text{:} \\ \#^{\mathcal{A}}_a\big(\mathbf{a}\tfrac{a}{j} \in \alpha \wedge \mathrm{atp}(a_j a) = \eta\big) \;\;=\;\; \#^{\mathcal{B}}_b\big(\mathbf{b}\tfrac{b}{j} \in \alpha \wedge \mathrm{atp}(b_j b) = \eta\big). \end{array} \tag{10}$$

Lemma 5.15. *For $k \geqslant 3$, if $(X_p)_{|p|<k}$ is a solution to* ISO$(k-1)$ *then for all $\mathbf{a} \in [n]^{k-1}$ and $\mathbf{b} \in [n]^{k-1}$:*

$$X_{\mathbf{ab}} > 0 \quad \Longrightarrow \quad \mathcal{A}, \mathbf{a} \equiv^{<k}_{\mathsf{C}} \mathcal{B}, \mathbf{b}.$$

Proof. By Corollary 5.11 we may assume that the given solution $X = (X_p)_{|p|<k}$ itself is good in the sense of Definition 5.7. It follows form CONT(1) that $\mathcal{A}$ and $\mathcal{B}$ have the same size, and we let $[n]$ be their vertex set. By COMP(2), X is supported by local isomorphisms, cf. Lemma 5.3. That the solution is good means that its lifting to tuple co-ordinates $\check{X}$, where $\check{X}_{\mathbf{a},\mathbf{b}} = X_p$ for $p = \{(a_i, b_i) : i < k\}$, induces $\check{X}$-related partitions of the vertex set of $\mathbb{I}^{(i)}(n, k-1)$ of the form

$$[n]^{k-1} = \dot{\bigcup}_s D_s \;\text{ and }\; [n]^{k-1} = \dot{\bigcup}_s D'_s$$

such that

(i) each partition is stable w.r.t. $\mathbb{I}^{(i)}$ for $i < k$;

(ii) $[n]^{k-1} = \dot{\bigcup}_s D_s$ is stable w.r.t. $A^{(i)}$ and $[n]^{k-1} = \dot{\bigcup}_s D'_s$ is stable w.r.t. $B^{(i)}$, for each $i < k$;

(iii) $\check{X}_{D_s D'_s} > 0$ so that $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism whenever $\mathbf{a}$ and $\mathbf{b}$ are from matching partition sets;

(iv) $\check{X}_{D_s D'_t} = 0$ for all $t \neq s$.

It suffices to exhibit a strategy for **II** that maintains the condition $X_p > 0$, or equivalently $\check{X}_{\mathbf{a},\mathbf{b}} > 0$. The argument is completely analogous to that in Lemma 4.8, for good solutions in the context of basic 1-dimensional fractional isomorphism. Consider tuples $\mathbf{a}$ and $\mathbf{b}$ of length $k-1$ such that $\check{X}_{\mathbf{a},\mathbf{b}} > 0$. It suffices to show that, for each $j < k$, **II** can choose a bijection ρ_j of $[n]$ (for a round played in component j) such that $a_j b_j \in \rho_j$ and for all pairs $ab \in \rho_j$

$$A_{a_j a} = 1 \;\Leftrightarrow\; B_{b_j b} = 1 \quad \text{ and } \quad \check{X}_{\mathbf{a}\frac{a}{j}, \mathbf{b}\frac{b}{j}} > 0.$$

The second condition precisely requires $\mathbf{a}\frac{a}{j}$ and $\mathbf{b}\frac{b}{j}$ to be from matching partition sets while the first condition is equivalent to

$$A^{(j)}_{\mathbf{a},\mathbf{a}\frac{a}{j}} = 1 \;\Leftrightarrow\; B^{(j)}_{\mathbf{b},\mathbf{b}\frac{b}{j}} = 1.$$

The existence of the desired bijection therefore follows directly from the properties of X as a good solution, which implies that the $\check{X}$-related partitions are equivalent stable partitions w.r.t. $A^{(j)}$ and $B^{(j)}$. Thus, for every partition index t,

$$\begin{aligned}\#_a(\mathbf{a}\tfrac{a}{j} \in D_t \wedge A_{a_j a} = 1) &= \#_{\mathbf{a}'}(\mathbf{a}' \in D_t \wedge A^{(j)}_{\mathbf{a},\mathbf{a}'} = 1) \\ &= \#_{\mathbf{b}'}(\mathbf{b}' \in D_t \wedge B^{(j)}_{\mathbf{b},\mathbf{b}'} = 1) = \#_b(\mathbf{b}\tfrac{b}{j} \in D_t \wedge B_{b_j b} = 1)\end{aligned}$$

so that the desired bijection can be pieced together from corresponding bijections between D_t and D'_t. □

The following should be contrasted with Theorem 5.9, which characterises C^k-equivalence in terms of $\mathrm{ISO}(k-1/2)$. That the half-step discrepancies constitute a proper gap in shown in Section 5.2 below.

Theorem 5.16. $\mathrm{ISO}(k-1)$ *has a solution if, and only if,* $\mathcal{A} \equiv^{<k}_{\mathsf{C}} \mathcal{B}$*.*

Proof. The last lemma settles one implication. For the converse implication, it remains to argue that $\mathsf{C}^{<k}$-equivalence suffices in place of C^k-equivalence to provide a solution to the Sherali–Adams relaxation of level $k-1$. We now let $\mathrm{tp}(\mathbf{a})$ stand for the $\mathsf{C}^{<k}$-type, or the $\mathsf{C}^{<k}$-equivalence class of the tuple $\mathbf{a}$. We may look at just tuples of length $k-1$, by trivial padding through repetition of the last component say. Put

$$\begin{aligned}&X_\emptyset := 1 \\ &X_p := \delta(\mathrm{tp}(\mathbf{a}), \mathrm{tp}(\mathbf{b})) \;/\; \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \\ &\qquad\qquad \text{for } p = \mathbf{ab},\ 0 < |p| \leqslant k-1.\end{aligned} \tag{11}$$

We know that $\mathsf{C}^{<k}$-equivalence refines C^{k-1}-equivalence, and that an assignment to X_p according to C^{k-1}-types of $(k-1)$-tuples was shown above to satisfy the continuity equations $\textsc{Cont}(\ell)$ of levels $\ell < k$, cf. Lemma 5.1. The same argument applies here to show that the refinement used here satisfies these equations.

For satisfaction of equations $\textsc{Comp}(\ell)$ of level $\ell < k$, however, we need to appeal to something less than the extension property that boosts $\mathbf{a}$ and $\mathbf{b}$ to k-tuples $\mathbf{a}a\hat{a}$ and $\mathbf{b}\hat{b}b$ of the same C^k-type, as we used in connection with (8) above.

Here as there, however, we only need to look at $p = \mathbf{ab}$ of size (up to) $k-2$ for which $\mathcal{A}, \mathbf{a} \equiv^{<k}_{\mathsf{C}} \mathcal{B}, \mathbf{b}$, because all other instances of the equation are trivially true with 0 on both sides. We fix such p.

Now, for any combination of $\mathsf{C}^{<k}$-types α and β of $(k-1)$-tuples and quantifier-free type η of a pair,

$$\begin{aligned}&\#^{\mathcal{A}}_{aa'}\big(\mathrm{tp}(\mathbf{a}a) = \alpha \wedge \mathrm{tp}(\mathbf{a}a') = \beta \wedge \mathrm{atp}(aa') = \eta\big) \\ = \;&\#^{\mathcal{B}}_{bb'}\big(\mathrm{tp}(\mathbf{b}b) = \alpha \wedge \mathrm{tp}(\mathbf{b}b') = \beta \wedge \mathrm{atp}(bb') = \eta\big).\end{aligned} \tag{12}$$

This follows from an analysis of the $\mathsf{C}^{<k}$-game from position $p = \mathbf{ab}$ through two rounds, in which the first player first gets the last pebble placed on any one of the possible choices for a, with responses b as provided by the second

player's bijection (in exactly the same number); then the first player plays on that last component again, and replaces it with any one of the choices he may have for a' and its match b' according to the second player's bijection (again, the same number of positive choices).

For given a and b, let now $\alpha := \mathrm{tp}(\mathbf{a}a)$ and $\beta := \mathrm{tp}(\mathbf{b}b)$. Then

$$\begin{aligned}
& \textstyle\sum_{a'} A_{aa'} X_{p^\frown a'b} \\
= \;& \textstyle\sum_{a'} A_{aa'}\, \delta(\mathrm{tp}(\mathbf{a}a'), \mathrm{tp}(\mathbf{b}b)) \;/\; \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}(\mathbf{b}b)) \\
= \;& \frac{\#^{\mathcal{A}}_{a'}\big(\mathrm{tp}(\mathbf{a}a') = \beta \wedge \mathrm{edge}(aa')\big)}{\#_{\mathbf{x}a'}(\mathrm{tp}(\mathbf{x}a') = \beta)} \\
= \;& \frac{\#^{\mathcal{A}}_{aa'}\big(\mathrm{tp}(\mathbf{a}a) = \alpha \wedge \mathrm{tp}(\mathbf{a}a') = \beta \wedge \mathrm{edge}(aa')\big)}{\#_{\mathbf{x}a'}(\mathrm{tp}(\mathbf{x}a') = \beta) \cdot \#_{a}(\mathrm{tp}(\mathbf{a}a) = \alpha)} \\
= \;& \frac{\#^{\mathcal{A}}_{aa'}\big(\mathrm{tp}(\mathbf{a}a) = \alpha \wedge \mathrm{tp}(\mathbf{a}a') = \beta \wedge \mathrm{edge}(aa')\big)}{\#_{a'}(\mathrm{tp}(\mathbf{a}a') = \beta) \cdot \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \cdot \#_{a}(\mathrm{tp}(\mathbf{a}a) = \alpha)}.
\end{aligned}$$

We transform this term further, using (12), a renaming of dummy variables in counting terms and the symmetry of the unique quantifier-free type η determined by $\mathrm{edge}(xy)$ in simple undirected graphs. The goal is to show equality with the corresponding term obtained for $\sum_{b'} X_{p^\frown ab'} B_{b'b}$. Equality (12) is used in the first step of these transformations, starting from the term just obtained:

$$\begin{aligned}
& \frac{\#^{\mathcal{A}}_{aa'}\big(\mathrm{tp}(\mathbf{a}a) = \alpha \wedge \mathrm{tp}(\mathbf{a}a') = \beta \wedge \mathrm{edge}(aa')\big)}{\#_{a'}(\mathrm{tp}(\mathbf{a}a') = \beta) \cdot \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{a})) \cdot \#_{a}(\mathrm{tp}(\mathbf{a}a) = \alpha)} \\
= \;& \frac{\#^{\mathcal{B}}_{bb'}\big(\mathrm{tp}(\mathbf{b}b) = \alpha \wedge \mathrm{tp}(\mathbf{b}b') = \beta \wedge \mathrm{edge}(bb')\big)}{\#_{b'}(\mathrm{tp}(\mathbf{b}b') = \beta) \cdot \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b})) \cdot \#_{b}(\mathrm{tp}(\mathbf{b}b) = \alpha)} \\
= \;& \frac{\#^{\mathcal{B}}_{bb'}\big(\mathrm{tp}(\mathbf{b}b') = \alpha \wedge \mathrm{tp}(\mathbf{b}b) = \beta \wedge \mathrm{edge}(bb')\big)}{\#_{b}(\mathrm{tp}(\mathbf{b}b) = \beta) \cdot \#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b})) \cdot \#_{b'}(\mathrm{tp}(\mathbf{b}b') = \alpha)} \\
= \;& \frac{\#^{\mathcal{B}}_{b'}\big(\mathrm{tp}(\mathbf{b}b') = \alpha \wedge \mathrm{edge}(bb')\big)}{\#_{\mathbf{x}}(\mathrm{tp}(\mathbf{x}) = \mathrm{tp}(\mathbf{b})) \cdot \#_{b'}(\mathrm{tp}(\mathbf{b}b') = \alpha)} \\
= \;& \textstyle\sum_{b'} B_{b'b}\, \delta(\mathrm{tp}^{<k}(\mathbf{b}b'), \mathrm{tp}^{<k}(\mathbf{a}a)) \;/\; \#_{\mathbf{x}x}(\mathrm{tp}(\mathbf{x}x) = \mathrm{tp}^{<k}(\mathbf{a}a)) \\
= \;& \textstyle\sum_{b'} X_{p^\frown ab'} B_{b'b}.
\end{aligned}$$

□

5.2 The gap

The following theorem shows that for every $k \geq 3$ the level of equivalence captured by the Sherali–Adams relaxation of fractional graph isomorphism of level $k-1$, i.e., $\equiv^{<k}_{\mathsf{C}}$, is strictly between C^{k-1}-equivalence and C^{k}-equivalence.

Theorem 5.17. *Let $k \geq 3$.*

1. *There are graphs $\mathcal{A}$ and $\mathcal{B}$ such that $\mathcal{A} \equiv_{\mathsf{C}}^{k-1} \mathcal{B}$ but $\mathcal{A} \not\equiv_{\mathsf{C}}^{<k} \mathcal{B}$.*

2. *There are graphs $\mathcal{A}$ and $\mathcal{B}$ such that $\mathcal{A} \equiv_{\mathsf{C}}^{<k} \mathcal{B}$ but $\mathcal{A} \not\equiv_{\mathsf{C}}^{k} \mathcal{B}$.*

We will use the bijective pebble game and weak bijective pebble game to prove the assertions of the lemma. To be able to deal with the two games more uniformly, we slightly change the presentation of the bijective k-pebble game in the following way. We now regard as positions sets of pairs of elements from $\mathcal{A}, \mathcal{B}$ of size $|p| \leq k-1$ (instead of size k in the original version). A single round of the game, starting in position p, is played as follows.

1. Player **II** selects a bijection f between the $\mathcal{A}$ and $\mathcal{B}$.

2. If $|p| = k-1$, player **I** selects a pair ab from the current position p to be removed.

3. Player **I** chooses a pair $a'b'$ from the bijection f to be added.

4. If $p^+ := p^\frown a'b'$ is a local isomorphism then the new position is

$$p' := \begin{cases} (p \backslash ab)^\frown a'b' & \text{if } |p| = k-1, \\ p^\frown a'b' & \text{if } |p| < k-1. \end{cases}$$

   Otherwise, the play ends and player **II** loses.

Player **II** wins a play if it lasts forever.

It is easy to see that this new version of the bijective k-pebble game is equivalent to the original version introduced on page 5 (also see page 32), in the sense that for all positions p of size at most $k-1$, player **I** (and also player **II**) has a winning strategy for the new game starting in position p if and only he has a winning strategy for the original game starting in position p. Essentially, we have just shifted the game by "half a round": instead of starting in a position p of size k, removing a pair from p to obtain an intermediate position p^- of size $k-1$, then choosing a bijection, then adding a pair to return to a position of size k and check if this position is a local isomorphism, in the new version we start in a position p of size $k-1$, choose a bijection, add a pair to p to obtain an intermediate position p^+ of size k, check if this is a local isomorphism, and then remove a pair to return to a position of size $k-1$. When we say "bijective k-pebble game" in the following, we always refer to the new version of the game.

This new way of looking at the k-pebble game highlights the difference between the game and its weak version: in the weak bijective k-pebble game, the first two steps are swapped, that is, player **I** first picks a pair ab and then player **II** selects a bijection. This is the only difference between the two games.

The proof of Theorem 5.17 is based on a well-known construction due to Cai, Fürer, and Immerman [6]. It will be convenient to discribe the construction for *multigraphs*, that is, graph that may have several "parallel" edges between the same pair of vertices. We denote the vertex set of a multigraph $\mathcal{G}$ by $V(\mathcal{G})$

and the edge set by $E(\mathcal{G})$. When we write $e = vw$, this merely indicates that e is an edge incident with v and w; there may be other edges linking this pair of vertices. For every vertex $v \in V(\mathcal{G})$, by $E(v)$ we denote the set of all edges incident with v. For every multigraph $\mathcal{G}$ with vertex set $V(\mathcal{G}) = \{v_1, \ldots, v_n\}$, we construct two structures $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$, which we call the *CFI-companions* of $\mathcal{G}$, as follows.[5] Both $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$ are coloured graphs whose vertices are coloured with $n + |E(G)|$ distinct colours C_v for $v \in V(\mathcal{G})$ and C_e for $e \in E(\mathcal{G})$. It will be convenient to call the vertices of the graphs $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$ *nodes*, to distinguish them from the *vertices* of $\mathcal{G}$.

For every $v \in V(\mathcal{G})$, the graph $\mathcal{X}(\mathcal{G})$ has nodes v^S, where S is a subset of $E(v)$ of even cardinality. For every edge e of $\mathcal{G}$, the graph $\mathcal{X}(\mathcal{G})$ has nodes e^0, e^1. The node set of $\widehat{\mathcal{X}}(\mathcal{G})$ is the same, except that for the vertex v_1 we take nodes v_i^S for the subsets of $E(v_1)$ of odd cardinality.

Nodes of the form v^S are called *vertex nodes* and nodes e^i *edge nodes*.

— The set of nodes $\mathcal{X}(\mathcal{G})$ is

$$\begin{aligned} &\{v_i^S \mid i \in [n], S \subseteq E(v_i) \text{ such that } |S| \equiv 0 \bmod 2\} \\ \cup\, &\{e^0, e^1 \mid e \in E(\mathcal{G})\} \end{aligned}$$

— The node set of $\widehat{\mathcal{X}}(\mathcal{G})$ is

$$\begin{aligned} &\{v_1^S \mid S \subseteq E(v_1) \text{ such that } |S| \equiv 1 \bmod 2\} \\ \cup\, &\{v_i^S \mid i \in [n] \setminus \{1\}, S \subseteq E(v_i) \text{ such that } |S| \equiv 0 \bmod 2\} \\ \cup\, &\{e^0, e^1 \mid e \in E(\mathcal{G})\} \end{aligned}$$

— The edges of both $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$ link vertex nodes v^S to edge nodes e^i for edges $e \in E(v)$ according to

$$\{v^S, e^i\} \text{ is an edge if } \begin{cases} i = 1 \text{ and } e \in S \\ i = 0 \text{ and } e \notin S \end{cases}$$

— In both $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$, the nodes of the form v^S are coloured C_v, and the nodes of the form e^i are coloured C_e.

Local isomorphisms between the coloured graphs $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$ are required to preserve the colours. Thus in the bijective k-pebble game or the weak bijective k-pebble game on $\mathcal{X}(\mathcal{G})$ and $\widehat{\mathcal{X}}(\mathcal{G})$, player **II** has to preserve colours and is thus forced to make sure that a node v^S is always mapped to a node $v^{S'}$ for some S' and that a node e^i is always mapped to a node $e^{i'}$.[6]

Let g be a local bijection or bijection from $\mathcal{X}(\mathcal{G})$ to $\widehat{\mathcal{X}}(\mathcal{G})$. We say that g is *colour-preserving* if for all vertices v of $\mathcal{G}$ and all S we have $g(v^S) = v^T$ for

[5]The graph $\widehat{\mathcal{X}}(\mathcal{G})$ will not only depend on $\mathcal{G}$, but also on the enumeration of its vertices, or rather, just on the choice of a *first vertex.* We choose not to highlight this dependence notationally.

[6]Colours can be eliminated by attaching gadgets encoding the colours (such as paths of different lengths) to the nodes.

some T, and for all edges e of $\mathcal{G}$ and all i we have $g(e^i) = e^j$ for some j. In the following, suppose that g is colour-preserving. Slightly abusing terminology, we say that a vertex v of $\mathcal{G}$ is in the domain of g if v^S is in the domain of g for some S. Similarly, we say that an edge e of $\mathcal{G}$ is in the domain of G if e^i is in the domain of g for some i.

We say that g is *vertex-consistent* if for all vertices v of $\mathcal{G}$ and all S, S', T, T' such that both v^S and $v^{S'}$ are in the domain of g and $g(v^S) = v^T$, $g(v^{S'}) = v^{T'}$ we have $S \triangle T = S' \triangle T'$. If g is vertex-consistent, then for all v in the domain of g we let $g_v := S \triangle T$ for some (and hence all) S, T such that v^S is in the domain of g and $g(v^S) = v^T$. Note that g_v determines $g(v^S)$ for all S, and that a position which fails to be vertex consistent would allow player **I** to win in one round played with the help of any pebble pair to spare.

Note that g, being a colour-preserving (local) bijection, is automatically *edge-consistent* in the sense that for all edges e of $\mathcal{G}$, if $g(e^i) = e^j$ and $g(e^{i'}) = e^{j'}$ then $i + j \equiv i' + j' \bmod 2$. In other words, $i = j$ iff $i' = j'$. This is clearly necessary for a colour-preserving bijection, which must map the colour $C_e = \{e^0, e^1\}$ in $\mathcal{X}(\mathcal{G})$ to colour $C_e = \{e^0, e^1\}$ in $\widehat{\mathcal{X}}(\mathcal{G})$. We let $g_e \in \{0, 1\}$ such that $g_e \equiv i + j \bmod 2$ for some (and hence for all) i, j with $g(e^i) = e^j$. If $g_e = 1$, then we say that g *flips* edge e.

We say that a (local) bijection g is *weakly consistent* if it is colour-preserving (and thus edge consistent), vertex-consistent, and for all vertices v and edges e in the domain of g we have $e \in g_v \Leftrightarrow g_e = 1$. Note that if g is weakly consistent then it is a (local) isomorphism.

We say that g is *strongly consistent* if it is weakly consistent and, in addition, for all edges $e = vw$ of $\mathcal{G}$, if both v and w are in the domain of g then $e \in g_v \Leftrightarrow e \in g_w$.

We say that a bijection h *consistently extends* g, or is a *consistent extension* of g, if it satisfies the following conditions (A)–(D).

(A) h is colour-preserving and vertex-consistent.

(B) h is an extension of g.

Note that if h satisfies (A) and (B), then g must be colour preserving and node consistent. Conversely, if g is colour preserving and node consistent, then condition (B) is equivalent to the condition that for all vertices v and edges e of $\mathcal{G}$ in the domain of g we have $g_v = h_v$ and $g_e = h_e$.

(C) For all vertices v of $\mathcal{G}$, if some edge e incident with v is in the domain of g, then $e \in h_v \Leftrightarrow g_e = 1$.

(D) For all edges e of $\mathcal{G}$, if some vertex v incident with e is in the domain of g, then $h_e = 1 \Leftrightarrow e \in g_v$.

Note that for g to have a consistent extension, it must be strongly consistent. However, even if g is strongly consistent it does not necessarily have a consistent extension, because g is only a local bijection, whereas h is a total bijection.

Note that player **I** can directly win the game from any position that fails to be strongly consistent, or whenever **II** proposes a bijection that fails to be a consistent extension of the current position. We may therefore, without loss of generality, restrict **II** to strongly consistent positions and consistent extensions.

Proof of Theorem 5.17 (1). Let $\mathcal{K}$ be the complete graph on k vertices. We fix some enumeration $v_1, \ldots, v_k$ of the vertex set of $\mathcal{K}$. For all $i \neq j$, we let e_{ij} be the edge between v_i and v_j.

We let $\mathcal{A} = \mathcal{X}(\mathcal{K})$ and $\mathcal{B} = \widehat{\mathcal{X}}(\mathcal{K})$ and show that $\mathcal{X}(\mathcal{K}) \equiv_{\mathsf{C}}^{k-1} \widehat{\mathcal{X}}(\mathcal{K})$, but $\mathcal{X}(\mathcal{K}) \not\equiv_{\mathsf{C}}^{<k} \widehat{\mathcal{X}}(\mathcal{K})$.

To prove that $\mathcal{X}(\mathcal{K}) \not\equiv_{\mathsf{C}}^{<k} \widehat{\mathcal{X}}(\mathcal{K})$, we give a winning strategy for player **I** in the weak bijective k-pebble game on $\mathcal{X}(\mathcal{K}), \widehat{\mathcal{X}}(\mathcal{K})$. In the first $k-1$ rounds of the game, player **I** can reach a position p with domain $v_2^{\emptyset}, \ldots, v_k^{\emptyset}$ and $p(v_i^{\emptyset}) = v_i^{S_i}$ for some sets S_i. That is,

$$p = \{v_2^{\emptyset} v_2^{S_2}, \ldots, v_k^{\emptyset} v_k^{S_k}\}.$$

Note that $p_{v_i} = \emptyset \triangle S_i = S_i$ for $2 \leq i \leq k$. For all i and all edges e of $\mathcal{K}$ we let $\varepsilon(i, e) = 1$ if $e \in S_i$ and $\varepsilon(i, e) = 0$ otherwise. In particular, $\varepsilon(i, e) = 0$ if v_i is not incident with the edge e. Without loss of generality, p is strongly consistent, and thus for $2 \leq i < j \leq k$ we have $\varepsilon(i, e_{ij}) = \varepsilon(j, e_{ij})$. Moreover, by the construction of $\widehat{\mathcal{X}}(\mathcal{K}_{k+1})$, all the sets S_i have even cardinality. Thus

$$0 \equiv \sum_{i=2}^{k} |S_i| \equiv \sum_{i=2}^{k} \sum_{e} \varepsilon(i, e) \equiv \sum_{i=2}^{k} \varepsilon(i, e_{1i}) \bmod 2.$$

Let T be the set of all edges e_{1i} with $e_{1i} \in S_i$. Then $|T|$ is even. To simplify the notation, we let $\varepsilon_i = \varepsilon(i, e_{1i})$ in the following.

In the next round of the game, player **I** starts by selecting the pair $v_2^{\emptyset} v_2^{S_2}$. Let f be the bijection selected by player **II**. Without loss of generality, f is a consistent extension of p. Thus by (D), f flips edge e_{12} if and only if $e_{12} \in p_{v_2} = S_2$. That is, $f(e_{12}^0) = e_{12}^{\varepsilon_2}$. Player **I** selects the pair $e_{12}^0 e_{12}^{\varepsilon_2}$, and the new position is

$$p' = \{e_{12}^0 e_{12}^{\varepsilon_2}, v_3^{\emptyset} v_3^{S_3}, \ldots, v_k^{\emptyset} v_k^{S_k}\}.$$

Note that $p'_{e_{12}} = \varepsilon_2$ In the next round of the game, player **I** starts by selecting the pair $e_{12}^0 e_{12}^{\varepsilon_2}$. Let f' be the bijection selected by player **II**. Without loss of generality, f' is a consistent extension of p'. Let $T' \subseteq E(v_1)$ such that $f'(v_1^{\emptyset}) = v_1^{T'}$ and $f'_{v_1} = T'$. By (C),

$$e_{12} \in f'_{v_1} = T' \Leftrightarrow \varepsilon_2 = 1 \Leftrightarrow e_{12} \in T. \tag{13}$$

Player **I** selects the pair $v_1^{\emptyset} v_1^{T'}$, and the new position is

$$p'' = \{v_1^{\emptyset} v_1^{T'}, v_3^{\emptyset} v_3^{S_3}, \ldots, v_k^{\emptyset} v_k^{S_k}\}.$$

Now **I** wins as p'' is not strongly consistent, which can be shown indirectly as follows. Suppose for contradiction that p'' were strongly consistent. Then, for $3 \leq i \leq k$, we would have $e_{1i} \in T' \Leftrightarrow e_{1i} \in S_i \Leftrightarrow e_{1i} \in T$. Combined with (13), this implies $T' = T$. However, $|T'|$ is odd by the construction of $\widehat{\mathcal{X}}(\mathcal{K})$, whereas $|T|$ is even.

To prove that $\mathcal{X}(\mathcal{K}) \equiv_{\mathsf{C}}^{k-1} \widehat{\mathcal{X}}(\mathcal{K})$, we give a winning strategy for player **II** in the variant of the bijective $(k-1)$-pebble game on $\mathcal{X}(\mathcal{K}), \widehat{\mathcal{X}}(\mathcal{K})$. It suffices to show that in every strongly consistent position of the game, **II** can maintain strong consistency. So let p be a strongly consistent position of size $|p| \leq k-2$. To define a consistent extension f of p, it suffices to specify f_v for all vertices v and f_e for all edges e of $\mathcal{K}$.

1. We start by letting $f_v = p_v$ for all vertices v in the domain of p and $f_e = p_e$ for all edges e in the domain of p.

2. For all edges e of $\mathcal{K}$ that are incident with at least one vertex v in the domain of p, we let $f_e = 1$ if $e \in p_v$ and $f_e = 0$ otherwise. We can do this consistently because p is strongly consistent.

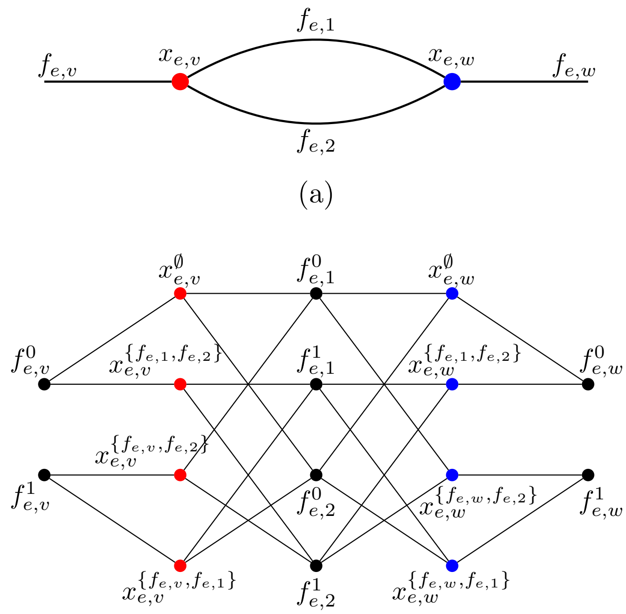
3. For all remaining vertices v of $\mathcal{K}$, we note that there is at least one edge $e = vw$ incident with v such that neither w nor e are in the domain of p (and hence f_e has not been defined yet). We choose a subset $S \subseteq E(v)$ such that for all edges $e' = vw' \in E(v)$ such that either e' or w' is in the domain of p we have $e' \in S \Leftrightarrow f_{e'} = 1$. Moreover, we choose such an S such that its cardinality is odd if $v = v_1$ and its cardinality is even otherwise. We have the freedom to choose the parity in this manner because we can add e to S without affecting the property $e' \in S \Leftrightarrow f_{e'} = 1$ for all edges $e' = vw' \in E(v)$ such that either e' or w' is in the domain of p.

   We let $f_v = S$.

4. Finally, for all edges e for which f_e has not yet been defined we let $f_e = 0$.

In the next round of the game, **II** selects f. Suppose that **I** selects $ab \in p$ to be removed and $a'b' \in f$ to be added. It is easy to prove that $p^+ = p^\frown a'b'$ is a local isomorphism and that the new position $p' = (p \setminus ab)^\frown a'b'$ is strongly consistent. The proof is by case distinction along the cases of the definition of the bijection f. It may seem that edges e for which f_e is defined in (iv) will cause problems, because for these edges the definition of f_e does not depend on the current position p at all. However, in the new position p' and even in the intermediate position p^+ such edges will not be incident with any vertex in the domain, so they will not affect strong consistency. $\square$

The proof of Theorem 5.17 (2) requires more preparation. Essentially, we will also play games on the CFI-companions of the complete graph $\mathcal{K}$, but we will insert certain "threshold gadgets" on the edges that require at least two pebbles to transport the information of whether an edge is flipped or not from one end of the edge to the other. The gadget is displayed in Figure 1(b); the name $\mathcal{T}_e$ of the gadget and the names of the vertices indicate that the gadget is intended to be inserted for an edge $e = vw$. Observe that the gadget is a CFI-companion of the multigraph, or rather: fragment of a multigraph, displayed in Figure 1(a). As for all CFI-companions, the nodes $x_{e,v}^S$ are coloured by a fresh colour, and so are the nodes $x_{e,w}^S$ as well as the edge-nodes $f_{e,v}^i$, $f_{e,1,}^i$, $f_{e,2}^i$,



(a)

(b)

Figure 1: Threshold gadget $\mathcal{T}_e$

$f^i_{e,w}$. The idea is to replace each edge $e = vw$ of some graph by the multigraph from Figure 1(a) by connecting $f_{e,v}$ to v and $f_{e,w}$ to w and then go to the CFI-companion of the new graph. The crucial property of the gadget is that player **I** needs two pairs of pebbles to transport information from one end of the gadget to the other end. To make this precise, we introduce this terminology: in the (weak) bijective k-pebble game on structures $\mathcal{A}$ and $\mathcal{B}$, we say that player **I** can *reach* position p' from position p if he has a strategy for the game starting in position p such that in each play that he plays according to this strategy, either he wins or a position $p'' \supseteq p'$ occurs. If **I** cannot reach position p' from position p, we say that **II** can *avoid* position p'. As usual, a position p of the game is a *winning position* for player **I** or **II** if the respective player has a winning strategy for the game starting in that position.

Lemma 5.18. *1. For the weak bijective* 3*-pebble game on* $\mathcal{T}_e, \mathcal{T}_e$*: any position* $\{f^i_{e,v}f^j_{e,v}, f^{i'}_{e,w}f^{j'}_{e,w}\}$ *such that* $i+j \not\equiv i'+j' \bmod 2$ *is a winning position for player* **I***.*

2. For the bijective 2*-pebble game on* $\mathcal{T}_e, \mathcal{T}_e$*: let* $i, j \in \{0,1\}$ *and let* $p = \{ab\}$ *be a vertex-consistent position such that* $x_{e,v}$ *and* $f_{e,v}$ *are not in the domain of* p *(that is,* a, b *are either of the form* $f^i_{e,w}$ *or* $x^S_{e,w}$ *or* $f^i_{e,j}$*); then player* **II** *can avoid position* $\{f^i_{e,v}f^j_{e,v}\}$ *from position* p*.*

Note that assertion (1) implies that **I** can reach position $\{f^i_{e,w}f^j_{e,w}\}$ from position $\{f^i_{e,v}f^j_{e,v}\}$ in the weak bijective 3-pebble game on $\mathcal{T}_e, \mathcal{T}_e$. This is because, if **I** selects $f^i_{e,w}$ in the first round of the game starting in position $\{f^i_{e,v}f^j_{e,v}\}$, then **II** has to answer with $f^j_{e,w}$; otherwise the position is $\{f^i_{e,v}f^j_{e,v}, f^i_{e,w}f^{j'}_{e,w}\}$ such that $i + j \not\equiv i + j' \bmod 2$, and **II** loses by (1).

Proof of Lemma 5.18. To prove (1), we give a winning strategy for **I** for the game starting in position $p = \{f^i_{e,v}f^j_{e,v}, f^{i'}_{e,w}f^{j'}_{e,w}\}$. In the first round, **I** first selects the pair $f^i_{e,v}f^j_{e,v}$. Suppose that **II** answers by selecting the bijection g. Without loss of generality we may assume that g is a consistent extension of p. Let $T \subseteq E(x_{e,v}) = \{f_{e,v}, f_{e,1}, f_{e,2}\}$ such that $g(x^{\emptyset}_{e,v}) = x^T_{e,v}$. Then $f_{e,v} \in T \Leftrightarrow i + j \equiv 1 \bmod 2$, because g is a consistent extension of p. Player **I** selects the pair $x^{\emptyset}_{e,v}x^T_{e,v}$, and the new position is

$$p' = \{x^{\emptyset}_{e,v}x^T_{e,v}, f^{i'}_{e,w}f^{j'}_{e,w}\}.$$

In the next round, **I** selects the pair $f^{i'}_{e,w}f^{j'}_{e,w}$ in the first step. Suppose that **II** answers by selecting the bijection g'. Let $T' \subseteq E(x_{e,w})$ be such that $g(x^{\emptyset}_{e,w}) = x^{T'}_{e,w}$. Then $f_{e,w} \in T' \Leftrightarrow i' + j' \equiv 1 \bmod 2$, because g' is a consistent extension of p. Player **I** selects the pair $x^{\emptyset}_{e,w}x^{T'}_{e,w}$, and the new position is

$$p' = \{x^{\emptyset}_{e,v}x^T_{e,v}, x^{\emptyset}_{e,w}x^{T'}_{e,w}\}.$$

Recall that $i + j \not\equiv i' + j' \bmod 2$. By symmetry, we may assume that $i + j \equiv 0 \bmod 2$ and $i' + j' \equiv 1 \bmod 2$. Then $f_{e,v} \notin T$, and as T is even, it follows that either $T = \emptyset$ or $T = \{f_{e,1}, f_{e,2}\}$. Similarly, either $T' = \{f_{e,w}, f_{e,1}\}$ or $T' = \{f_{e,w}, f_{e,2}\}$. Thus there is a $j \in \{1, 2\}$ such that $f_{e,j} \in T \triangle T'$. Hence the position p' is not strongly consistent, and therefore Player **I** wins the game.

To prove (2), we give a strategy for **II** that avoids position $\{f^i_{e,v}f^j_{e,v}\}$ from position p in the bijective 2-pebble game on $\mathcal{T}_e, \mathcal{T}_e$. A position p' is *good* if it is vertex-consistent and satisfies the following two conditions.

(E) If $x_{e,v}$ is in the domain of p', then $f_{e,v} \in p_{x_{e,v}} \Leftrightarrow i + j \equiv 0 \bmod 2$.

(F) If $f_{e,v}$ is in the domain of p', then $p_{f_{e,v}} \not\equiv i + j \bmod 2$.

Recall that positions in the 2-pebble game have size 1 and thus are strongly consistent if and only if they are vertex-consistent. Note that the initial position p is good. It is easy to prove (by an extensive case analysis) that in any good position, **II** can play the next round of the game in such a way that the position after the round is good again. □

Proof of Theorem 5.17 (2). Let $\mathcal{H}$ be the multigraph obtained from the complete k-vertex graph $\mathcal{K}$ by replacing every edge $e = vw$ by the multigraph displayed in Figure 1(a), where edge $f_{e,v}$ is connected to v and edge $f_{e,w}$ is connected to w. Note that

$$V(\mathcal{H}) = V(\mathcal{K}) \cup \{x_{e,v}, x_{e,w} \mid e = vw \in E(\mathcal{K})\},$$
$$E(\mathcal{H}) = \{f_{e,v}, f_{e,w}, f_{e,1}, f_{e,2} \mid e = vw \in E(\mathcal{K})\}.$$

To define $\widehat{\mathcal{X}}(\mathcal{H})$, we fix some enumeration of $V(\mathcal{H})$ where the vertex $v_1 \in V(\mathcal{K})$ comes first. (Again we assume that $V(\mathcal{K}) = \{v_1, \dots, v_k\}$.)

We let $\mathcal{A} = \mathcal{X}(\mathcal{H})$ and $\mathcal{B} = \widehat{\mathcal{X}}(\mathcal{H})$. Note that $\mathcal{A}$ is obtained from $\mathcal{X}(\mathcal{K})$ by replacing, for every edge $e \in E(\mathcal{K})$, the vertices e^0, e^1 by a threshold gadget $\mathcal{T}_e$, and $\mathcal{B}$ is similarly obtained from $\widehat{X}(\mathcal{K})$.

We first prove that player **I** has a winning strategy for the bijective k-pebble game on $\mathcal{A}, \mathcal{B}$.

Let us call an edge $e = vw \in E(\mathcal{K})$ *inconsistent* in a position p of the game if both v and w are in the domain of p and $f_{e,v} \in p_v \not\Leftrightarrow f_{e,w} \in p_w$. Note that if some edge e is inconsistent in a position p then **I** can reach position $\{f^0_{e,v}f^1_{e,v}, f^0_{e,w}f^0_{e,w}\}$ (if $f_{e,v} \in p_v$ and $f_{e,w} \notin p_w$) or position $\{f^0_{e,v}f^0_{e,v}, f^0_{e,w}f^1_{e,w}\}$ (if $f_{e,v} \notin p_v$ and $f_{e,w} \in p_w$). Then by Lemma 5.18 (1), **I** wins the game. Thus player **II** needs to avoid inconsistent edges.

The winning strategy for player **I** in the bijective k-pebble game on $\mathcal{A}, \mathcal{B}$ is as follows. In the first $k-1$ rounds of the game he reaches a position p with domain $v^\emptyset_2, \dots, v^\emptyset_k$ and $p(v^\emptyset_i) = v^{S_i}_i$ for some sets S_i. That is,

$$p = \{v^\emptyset_2 v^{S_2}_2, \dots, v^\emptyset_k v^{S_k}_k\}.$$

For all $i \geq 2$ and all edges $e = v_i w \in E(\mathcal{K})$ we let $\varepsilon(i,e) = 1$ if $f_{e,v_i} \in S_i$ and $\varepsilon(i,e) = 0$ otherwise. For edges e that are not incident with v_i we let $\varepsilon(i,e) = 0$. If there is some edge e_{ij} of $\mathcal{K}$ such that $\varepsilon(i,e_{ij}) \neq \varepsilon(j,e_{ij})$, then e_{ij} is inconsistent, and player **I** wins the game. Moreover, all the sets S_i have even cardinality. Thus

$$0 \equiv \sum_{i=2}^{k} |S_i| \equiv \sum_{i=2}^{k} \sum_{e} \varepsilon(i,e) \equiv \sum_{i=2}^{k} \varepsilon(i, e_{1i}) \mod 2.$$

Thus the set of all edges e_{1i} with $f_{e_{1i},v_i} \in S_i$ is even.

Let g be the bijection selected by player **II** in the next round of the game, and let $T \subseteq E(v_1)$ such that $g(v^\emptyset_1) = v^T_1$. Then T is odd, and thus there is some $i \in \{2, \dots, k\}$ such that for the edge $e := e_{1i} = v_1 v_i$ we have $f_{e,v_1} \in T \Leftrightarrow f_{e,v_i} \notin S_i$. Player **I** selects some pair $v^\emptyset_j v^{S_j}_j$ for $j \neq i$ to remove and the pair $v^\emptyset_1 v^T_1$ to add. The new position p' contains the pairs $v^\emptyset_1 v^T_1$ and $v^\emptyset_i v^{S_i}_i$. Thus the edge e_{1i} is inconsistent in this position, and player **I** wins.

Let us now prove that player **II** has a winning strategy for the weak bijective k-pebble game on $\mathcal{A}, \mathcal{B}$. For a vertex-consistent position p of the game and an edge $e = vw \in E(\mathcal{K})$, we let $p \restriction \mathcal{T}_e$ be the set $\{ab \in p \mid a, b \in V(\mathcal{T}_e)\}$ together with the following pairs:

- $f^0_{e,v}f^0_{e,v}$ if v is in the domain of p and $f_v \notin p_v$,
- $f^0_{e,v}f^1_{e,v}$ if v is in the domain of p and $f_v \in p_v$,
- $f^0_{e,w}f^0_{e,w}$ if w is in the domain of p and $f_w \notin p_w$,
- $f^0_{e,w}f^1_{e,w}$ if w is in the domain of p and $f_w \in p_w$.

We view $p \upharpoonright \mathcal{T}_e$ as a position of the weak bijective k-pebble game on $\mathcal{T}_e, \mathcal{T}_e$.

We say that edge $e = vw$ is *flipped* in position p if $p \upharpoonright \mathcal{T}_e$ is nonempty and **I** can reach $\{f^0_{e,v} f^1_{e,v}\}$ from $p \upharpoonright \mathcal{T}_e$ in the weak bijective k-pebble game on $\mathcal{T}_e, \mathcal{T}_e$. The edge e is *straight* in position p if $p \upharpoonright \mathcal{T}_e$ is nonempty and **I** can reach $\{f^0_{e,v} f^0_{e,v}\}$ from $p \upharpoonright \mathcal{T}_e$ in the weak bijective k-pebble game on $\mathcal{T}_e, \mathcal{T}_e$. Observe that, as discussed in connection with Lemma 5.18 (1), if e is flipped, then **I** can reach $\{f^0_{e,w} f^1_{e,w}\}$ as well, and similarly, if e is straight, then **I** can reach $\{f^0_{e,w} f^0_{e,w}\}$. Moreover, if $p \upharpoonright \mathcal{T}_e$ is nonempty then e is either straight or flipped.

We say that a vertex $v \in V(\mathcal{K})$ is *trapped* in a vertex-consistent position p if it satisfies the following conditions:

(G) for all edges $e = vw \in E(\mathcal{K})$ incident with v, the position $p \upharpoonright \mathcal{T}_e$ is nonempty.

(H) the set S of all $f_{e,v}$ such that e is flipped in position p has the wrong parity, that is, $|S|$ is even if $v = v_1$ and $|S|$ is odd otherwise.

(I) there is an edge $e = vw \in E(\mathcal{K})$ such that either $f_{e,v}$ or $x_{e,v}$ is in the domain of p.

Observe that if some vertex is trapped in a position p of the weak bijective k-pebble game, then this position is a winning position for player **I**. (We will not use this observation and hence we omit a proof.) Let us call position p *good* if it satisfies the following conditions:

(J) p is strongly consistent;

(K) for all $e \in E(\mathcal{K})$, player **II** has a winning strategy for the weak bijective k-pebble game on $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$;

(L) no vertex $v \in \mathcal{K}$ is trapped in position p.

Note that, by Lemma 5.18 (1), if p is good, then for every edge $e = vw \in E(\mathcal{K})$, if both v and w are in the domain of p then $f_{e,v} \in p_v \Leftrightarrow f_{e,w} \in p_w$.

We claim that in any good position, **II** can play the next round of the game in such a way that the position after the round is good again. We have to define a bijection g for player **II**, which is done in (M)–(R) below. Since the node sets of $\mathcal{A}$ and $\mathcal{B}$ are the disjoint unions of the sets of vertex nodes v^S for $v \in V(\mathcal{K})$ and the node sets of the T_e for $e \in E(\mathcal{K})$, it suffices to define g_v for every $v \in V(\mathcal{K})$, which determines $g(v^S)$ for each S, and the restriction of g to $\mathcal{T}_e$ for every $e \in E(\mathcal{K})$.

Let p be the given good position. If $|p| < k-1$, let $p^- = p$, and if $|p| = k-1$, let $ab \in p$ be the pair selected by player **I** in the first step of the next round, and let $p^- = p \setminus ab$.

(M) For every $v \in V(\mathcal{K})$ such that v is in the domain of p we let $g_v = p_v$.

An edge $e = vw \in E(\mathcal{K})$ *requires attention at* v if v is not in the domain of p and for all edges $e \neq e'$ that are incident with v, the restriction $p^- \upharpoonright \mathcal{T}_{e'}$ is nonempty. Note that there is at most one pair (e, v) such that e requires attention at v and that $|p \upharpoonright \mathcal{T}_e| \leq 1$ if e requires attention. This follows from the fact that $|p^-| \leq k-2$ and the degree of all vertices of $\mathcal{K}$ is $k-1$.

Suppose that $e = vw$ requires attention at v. Let S' be the set of all $f_{e',v}$ such that e' is flipped in p^-. If $v \neq v_1$ and $|S'|$ is odd or $v = v_1$ and $|S'|$ is even, we let $S = S' \cup \{f_{e,v}\}$; otherwise, we let $S = S'$. The set S determines whether e must be flipped or not. Without loss of generality, let us assume that $f_{e,v} \in S$, that is, e must be flipped. If neither $f_{e,v}$ nor $x_{e,v}$ are in the domain of p, then by Lemma 5.18 (2) player **II** can avoid position $\{f^0_{e,v} f^0_{e,v}\}$ in the bijective 2-pebble game on $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$. If $f_{e,v}$ is in the domain of p then $p_{f_v} = 1 \Leftrightarrow f_{e,v} \in S$ and if $x_{e,v}$ is in the domain of p then $f_{e,v} \in p_{x_{e,v}} \Leftrightarrow f_{e,v} \in S$; otherwise v would be trapped in position p, which contradicts p being a good position. In particular, this implies that in both cases player **II** can avoid position $\{f^0_{e,v} f^0_{e,v}\}$ in the bijective 2-pebble game on $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$. This enables us to define the restriction of the bijection g to $V(\mathcal{T}_e)$.

(N) If $e = vw \in E(\mathcal{K})$ requires attention at v, then we determine the set S as above. If $f_{e,v} \in S$, we choose the restriction of g to $V(\mathcal{T}_e)$ according to a strategy for player **II** in the bijective 2-pebble game on $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$ that avoids $\{f^0_{e,v} f^0_{e,v}\}$. If $f_{e,v} \notin S$, we choose the restriction of g to $V(\mathcal{T}_e)$ according to a strategy for player **II** in the bijective 2-pebble game on $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$ that avoids $\{f^0_{e,v} f^1_{e,v}\}$.

(O) For every $e = vw \in E(\mathcal{K})$ such that e does not require attention and $p \upharpoonright \mathcal{T}_e$ is nonempty, we choose the restriction of g to $V(\mathcal{T}_e)$ according to a winning strategy for **II** in the weak bijective k-pebble game $\mathcal{T}_e, \mathcal{T}_e$ starting in position $p \upharpoonright \mathcal{T}_e$. If $|p \upharpoonright \mathcal{T}_e| = k-1$, we assume that in the first step **I** selects the unique pair in $(p \upharpoonright \mathcal{T}_e) \setminus (p^- \upharpoonright \mathcal{T}_e)$.

(P) For every $e = vw \in E(\mathcal{K})$ such that e does not require attention and $p \upharpoonright \mathcal{T}_e$ is empty, we let the restriction of g to $V(\mathcal{T}_e)$ be the identity mapping.

It remains to define $g_v \in V(\mathcal{K})$ for $v \in V(\mathcal{K})$ that are not in the domain of p.

(Q) If $v \in V(\mathcal{K})$ is not in the domain of p and there is some edge $e = vw$ that requires attention at v, then we define the set S as above and let $g_v = S$.

(R) If $v \in V(\mathcal{K})$ is not in the domain of p and there is no edge that requires attention at v, there is an edge $e = vw \in E(\mathcal{K})$ such that $p \upharpoonright \mathcal{T}_e = \emptyset$. We choose a set $S \subseteq E(v)$ such that for all $e' = vw'$ with nonempty $p \upharpoonright \mathcal{T}_{e'}$ we have $f_{e',v} \in S \Leftrightarrow p$ flips e'. By adding $f_{e,v}$ if necessary, we can choose S such that $|S|$ has the right parity (even if $v \neq v_1$ and odd if $v = v_1$). We let $g_v = S$.

It is easy to see that if player **II** selects this bijection g, then regardless of which pair $a'b'$ player **I** selects, $p^\frown a'b'$ will be a local isomorphism and the new position $p^{-\frown} a'b'$ will again be good. Again proof consists of a case distinction along the cases of the definition of the bijection g in (M)–(R). □

5.3 Boolean arithmetic and L^k-equivalence

We saw in Section 4.2 that equations, which are direct consequences of the basic continuity and compatibility equations w.r.t. the adjacency matrices A and B, may carry independent weight in their boolean interpretation. This is no surprise, because the boolean reading is much weaker, especially due to the absorptive nature of $\vee$, which unlike $+$ does not allow for inversion. $AX = XB$ for doubly stochastic X and $A, B \in \mathbb{B}^{n,n}$ implies $A^c X = XB^c$. Similarly, we found in part (a) of Lemma 5.3 that the continuity equations guarantee that solutions are supported by local bijections, under real arithmetic; this also fails for boolean arithmetic.

We now augment the boolean requirements by corresponding boolean equations that express

(a) compatibility also w.r.t. A^c and B^c, as in boolean fractional isomorphism,

(b) the new constraint $X_p = 0$ whenever p is not a local bijection.

In the presence of the continuity equations, which force monotonicity, it suffices for (b) to force $X_{aa'bb'} = 0$ for all $a, a' \in [m]$, $b, b' \in [n]$ such that $a = a' \not\Leftrightarrow b = b'$. This is captured by the constraint Match(2) below. Together with the continuity and compatibility equations, Match(2) then implies that $X_p = 0$ unless p is a local isomorphism, just as in the proof of part (b) of Lemma 5.3, also in terms of boolean arithmetic.

So we now use the following boolean version of the Sherali–Adams hierarchy ISO$(k-1)$ and its variant ISO$(k-1/2)$ for $k \geq 2$.

B-ISO$(k-1)$

$$\left.\begin{array}{l} X_\emptyset = 1 \quad \text{and} \\ X_p = \sum_{b'} X_{p\frown ab'} = \sum_{a'} X_{p\frown a'b} \\ \text{for } |p| < k, a \in [m], b \in [n] \end{array}\right\} \quad \textsc{Cont}(\ell) \text{ for } \ell < k$$

$$\left.\begin{array}{l} X_{ab\frown ab'} = 0 = X_{ab\frown a'b} \\ \text{for } a \neq a' \in [m], b \neq b' \in [n] \end{array}\right\} \quad \textsc{Match}(2)$$

$$\left.\begin{array}{l} \sum_{a'} A_{aa'} X_{p\frown a'b} = \sum_{b'} X_{p\frown ab'} B_{b'b} \\ \text{for } |p| < k-1, a \in [m], b \in [n] \end{array}\right\} \quad \textsc{Comp}(\ell) \text{ for } \ell < k$$

$$\left.\begin{array}{l} \sum_{a'} A^c_{aa'} X_{p\frown a'b} = \sum_{b'} X_{p\frown ab'} B^c_{b'b} \\ \text{for } |p| < k-1, a \in [m], b \in [n] \end{array}\right\} \quad \textsc{Comp}(\ell)^c \text{ for } \ell < k$$

For B-ISO$(k-1/2)$ we require Cont(ℓ) for all $\ell \leqslant k$, i.e., also for $\ell = k$.

Remark 5.19. *The systems* B-ISO$(k-1)$ *and* B-ISO$(k-1/2)$ *consist of linear boolean equations and can be solved in polynomial time.*

For this observe that the systems B-ISO$(k-1)$ and B-ISO$(k-1/2)$ consist of equations of the following forms:

$$\sum_{i\in I} X_i = \sum_{j\in J} X_j, \tag{14}$$

$$\sum_{i\in I} X_i = 0, \tag{15}$$

$$\sum_{i\in I} X_i = 1. \tag{16}$$

Those of type (15) are actually subsumed by those of type (14) with $J = \emptyset$. It is an easy exercise to prove that such systems of linear boolean equations can be solved in polynomial time.

The *weak* k-pebble game is the straightforward adaptation of the weak bijective k-pebble game to the setting without counting. A single round of the game is played as follows.

1. If $|p| = k-1$, player **I** selects a pair $ab \in p$;
   if $|p| < k-1$, this step is omitted.

2. Player **I** chooses an element a' of $\mathcal{A}$ or b' of $\mathcal{B}$.

3. Player **II** must respond with an element b' of $\mathcal{B}$ or a' of $\mathcal{A}$, respectively, such that aa' is an edge of $\mathcal{A}$ if, and only if, bb' is an edge of $\mathcal{B}$.

4. If $|p| < k-1$, then the new position is $p' := p^\frown a'b'$;
   if $|p| = k-1$, then the new position is $p' := (p \backslash ab)^\frown a'b'$.

II loses if she cannot respond in step (3) or if the resulting position p' fails to be a local isomorphism.

We denote weak k-pebble equivalence as in $\mathcal{A} \equiv_{\mathsf{L}}^{<k} \mathcal{B}$ and extend this to $\mathcal{A}, \mathbf{a} \equiv_{\mathsf{L}}^{<k} \mathcal{B}, \mathbf{b}$ for tuples $\mathbf{a}, \mathbf{b}$ of the same length $< k$. We sketch a proof of the following, which is a boolean analogue of the correspondences between half-step levels of Sherali–Adams and C^k- and $\mathsf{C}^{<k}$-equivalence established in Section 5.1.

Theorem 5.20. B-ISO$(k-1/2)$ *has a solution (w.r.t. boolean arithmetic) if, and only if,* $\mathcal{A} \equiv_{\mathsf{L}}^{k} \mathcal{B}$.

Theorem 5.21. B-ISO$(k-1)$ *has a solution (w.r.t. boolean arithmetic) if, and only if,* $\mathcal{A} \equiv_{\mathsf{L}}^{<k} \mathcal{B}$.

Towards the proofs of the critical directions, viz., from solutions to equivalences mediated by pebble games, we want to pass from given solutions to induced *good* solutions, from which strategies can be directly extracted. These are characterised in the boolean case by conditions that are analogous to those of Definition 5.7 for the real case; good solutions are induced by arbitrary solutions in a manner that is analogous to our findings in Corollaries 5.8 and 5.11, essentially through reductions via liftings to tuple co-ordinates.

The relevant liftings of equations to tuple co-ordinates are also analogous to those in the real case, now including compatibility equations for the complements of the edge relations in $\mathcal{A}$ and $\mathcal{B}$. We leave out Match(2), whose lifting says that $\check{X}$ is supported by local bijections.

$$\left.\begin{array}{l}\sum_{\mathbf{a}'} \check{X}_{\mathbf{a}'\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a}\mathbf{b}'} = 1 \\[2ex] \sum_{\mathbf{a}'} \mathbb{I}^{(i)}_{\mathbf{a}\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'} \mathbb{I}^{(i)}_{\mathbf{b}'\mathbf{b}} \\ \text{for all } \mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell, \text{ and all } i \in [\ell] \end{array}\right\} \quad \text{lifting of } \textsc{Cont}(\ell'), \ell' \leqslant \ell$$

$$\left.\begin{array}{l}\sum_{\mathbf{a}'} A^{(i)}_{\mathbf{a},\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'} B^{(i)}_{\mathbf{b}',\mathbf{b}} \\ \text{for all } \mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell, \text{ and all } i \in [\ell] \end{array}\right\} \quad \text{lifting of } \textsc{Comp}(\ell'), \ell' \leqslant \ell$$

$$\left.\begin{array}{l}\sum_{\mathbf{a}'} (A^c)^{(i)}_{\mathbf{a},\mathbf{a}'} \check{X}_{\mathbf{a}',\mathbf{b}} = \sum_{\mathbf{b}'} \check{X}_{\mathbf{a},\mathbf{b}'} (B^c)^{(i)}_{\mathbf{b}',\mathbf{b}} \\ \text{for all } \mathbf{a} \in [m]^\ell, \mathbf{b} \in [n]^\ell, \text{ and all } i \in [\ell] \end{array}\right\} \quad \text{lifting of } \textsc{Comp}(\ell')^c, \ell' \leqslant \ell$$

Here the matrices $(A^c)^{(i)}$ are the lifting of A^c to tuple co-ordinates, just as the $A^{(i)}$ are the familiar liftings of A, as introduced for Lemma 5.10, for $i \in [\ell]$:

$$(A^c)^{(i)}_{\mathbf{a},\mathbf{a}'} = \prod_{j \neq i} \delta(a_j, a'_j) \; A^c_{a_i a'_i}.$$

As the relationship between the edge relations $(A^c)^{(i)}$ and $A^{(i)}$ is not one of complementation over $[m]^\ell$, the commutativity conditions for $\check{X}$ in Comp(ℓ) and Comp$(\ell)^c$ do not give rise to *bi-stable* boolean equivalent partitions as in the boolean variant of fractional isomorphism. Instead, the lifting to tuple co-ordinates of a good boolean solution for Comp(ℓ) and Comp$(\ell)^c$ induces partitions that are just *boolean stable* and *boolean equivalent*, but simultaneously so, for $(A^c)^{(i)}/(B^c)^{(i)}$ and $A^{(i)}/B^{(i)}$. Similarly the lifting of a boolean solution to the continuity equations that is supported by local bijections induces good solutions with partitions that are just *boolean stable* and *boolean equivalent* w.r.t. the $\mathbb{I}^{(i)}$. It turns out that these are precisely the conditions that support strategies for the second player in the corresponding k-pebble games.

Let us say that partitions of the vertex sets $[m]^\ell = \dot{\bigcup}_s D_s$ and $[n]^\ell = \dot{\bigcup}_s D'_s$ are *equivalent* and *boolean stable* w.r.t. edge relations E on $[m]^\ell$ and E' on $[n]^\ell$ if for all partition indices s, t, and all $\mathbf{a} \in D_s, \mathbf{b} \in D'_s$,

$$\{\mathbf{a}' \in D_t \colon (\mathbf{a}, \mathbf{a}') \in E\} \neq \emptyset \;\Leftrightarrow\; \{\mathbf{b}' \in D'_t \colon (\mathbf{b}, \mathbf{b}') \in E'\} \neq \emptyset.$$

We shall apply this notion to the undirected reflexive edge relations of the $\mathbb{I}^{(i)}$, where the condition becomes

$$\{a \in [m] \colon \mathbf{a}\tfrac{a}{i} \in D_t\} \neq \emptyset \;\Leftrightarrow\; \{b \in [n] \colon \mathbf{b}\tfrac{b}{i} \in D'_t\} \neq \emptyset;$$

and to the symmetric and irreflexive edge relations $A^{(i)}/B^{(i)}$ and $(A^c)^{(i)}/(B^c)^{(i)}$, for which the combination of the conditions

$$\{a \in [m] \colon A_{a_i a} = 1 \wedge \mathbf{a}\tfrac{a}{i} \in D_t\} \neq \emptyset \;\Leftrightarrow\; \{b \in [n] \colon B_{b_i b} = 1 \wedge \mathbf{b}\tfrac{b}{i} \in D'_t\} \neq \emptyset,$$
$$\{a \in [m] \colon A_{a_i a} = 0 \wedge \mathbf{a}\tfrac{a}{i} \in D_t\} \neq \emptyset \;\Leftrightarrow\; \{b \in [n] \colon B_{b_i b} = 0 \wedge \mathbf{b}\tfrac{b}{i} \in D'_t\} \neq \emptyset$$

becomes the natural lifting of bi-stability and equivalence conditions for boolean fractional isomorphism.

Definition 5.22. A boolean solution $X = (X_p)_{|p|\leqslant \ell}$ to $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$ is *good* if its lifting $\check{X} = (\check{X}_{\mathbf{a},\mathbf{b}})$ to tuple co-ordinates is a good boolean solution to the equations $\textsc{Comp}[\mathbb{I}^{(i)}(m,\ell), \mathbb{I}^{(i)}(n,\ell)]$ (simultaneously for all $i \in [\ell]$) in the sense of Definition 4.7.

We obtain the analogue of Corollary 5.8, which can also be proved in complete analogy, simply by specialisation to boolean arithmetic, which can then be used to prove the critical direction in Theorem 5.20.

Lemma 5.23. *Any boolean solution $X = (X_p)_{|p|\leqslant \ell}$ to $\textsc{Cont}(\ell')$ for $\ell' \leqslant \ell$ that is supported by local isomorphisms between $\mathcal{A}$ and $\mathcal{B}$, induces a solution $X' = (X'_p)_{|p|\leqslant \ell}$ that is* good *in the sense of Definition 5.22, and is non-zero where X is.*

Now we are ready to prove the theorem.

Proof of Theorem 5.20. We start with the implication from right to left. If $\mathcal{A} \equiv^k_{\mathsf{L}} \mathcal{B}$ we put, for $p = \mathbf{ab}$ of size $|p| \leqslant k$,

$$X_p := \begin{cases} 1 & \text{if } \mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}, \\ 0 & \text{else.} \end{cases}$$

Clearly this assignment satisfies $\textsc{Match}(2)$, and one easily checks that it also satisfies the boolean continuity equations $\textsc{Cont}(\ell)$ for $\ell \leqslant k$. For the boolean compatibility equations $\textsc{Comp}(\ell)$ and $\textsc{Comp}(\ell)^c$ for $\ell < k$, let us check, for instance, an equation $\textsc{Comp}(k-1)$. The non-trivial case is that of $p = \mathbf{ab}$ where $\mathbf{a} \in [n]^{k-2}$ and $\mathbf{b} \in [m]^{k-2}$ are such that $\mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}$ so that $X_p = 1$. Consider the instance of equation $\textsc{Cont}(k-1)$ for $a \in [m], b \in [n]$:

$$\sum_{a'} A_{aa'} X_{p^\frown a'b} = \sum_{b'} X_{p^\frown ab'} B_{b'b}.$$

Since $\mathcal{A}, \mathbf{a} \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}$, there is a $\hat{b} \in [m]$ such that $\mathcal{A}, \mathbf{a}a \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}\hat{b}$. Suppose the left-hand side of the equation evaluates to 1. This means that there is an edge in $\mathcal{A}$ from a to some a' for which $X_{p^\frown a'b} = 1$, i.e., for which $\mathcal{A}, \mathbf{a}a' \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}b$.

In other words, there is an edge in $\mathcal{A}$ from some a' for which $\mathcal{A}, \mathbf{a}a' \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}b$ to some a for which $\mathcal{A}, \mathbf{a}a \equiv^k_{\mathsf{L}} \mathcal{B}, \mathbf{b}\hat{b}$. So every realisation of the L^k-type of $\mathcal{B}, \mathbf{b}b$ has an edge between b and some b' where $\mathcal{B}, \mathbf{b}b' \equiv^k_{\mathsf{L}} \mathcal{A}, \mathbf{a}a$, which implies that the right-hand side of the equation evaluates to 1, too.

For the implication from left to right in part (b) we extract a strategy for player **II** in the k-pebble game from a good solution as provided in Lemma 5.23. As discussed above, any good solution is supported by local isomorphisms, whence it suffices for **II** to maintain the condition that $\check{X}_{\mathbf{a},\mathbf{b}} = 1$, or, equivalently, that the pebbled tuples are in matching partition sets. This can be achieved for rounds played in the j-th component, because the partitions induced by the lifting of the good solution are boolean equivalent and stable w.r.t. the edge relation $\mathbb{I}^{(j)}$. □

We turn to B-ISO$(k-1)$ and the situation of Theorem 5.21, where the higher levels of the compatibility equations matter. For the analogue of Corollary 5.11 we also need to reason that any solution to B-ISO$(k-1)$ is supported by local isomorphisms. Support by local bijections is clear, because that is explicitly demanded by Match(2). For the strengthening to local isomorphy, we may reason on the basis of Comp(2) exactly as for Lemma 5.3 (b). The rest of the proof of the lemma is again strictly analogous to the argument for Corollary 5.11.

Lemma 5.24. *Let $k \geqslant 3$. Any boolean solution $X = (X_p)_{|p|<k}$ to* B-ISO$(k-1)$ *induces a boolean solution $X' = (X'_p)_{|p|<k}$ to* B-ISO$(k-1)$ *that is supported by local isomorphisms and is* good *in the sense that its lifting $\check{X}'$ to tuple coordinates is a good simultaneous boolean solution to the following equations for all $i < k$:*

$$\text{Comp}[\mathbb{I}^{(i)}(m, k-1), \mathbb{I}^{(i)}(n, k-1)], \text{Comp}[A^{(i)}, B^{(i)}], \text{Comp}[(A^c)^{(i)}, (B^c)^{(i)}],$$

and thus induces $\check{X}'$-related partitions of $[m]^{k-1} = \dot{\bigcup}_s D_s$ and $[n]^{k-1} = \dot{\bigcup}_s D'_s$ such that

(i) *these partitions are boolean equivalent and stable w.r.t. the edge relations of the $\mathbb{I}^{(i)}$;*

(ii) *these partitions are boolean equivalent and stable w.r.t. the liftings of the edge relations $A^{(i)}/B^{(i)}$ as well as $(A^c)^{(i)}/(B^c)^{(i)}$;*

(iii) *$\check{X}'_{D_s D'_s} = 1$ for all s;*

(iv) *$\check{X}'_{D_s D_t} = 0$ for all $s \neq t$.*

In particular, $\mathbf{a} \mapsto \mathbf{b}$ is a local isomorphism between $\mathcal{A}$ and $\mathcal{B}$ for $\mathbf{a}$ and $\mathbf{b}$ from matching partition sets. Moreover, X' is non-zero where the given X is.

We are now ready to prove Theorem 5.21.

Proof of Theorem 5.21. For the direction from right to left, suppose that $\mathcal{A} \equiv^{<k}_{\mathsf{L}} \mathcal{B}$ and let $X_\emptyset := 1$ and, for $\mathbf{a} \in [n]^{k-1}$ and $\mathbf{b} \in [m]^{k-1}$, $X_{\mathbf{ab}} := 1$ iff $\mathcal{A}, \mathbf{a} \equiv^{<k}_{\mathsf{L}} \mathcal{B}, \mathbf{b}$. It is clear that this assignment satisfies Match(2) and Cont(ℓ) for $\ell < k$. Consider then an instance of Comp(ℓ) for $\ell < k$,

$$\sum_{a'} A_{aa'} X_{p^\frown a'b} = \sum_{b'} X_{p^\frown ab'} B_{b'b}, \tag{17}$$

where $a \in [n], b \in [m]$, $|p| < k-1$, $p = \mathbf{ab}$. Let us assume that $|p| = k-2$; this is the most difficult case. If $X_p = 0$ then $X_{p^\frown a'b'} = 0$ for all $a'b'$, and thus equation (17) is trivially satisfied. So assume $X_p = 1$, that is, $\mathcal{A}, \mathbf{a} \equiv^{<k}_{\mathsf{L}} \mathcal{B}, \mathbf{b}$. Suppose for instance that the left-hand side of equation (17) evaluates to 1, i.e., that there is some a' adjacent to a in $\mathcal{A}$ for which $\mathcal{A}, \mathbf{a}a' \equiv^{<k}_{\mathsf{L}} \mathcal{B}, \mathbf{b}b$. Consider the weak k-pebble game in position $\mathbf{a}a'\mathbf{b}b$. Assume player **I** selects the pair $a'b$ in the first step of the next round and selects a in the second step. Let b' be the answer of **II** when she plays according to her winning strategy. Then $\mathbf{a}a'a \mapsto \mathbf{b}bb'$ is a local isomorphism and the new position $\mathbf{a}a\mathbf{b}b'$ is a winning position for player **II**, that is, $\mathcal{A}, \mathbf{a}a \equiv^{<k}_{\mathsf{L}} \mathcal{B}, \mathbf{b}b'$. Since $\mathbf{a}a'a \mapsto \mathbf{b}bb'$ is a local

isomorphism and aa' is an edge of $\mathcal{A}$, the pair bb' is an edge of $\mathcal{B}$ and thus $B_{b'b} = 1$. Since $\mathcal{A}, \mathbf{a}a \equiv_{\mathsf{L}}^{<k} \mathcal{B}, \mathbf{b}b'$, we have $X_{p\hat{\ }ab'} = 1$. Thus the right-hand side of equation (17) evaluates to 1 as well.

For the direction from left to right we extract a strategy for **II** in the weak k-pebble game from a good solution X and its lifting $\check{X}$ as provided in Lemma 5.24. Again, the strategy for **II** is to maintain the condition that $\check{X}_{\mathbf{a},\mathbf{b}} = 1$. In addition, in a round played on the j-th component, the old and new positions of the j-th pebble must be linked by an edge in $\mathcal{A}$ if, and only if, they are linked by an edge in $\mathcal{B}$. This can be achieved because the partitions induced by the lifting of the good solution are simultaneously boolean equivalent and stable w.r.t. $A^{(j)}/B^{(j)}$ and $(A^c)^{(j)}/(B^c)^{(j)}$. □

Remark 5.25. *For all $k \geqslant 3$, $\equiv_{\mathsf{L}}^{k-1}$, $\equiv_{\mathsf{L}}^{<k}$, $\equiv_{\mathsf{L}}^{k}$ form a strictly increasing hierarchy of discriminating power.*

Proof. The examples for the gaps between $\equiv_{\mathsf{C}}^{k-1}$, $\equiv_{\mathsf{C}}^{<k}$, $\equiv_{\mathsf{C}}^{k}$ given in Section 5.2, are in fact good in the setting without counting. The strategy analysis given there does not involve counting in any non-trivial manner. □

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